A QUANTUM MEASUREMENT MODEL OF REACTION-TRANSPORT SYSTEMS

BY

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DISSERTATION

Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Nuclear Engineering
in the Graduate College of the
University of Illinois at Urbana-Champaign, 2018

Urbana, Illinois

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Abstract

This research develops a mesoscopic quantum measurement theoretic foundation for neutron transport theory in the presence of delayed fission and compound scattering processes. Specifically, we construct a quantization of the Pál-Bell equation of stochastic neutron transport theory from a quantum stochastic calculus for particle detection in quantum fields. This enables us to formulate a quantum theory of mesoscopic neutron transport physics that explicitly incorporates both transport mechanisms and resonance scattering into a single quantum stochastic process. The quantum stochastic process representation is shown to have a unique, trace-norm convergent perturbation expansion in the number of observed reaction events. This expansion result, and the proofs that lead to it, help to establish a variety of approximation methods that are applied to nuclear data assimilation and neutron thermalization problems.

Acknowledgments

There are incredible people who made this work possible. I started asking questions that ultimately led to this work almost 10 years ago. Since then I have had the benefit of insight and incredible unwavering support from my advisor, Roy Axford. Marius has been an amazing teacher and an inspiring analyst. Rizwan has been a continually supportive friend and mentor. Joyce helped me to be patient and keep working to solve problems when it felt impossible. My Mom has always helped me to stay realistic about the research and writing process. My friends, family, teachers, and colleagues have all been supportive and encouraging. Without all of them this would not have been possible. This research was performed in part using funding received from the DOE Office of Nuclear Energy's Nuclear Energy University Programs.

Table of Contents

Chapter 1

Introduction

This research into a measurement theory for reaction-transport systems is motivated by an apparent deficit in quantum mechanical foundations for neutron transport theory. This shortcoming manifests itself in four related difficulties in current nuclear engineering research. First, there is currently no way to represent scattering and transport processes in one reference system so that uncertainty can be propagated from resonance scattering models to the induced reaction-transport systems without violating consistency constraints. Second, there is no obvious procedure for adding corrections to nuclear reaction-transport theories for mesoscopic systems (where generalized law of large numbers arguments are more difficult to justify). Third, there is currently no quantum mechanical method for studying multi-time correlations that incorporate the dynamical transmutation of the nuclear medium. Finally, there is no sufficiently general measurement theory for describing reaction-transport systems.

Solving the measurement theory problem turns out to be the key to understanding the other challenges, as quantum mechanics is fundamentally a theory of measurement. We will adopt an entirely measurement-centric approach and invoke quantum measurement theoretic ideas to arrive at a phenomenological theory that explicitly couples reactive scattering and transport mechanisms through a shared topology. That is, we will derive a quantum reaction measurement theory that allows us to calculate quantum transport probabilities directly from a practical nuclear reaction model. Moreover, it turns out that the variety of practical nuclear models that this technique applies to is quite large. The power of this approach comes from the fact that it is grounded in precise mathematical results (that lend themselves to constructive approximation) as well as a clearly articulated set of empirical goals. Moreover, this framework emphasizes approximation features that are critical to the practical application of nuclear models to real nuclear engineering systems.

The core of this work focuses on the development of a quantum stochastic process (QSP) based measurement theory for continuous absorption and decay counting. We will accomplish this in three steps. We begin, in chapter 3, by examining the classical theory of stochastic neutronics in order to identify the reaction observables that need to be modeled in order to the develop a successful quantum theory. Using these ideas we will develop a set of general assumptions and quantum measurement heuristics in chapter

4. Finally, in chapter 5, we will establish that any self-consistent quantum reaction-transport model that conforms to our assumptions induces a unique QSP that is fully equivalent. This will allow us to discuss physical interpretation of the quantum theory in terms of classically familiar structures in chapter 6.

We will directly apply the resulting theory to two interesting model cases: (1) particle number conserving neutron thermalization with compound elastic processes and (2) particle number non-conserving processes in the presence of a discrete and finite number of reactive nuclei. Both introduce substantive limitations and a rigorous analysis of the passage to a thermodynamic-like scaling limit for non-conserving processes will require additional analysis of a class of processes that we discuss in future work.

Chapter 2

Review of Literature

This chapter will provide a review of the key research and ideas that will be used throughout the remainder of the work. We will begin with a survey of neutron physics for reactor analysis. This review will compare the main methods used in the study neutron transport dynamics. We will also review some techniques from statistical mechanics and quantum field theory that provide a foundation for our analysis. Finally, we will provide a summary of the key definitions and results that we will be using from functional analysis and quantum measurement theory. This last section assumes a knowledge of real analysis at the level of a second graduate course in linear analysis.

2.1 Neutron Transport

The primary goal of this work is to investigate the propagation of approximations between nuclear reaction models and neutron transport models. This analysis readily generalizes to other deterministically propagating and locally scattering particle systems, like plasmas, through the introduction of global mean field potentials in the classical inter-collision trajectory. However, for simplicity we will exclusively discuss dynamical neutron fields as they posses a very small self-interaction probability and approximately piecewise linear trajectories on individual paths. We will provide a brief focused review of the history of neutron transport theory and nuclear reactor physics.

2.1.1 Neutron Transport Physics

To begin with, we will consider some of the neutron physics that is important in macroscopic nuclear systems. We will attempt to describe a dynamical neutron population model with enough generality to cover a variety of engineering applications: nuclear reactors, cold neutron imaging systems, and subcritical containment systems. Unlike the situations to which we can directly apply the Boltzmann equation, in the applications above, the dominant interaction is not with members of the same particle species. Instead, neutrons interact primarily with a condensed matter medium. The neutron-neutron scattering cross section

is so small that it is negligible below particle densities found primarily in stellar phenomena.

The main consequence of this is that a PDE similar to the linearized model for the Boltzmann kinetics is a very accurate approximating model for neutron density mean field dynamics. This governing equation is called the linear neutron transport equation. We will focus on neutrons interacting exclusively with a medium and influencing each other through only though how they alter the medium. Although there is a great deal to say about models of the environment (particularly in imaging applications), we only require the notion that the medium is made of atoms with densities typical of condensed matter and that neutrons interact exclusively with the nuclear core of these atoms.

We can construct a useful geometric picture of the environment that neutrons live in. There are very small regions where collisions can occur at all. A large nuclear radius (say for Uranium) is about 10^{-13} cm. A small atomic radius (say for He) is between 10^{-9} and 10^{-8} cm. Thus each atomic diameter is between 10000 and 100000 nuclear diameters across. Moreover the volume ratio scales as the cube of the radius ratio. So, there is between 10^{12} and 10^{15} times as much non-nuclear volume as there is nuclear volume. Since the nuclear potential is so short ranged and the neutron is net neutral, even a short distance away from the nucleus of an atom, neutrons will propagate by the dynamics of quantum wavepackets in a zero potential. That is, all of the non-nuclear matter is effectively free space to a neutron. The distances between collisions are so large relative to nuclear interaction distances that we can often approximate the neutrons as propagating classically between collisions. [33]

Justifying and qualifying this semi-classical model relative to a fully quantum problem takes great care and is a significant approximation problem in the theory of neutron optics. One may consult section 6.2.2 and p.367 of [19] for a salient discussion of the Fermi pseudo-potential and the Born approximation, [117] for a careful beam averaging and bound state energy analysis of neutron scattering fields. There are related discussions of coherent state dynamics in chapter 1 of [1] and "Collision Theory" chapters 3 and 4 [65]. Understanding how to include scattering spaces in a global transport space is of critical significance in attempting to describe the measurement topology that connects scattering and transport models. In some sense, we will spend all of chapters 4 and 5 discussing the mathematical structure of this problem in terms of quantum stochastic integrals. For now, we will focus on the physics described in conventional analyses of neutron transport and treat all neutrons as being in minimum uncertainty states outside of purely local collision events. As such, we will approximate neutrons as evolving classically between collisions and existing in definite position and momentum states on macroscopic scales. This is typical of the assumptions used in constructing neutron transport theories. [20], [136]

The vast distances between scattering centers and the small radii relative to neutron speeds suggests

that we can also fairly comfortably invoke the standard Möller wave operator scattering approximation for the interaction events.[125] In this approximation, we map interaction states to free states by extending the collision over an infinite amount of time relative to the nuclear direct transit time. This is an asymptotic approximation in interaction distances and time scales. We treat collision events as instantaneous and spatially point-like relative to macroscopic distances. Using the classical free propagation approximation in conjunction with this, we arrive at a pin ball-like picture of neutron kinematics. Neutrons move in straight lines over long distances between collision centers. When they arrive at a collision center, they abruptly change direction and energy without changing position. In principle, these scattering centers can be oscillating or flowing (generally slowly) relative to one another, with some minimum separation distance. If our goal is to analyze diffraction physics for problems of neutron optics then we need to retain much of the condensed matter physics that governs the motion of scattering centers. On the other hand, by treating the scattering centers as forming a continuous scattering medium in a scaling (or collision rate averaging [33] p.2) approximation, we can arrive back at a simple linear Monte Carlo particle simulation for non-reacting particles.

Regardless of how we choose to address the dynamics of the scattering centers, we need to understand the implications of the fact that we are now dealing with non-conservative collisions. Specifically, by working on problems where neutrons interact with a medium composed of nuclei (including neutrons) that are not explicitly part of our model, we need to incorporate nonconservative collision outcomes to describe nuclear reactions: absorption, decay, induced fission, compound elastic scattering and compound inelastic scattering.

When a neutron arrives at a scattering center, a conservative two-body quantum scattering problem involves the neutron evolving for a finite time by an interaction propagator that is radically different from the free evolution. However, when the neutron exits the scattering event, it still exists, the internal structure of the scattering nucleus is left unchanged, and energy is conserved between the neutron and the colliding nucleus (up to the coupling effects to the rest of the medium). This is a valid description of many scattering processes (for example, neutron thermalization in water). However, it does not describe what happens when a neutron collides with a complex nucleus such as Xenon-135. In this case, the neutron enters into a complex and highly coupled interaction with the constituent bound nucleons that comprise the nucleus. It is possible for the neutron to redistribute its incident energy among the other nucleons in such a way that none of them can escape from the joint potential well. From the perspective of the external neutron field, the scattered neutron was annihilated. Since we know that it has been incorporated into a nucleus, we will usually choose the word absorbed.

The environment in a nuclear system is often composed partly of unstable nuclei such as Plutonium-239.

These nuclei can "boil off" neutrons or alpha particles to stabilize, which we will refer to as a decay event. However, sometimes their instabilities are so severe that they decay by spontaneous fission, breaking into (usually) two large clusters that are individually both much smaller than the source nucleus. This event involves the release of tremendous kinetic energy and is highly disruptive to the structure of the surrounding medium. [41] We will generally treat these as one class of events for the purposes of stochastic neutron transport modeling. From the perspective of the external neutron field, one or more neutrons is created in this process and no collision was required to make it possible. This motivates us to generalize our notion of a collision to include creation events in the absence of any neutrons from the external neutron field. Accounting for these events typically necessitates the inclusion of a source term in our models. [20]

Induced fission reactions combine the idea of an absorption and a decay. An incident neutron from the neutron field is absorbed at a scattering site and some random quantity of time later, there is a decay involving a release of energy and typically one or more neutrons at the same site. [145] The distribution of delay times is strongly multimodal with a large peak around nearly instantaneous times and one or more (generally) smaller peaks much later. This gives rise to a wide variety of useful approximations to the system dynamics based on the distribution of these peaks and has implications for approximating Laplace transforms. [3] From the perspective of the external neutron field, each collision results in the creation of one or more new neutrons over a range of delayed times.

Finally, compound scattering events involve colliding neutrons entering into a complex mixed state involving the nucleons of the nucleus for a usually short time but not macroscopically instantaneous. During this time the nucleus is evolving by a highly coupled and complex dynamics without settling into the kind of equilibrium observed in an absorption reaction. Instead, the incident neutron (for symmetry reasons this distinction is disingenuous) typically enters into an excited state of the nucleus and scatters through a couple other states before exiting to a free state again. However, this process can result in stimulated emission of additional neutrons or simply a lack of energy conservation by scattering out while internal degrees of freedom in the nucleus are excited. If the structure of the nucleus is changed by the collision it is called an inelastic collision. If all kinetic energy is conserved between the entrance and exit states, it is called elastic. From the perspective of the external neutron field, this is a collision that occurs with macroscopically large time delays, possible secondary neutron creation, and a distinctive energy and directional correlation signature as compared with direct potential scattering. [59]

In summary, we have expanded the standard Boltzmann reaction kinetics by the addition of interactions in the presence of one or even zero neutrons. We have added neutron creation processes, neutron destruction processes, and time delayed collisions with distinctive transition probability kernels. This new transport

process does not preserve particle number and does not have purely instantaneous collisions. Several approximate models have been constructed for describing the evolution of a macroscopic neutron field in the presence of these reaction processes and we will be proposing a new one that builds on the success of existing methodologies.

2.1.2 Neutron Balances and Linear Transport Models

The multiplication of neutrons in a fission system was identified as a branching process by Fermi and Feynman at the dawn of nuclear science. [48],[54] However, at that time there were neither the computational resources nor the mathematical technologies required to effectively analyze time-dependent fluctuations in spatially heterogeneous nuclear systems. As such, design choices were constrained in such a way that nuclear systems could to be characterized almost completely in terms of the expected stationary neutron population.

We formulate a governing equation for modeling the expected population as a position and velocity (i.e. phase space) dependent density function. This governing equation can take a number of equivalent forms including both integral and integrodifferential transport type equations. Throughout this section, two assumptions will be applied without further comment. First, since this is essentially classical and approximately non-relativistic outside of collisions and cross sections are calculated in a momentum representation, we will use $p = mv = \sqrt{2mE}$ to move between energy, velocity and momentum in our transport model. Second, since neutrons are neutral particles we will use constant velocity kinematics (piecewise linear motion) between collisions. That is, for a given neutron trajectory $x(t)$, $x(t + \Delta t) = x(t) + v\Delta t$ is valid for all time intervals $(t, t + \Delta t]$ that do not include a collision event.

In transport models for neutron populations, we are primarily interested in estimating different nuclear reaction rates since these are the basis of all neutron detection measurements. This will motivate several of our key definitions in this section. First, we will denote the phase space density of paths as $n(\bar{x}, \bar{v}, t)$. When this is integrated over a region of phase space, it gives the total expected number of neutrons (or as is classically equivalent, neutron paths) in that phase space volume at that time. Moreover, $vn\Delta t$ can be integrated over a region of phase space to obtain the total path length traveled in that region of phase space in $[t, t+\Delta t]$. In section 2.1.1, we reverenced a scaling limit (described in both Davison [33] and Parks [117]) of local interaction probability averages applied to the environment in order to approximate it as a continuous field. This approximation enforces a proportionality between the reaction rate and the total path length traveled in a volume of phase space. The macroscopic cross section for a given collision outcome $\Sigma(\bar{v}, \bar{x}, t)_r$ is the field of local proportionality constants for calculating the aggregate reaction rate in a volume. This is the relevant transport coefficient for a neutron transport model. However, we can see that by the time

we have defined the primitive quantities of the theory in this framework, we have already obscured the true connection to the microscopic cross sections of scattering experiments.

The linear transport equation derives its validity from a principle of neutron accounting that mimics the measure theoretic decomposition of a probability space by a union of disjoint sets.

$$\Omega = \bigsqcup_i X_i \tag{2.1.2.1}$$

$$\mu(\Omega) = \sum_i \mu(X_i) \tag{2.1.2.2}$$

This parallel is not an accident, as we will see in our discussion of the backward Kolmogorov formulation of the Pál-Bell equation. Heuristically, this comes down to enumerating possible collision outcomes along a family of adjacent neutron paths and then using the expected single event rates to estimate the rate of change in the neutron flux. For example, in order for a neutron to be removed from a given region of phase space in our system (and thus no longer contribute to the expected total path length in that volume), it must either propagate across the boundary of the region by moving with one of the velocities in the momentum region or it must be removed by a collision mechanism. Similarly, for a neutron to be added to a region, it must either propagate in across the boundary by moving with one of the velocities in the momentum region, or be added by a collision mechanism (or decay). Thus, the expectation for a time evolved neutron phase space density (along a cone of characteristic neutron paths) can be constructed as sum of expected contributions from different reaction processes. This line of reasoning immediately suggests a tacit invocation of a generalizes Law of Large Numbers as part of our continuum scaling limit. [83] However, for now, we will focus on the limiting or heuristic form.

In order to make this neutron balance principle concrete, we will begin by recalling a standard monochromatic beam attenuation model which employs the same scaling limit for a reactive medium that we referenced above that makes collisions spatially and temporally point-like. In this model, we consider a single velocity (v) beam penetrating into a material and attempt to describe how much of the beam penetrates to a given distance in the material without scattering even once. This quantity, vn_u, is called the uncollided flux. To find this, we estimate the amount that the beam flux does change by over the distance $|x_2 - x_1|$ by comparing the number of neutrons passing the x_1 plane per unit time to the number of neutrons passing the x_2 plane per unit time. This is achieved by considering the particle current vn_u passing through an area A_{section} equal to the cross sectional area of the beam. Under steady state conditions, this difference between $vn_u(x_1)A_{\text{section}}$ and $vn_u(x_2)A_{\text{section}}$ (i.e. the number of neutrons passing through x_1 and x_2 respectively) equals the number of collisions that occur in the subtended beam volume. We can formulate this as an

equation

$$vn_u(x_2,v,t)A_{\text{section}} - vn_u(x_1,v,t)A_{\text{section}} = -\int_{A_{\text{section}}}\int_{x_1}^{x_2}\Sigma(v,x)vn_u(x,v,t)\mathrm{d}x\mathrm{d}S \tag{2.1.2.3}$$

Now using the fact that the beam is uniform in the plane perpendicular to its direction of propagation, we find that by defining $\psi_u = vn_u$

$$\psi_u(x_2,v,t) - \psi_u(x_1,v,t) = -\int_{x_1}^{x_2}\Sigma(v,x)\psi_u(x,v,t)\mathrm{d}x \tag{2.1.2.4}$$

and solving the resulting integral equation, we fine that the uncollided flux for a monochromatic beam is given by

$$\psi_u(x,v,t) = \exp\left(-\int_{x_1}^{x}\Sigma(v,x')\mathrm{d}x'\right)\psi_u(x_1,v,t) \tag{2.1.2.5}$$

This can be interpreted to mean that the uncollided phase space density of a particle beam decreases exponentially along a fixed neutron trajectory $x(t) = vt$.

This reduced model will be our starting point for a derivation of the neutron transport equation for two reasons. First, it allows us to generalize our intuition from a simple model. Second, it emphasizes the scattering process and piecewise linear trajectory as the generator of an evolution without involving any discussion of currents on bounding surfaces or interpreting weak derivatives as would be required by a direct construction of the integrodifferential form. [31] In essence, what follows is a direct justification of the integral form of the transport equation.

We take ψ to be differentiable function of both phase space and time variables. If we accept that the true phase space path length density is being approximated by a scaling limit of local averages in this model, then this assumption is reasonable. In this case, we can consider a sufficiently narrow energy band from a cone of sufficiently small solid angle in momentum space so as to have the measure be approximated as well as we like by the flux at a single representative velocity. Since the phase space is Euclidean (and so locally compact) and the density is differentiable, we can construct the measure of phase space volume out of a union of sufficiently small phase space cells where we use a single representative value for the velocity in our evaluation of the flux. (we are essentially using a Riemann sum approximation here) With this in mind, we will take the product of a small band of a narrow cone in momentum space with a cube in coordinate space and set this as our basic phase space cell.

Now, to construct an equation for the total phase space density n, we will attempt to estimate the phase space density in a phase cell centered at $(x + v\Delta t, v)$ at time $t + \Delta t$ from a knowledge of the phase space

density in a phase cell centered at (x, v) at a time t. By combining this approximation scheme across all phase cells in the system, this amounts to estimating the phase space density at a later time from knowledge of its state at one specific earlier time without any reference to earlier or later states. That is, we are constructing the Markovian evolution of the phase space density for the expected number of neutron paths.

$$\begin{aligned} n(\bar{x}+\bar{v}\Delta t, \bar{v}, t+\Delta t)\Delta V_{\text{xCell}}\Delta V_{\text{vCell}} = \\ \exp\left(-\int_{\bar{x}}^{\bar{x}+\bar{v}\Delta t}\Sigma(\bar{v}, \bar{x}+\bar{v}\tau)\mathrm{d}|\bar{x}+\bar{v}\tau|\right) n(\bar{x}, \bar{v}, t)\Delta V_{\text{xCell}}\Delta V_{\text{vCell}} + \\ S(\bar{x}, \bar{v}, t)\Delta V_{\text{xCell}}\Delta V_{\text{vCell}} \end{aligned} \tag{2.1.2.6}$$

Note that since $\bar{v}$ and $\bar{x}$ are fixed in the above formula, the integral over the cross section is actually a one dimensional line integral parametrized by the τ parameter and expressed as norms of vector differences. Since $\bar{x}$ is a fixed vector this can be dropped from the differential. The measure thus transforms to $|\bar{v}|\mathrm{d}\tau = v\mathrm{d}\tau$. Also, $\Delta V_{\text{xCell}}\Delta V_{\text{vCell}}$ is the phase cell volume and only serves to remind us that this is actually a relationship between terms in approximations to integrals at different times. Finally, S is a source function and is presently a placeholder for reaction rates associated to collisions that add neutrons to the phase cell of interest. We will introduce these terms into 2.1.2.6 to establish a measure theoretic version of the classical neutron transport equation before constructing finite differences to obtain the standard integrodifferential form.

First, we will consider the processes that are globally conservative. Specifically, we will focus on direct elastic scattering events. For the purpose of describing scattering, we will often think of the phase space as a fiber bundle. Collisions occur locally in coordinate space, so the velocity space associated to a particular point in the coordinate space will be the system that we are conserving particles in. We argued at the start of this section that the form of the reaction rate density for a specified process at fixed incident velocity $\bar{v'}$ and position $\bar{x}$ is given by

$$\Sigma_r(\bar{v'} \to \bar{v}, \bar{x})\psi(\bar{x}, \bar{v'}, t) = \Sigma_r(\bar{v'} \to \bar{v}, \bar{x})n(\bar{x}, \bar{v'}, t)v' \tag{2.1.2.7}$$

This is an event density on phase space and we want to account for all of scattering events that result in a particle scattering into the phase cell of interest. The first term on the right hand side of 2.1.2.6 is the purely uncollided phase space density. So, any particle that undergoes a collision, including one that leaves the particle in the same phase cell (forward scattering), is removed from the uncollided total. In order to estimate the total phase space density, we need to include scattering contributions from all velocities

(including the target phase cell of interest) that contribute to the flux in the phase cell of interest. Thus, the elastic scattering rate into the phase cell as $\Delta t \to 0$ is given in our Riemann approximation by

$$\int_{\mathbb{R}^3} v' \Sigma_r(\bar{v'} \to \bar{v}, \bar{x}) n(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' \tag{2.1.2.8}$$

In order to account for the uncollided contribution from this to the flux in a phase cell centered at $(x+v\Delta t, v)$ at time $t + \Delta t$, we will have to integrate the attenuation discounted contributions to this from in-scattering rates at each time in $[t, t + \Delta t]$. (cf. (18) p.47 of [20]))

$$\int_0^{\Delta t} \exp\left(- \int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau \right) \int_{\mathbb{R}^3} v' \Sigma_r(\bar{v'} \to \bar{v}, \bar{x} + \bar{v}\tau') n(\bar{x} + \bar{v}\tau', \bar{v'}, t + \tau') \mathrm{d}^3 v' \mathrm{d}\tau' \tag{2.1.2.9}$$

There are a few interpretive notes to make here. First, the outer time integral actually accumulates the discounted in-scattering contributions from all times in the interval $[t, t + \Delta t]$ since τ' is an integration parameter taking values in the interval of the increment and n is evaluated at $t + \tau'$ while all other functions depend on the increment only. Second, the exponential integrating factor is the uncollided flux discounting function with the change of variables described above. Finally, this contribution to the flux at the new point in space and time depends on all values of the flux along the path in time and space between the two phase cells of interest, but it depends on no values of the flux outside of this path. This implies that the stochastic evolution is Markovian.

Now we come to the non-conservative collision terms: fission, inelastic scattering and decay from existing sources. The nearly instantaneous (prompt) reaction terms will be handled very similarly to the elastic scattering term but with modifications sensitive to the specific physics of the different processes. In the fission term, we introduce an energy dependent neutron multiplicity product to account for the variable expected number of neutrons added from a fission induced at a given energy $\nu(E')$. There is also an energy distribution for the added particles that is approximately independent of the creation probability and expected count $\chi(E)$. Finally, we define β as the fraction of all neutrons created across all precursor species that are delayed by a macroscopically significant amount of time (i.e. the delayed neutron fraction). Conversely, $(1 - \beta)$ is the prompt neutron fraction. We treat β as statistically independent of all details of the creation process. Thus, the contribution to the total phase space density from neutrons promptly born with an energy $E = mv^2/2$ is given by

$$(1 - \beta) \frac{\chi(E)}{4\pi} \int_{\mathbb{R}^3} \nu(E') \Sigma_f(\bar{v'}, \bar{x}) v' n(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' \tag{2.1.2.10}$$

Similarly, promptly inelastically scattered particles have an approximately isotropic angular exit distribution but $\nu \equiv 1$

$$\frac{1}{4\pi}\int_{\mathbb{R}^3} \Sigma_{IS}(\bar{v'} \to E, \bar{x}) v' \psi(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' \tag{2.1.2.11}$$

Finally, delayed emission terms are handled by coupling to a first order spatial kinetics differential equation. (cf. [137] p.603) This implements a very simple delay model in which the time-dependent decay probability is given by a Poisson process (with parameter λ) is independent of the absorption reaction. Let i be a precursor group index, then the model is given in terms of a precursor spatio-temporal density $C_i(\bar{x}, t)$ with decay constant λ_i and creation fraction β_i such that $\beta = \sum_i \beta_i$ and

$$S_{\text{delayed,local}} = \sum_i \lambda_i(\bar{x}) \chi_i(\bar{x}, E) C_i(\bar{x}, t) \tag{2.1.2.12}$$

$$\frac{\partial C_i(\bar{x}, t)}{\partial t} = -\lambda(\bar{x}) C_i(\bar{x}, t) + \beta_i \int_{\mathbb{R}^3} \nu(E') \Sigma_f(\bar{v'}, \bar{x}) v' n(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' \tag{2.1.2.13}$$

This first order decay model combines with the transport equation to introduce a delay between deterministic free propagations on some subset of neutrons. Precursor groups can also be used to represent compound scattering neutrons that do not involve fissions. However, primarily they are used as a way of dividing up the delay kinetics into manageable subsproblems.

In practice, experiments generally reveal a small number of dominant modes to the time delay distribution. For example, the U-235 distribution reveals six major peaks [78] between 0.0127s^{-1} and 3.88s^{-1}. For the purposes of this conventional formulation of neutron transport, we will stick to this mode-averaged formulation. However, it is valuable to recognize that the decay time is really an $\mathbb{R}_+$-valued random variable associated with emitted neutron times (by extension internal processes that occur during fission events). We will use this complication in extending the fission model for the case of stochastic neutronics.

With these additional processes accounted for, we can build them into our phase space density evolution model using the same flux discounting by optical length exponents argument that we did to justify the direct elastic scattering term. Specifically, for each source term $S_i(\bar{x}, \bar{v}, t)$ we will introduce a discounted integral over the uncollided contributions:

$$S_i(\bar{x}, \bar{v}, t) = \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) S_{i,\text{local}}(\bar{x} + \bar{v}\tau', \bar{v}, t + \tau') \mathrm{d}\tau' \tag{2.1.2.14}$$

Now, we can evaluate the total contribution from each of the non-conservative collision terms:

$$S_{\text{fission}}^{\text{prompt}} = \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) (1-\beta)\frac{\chi(E)}{4\pi} \int_{\mathbb{R}^3} \nu(E')\Sigma_f^{\text{prompt}}(\bar{v'}, \bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') v' n(\bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') \mathrm{d}^3 v' \mathrm{d}\tau' \quad (2.1.2.15)$$

$$S_{\text{inelastic}} = \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \frac{1}{4\pi} \int_{\mathbb{R}^3} \Sigma_{IS}(\bar{v'} \to E, \bar{x} + \bar{v}\tau') v' n(\bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') \mathrm{d}^3 v' \mathrm{d}\tau' \quad (2.1.2.16)$$

$$S_{\text{delayed}} = \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \sum_i \lambda_i(\bar{x} + \bar{v}\tau')\chi_i(\bar{x} + \bar{v}\tau', E) C_i(\bar{x} + \bar{v}\tau', t+\tau') \mathrm{d}\tau' \quad (2.1.2.17)$$

Finally, combining all of these non-conservative contributions into 2.1.2.6, we find a transport evolution equation connecting phase cells along contributing transport paths. The result is valid over an arbitrary time interval

$$\begin{aligned}
\psi(\bar{x} + \bar{v}\Delta t, \bar{v}, t + \Delta t)\Delta V_{\text{xCell}}\Delta V_{\text{vCell}} = \\
&\exp\left(-\int_0^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) n(\bar{x}, \bar{v}, t)\Delta V_{\text{xCell}}\Delta V_{\text{vCell}} \\
&+ \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \ldots \\
&\int_{\mathbb{R}^3} v' \Sigma_{\text{ES}}(\bar{v'} \to \bar{v}, \bar{x} + \bar{v}\tau') n(\bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') \mathrm{d}^3 v' \mathrm{d}\tau' \Delta V_{\text{xCell}}\Delta V_{\text{vCell}} \\
&+ \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \ldots \\
&(1-\beta)\frac{\chi(E)}{4\pi} \int_{\mathbb{R}^3} \nu(E')\Sigma_{\text{fission}}^{\text{prompt}}(\bar{v'}, \bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') v' n(\bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') \mathrm{d}^3 v' \mathrm{d}\tau' \Delta V_{\text{xCell}}\Delta V_{\text{vCell}} \\
&+ \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \ldots \\
&\frac{1}{4\pi} \int_{\mathbb{R}^3} \Sigma_{\text{IS}}(\bar{v'} \to E, \bar{x} + \bar{v}\tau') v' n(\bar{x} + \bar{v}\tau', \bar{v'}, t+\tau') \mathrm{d}^3 v' \mathrm{d}\tau' \Delta V_{\text{xCell}}\Delta V_{\text{vCell}} \\
&+ \int_0^{\Delta t} \exp\left(-\int_{\tau'}^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \ldots \\
&\sum_i \lambda_i(\bar{x} + \bar{v}\tau')\chi_i(\bar{x} + \bar{v}\tau', E) C_i(\bar{x} + \bar{v}\tau', t+\tau') \mathrm{d}\tau' \Delta V_{\text{xCell}}\Delta V_{\text{vCell}} \quad (2.1.2.18)
\end{aligned}$$

Note that the absorption discounting is how we account fo the loss terms that generate the ith precursor

as a fraction β_i as well as a prompt events. We will briefly compare this result to the standard forms of the transport equation that have been extensively tested against experiments as check on the validity of our reasoning. If we set $t = 0,\ \Delta t = t$ then we immediately recover the standard Integral transport equation as a Volterra equation of the second kind. (compare to [20] p.47) This confirms that our formulation of the problem in terms of attenuated mono-energetic beams generated from collision and decay sources is at least valid for modeling average behavior.

On the other hand, if we let $\Delta t \to 0$ then we can recover the integrodifferential construction of transport. In this limit, the collision and decay terms can be approximated by standard Lebesgue differentiation arguments. We accomplish this by dividing all terms by Δt and noting that the outer τ' integrals converge to the value of the integrand with $\Delta t = 0$, which is just the standard form of the collision and decay terms. Now we turn our attention to the uncollided flux exponent. The locally averaged and scaled macroscopic cross section can be taken to be continuous. So, for $\Delta t << 1/v$, we can approximate the cross section integral as

$$\exp\left(-\int_0^{\Delta t} \Sigma(\bar{v}, \bar{x} + \bar{v}\tau) v \mathrm{d}\tau\right) \sim e^{-v\Delta t \Sigma(\bar{v},\bar{x})} \sim 1 - v\Delta t \Sigma(\bar{v}, \bar{x})$$

As there is no additional Δt dependence in the uncollided phase space density term (propagated from the source phase cell at $(\bar{x}, \bar{v})$), this is a perfectly good first order term. The only terms left to make sense of in this limit are the unscaled phase space density in the source and target phase cells. That is, the left hand side of the transport equation and the unital term in the uncollided phase space density expansion on the right hand side. However, this is exactly the finite difference approximation to the total material derivative which we can evaluate as $\Delta t \to 0$ using either standard Taylor expansions from continuum mechanics or differential geometric change of tangent vector basis (depending on your taste).

$$\frac{n(\bar{x} + \bar{v}\Delta t, \bar{v}, t + \Delta t) - n(\bar{x}, \bar{v}, t)}{\Delta t} \to \frac{\partial n(\bar{x}, \bar{v}, t)}{\partial t} + \bar{v} \cdot \nabla_{\bar{x}} n(\bar{x}, \bar{v}, t) \tag{2.1.2.19}$$

Substituting these first order approximations in to our integral equation, we obtain the standard form of the transport equation,

$$\begin{aligned}\frac{\partial n(\bar{x}, \bar{v}, t)}{\partial t} + \bar{v} \cdot \nabla_{\bar{x}} n(\bar{x}, \bar{v}, t) + v\Sigma(\bar{v}, \bar{x})\psi(\bar{x}, \bar{v}, t) = \\ \int_{\mathbb{R}^3} v' \Sigma_{\mathrm{ES}}(\bar{v'} \to \bar{v}, \bar{x}) n(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' + (1 - \beta)\frac{\chi(E)}{4\pi} \int_{\mathbb{R}^3} \nu(E') \Sigma_{\mathrm{fission}}(\bar{v'}, \bar{x}) v' n(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' + \\ \frac{1}{4\pi} \int_{\mathbb{R}^3} \Sigma_{\mathrm{IS}}(\bar{v'} \to E, \bar{x}) v' n(\bar{x}, \bar{v'}, t) \mathrm{d}^3 v' + \sum_i \lambda_i(\bar{x}) \chi_i(\bar{x}, E) C_i(\bar{x}, t)\end{aligned} \tag{2.1.2.20}$$

This is the most commonly cited form of the linear transport equation, although the right hand side is often rolled up into a single source term identified as a collision integral to reinforce the conceptual parallel between this equation and the Boltzmann equation.

We have been working from a physical model outlined in section 2.1.1 for describing the essential dynamics of a transport system. In the heuristic derivation above, we used a classical path interpretation of this to construct a phase space density evolution equation that includes no fluctuations. This is evident in integral form which is expressly formulated in terms of a classical propagator applied to the phase space density in the nearby source cells. By choosing our target phase space cell to be sufficiently small in the range of momenta that is includes, we are able to restrict the number of contributing source phase space cells to a specific region of coordinate space constrained by the deterministic flow. In a sense, we have incorporated a model for the phase space propagator in our choice of phase space cells to compare. By contrast, in both the classical and field-theoretic derivations of the Boltzmann equation, we begin from a many-body governing equation and explicitly construct approximations to the expected particle density.

The interpretive details disguise a very similar mathematical approach. Indeed, the field theoretic methods deployed by the Brussels school make extensive use of a propagator for the single particle density approximated by a fluctuation free propagator plus an collision integral term. [5] This explains the appearance of similar streaming terms in both the neutron transport equation and in the Boltzmann kinetics. In fact, this inter-collision determinism specifies a very large class of stochastic processes that can be reduced to similar looking kinetic equations. In this light, we see that most kinetic models can be understood as perturbation formulas where the process is generated by a potential distorted streaming term and a collision term.

For many systems, the streaming term is determined using prior knowledge of the free system obtained from simple experiments. The essence of the model is then stored in the collision dynamics. That is to say, transport physics is fundamentally a direct consequence of scattering physics. Some authors have identified this link to be a result of ideas from chaos theory. [62] This seems to be a needlessly opaque justification that contributes very little to the development of approximation methodologies. We will argue that the link between scattering and transport can be made most transparent and most amenable to direct computation through the formulation of a reaction-transport measurement model.

2.1.3 Stochastic Neutron Transport and Branching Process Models

Linear Transport Theory as we have presented it above has a critical weakness. Specifically, a linear transport theory does not provide a probabilistic model for neutron neutron number since we can't assign probabilities

to each neutron count in each volume based on the solution to a linear transport equation. The solution to a linear transport equation can only provide an estimate for the the expected path length traveled per unit volume per unit time or equivalently an expected reaction rate per unit volume. In order to access this kind of information we need to build a more general model for the probabilistic behavior underlying a linear transport theory.

Linear transport behavior is the consequence of a generalized law of large numbers applied to a nonlinear Markov process. [83] As such, deviations from the mean behavior should have very small amplitude under most conditions realized in existing reactors. However, when neutron populations are small or when material properties are changing rapidly, this expectation can be badly violated. This limitation was understood by the first nuclear scientists but linear transport theory still proved to be a useful approximation for solving a wide variety of experimental design problems.

In order to address the deficiency of not being able to model fluctuation phenomena, Bell (and separately Pál) proposed a stochastic neutron transport framework in the early 1960s [10] that was strongly influenced by Chandrasekhar's [23] and Chakrabarty's work on photon-electron cascades in the 1950s. [68],[122] Due to the enormous size and carefully engineered long timescales common to commercial reactors, much of the analytical engineering work since has focused on the approximate solution of deterministic transport models. However, the stochastic theory is the most relevant classical starting point for our work. We will discuss the spatially-dependent theory from a measurement theoretic perspective in some detail in chapter 3. However, it is worth highlighting some of the structure of the model and its similarities to the deterministic theory.

The essential idea is to construct a state space that includes both reaction events and particle number distributions for each volume. By allowing events that correspond to any arbitrary reaction volume, we effectively have a continuous state space even though particle numbers and reaction counts are discrete. We assume a Markovian evolution which is equivalent to a Chapman-Kolmogorov evolution equation in the case of a continuous state space.[134] This equation can most easily be defined in terms of the propagators starting from a single particle state and evolving through a multi-particle intermediate state to a multi-particle final state:

$$G_j \equiv \prod_{j=1}^{n_2} \mathscr{V}_D \times \mathscr{O}$$

$$\mathrm{d}\bar{u}_2^{n_2} \equiv \prod_{j=1}^{n_2} \mathrm{d}u_2^j$$

$$T((u_3^l)_{l=1}^{n_3}, t_3|u_1, t_1) = \sum_{n_2 \in \mathbb{N}} \iiint_{G_j} \mathrm{d}\bar{u}_2^{n_2} T((u_3^l)_{l=1}^{n_3}, t_3|(u_2^j)_{j=1}^{n_2}, t_2) T((u_2^j)_{j=1}^{n_2}, t_2|n_1, u_1, t_1)$$

We begin by splitting off the set on which no reactions occur. Let $T_0(u_3, t_3|u_1, t_1)$ be the evolution of the

system with no collisions from u_1, t_1 to u_3, t_3. The contribution from sets with one or more collisions are further divided up based on the type i of the first collision. Thus, we split the propagator at the collision event time t into an evolution including one collision of type i at time t and subsequent decays back to a randomly distributed free state at a later time t', given by $T_1^i((u_2^j)_{j=1}^{n_2}, t, (t'_j)_{j=1}^{n_2}|u_1, t_1)$ and any remaining full evolution past that point. By incorporating the first collision time and process duration as state parameters in purely heuristic manner, we obtain a Backward Chapman-Kolmogorov equation.

$$T(n_3, u_3, t_3|u_1, t_1) = T_0(u_3, t_3|u_1, t_1)\delta_{n_3,1} + \sum_i \int_{t_1}^{t_3} \mathrm{d}t \iiint_t^{t_3} \mathrm{d}t'_j \sum_{n_2 \in \mathbb{N}} \iiint_{G_j} \mathrm{d}\bar{u}_2^{n_2}\, T(n_3, u_3, t_3|(u_2^j)_{j=1}^{n_2}, t')T_1^i((u_2^j)_{j=1}^{n_2}, t, (t'_j)|u_1, t_1)$$

We can put this in a form that is typical of PDMP theory by viewing collisions as a point process contribution to an otherwise smooth flow. Specifically, we can introduce a single step transition rate $W_i((u_3^l)_{l=1}^{n_3}|u_2; t)$ for each transition type i. Moreover, to enforce consistency constraints relating the flow to the reaction timestamp and location, we introduce delta distributions into our T_1 operator. Namely, with $u'_2 = (x_2, k_2)$ and $u'_1 = (x_2, k_1)$ for each of the participating particles

$$T_1^i((u_2^{j,'})_{j=1}^{n_2}, t|u_1, t_1) = W_i((u_2^{j,'})_{j=1}^{n_2}; (t'_j)_{j=1}^{n_2}|u'_1; t)T_0(u'_1, t|u_1, t_1)\delta\left(\bar{x_2} - \bar{x_1} - \frac{\bar{k_1}}{m_n}(t - t_1)\right)$$

Note that we have decomposed the Chapman-Komogorov equation for the particle number probability density in each volume into a collection of gain and loss terms by partitioning the first reaction event into the set of possible reaction mechanisms. The result is a generator for a measure-valued branching Markov process for the neutron field. The Markovian assumption is an approximation since the model fails to include dynamic information about the medium. However, since the model is typically used over very short time scales, this is often an acceptable approximation. [122] This can be further refined by the following observations,

$$T_0(u_2, t_3|u_1, t_1) = \exp\left(-\int_{t_1}^{t_3} \mathrm{d}t \iiint_t^{t_3} \prod_{j=1}^{n_2} \mathrm{d}t'_j \int_{\mathscr{O}} \prod_{j=1}^{n_2} \mathrm{d}k_2^j \sum_i \sum_{n_2} W_i((u_2^j)_{j=1}^{n_2}; (t'_j)_{j=1}^{n_2}|u'_1; t)\right)$$

and

$$C_\ell^{(m_\ell, m'_\ell)} \equiv \frac{m_\ell!}{m'_\ell!(m_\ell - m'_\ell)!} e^{-\lambda_\ell(m_\ell - m'_\ell)(t_3 - t)}$$

$$\int_{t_1}^{t_3}\mathrm{d}t\iiint_{t}^{t_3}\mathrm{d}t^{n_2,'}\iiint_{\mathscr{O}}\mathrm{d}\bar{k}_2^{n_2}\,T((u_3^l)_{l=1}^{n_3},t_3|(u_2^{j,'})_{j=1}^{n_2},(t_j')_{j=1}^{n_2})$$

$$D_{\text{fission}}((u_2^{j,'})_{j=1}^{n_2},u_1',t,(t_j')_{j=1}^{n_2})Q_{\text{fission}}(t,u_1')T_0(u_1',t|u_1,t_1)$$

$$=\int_{t_1}^{t_3}\mathrm{d}t\sum_{n_2=1}^{N}\sum_{\substack{(m_0,\ldots,m_\ell,\ldots,m_M)\\ m_0+\cdots+m_\ell+\cdots+m_M=n_2}}f((\nu_\ell)_\ell=(m_\ell)_\ell|k_1)Q_{\text{fission}}(t,u_1')T_0(u_1',t|u_1,t_1)$$

$$\sum_{\substack{(n_{3,\ell})_1^M\\ \sum_i n_{3,\ell}=n_3}}\prod_{\ell=0}^{M}\sum_{m_\ell'=0}^{m_\ell}C_\ell^{(m_\ell,m_\ell')}\sum_{\substack{(n_{\ell,i})_1^{m_\ell'}\\ \sum_i n_{\ell,i}=n_{3,\ell}}}\prod_{i=1}^{m_\ell'}\left(\int_t^{t_3}\mathrm{d}t_i'\int_{\mathscr{O}}\mathrm{d}k_{2,i}\,T(n_{\ell,i},u_3,t_3|u_{2,i}',t_i')w_{\text{fission}}^{\ell}(k_{2,i})\lambda_\ell e^{-\lambda_\ell(t_i'-t)}\right)$$

The entire model that we have described up to this point has been for the evolution of a multiparticle state from a single particle. This is essentially a phase space dependent version of the idea of trees from the theory of Galton-Watson processes. As such, we can build a theory of many particle transport systems from a collection of independent trees by using generating functions and an assumption about the boundedness of transition rates. The result is the fundamental model of stochastic neutronics: the Pál-Bell equation.

$$\frac{\partial g(t_0,\bar{u}_0;t,z)}{\partial t_0}-Q(t_0,\bar{r}_0,\bar{v}_0)g(t_0,\bar{u}_0;t,z)+\bar{v}_0\cdot\nabla_{\bar{r}_0}g(t_0,\bar{u}_0;t,z) \tag{2.1.3.1}$$

$$+Q_s(t_0,\bar{r}_0,\bar{v}_0)\int_{\mathscr{O}}\mathrm{d}^3v'w_s(\bar{v}_0,\bar{v}')g(t_0,\bar{r}_0,\bar{v}';t,z) \tag{2.1.3.2}$$

$$+Q_f(t_0,\bar{r}_0,\bar{v}_0)q[\bar{s}(t_0,\bar{r}_0,\bar{v}_0;t,z)|\bar{v}_0]+Q_a(t_0,\bar{r}_0,\bar{v}_0)=0 \tag{2.1.3.3}$$

We quote this, in its most general form, directly from [122]. The source terms and the initial condition that the generator function satisfies are then related to the particular reaction volume. In the usual way of generators, moments of the particle count distribution in the reaction volume can be computed from the derivatives of g. This model is sufficient for a wide range of concrete applications involving neutron noise.

Although a great deal has been added to this model relative to the deterministic neutron transport equation, we can still see key patterns emerging in its construction. It has a division among reaction types. It has time dependent decay distributions from the medium into the neutron population. It has free streaming that looks like translation but decays off like linear attenuation. Finally, it has point-like collision events with a distribution that is absolutely continuous with respect to the Lebesgue measure on phase space. These properties and the relationship between particle counting and reaction counting will be the focus of intensive examination in chapter 3. However, most of those technical results can already be found in the literature (in particular the excellent text [122] by Pál and Pázsit). My contribution in chapter 3 is primarily a reformulation in terms of reaction events where particle number density is merely an accounting mechanism rather than the converse. We will use this reformulation in later chapters to build a quantum

stochastic theory of reaction counting.

2.1.4 Neutron Optics and Slow Neutron Scattering

So far we have discussed neutron field dynamics in terms of the evolution of particle path distributions evolving in response to asymptotic approximations to individual particle dynamics. A very different perspective on the dynamics of the neutron field can be obtained by looking at the neutron field as a matter wave scattering off of nuclear obstacles. This point of view has been used predominantly in neutron-based microscopy and neutron thermalization.[19] Although this formulation is inherently quantum mechanical and diffraction effects can be modeled directly, the particle number and the reaction number are not well-defined and measurements are assumed to be made far from the interaction region.

This framework is best understood by comparison to wave optics of photons. The square amplitude of the (neutron) matter wave is taken to be a measure of the local field intensity (particle density). The interaction dynamics with the medium are modeled as complex wave scattering from a lattice of Fermi pseudopotentials. The comparison to electromagnetic wave scattering is obvious and thoroughly studied.[19], [99], [117] This line of research has formed the basis of a litany of cold neutron technologies, from neutron interferometers to neutron diffraction microscopy. [60]

We will now outline a simple formulation of this as a scattering theory. In particular, we will use some standard results of time-independent scattering theory and optical potential modeling. This construction will prove helpful in interpreting our main results in chapter 6.

We consider a free evolution Hamiltonian $\boldsymbol{H}_0 = -1/(2m)\Delta$ and an interaction potential $V(\bar{r})$ yielding a full Hamiltonian $\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{V}$. This can be used to define a scattering theory incorporating contributions from multiple spatially isolated sources. In this way, the neutron optical theory can be used for neutron diffraction studies by way of the classical formulas. We represent a macroscopic neutron wave as an incident beamlet having spatial extent and a normalized total distribution using a function $\psi_0(\bar{r})$. We suppose that this macroscopic wave packet is incident on a volume containing multiple nuclei and we study its time evolution. The traditional ideas for describing the scattering of macroscopic wave packets can be found in Goldberger and Watson[65], a mathematically precise formulation in terms of spectral representations and Fourier transforms is given in Prugovecki's text[125], while applications to neutron optics can be found in any number of traditional texts but most of them are nicely compiled in the encyclopedic and very modern text by Byrne[19]. The essential idea is that we can define a Green's operator $\boldsymbol{G}(\xi)$ for any Hamiltonian $\boldsymbol{H}$ as the negative of its resolvent.

Let,

$$\boldsymbol{G}(\xi) = -\left(\boldsymbol{H} - \xi\right)^{-1} \tag{2.1.4.1}$$

and

$$\boldsymbol{G}_0(\xi) = -\left(\boldsymbol{H}_0 - \xi\right)^{-1} \tag{2.1.4.2}$$

Both of these operator valued functions support spectral representations in the usual way for self-adjoint operators and also using the derived integral operator representations on L_2. In particular,[125]

$$(\boldsymbol{G}_0(\xi)\psi_0)(\bar{r}) = \int_{\mathbb{R}^3} \mathrm{d}^3 r' G_0(\bar{r}, \bar{r}'; \xi)\psi_0(\bar{r}') \tag{2.1.4.3}$$

where

$$G_0(\bar{r}, \bar{r}'; \xi) = \frac{-m}{2\pi|\bar{r} - \bar{r}'|} e^{i(2\pi\xi)^{1/2}|\bar{r} - \bar{r}'|} \tag{2.1.4.4}$$

This result can be obtained directly by Fourier transform. Incorporating some theory of integral operators, we can prove that the full Green's function can be computed from the free Green's function by using a Fredholm Expansion. In order to make the implications for our problem concrete, we allow ψ_0 to be a reaction state and then compute the corresponding time advanced state (i.e. the scattering state that it maps to as the scattering process proceeds to its completion) from the Lippman-Schwinger equation,

$$\psi(\bar{r}) = \psi_0(\bar{r}) + \int \mathrm{d}^3 k \tilde{\psi}_0(\bar{k}) \int \mathrm{d}^3 r' G_0(\bar{r}, \bar{r}'; k^2/(2m)) V(\bar{r}')\Phi_k(\bar{r}') \tag{2.1.4.5}$$

where

$$\psi(\bar{r}') = \int \mathrm{d}^3 k \tilde{\psi}_0(\bar{k})\Phi_k(\bar{r}') \tag{2.1.4.6}$$

This can be simplified by studying an equation for the transform functions (also known as distorted plane waves, see [125] sections V.4-V.6), in which case this reduces to

$$\Phi_k(\bar{r}) = \frac{e^{i\bar{k}\cdot\bar{r}}}{(2\pi)^{3/2}} + \int \mathrm{d}^3 r' G_0(\bar{r}, \bar{r}'; k^2/(2m)) V(\bar{r}')\Phi_k(\bar{r}') \tag{2.1.4.7}$$

This says that plane waves in the interacting state are transformed into distorted plane waves in the outgoing free state by the scattering process. Moreover, we find that these distorted plane waves are unnormalized solutions of the Schrödinger equation. This transition is enough information to compute the angle dependent scattering amplitudes f that we measure in the far field as $|f|^2$ for sufficiently finely resolved incident

wavepackets. Indeed, we find that [19] [125]

$$f_k(\theta,\phi) = \frac{-m}{2\pi}\int \mathrm{d}^3 r' e^{-ik\bar{r}'\cdot\frac{\bar{r}}{r}} V(\bar{r}')\Phi_k(\bar{r}') \equiv -(2\pi)^2 m \left\langle k\bar{\omega}\right| \boldsymbol{T} \left|\bar{k}\right\rangle \tag{2.1.4.8}$$

where $\frac{\bar{r}}{r} = \bar{\omega}$. This yields a definition for the $\boldsymbol{T}$ matrix in terms of the distorted plane wave eigenfunctions. We can use this to directly compute observable quantities in a slow neutron scattering theory. In particular, suppose we are considering a domain with a finite number of nuclei having known elastic scattering potentials $V_j(\bar{r}-\bar{r}_j)$ localized around well separated scattering centers $\bar{r}_j$. Then we can represent the Lippmann-Schwinger equation as a sum of scattering terms due to each nucleus.

$$\Phi_k(\bar{r}) = \frac{e^{i\bar{k}\cdot\bar{r}}}{(2\pi)^{3/2}} + \sum_{j=1}^{N_m}\int \mathrm{d}^3 r' G_0(\bar{r},\bar{r}';k^2/(2m))V_j(\bar{r}'-\bar{r}_j)\Phi_k(\bar{r}') \tag{2.1.4.9}$$

From this point of view, a scattered neutron field can be directly computed from an initial field and a model potential for the system of nuclei. This kind of calculation can be seen as a kind of single scattering event. Although the multiple centers are included in the scattering calculation, they are treated as being separated from one another by a finite distance. This is appropriate to a diffraction measurement, but fundamentally at odds with any measurements that would involve repeated absorption and decay. However, by making the potential complex, we can construct an optical model that includes effective absorption along with elastic scattering. This somewhat extends the scope of the model to account for lossy systems and quantum uncertainty in position and momentum, but it is still not appropriate to describing a transport process in an evolving medium. [132],[19],[117]

It is valuable to note that the calculation we have referenced here provides the best point of comparison for interpretation of a single scattering event in the class of models that we construct in section 6.1.4. In fact, the model that we are building can be thought of as a reaction centric quantization of the Pàl-Bell equation where consistency with slow neutron scattering formulas is required to first-order in a Born approximation, where we expand $\Phi_k(\bar{r}')$ using a power series in V.

2.1.5 Field Theoretic Models of Neutron Physics

In the mid 1960s, a nonequilibirum quantum field theoretic framework was developed by Osborn and Yip for analyzing the dynamics of neutrons in a non-conservative medium. [115],[114] This framework attempts to resolve many of the limitations implicit in classical theories of neutron transport. First, it provides a quantum mechanical foundation for describing the evolution of neutron fields in the presence of a scattering medium while allowing for a variable and finite number of neutrons. Second, the theory includes many-body potential

operators that (hypothetically) could form a link to the underlying neutron scattering theory. Third, the theory allows for the calculation of multiplet densities (a feature that BBGKY theory and Baym's work on quantum kinetics achieved for the field theoretic Boltzmann kinetics).[8] Finally, the Osborn and Yip thepry resolves the superficial contradictions between the particle and wave formulations of the neutron field evolution. [114]

These remarkable successes are common to most quantum field theoretically grounded kinetic theories. However, this framework also exhibits some limitations that are common to most QFT theories. The first assumption is that there exists a second quantized Hamiltonian theory that can be used to describe the evolution of the neutron field. There are many situation where this can be constructed for suitably defined quantum stochastic processes[119] or in the representation of bounded linear operators on a Fock space[12]. For a generic unbounded process on a Fock space it is not obvious that this is possible. This can be seen from the divergence of the vacuum state energy in every quantum field theory with a quadratic Lagrangian that admits a potentially infinite number of particles.

It is possible to resolve the divergence problem using renormalization group methods (such as in QED) by incorporating the divergent interaction sum into the particle definition as an effective mass or into the potential as an effective potential. In low energy nuclear interactions, this resolution is not possible due to divergences in the potential that are necessary for representing the effective interaction outside of the QCD regime. [42] Moreover, the standard alternative of using the resummation of ladder diagrams to obtain a Galitskii integral equation for the scattering amplitude [52] has been shown to have valid first order corrections but possess divergent second order corrections for the definition of reaction cross sections in the presence of noise. Ultimately, the approximate nuclear potentials that have been studied to date are not amenable to renormalized quantum field theoretic methods at low to medium reaction energies. The meaning of any formulas expressed in terms of these unknown but supposedly globally valid potentials will necessarily remain opaque in the absence of a practical approach to phenomenological modeling.

The second assumption is that there is a fundamental separation of the nuclear scale (where neutrons have a finite width) and the transport scale (where neutrons are point like). In Osborn and Yip's theory, this is achieved through the use of cell-functions to define the neutron number distribution. ([115] p.10) This is analogous to choosing a disjoint collection of volumes in the stochastic neutron transport theory and performing a neutron counting analysis on them simultaneously.

We also note that the cell function analysis appears to be a special case of the approximate phase space instrument that we will introduce in section 4.2. However, Osborn and Yip go on to employ the creation and annihilation operators for number representation (in cell coordinates) to obtain the resulting spinor field

decomposition of the Hamiltonian. This introduces a spatial discretization that is fixed and will make it difficult to describe scattering processes in a continuous way that can be compared to neutron diffraction.

The third assumption is that collision processes are concluded on a time scale that is asymptotically small relative to the mean time between collisions. (cf. [114] p.18) This fails unambiguously for typical nuclear reaction systems as compound reactions (especially those related to delayed fission neutron emissions) can have lifetimes on the order of seconds, which is more than sufficient for particles to cover the mean free path length at thermal velocities. We can resolve this by making compound states into sequential but distinct death and birth processes. However, this raises further issues about the Hermitian nature of the Hamiltonian (even on a Fock space) and symmetries of the underlying model if we are to have any hope of retaining correlations in the locations associated to compound reaction.

Realistically, in order to resolve the time scale disassociation between different processes, we will need to allow the generator of our system's evolution to be positive and contractive rather than Hermitian. This issue and its relation to time's arrow has been discussed at great length in philosophical contexts throughout the history of quantum statistical mechanics. It is interesting to note that, from a purely mathematical perspective, it is certainly possible to dilate a quantum stochastic process for absorption and decay processes (that is not Hermitian on the natural Hilbert space) into a proper unitary evolution on a larger Hilbert space.[135]

These issues imply that, in spite of the successes of field-theoretic methods in studying particle conserving Boltzmann kinetics, a different approach is required in order to use this kind of theory in a computable model of neutron dynamics in a reactor. The physical heuristics behind Osborn and Yip's model are very useful. However, in order to tackle the nuclear data assimilation problem, we require a more detailed analysis of the connection to scattering theory, a process governed by a non-unitary evolution, and a more thorough discussion of the nature of the neutron field and the states involved in the field quantization. These three are not actually distinct problems but are all manifestations of the fact that we have not identified a quantum measurement model for describing the interaction between the neutron field and the medium or what we consider to be observable in this system.

2.2 Non-Equilibrium Statistical Mechanics and Many-Body Physics

In the previous section, we outlined the standard theories of neutron scattering and transport physics and we identified their relative strengths and limitations. We will now delve into some of the quantum and classical

non-equilibrium statistical mechanics that form the conceptual foundation of this work. This will evolve in three stages that provide us different kinds of justifications for the assumptions we will make later. We will begin by examining the problem of particle localization and its implications for symmetrization and classical approximation. We will then review some key observations from the large body of non-equilibrium field theory that grew out of the work of the Brussels school. Finally, we will analyze some famous expansions related to the number of collisions in a scattering system.

2.2.1 Localization and Symmetrization

The most elementary question that needs to be addressed is, "what is a particle in our theory?" The complexity of this question stems from two competing concerns. The first consideration is that we want the particles of our scattering theory to be the particles that we count in our reaction-transport theory. To this end, the immediate answer for a transport theory is that our particles are free neutrons represented as macroscopic wave packets in L_2. However, this raises two issues.

First, we find that in many quantum contexts (e.g. in nuclei) distinguishability breaks down and states must be represented as symmetrized or anti-symmetrized tensor products of multi-particle states. [51] At the same time, it is possible to isolate structures associated to the separate but indistinguishable nucleons even inside the nucleus.[88] The problem is further complicated by the fact that individual neutrons that decay with temporal uncertainty from an oscillating atom can have a position-momentum wave packet with a macroscopic scale. This implies that the effective radius of a free neutron is not necessarily a guide to the phase space uncertainty that we must associate to it. This requires a knowledge of the system dynamics. Thus, the application of standard measures of clustering that work well in a pure scattering experiment setting may not be a good guide to characterizing single particle volumes in a transport setting.

This issue has been studied in some detail for quantum gases.[111] It turns out that we can substitute localization for classicality to obtain a quantized Maxwell-Boltzmann statistics. This introduces exchange degeneracies for computing the equilibrium energy distribution. However, since we don't use energy distributions directly, we simply find that we are (approximately) freed from the obligation to account for symmetrization terms when neutrons are not in bound states with other nucleons. This is a significant simplification and we will make liberal use of it even though we will indicate how one would restore these symmetrization terms if the situation demanded it.

The second consideration relating to the definition of a particle is that of using bare versus dressed particles in a quantum field theory. We find that, for many practical calculations in quantum fields, it is useful to define the particle as its natural form transformed by an effective interaction. This makes it easier

to calculate in the interaction representation. This is a complex consideration and much harder to address than the first issue. We will return to this in our discussion of Galitskii integral equations. However, we will generally avoid the issue by assuming that this is incorporated into the model through the choice of L_2 representation for interaction potentials. This is clear abdication of responsibility for considering the relationship to high energy nuclear interaction models. However, in a practical sense, the techniques of nuclear data analysis for complex nuclear processes exist separately from the high energy QCD methods. Indeed, there are effective field theories for developing and fitting nucleon-nucleon potentials and it is possible to use these to model more complex nuclear dynamics as sums over pair potentials.[50] However, from a practical standpoint, the results of these analyses are ultimately cast in the terms of simpler phenomenological theories (such as optical models) when they are used in nuclear data analysis. As such, we can reasonably ignore this issue for the purposes of developing our theory and simply accept our naive definition in terms of single neutron wavepackets in phase space.

2.2.2 Collisions, Propagation, and Classical Field Theories

We will now discuss some of the work done by the Brussels school on classical field theories of non-equilibrium statistical mechanics. The analyses we will reference were developed to study models in the BBGKY hierarchy such as the Vlasov equation and the Boltzmann equation. This approximation scheme will help to illuminate the dynamical origins of the streaming and collision terms in the neutron transport equation and their implications for the evolution of macroscopic phenomena.

We will outline a conventional derivation of the BBGKY hierarchy from the N-particle Liouville equation that closely follows Balescu.[5] There are many equally good references regarding this technique, which has its origin in Prigogine's field theoretic approach to non-equilibrium dynamics. [124] However, Balescu's particular perspective meshes well with the collision expansion framework that we will develop as a quantum measurement theory.

The Liouville equation governs the evolution of a classically propagated phase space distribution function $F(q_1, \ldots, q_n, p_1, \ldots, p_n)$ (a microscopic dynamical field), which is defined by the property that it agrees with the full classical system on all measured system quantities (macroscopic dynamical fields). Every microscopic dynamical function $b(\bar{p}, \bar{q})$ evolves classically according to its Poisson bracket (which includes sums over all $6n$ degrees of freedom in a typical system of interest)

$$\partial_t b(q,p;t) = [b,H]_{\mathrm{P}} = \sum_{j=1}^{3n} \left(\frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j} \right) b(q,p;t) \tag{2.2.2.1}$$

We can construct a formal solution in terms of a classical propagator applied to an initial distribution.

$$b(q,p;t) = e^{[H]t} b(q,p;0) \tag{2.2.2.2}$$

This is fairly easy to show for typical quantities like the average kinetic energy. However, this is valid (in a weak sense that will be made clear) even for expressing the evolution of atomistic particle densities such as appear in Klimontovich representation of a transport process $\rho(x) \equiv \sum_i c_i \delta(q_i - x)\delta(p_i - x)$.[81] This is a model for the exact microscopic physics of the full many-body system. We take as given that almost all practically measurable quantities in classical statistical mechanics are of the form of a phase space average over equiprobable system configurations corresponding to a known measurement.

We claim that, for every macroscopic dynamic field $B(x,t)$, there exists a time dependent distribution function $b(q,p;x,t)$ on $\mathbb{R}^{6n}$ that is $L_1 \bigcap L_2$-integrable and normalized in L_1 such that it can be used to define a functional on the space of microscopic dynamical fields:

$$B(x,t) \equiv \langle b(q,p;x,t) \rangle = \int \mathrm{d}^{3n}p \; \mathrm{d}^{3n}q \; b(q,p;x,t) F(q,p) \tag{2.2.2.3}$$

Since, this must hold at $t = 0$, this is effectively an average over microscopic configurations that would have resulted in the observed values for all macroscopic quantities that are measured. The existence of such a function can be supported by an application of a suitable generalization of the Riesz-Frechet Representation Theorem, namely the Lax-Milgram Lemma. [91] Lets look at a relatively concrete example of constructing a physically meaningful distribution function. For any given measurement (and measurement uncertainty interval), there is a set of points in the phase space that is of significant Lebesgue measure, which would correspond to an observed measurement. If we have made multiple measurements and require that they all hold simultaneously, we can simply take the intersection of the corresponding observation sets. Then F can be taken to be a scaled characteristic function on these sets (with some cutoff or exponential decay over extreme values of unbounded sets based on a model of the configuration formation process). This representation can be seen as an application of the Equi-Probability Principle of statistical thermodynamics. We can further smooth this restricted uniform distribution function into an infinitely-differentiable function by using a gaussian mollifier (if necessary). In a classical setting, the smooth approximation can be made so sharp that there is no meaningful affect on the value of any of the measurement integrals. We will use this linear measurement construction in chapter 3 to reformulate the Pál-Bell equation into a convenient form for quantization.

Finally, we note that certain quantities like temperature, particle number, volume and pressure are

used as model parameters in an equilibrium expression for F. To the extent that they are treated this way (rather than as $\langle p\partial_p H\rangle$), these important measurements cannot really be seen as both an average like equation 2.2.2.3 and a distributional parameter. This distinction between measurable thermal parameters like (T, P, V, N) and measurable mechanical quantities representable by equation 2.2.2.3 is important to technical approximation theories of statistical mechanics. [5], [120], [141], [150] For our purposes, this observation is mostly significant because it is a reminder that not all measurable quantities are equally representable in all theories.

We will now construct an explicit evolution equation for the distribution function. Viewed as an inner product on the square-integrable functions defined on the $6n$-dimensional phase space, we can use the fact that the classical propagator is a unitary operator in phase space to transfer its adjoint onto the distribution function F without changing the integral. Thus, we arrive at a formula for modeling our collection of measurements

$$B(x,t) = \int \mathrm{d}^{3n}p\ \mathrm{d}^{3n}q\ b(q,p;x,0)e^{-[H]t}F(q,p) \tag{2.2.2.4}$$

This motivates a transition from a Heisenberg-like representation, where we average a time dependent measurement over a space of possible configurations consistent with an initial value distribution, to a Schrödinger-like representation where the time dependence is on the distribution of system configurations. In this perspective, $b(q,p;x,0)$ is a measurement prescription associated to a given set of values for the $6n$ microscopic phase space variables. By defining $F(q,p;t) \equiv e^{-[H]t}F(q,p)$ we obtain an evolution equation for the microscopic dynamical function that we are interpreting as a probability distribution of microscopic system states. This equation is the classical Liouville equation:

$$\partial_t F(q,p;t) = LF(q,p;t) \tag{2.2.2.5}$$

$$LF(q,p;t) \equiv [H(q,p), F(q,p;t]_{\mathrm{P}} = \sum_{j=1}^{3n}\left(\frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j} - \frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j}\right)F(q,p;t) \tag{2.2.2.6}$$

Using a binary interaction hamiltonian,

$$H = H_0 + H' \tag{2.2.2.7}$$

$$H_0 = \sum_j \frac{|p_j|^2}{2m} \tag{2.2.2.8}$$

$$H' = \sum_{j=1}^{n}\sum_{k<j} V(\bar{q}_j, \bar{q}_k) \tag{2.2.2.9}$$

We obtain an explicit form for LF,

$$L = \sum_{j=1}^{3n} \frac{\partial H_0}{\partial p_j}\frac{\partial}{\partial q_j} + \sum_{j=1}^{3n} \frac{\partial H'}{\partial q_j}\frac{\partial}{\partial p_j} \tag{2.2.2.10}$$

$$= \sum_{j=1}^{3n} \frac{-\bar{p_j}}{m} \cdot \nabla_{\bar{q}_j} + \sum_{j=1}^{n} \nabla_{\bar{q}_j} \left(\sum_{k<j} V(\bar{q}_j, \bar{q}_k) + \sum_{k>j} V(\bar{q}_k, \bar{q}_j) \right) \cdot \nabla_{\bar{p}_j} \tag{2.2.2.11}$$

The first term will become the streaming term in the Boltzmann equation while the second term will give rise to mean field path corrections and localized scattering terms.

This can be recast in terms of a reduced distribution function by way of the BBGKY hierarchy. The essential insight here is that the expressions that we use to calculate the macroscopic dynamical functions are symmetric in the identical particles that make up the Boltzmann gas and can be recast in terms of only the first few s-particle distribution functions where $s = 1, \ldots, n$. Specifically, we define a reduced distribution function which inherits the identical particle index permutation symmetry of the full distribution function and describes the marginal distribution associated to the first s particles.

$$f_s(q_1, p_1, \ldots, q_s, p_s) = \frac{n!}{(n-s)!} \int \mathrm{d}^3 q_{s+1}\, \mathrm{d}^3 p_{s+1} \ldots \mathrm{d}^3 q_n\, \mathrm{d}^3 p_n F(q_1, p_1 \ldots, q_s, p_s, q_{s+1}, p_{s+1} \ldots, q_n, p_n) \tag{2.2.2.12}$$

we then decompose the dynamical microscopic function into a sum of symmetric non-additive (i.e. those that do not depend on their parameters additively) functions,

$$b(q_1, p_1, \ldots, q_n, p_n) = b_0 + \sum_{j=1}^{n} b_1(q_j, p_j) + \sum_{k=1}^{n} \sum_{j<k} b_2(q_j, p_j, q_k, p_k) + \ldots b_n(q_1, p_1, \ldots, q_n, p_n) \tag{2.2.2.13}$$

We then use the permutation symmetry to reduce the macroscopic dynamical function to a sum of identical integrals on the first s particles with the multiplicity getting absorbed into the normalization of the reduced distribution function.

$$\langle b(q, p; x, t) \rangle = \sum_{s=1}^{n} \frac{1}{s!} \int \mathrm{d}^{3s} p\, \mathrm{d}^{3s} q\, b_s(q_1, p_1, \ldots, q_s, p_s) f_s(q_1, p_1, \ldots, q_s, p_s) \tag{2.2.2.14}$$

Thus, calculation of macroscopic dynamical functions that can be experimentally measured is reduced to a knowledge of the reduced distribution function integrals, each of which will behave like a macroscopic

dynamical function in its own right. Based on the fact that the full distribution F satisfies the Liouville equation, then for zero flux or periodic boundary conditions or in the thermodynamic limit, we can construct a hierarchy of equations for the reduced densities. The result can only be established as a convergent approximation to the Liouvillian dynamics in the thermodynamic limit. The thermodynamic limit is realized as the particle number becomes infinite but the density remains finite and characterizes the "bulk" behavior of a system. [141], [13] The resulting model is known as the BBGKY hierarchy, for which the single particle density is seen to be the solution of the first order linear differential equation

$$\partial_t f_1(\bar{q}_1, \bar{p}_1) = -\frac{\bar{p}_1}{m} \cdot f_1(\bar{q}_1, \bar{p}_1) + \int \mathrm{d}^3 p_2 \, \mathrm{d}^3 q_2 (\nabla_{q_1} V(|\bar{q}_1 - \bar{q}_2|)) \cdot (\nabla_{p_1} - \nabla_{p_2}) f_2(\bar{q}_1, \bar{p}_1, \bar{q}_2, \bar{p}_2) \tag{2.2.2.15}$$

while the s-particle density for $s > 1$ is given as the solution of

$$\begin{aligned} \partial_t f_s(\bar{q}_1, \bar{p}_1, \ldots, \bar{q}_s, \bar{p}_s) = &- \sum_{j=1}^{s} \frac{\bar{p}_j}{m} \cdot f_s + \sum_{k=1}^{s} \sum_{j<k} (\nabla_{q_j} V(|\bar{q}_j - \bar{q}_k|)) \cdot (\nabla_{p_j} - \nabla_{p_k}) f_s \\ &+ \sum_{j=1}^{s} \int \mathrm{d}^3 p_{s+1} \, \mathrm{d}^3 q_{s+1} (\nabla_{q_j} V(|\bar{q}_j - \bar{q}_{s+1}|)) \cdot (\nabla_{p_j} - \nabla_{p_{s+1}}) f_{s+1}(\bar{q}_1, \bar{p}_1, \ldots, \bar{q}_{s+1}, \bar{p}_{s+1}) \end{aligned} \tag{2.2.2.16}$$

Note that the collision probability for the one particle reduced distribution function is expressed in terms of the two particle distribution function, which in turn is characterized in terms of the 3 particle distribution function and so on. (cf. [5] section 4.2-4.3) The BBGKY Hierarchy is a significant result in the history of non-equilibrium theory. For our purposes, it is mostly significant because we can use it to express a perturbation theory of correlation functions in terms of multi-particle interactions. As in quantum field theory, we can rewrite the reduced distribution function hierarchy as a one particle distribution function and a collection of "connected" multi-particle correlation functions.

By applying this process to the BBGKY hierarchy and canceling terms using the $s = 1$ equation, we obtain factorized expressions for the first two BBGKY equations. Let

$$D_j = \partial_t + \bar{v}_j \cdot \nabla_{q_j} \tag{2.2.2.17}$$

$$D_{jk} = \partial_t + \bar{v}_j \cdot \nabla_{q_j} + \bar{v}_k \cdot \nabla_{q_k} \tag{2.2.2.18}$$

$$L_{jk} = (\nabla_{q_j} V(|\bar{q}_j - \bar{q}_k|)) \cdot (\nabla_{p_j} - \nabla_{p_k}) \tag{2.2.2.19}$$

then the governing equation for the single particle distribution function is

$$D_1 f(x_1; t) = \int_{\mathbb{R}^6} \mathrm{d}x_2 [L_{12} f(x_1; t) f(x_2; t) + L_{12} g_2(x_1, x_2; t)] \tag{2.2.2.20}$$

while the governing equation for the two-particle correlation function is

$$D_{12}g_2(x_1,x_2;t) = L_{12}f(x_1;t)f(x_2;t) + L_{12}g_2(x_1,x_2;t) + \int_{\mathbb{R}^6} \mathrm{d}x_3[L_{13}(f_1(x_1;t)g_2(x_2,x_3;t) + f_1(x_2;t)g_2(x_1,x_3;t)) + (L_{13}+L_{23})(f_1(x_3;t)g_2(x_1,x_2;t) + g_3(x_1,x_2,x_3;t))] \quad (2.2.2.21)$$

These are nonlinear governing equations for the connected components of the first two joint particle distribution functions. Therefore, they are easier to compute approximate solutions for but more difficult to characterize analytically than the original Liouville equation.

The Liouville equation acts on a very large number of variables and is not numerically solvable by standard methods. By virtue of its linearity and the simple way it acts on those variables, it is relatively easy to characterize functional analytic approximation schemes and the spaces of functions that they work on by using simple tools from the theory of linear operators. However, the link between the macroscopic state that would be measured in practice and the microphysics is obscured by complexity.

Conversely, the reduced model (2.2.2.21) is more computationally tractable and clarifies the mechanism by which local physics drives macroscopic correlations. However, it does so at the cost of functional analytic clarity (since the theory of linear operators only applies indirectly).

We will now interpret the reduced model for one and two particle distributions. The free dynamics are the result of ignoring all interaction terms L_{jk}. The free dynamics evolve the reduced distribution function representation of the system according to the classical paths that the individual particles would take in the absence of any other particles. For charged particles we would need to account for the presence of external fields. However, for unpolarized neutrons is suffices to take the free dynamics as,

$$D_1 f(x_1;t) = 0 \quad (2.2.2.22)$$

$$D_{12}g_2(x_1,x_2;t) = 0 \quad (2.2.2.23)$$

this yields a propagator that is nearly trivial

$$f(\bar{q}_1,\bar{v}_1;t) = U_1^0(t)f(\bar{q}_1,\bar{v}_1;0) \equiv e^{-t\bar{v}_1\cdot\nabla_{q_1}}f(\bar{q}_1,\bar{v}_1;0) \quad (2.2.2.24)$$

However, this is recognizable as the infinitesimal generator representation of the translation operator by

standard Lie group arguments. Consequently, we have a translation representation of the free propagator

$$f(\bar{q}_1, \bar{v}_1; t) = f(\bar{q}_1 - \bar{v}_1 t, \bar{v}_1; 0) \tag{2.2.2.25}$$

By the same group representation argument we obtain a free propagator translation representation for the 2 particle correlation function:

$$g_2(\bar{q}_1, \bar{r}_{21}, \bar{v}_1, \bar{v}_{21}; t) = g_2(\bar{R} - \bar{V}t, \bar{r}_{21} - \bar{v}_{21}t, \bar{V}, \bar{v}_{21}; 0) \tag{2.2.2.26}$$

Note that these only hold as exact expressions for the free dynamics. We can interpret this to mean that when the reduced distribution function or the correlation function undergoes an evolution by a free propagator, the distributional mass propagates through the state space along a characteristic curve (namely, the $\nabla V = 0$ constant momentum trajectories). This is consistent with the conventional analysis of first order partial differential equations.

This would also be the expected dynamics of a solitary classical particle, moving in a vacuum. In order to get further insight into the dynamics that will influence the evolution of the distribution function in the case of Boltzmann kinetics, we will need to analyze a formal solution to the full two body problem. This will be done in three stages: (1) the two-body propagator equation, (2) its use in analyzing a simplified correlation function equation, and (3) its interpretation as a scattering model. We begin by supposing that the connected two-particle correlation function satisfies a simplified dynamics relative to equation (2.2.2.21). Specifically, suppose that we can represent the evolution in terms of a linear operator acting on g_2 alone and a source term:

$$(D_{12} - L_{12})\, g_2(\bar{q}_1, \bar{r}_{21}, \bar{v}_1, \bar{v}_{21}; t) = S(\bar{q}_1, \bar{r}_{21}, \bar{v}_1, \bar{v}_{21}; t) \tag{2.2.2.27}$$

subject to some initial distribution belonging to a nice space and decay rate based boundary conditions at infinity compatible with our original Liouville equation constraints. Then it is well known that we can obtain a formal solution by application of Green's function (semigroup) methods. Convergence and uniqueness of the resulting solution are separate questions that we will set aside for now. As is so often the case in field theory, we will proceed by ignoring many of the analytic properties of our approximations until we arrive at something well-defined. Our goal here is still essentially heuristic, in spite of the level of detail in these

arguments. As such, we define a propagator equation,

$$\partial_t G_{12}(t) = \left(\bar{V} \cdot \nabla_R + \bar{v}_{21} \cdot \nabla_{\bar{r}_{21}} + L_{12}\right) G_{12}(t) \tag{2.2.2.28}$$

$$G_{12}(0) = \mathbb{I} \tag{2.2.2.29}$$

Then, we can show that

$$g_2(t) = G_{12}(t)g_2(0) + \int_0^t \mathrm{d}\tau G_{12}(\tau) S(\bar{q}_1, \bar{r}_{21}, \bar{v}_1, \bar{v}_{21}; t-\tau) \tag{2.2.2.30}$$

How do we interpret this result? First, we can observe that G_{12} satisfies the propagator equation for the two-body dynamical Liouville equation. However, this is precisely the model for a two body collision and in the absence of any other interactions, the two-body Liouville equation would represent precisely one collision and would correspondingly decay to isolated free states for large times. (cf. classical potential scattering theory or born approximated quantum scattering) This is significant because we note that the differential equation 2.2.2.28 also agrees with the full BBGKY two-particle propagator equation without three-body contributions, given by equation (2.2.2.16) for $s = 2$ in the absence of three body interactions. The neglect of three-body terms can be justified by low density asymptotics. The common propagator governing equation indicates that both solutions have the same decay properties for **the same initial localization**. As such, the exponential decay of the solution of the scattering problem (2.2.2.28) to $f(x_1)f(x_2)$ indicates that action of the BBGKY propagator on $f_2(x_1, x_2; t)$ leads to an exponential decay to $f(x_1)f(x_2)$ and, consequently, an exponential decay of $g_2(x_1, x_2; t) \to 0$. Therefore, at large times, $G_{12}(t)g_2(0) \to 0$. Moreover, as the mass of the single particle states becomes separated under the action of the propagator, the interaction through a short range central potential dies off exponentially. Thus, it follows from the fact that L_{12} is the Liouvillian two-body interaction term, that for pairwise potential scattering, the potential scattering contribution for intermediate to large times becomes strongly subdominant to the contribution at early times

$$\int_{\tau_c}^{\infty} \mathrm{d}t L_{12} G_{12}(t) L_{12} f_2(t) << \int_0^{\tau_c} \mathrm{d}t L_{12} G_{12}(t) L_{12} f_2(t) \tag{2.2.2.31}$$

Formula 2.2.2.30 forms the basis of a laplace-type asymptotic integral approximation for equation (2.2.2.30). [11] This result supports the schematic observation that the distributional mass of the interacting particles becomes widely separated at large times while the interaction domain remains localized around each of the separate wavepackets. Moreover, this connects back to our earlier observations about particle localization.

Following Balescu in this section, we have constructed a BBGKY hierarchy decomposition of the full

system dynamics into a sequence of correlation functions that are assumed to be of decreasing importance. Specifically, the higher order correlation functions are assumed to have decaying amplitude and thus a decaying impact on their prediction for macroscopic measurements through the integral representation 2.2.2.3 and 2.2.2.14. This is why the Boltzmann equation becomes such a powerful tool for the analysis of macroscopic measurements. Moreover, this approximation scheme has revealed a microscopic origin to dynamical features of macroscopic measurements. A similar analysis is possible for quantum mechanical systems by expanding Green's operators. [87] [8]

When we apply this to number density measurements for the gas being studied we can see that the propagation of density waves has two distinct origins that are sometimes referred to as the zero sound and the second sound. [101] By introducing an exclusively two-body interaction Hamiltonian we were able to construct a form of the Liouville equation 2.2.2.10 that already exhibited some of the essential structure of the two drivers of sound propagation. In particular, we isolated a streaming term and a collision term. Some density wave propagation exists in the absence of collisions and can be understood purely as streaming in a potential 2.2.2.25. This is sufficient for modeling macroscopic density evolution only in zero temperature systems like simple models of quantum liquids. [128],[101] In finite temperature systems, the collision physics 2.2.2.30 introduce a significant complication and need to be accounted for carefully because of the potentially large individual amplitude of the scattering events. This last point is the main subject of discussion in the next section.

2.2.3 Scattering Count Expansions

This section is devoted to a brief survey of important methods for constructing expansions in the number of scattering events that occur in a given time interval. We will ignore the family of non-perturbative methods that came out of the study of Anderson Localization [39],[73] because they are difficult to connect meaningfully to our methodology. Instead, we will focus on the older field theoretic methods used in the renormalization of cross sections by virtual processes as these hew closer to the point of view that we will ultimately adopt for a reaction counting quantum stochastic process. This discussion will begin with a brief review of the interaction representation and perturbative expansions of time ordered exponents. We will then address the fact that phenomenological nuclear potentials don't need to have an intrinsic small parameter and how this can be partially overcome by the Galitskii integral equation. Finally, we will discuss the cluster expansions of constructive quantum field theory (that we tacitly invoked in the last section) as they are a powerful tool for understanding the relationships between different trees in a more general quantum branching process.

Interaction Representation and Time-Dependent Perturbation Theory

We will begin with a conventional discussion of the interaction representation and time-ordered exponents that can be found in any basic text on quantum mechanics. [133],[7] This will furnish a simple, well-studied prototype for the time-dependent perturbation expansion that this research revolves around. We begin from a Hamiltonian with a free and a perturbative part,

$$\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{V} \tag{2.2.3.1}$$

We allow all vectors to transform continually in time according to the free propagator $\boldsymbol{U}^0_{\Delta t}$, which satisfies the semigroup equation

$$\boldsymbol{U}^0_{t-t_0} = e^{-i(t-t_0)\boldsymbol{H}_0} \tag{2.2.3.2}$$

Interaction representation vectors thus take the form

$$|\psi_I(t)\rangle = \boldsymbol{U}^{0,*}_t |\psi(t)\rangle \tag{2.2.3.3}$$

This, in principle, unwinds the effect of the free evolution over each interval so that the vector is relatively static in that it only evolves in response to potential induced transitions. We can imagine this as a process that already takes into account all of the free dynamics as part of the vector and operator definitions so that the only thing that needs to be computed is the change due to collisions. In order for this representation to leave all of the expectation values intact, we need to also transform any operator that acts on the vector by

$$\boldsymbol{A}_I(t) = \boldsymbol{U}^{0,*}_t \boldsymbol{A} \boldsymbol{U}^0_t \tag{2.2.3.4}$$

so that

$$\langle\psi(t)| \boldsymbol{A} |\psi(t)\rangle = \langle\psi_I(t)| \boldsymbol{A}_I(t) |\psi_I(t)\rangle \tag{2.2.3.5}$$

and

$$\boldsymbol{V}_I(t) = \boldsymbol{U}^{0,*}_t \boldsymbol{V} \boldsymbol{U}^0_t \tag{2.2.3.6}$$

then we can define an interaction representation propagator $\boldsymbol{U}^I_t$ that evolves a vector in the interaction representation

$$|\psi_I(t)\rangle = \boldsymbol{U}^I_t |\psi_I(0)\rangle \tag{2.2.3.7}$$

we find that the interaction propagator satisfies

$$\frac{\mathrm{d}\boldsymbol{U}_t^I}{\mathrm{d}t} = -i\boldsymbol{V}_I(t)\boldsymbol{U}_t^I \tag{2.2.3.8}$$

so that our effective Hamiltonian is now $\boldsymbol{V}_I(t)$. Since this is not a time independent generator of the semigroup, we arrive at an integral equation rather than a pure exponential representation

$$\boldsymbol{U}_t^I = \boldsymbol{I} - i\int_0^t \mathrm{d}t'\boldsymbol{V}_I(t')\boldsymbol{U}_{t'}^I \tag{2.2.3.9}$$

Now using the fact that $\boldsymbol{U}_t = \boldsymbol{U}_t^0\boldsymbol{U}_t^I$, we obtain

$$\boldsymbol{U}_t = \boldsymbol{U}_t^0 - i\int_0^t \mathrm{d}t'\boldsymbol{U}_{t-t'}^0\boldsymbol{V}\boldsymbol{U}_{t'} \tag{2.2.3.10}$$

A parallel can be seen to the Forward Chapman-Kolmogorov equation (or with a little more imagination, the Lippman-Schwinger equation). However, this version is non-commutative and only applies to conservative systems that possess a reversible (unitary) evolution. Moreover, the existence of a solution is by no means obvious. The usual formal solution is given by a time ordered exponent

$$\boldsymbol{U}_t^I = T(e^{\int_0^t \mathrm{d}t'\boldsymbol{V}_I(t')}) \tag{2.2.3.11}$$

where the integrals are made to apply over domains such that the temporally later interactions are always further left in the product. This motivates the generalized path integral form of correlation generators used in perturbative quantum field theory. (see, for example, the Gell-Mann and Low theorem)[150],[58],[52] Moreover, the analogy to a Chapman-Kolmogorov equation suggests a link between potentials and probability distributions via a path integral type representation. This idea was brought into a precise form via Feynman-Kac type theorems for self-adjoint Feller operators. [36],[98],[43],[109] Clarifying this analogy proves to be a significant technical feat but it forms a profound link between stochastic processes, interacting particle systems, Banach spaces, and quantum mechanics. The simplest example is for diffusion operators and Wiener processes.[139] The results of this theory can be found in any advanced text on probability theory and stochastic integration. Although we will adopt a different methodology for studying the quantization of our stochastic neutron transport processes, path integral quantization has a long history of successfully quantizing complex systems by exploiting the simplicity of Lagrangian representations for classical paths.[80]

The formula 2.2.3.10 motivates a point of view about transport processes that will prove very fruitful once

it is correctly formalized. Specifically, it suggests that an evolution can be broken into a chain of free evolutions and interactions. Although this idea is appealing, the expansion implied by 2.2.3.11 is only convergent in a weak coupling approximation. In particular, $\boldsymbol{V}$ must induce a small transition probability (for example by having a small total norm). The naive interpretation of $\boldsymbol{V}$ as the one particle interaction potential can be used effectively for many purposes. For example, in kinetic theory of low density plasmas, the dynamics are dominated by weak long range potentials. However, for hard core potentials and strongly repulsive nuclear potentials this approach cannot be justified. This raises the question, "is there a diagrammatically similar expansion procedure that can be shown to be convergent for strong potentials in low density gases?" As we will show next, the answer is a conditional yes that will further motivate the construction that we use for reaction measurement operators in chapter 5.

T Approximation

We can build on the interaction representation based perturbation theory by moving from an expansion in orders of the potential operator $\boldsymbol{V}$ to orders of the scattering amplitude f. Even when dealing with strong repulsive potentials (such as those for nuclear collisions at very small ranges), the scattering amplitude is a small quantity. This can be applied to the analysis of a translation invariant imperfect fermi gas. (cf. [52] p.128) In this context, we can build a scattering theory based on the idea of a particle scattering off of the medium (which consists of an infinite number of particles). This is accomplished by resumming ladder diagrams. Ladder diagrams consist of those Feynman diagrams arrived at by expanding the scattering amplitude and coupling it to virtual excitations in the medium where the particle that couples to the scattering amplitude is a real particle and not a hole. This all comes from the forward propagating part of the perturbatively expanded Feynman propagator.

Applying this technique to the two particle interaction potential yields a procedure for computing the effective interaction $\boldsymbol{\Gamma}(p_1, p_2; p_3, p_4)$ between the two particles when you account for contributions due to participation of intermediate states involving the dynamic medium. The result is a renormalized integral equation called the Bethe-Salpeter equation

$$\boldsymbol{\Gamma}(p_1, p_2; p_3, p_4) = \boldsymbol{U}_0(p_1 - p_3) + \frac{i}{(2\pi)^4} \int \mathrm{d}^4 q \boldsymbol{U}_0(q) \boldsymbol{G}_0(p_1 - q) \boldsymbol{G}_0(p_2 + q) \boldsymbol{\Gamma}(p_1 - q, p_2 + q; p_3, p_4) \quad (2.2.3.12)$$

by introducing effective wave functions we can reduce this to an expansion in integrals over products of free particle scattering amplitudes that is referred to alternately as Galitskii's integral equations[52], the T approximation[8], or the Ladder diagram expansion. This justifies the effective renormalization to first order of the scattering cross section in the presence of a dynamic medium. This technique has been used in the

study of nuclear matter and quantum liquids.

Fundamentally, this is of interest to us because it provides a justification for dominating repeated scattering processes against a medium by replacing pure potential interactions with their resummation in the form of full scattering events. This is achieved by introducing a coupling through the T matrix rather than $\boldsymbol{V}$ itself. We will use this observation in our construction of example reaction transition operators in chapter 6.

Cluster Expansions

We now come to the topic of cluster expansions. As we noted, there is a standard approach to this problem using classical generating functions for independent trees in the stochastic neutronic theory. However, in the general quantum field theory, a more technical method is necessary. The full technique can be understood by studying the work done in constructive quantum field theory on cluster expansions. [64],[63],[98] For simplicity, we will focus on the combinatorial part of the technique (rather than the analytic decay estimates) as applied to classical correlation functions. A simple variation on this method appears in any of the standard texts on non-equilibrium physics that were produced by the Brussels school. For the sake of continuity with our earlier discussion, we follow the formulation in Balescu. [5]

In order to make this process reasonably precise, we need to explain what we mean by connected multi-particle correlation functions. If we think of the reduced distribution functions as governing the joint distribution of $2s$ random vectors then fully independent particle motion (i.i.d random variables by symmetry) would be formally equivalent to factorization of the probability density. Thus, following the notation of Balescu (where in $(\bar{q_k}, \bar{p_k}) = x_k$),

$$f_s^{\text{unc}}(x_1, \ldots, x_s; t) = \prod_{k=1}^{s} f_1(x_k; t) \tag{2.2.3.13}$$

is the uncorrelated (independent particle) density. With this observation we can define a two particle correlation function,

$$f_2(x_1, x_2; t) = f_1(x_1; t) f_1(x_2; t) + g_2(x_1, x_2; t) \tag{2.2.3.14}$$

Here, g_2 is the connected contribution to the two particle joint density. In a practical sense, this just means that this part of the density is non-factorizable in its phase space arguments. However, the name comes from the diagrammatic representation of perturbation series as graphs.

We can extend this definition to correlation functions for $s > 1$. However, it requires that we account for all lower order factorizations and not just a complete lack of correlation. Essentially, we are noting that it is

possible for any lower order correlation to contribute structure to a higher order correlation. For Δ a given partition of the set $\{1,\ldots,s\}$ and σ_Δ being the permutation required to swap the indices from the first j_k indices in to the right values in order to match up with Δ

$$f_s(x_1,\ldots,x_s;t)=\sum_{\Delta}\prod_{\substack{\sigma_\Delta(\{1,\ldots,j_k\})\in\Delta\\ \sum_k j_k=s}} g_{j_k}(x_{\sigma_\Delta(1)},\ldots,x_{\sigma_\Delta(j_k)};t)+g_s(x_1,\ldots,x_s;t) \tag{2.2.3.15}$$

For example,

$$\begin{aligned} f_3(x_1,x_2,x_3;t) = {} & f_1(x_1;t)f_1(x_2;t)f_1(x_3;t)+ \\ & f_1(x_1;t)g_2(x_2,x_3;t)+f_1(x_2;t)g_2(x_1,x_3;t)+f_1(x_3;t)g_2(x_1,x_2;t)+ \\ & g_3(x_1,x_2,x_3;t) \end{aligned} \tag{2.2.3.16}$$

This expansion in connected substructures with a residual is commonly referred to as a cluster representation or cluster expansion. It can also be justified algebraically for any system instantaneously governed by a Gibbs measure, by comparing a perturbative expansion of the free energy $\ln(Z)$ to the path integral definition of the correlation functions.([150] p.160, [80] p.288) This is valid for quantum field theories and by wick rotation it is also applicable to statistical field theories. If we consider this as a recursive definition and do not substitute these expressions back in to one function then we do not need to address questions about the convergence of the resulting cluster series that can only be answered affirmatively for special cases in the thermodynamic limit. Some discomfort with the treatment of divergences in standard quantum field theories is warranted but convergence results for the Meyer Cluster Expansion are also well established in classical statistical mechanics and constructive field theory for systems representable by a Gibbs Measure in a thermodynamic limit. (cf. chapter 2 and chapter 18 of [64]) This approach is valid far from critical points. (cf. [53], [150]) Specifically, this is a useful approach under the same circumstances when the mean field theory of quantum fields is an accurate approximation to the system of interest.

2.3 Quantum Measurement Theory

In this final section of the review of literature, we will provide the standard technical definitions of the ideas of an Operation, an Instrument, and a Quantum Stochastic Process (QSP). The relationship between these measurement theory definitions can be understood loosely as follows. An Operation is the transformation that happens when a measurement event occurs. An Instrument is a function mapping all possible measure-

ment events to Operations for a particular non-ideal measurement process. A Quantum Stochastic Process is a family of instantaneous Instruments connected through a time index in the manner of a stochastic process to provide a measure on events in both the measurement space and in time. Before we get down to the business of making this more precise, we will briefly summarize some motivations.

The most fundamental fact about quantum mechanics is that it is a theory of measurement where the act of measuring can change the underlying quantity to be measured. Although this fact is often presented with diminished significance relative to discussions of complex wave equations and uncertainty principles, the measurement theoretic character of quantum mechanics is the foundation of both the beautiful functional analytic character of quantum mechanics and the most potent physical intuitions for understanding what makes quantum mechanics distinct from its classical analogue.[146]

One of the greatest short comings of traditional quantum mechanics is the inability to represent non-conservative dynamics or classically imperfect a priori information. This led to a number of powerful technical formulations of quantum statistical mechanics. [95] [143] [8] However, building on von Neumann's work, a careful analysis of the measurement problem itself reveals a particular approach to the theory of open quantum systems that is directly connected to practical questions of what can be measured and the structure of noise distributions. [86] [15] For clarity, we will distinguish this approach from other common approaches to quantum statistical mechanics by referring to it as "quantum measurement theory". Modern treatments of quantum measurement theory tend to be explicit in their connection with the application of statistics to experimental problems. [16] [147] [71] This offers another motivation for the decision to use this formalism over other formalisms that are generally easier to use.

In spite of the fundamental role of measurement in quantum theory, even technically detailed references on the traditional theory of quantum mechanics spend very little time characterizing how a quantum measurement changes the measured system. [125] By contrast, in the theory of quantum measurement, it is paradigmatic that a large class of quantum evolutions can be understood as the combination of a Hamiltonian evolution with the back-action of a continuous measurement on a system. This effort to include the effect of repeated measurements explicitly in the system model leads to substantial mathematical extensions of the traditional theory.

In order to make this comparison explicit, we will begin by examining the standard measurement ideas of traditional quantum mechanics. In the correspondence statements of traditional quantum mechanics, a clear distinction is made between preparatory and determinative measurements. [125] The preparatory measurement can be described in terms of an arbitrary prepared "state of the system" (represented as a vector in a Hilbert space) at the end of the preparatory measurement. This vector is given as $|\psi\rangle$. The determinative

measurement is described as a predicted meter reading expressed as an observable operator $\boldsymbol{O}$ evaluated against a prepared vector $|\psi\rangle$ as $\langle\psi|\,\boldsymbol{O}\,|\psi\rangle$. In this theory, a study of spectral integral representations reveals that the back-action of any approximate position measurement can be understood as projection operator realized as multiplication by an indicator function in an L_2 representation. Generally then, a collection of commuting preparatory measurements act on the system vector through a projection. [125] Although this measurement model sufficient for the application of simple constructions like Fermi's Golden Rule, the resulting picture provides us relatively little information about how the system is changed by a more general lossy measurement. This is especially true when that measurement is not instantaneous. This raises many questions about if it is possible for a measurement to be both preparatory and determinative (see studies of the quantum Zeno effect [16]) or what approximate simultaneous measurements of non-commuting random variables look like. The answers to these questions are indirectly essential to any quantum theory of reaction-transport. As such, we will require a more general formalism based on the density matrix operator.

The traditional quantum theory can only encode the so called pure states for the description of quantum systems. In order to describe a more general class of processes, we will need to work with trace class operators in the state space of a Hilbert space as our system representation, rather than vectors in a Hilbert space. This will introduce a wide array of mathematical challenges for which there are corresponding answers that enrich the set of possible systems described by a quantum measurement theory. Most basically, the vector space of Trace class operators on a Hilbert space is a Banach space rather than a Hilbert space. Many powerful ideas from functional analysis are preserved, including a kind of relative of Riesz representation for functionals along with a spanning criterion, a spectral representation theorem for trace class operators, and the Riesz functional calculus. However, much of the traditional unitary group theory that we rely on for describing system evolutions is now out of bounds. Instead, we must rely on the much more delicate theory of strongly continuous semigroups on Banach spaces. This is both essential and liberating when it comes to modeling. Most importantly, any general theory of quantum measurement worth the name should be able to represent irreversible processes. A traditional quantum theory clearly can't manage this since it is built on unitary group evolutions that are, by definition, reversible. [91]

2.3.1 Review of Functional Analysis

We begin by specifying a separable Hilbert space $\mathscr{H}$ as the vector space of states of the underlying quantum system. To this Hilbert space, we associate a Banach space over $\mathbb{C}$: the space of bounded linear operators $\mathscr{L}(\mathscr{H})$ in the uniform operator norm $\|\boldsymbol{A}\| = \sup_{\substack{\|x\|_{\mathscr{H}}=1 \\ x\in\mathscr{H}}} \|\boldsymbol{A}x\|_{\mathscr{H}}$. As a closed subspace of these operators, we have the compact operators $\mathscr{C}(\mathscr{H})$ defined by the property that it is the norm closure of the finite rank

operators in $\mathscr{L}(\mathscr{H})$. That is, for every compact operator, there is a sequence of matrices that eventually becomes arbitrarily close to the compact operator in the uniform norm. The equivalence of this definition to more generally useful topological definitions can be proven using the Riesz functional calculus for projection operators and integration paths forming loops around the isolated eigenvalues of the spectrum. It is an important fact that every compact operator has a countable number of eigenvalues λ_k, each with finite multiplicity and at most one accumulation point at 0. Moreover, any operator with such a spectrum is compact. Finally, for every compact operator on a Hilbert space, we can define an absolute value $|\boldsymbol{A}| = (\boldsymbol{A}^*\boldsymbol{A})^{1/2}$ using the functional calculus and it follows that the absolute value is also compact. A positive compact operator has exclusively positive eigenvalues and a single maximal eigenvalue. This allows us to define a new norm. [91]

Definition 2.3.1. *Trace Norm and Trace Class*

For any $\boldsymbol{A} \in \mathscr{C}(\mathscr{H})$, we can arrange the countable set of eigenvalues including multiplicity in descending order. If $(\lambda_k)_{k\in\mathbb{N}}$ are the suitably ordered eigenvalues including multiplicity of $|\boldsymbol{A}|$ then the trace norm is defined to be

$$\|\boldsymbol{A}\|_{\mathrm{Tr}} = \sum_k \lambda_k \tag{2.3.1.1}$$

The linear subspace of compact operators with finite trace norm is closed in the trace norm and forms a Banach space that is usually called the space of trace class operators. This Banach space is assigned the symbol $\mathscr{T}(\mathscr{H})$

$\mathscr{T}(\mathscr{H})$ (and in particular its positive symmetric cone $\mathscr{T}_+(\mathscr{H})$) turns out to have the same significance for quantum statistical mechanics that the Hilbert space of wave functions has in quantum mechanics. [91] [125] Moreover, $\mathscr{T}(\mathscr{H})$ has many nice properties that make it pleasant to work with. This can be understood as a consequence of the fact that trace class operators behave very similarly to finite dimensional matrices and the trace norm is the trace (i.e. the sum of diagonal elements) of the absolute value of such matrices. For positive matrices, the trace norm is the finite dimensional trace of the matrix itself. In order to make this connection explicit, we define a trace for infinite dimensional systems that extends the finite dimensional definition in a natural way.

Definition 2.3.2. *Trace*

Any separable Hilbert space $\mathscr{H}$ has a countable orthonormal basis. For any choice of orthonormal basis $|\psi_k\rangle$ and any trace class operator $\boldsymbol{A}$, we define the trace to be the linear functional $\mathrm{Tr}\,[\cdot] : \mathscr{T}(\mathscr{H}) \to \mathbb{C}$ by

$$\mathrm{Tr}\,[\boldsymbol{A}] = \sum_k \langle \boldsymbol{A}\psi_k, \psi_k\rangle \tag{2.3.1.2}$$

Based on these definitions, we have some key properties to enumerate that we will use frequently throughout this text. These results can be found in any standard text on functional analysis or operator theory. [91] [26] They also appear in some form in most references on mathematical quantum mechanics given the enormous power of these tools for studying quantum statistical mechanical systems. [32] [125]

Remark Trace Norm Properties

This linear functional is independent of the choice of basis and satisfies the norm bound

$$|\mathrm{Tr}\left[\boldsymbol{A}\right]| \leq \|\boldsymbol{A}\|_{\mathrm{Tr}} \tag{2.3.1.3}$$

If $\boldsymbol{A} \in \mathscr{T}_{+}(\mathscr{H})$ then by Lidskii's Trace formula [91] we have

$$\mathrm{Tr}\left[\boldsymbol{A}\right] = \|\boldsymbol{A}\|_{\mathrm{Tr}} \tag{2.3.1.4}$$

If $\boldsymbol{A} \in \mathscr{T}_{\mathrm{S}}(\mathscr{H})$ (the closed cone of symmetric compact operators $\boldsymbol{A}^{*} = \boldsymbol{A}$), then for $\boldsymbol{A}_{+}$ and $\boldsymbol{A}_{-}$ the positive and negative parts constructed in the usual way from the absolute value

$$\|\boldsymbol{A}\|_{\mathrm{Tr}} = \|\boldsymbol{A}_{+}\|_{\mathrm{Tr}} + \|\boldsymbol{A}_{-}\|_{\mathrm{Tr}} \tag{2.3.1.5}$$

Remark Trace Class Algebraic Ideal Properties

As noted above, the trace is a linear functional, so $\forall \alpha_1, \alpha_1 \in \mathbb{C}$ and $\forall \boldsymbol{A}, \boldsymbol{B} \in \mathscr{T}(\mathscr{H})$

$$\mathrm{Tr}\left[\alpha_1 \boldsymbol{A} + \alpha_2 \boldsymbol{B}\right] = \alpha_1 \mathrm{Tr}\left[\boldsymbol{A}\right] + \alpha_2 \mathrm{Tr}\left[\boldsymbol{B}\right] \tag{2.3.1.6}$$

Trace Class operators form a two-sided algebraic ideal in $\mathscr{L}(\mathscr{H})$. That is, $\forall \boldsymbol{A} \in \mathscr{T}(\mathscr{H})$ and $\forall \boldsymbol{B} \in \mathscr{L}(\mathscr{H})$, $\boldsymbol{AB} \in \mathscr{T}(\mathscr{H})$ and $\boldsymbol{BA} \in \mathscr{T}(\mathscr{H})$ and

$$\|\boldsymbol{AB}\|_{\mathrm{Tr}} \leq \|\boldsymbol{A}\|_{\mathrm{Tr}} \|\boldsymbol{B}\| \tag{2.3.1.7}$$

$$\|\boldsymbol{BA}\|_{\mathrm{Tr}} \leq \|\boldsymbol{A}\|_{\mathrm{Tr}} \|\boldsymbol{B}\| \tag{2.3.1.8}$$

Operator order can be permuted within the trace so long as at least one of the operators belongs to the trace class. That is, $\forall \boldsymbol{A} \in \mathscr{T}(\mathscr{H})$ and $\forall \boldsymbol{B} \in \mathscr{L}(\mathscr{H})$,

$$\mathrm{Tr}\left[\boldsymbol{AB}\right] = \mathrm{Tr}\left[\boldsymbol{BA}\right] \tag{2.3.1.9}$$

This is significant because it allows us to get around non-commutativity inside of our linear functionals.

Remark Trace Class Duality Properties

The Trace can be used to define an inner product between Hilbert-Schmidt class operators $S(\mathscr{H})$

$$\langle \boldsymbol{A}, \boldsymbol{B} \rangle_{\mathrm{HS}} = \mathrm{Tr}\left[\boldsymbol{A}^* \boldsymbol{B}\right] \tag{2.3.1.10}$$

Thus by a Riesz-Frechet representation, every linear functional on the Hilbert-Schmidt class operators can by represented by tracing against a Hilbert-Schmidt class operator. We express this by saying that $S(\mathscr{H})$ is its own dual space, $S(\mathscr{H})^* = S(\mathscr{H})$.

We can build on this idea of the trace as playing an analogous role to that of the integral in L_p spaces. For any $\boldsymbol{X} \in \mathscr{T}(\mathscr{H})$, we can define a linear functional on any closed subspace of the bounded operators by

$$\ell(A) = \mathrm{Tr}\left[XA\right], \forall \boldsymbol{A} \in \mathscr{L}(\mathscr{H}) \tag{2.3.1.11}$$

Conversely, we can define a linear functional on any closed subspace of the trace class operators by,

$$\ell(X) = \mathrm{Tr}\left[XA\right] \tag{2.3.1.12}$$

By the trace bounding inequality, 2.3.1.7, any such functional is uniformly bounded and so continuous. It is possible to turn these maps into isometries by choosing the source and target spaces suitably. This yields two powerful facts:

In the sense described above, the dual space of the compact operators is the trace class operators,

$$\mathscr{C}(\mathscr{H})^* = \mathscr{T}(\mathscr{H}) \tag{2.3.1.13}$$

In the sense described above, the dual space of the trace class operators is the full Banach algebra of bounded operators,

$$\mathscr{T}(\mathscr{H})^* = \mathscr{L}(\mathscr{H}) \tag{2.3.1.14}$$

Finally, we note that these dual relationships are compatible with the spectral definition of operator partial ordering. In particular,

$$\boldsymbol{X} \in \mathscr{T}_+(\mathscr{H}) \iff \mathrm{Tr}\left[XY\right] \geq 0, \ \forall \boldsymbol{Y} \in \mathscr{L}_+(\mathscr{H}) \tag{2.3.1.15}$$

and

$$\boldsymbol{X} \in \mathscr{L}_+(\mathscr{H}) \iff \mathrm{Tr}\,[XY] \geq 0,\ \forall \boldsymbol{Y} \in \mathscr{T}_+(\mathscr{H}) \tag{2.3.1.16}$$

One facet of functional analytic approximation that is frequently overlooked in physics texts is the nuanced distinction between different kinds of convergence. In particular, the topological structure of infinite dimensional spaces can become fairly subtle even when speaking coarsely about convex sets in homogeneous vector spaces. This is in stark contract to the situation we are accustomed to from finite dimensional theories where all manner of convergence looks more or less the same. Since we are interested in building a theory of scaling limits on top of this, we do not have the luxury of ignoring topology. We need to speak precisely about what kind of convergent sequence we are talking about (we will mostly be able to avoid issues related to nets by working on separable Hilbert spaces). Fortunately, although different methods of proving convergence will be more suitable in different situations, for the most part, we will only need to distinguish between uniform convergence and ultraweak convergence. This will be made clear in the remark below.

Definition 2.3.3. *Sequential Operator Convergence*

Norm Convergence (or Uniform) of a Sequence of Operators $(\boldsymbol{X_n})_{n\in\mathbb{N}}$ *to an operator* $\boldsymbol{X}$

$$\lim_n \|\boldsymbol{X_n} - \boldsymbol{X}\| = 0 \tag{2.3.1.17}$$

Strong Convergence of a Sequence of Operators $(\boldsymbol{X_n})_{n\in\mathbb{N}}$ *to an operator* $\boldsymbol{X}$

$$\lim_n \|\boldsymbol{X_n}x - \boldsymbol{X}x\|_{\mathscr{H}} = 0\ \forall x \in \mathscr{H} \tag{2.3.1.18}$$

Weak Convergence of a Sequence of Operators $(\boldsymbol{X_n})_{n\in\mathbb{N}}$ *to an operator* $\boldsymbol{X}$ *(Sequential Convergence in the Weak Operator Topology)*

$$\lim_n \langle \boldsymbol{X_n}x - \boldsymbol{X}x, y\rangle_{\mathscr{H}} = 0\ \forall x, y \in \mathscr{H} \tag{2.3.1.19}$$

Ultraweak (or Weak Convergence on* $\mathscr{T}(\mathscr{H})^*$*) of a Sequence of Operators* $(\boldsymbol{X_n})_{n\in\mathbb{N}}$ *to an operator* $\boldsymbol{X}$

$$\lim_n \mathrm{Tr}\,[\boldsymbol{X_n}\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{Y}] = 0\ \forall \boldsymbol{Y} \in \mathscr{T}(\mathscr{H}) \tag{2.3.1.20}$$

Remark Sequential Convergence Equivalencies

Norm Sequential Convergence implies Strong Sequential Convergence implies Weak Sequential Convergence

Ultraweak convergence implies weak convergence

By Alaoglu the unit ball is ultraweak compact. It follows that the inclusion map is a bijective homeomorphism between the weak and ultraweak unit balls. Therefore, we find that the unit ball is both weak and ultraweak compact and weak also implies ultraweak on norm bounded sets of operators.

Finally, for increasing countable sequences of operators, then weak and ultraweak are also equivalent to strong convergence of the sequence to its least upper bound. Thanks to the uniform boundedness principle, we will usually be able to use of this simple type of convergence for the studying the continuity of quantum processes. In particular, we will refer to maps that are continuous with respect to every such increasing, norm bounded, ultraweak convergent sequence, as *Normal linear maps.*

It is important to note that these other types of convergence are not directly equivalent to uniform convergence.

We are now prepared to introduce the primary spaces that we will define most of our processes on.

Definition 2.3.4. *States and State Spaces*

The state space, $\mathscr{T}_{\mathrm{S}}(\mathscr{H})$, associated to a fixed Hilbert Space $\mathscr{H}$ are the Trace Class operators $\boldsymbol{A} : \mathscr{H} \to \mathscr{H}$ such that $\boldsymbol{A}^* = \boldsymbol{A}$.

The positive cone of the state space, $\mathscr{T}_{+}(\mathscr{H})$, consists of those $\boldsymbol{A} \in \mathscr{T}_{\mathrm{S}}(\mathscr{H})$ such that $\sigma(\boldsymbol{A}) \geq 0$ or, equivalently, $\langle \boldsymbol{A}\psi, \psi \rangle \geq 0 \ \forall \psi \in \mathscr{H}$. Any symmetric trace class operator can be represented as a difference of positive elements.

Those elements $\boldsymbol{X} \in \mathscr{T}_{+}(\mathscr{H})$ such that $\mathrm{Tr}\left[\boldsymbol{X}\right] = 1$ are called states. Arbitrary elements of this convex set are called density matrices or mixed states, while the extreme points of the set are called pure states and take the form $|\psi\rangle \langle\psi|$ where $\psi \in \mathscr{H}$ and $\|\psi\|_{\mathscr{H}} = 1$.

States facilitate a number of very useful representations and decompositions. The most important of these for answering a variety of practical questions is the Spectral Representation. Indeed, most calculations in quantum mechanics that invoke a "resolution of identity" are actually using a spectral representation in disguise. There are many theorems that fall under this name for different classes of operators. We will quickly review some of the highlights, but entire books are devoted to this subject. [91] [40] [77]

Remark Spectral Representation of Compact Symmetric Operators on a Hilbert Space

The spectrum of a linear operator $\boldsymbol{C}$ relative to a given unital operator algebra $\mathscr{B}$, is the subset of the complex plane $\sigma_{\mathscr{B}}(\boldsymbol{C}) \subset \mathbb{C}$ such that for each $\lambda \in \sigma_{\mathscr{B}}(\boldsymbol{C})$ there does not exist an inverse operator $\boldsymbol{T} \in \mathscr{B}$ such that $\boldsymbol{T}(\boldsymbol{C} - \lambda\mathbb{I}) = (\boldsymbol{C} - \lambda\mathbb{I})\boldsymbol{T} = \mathbb{I}$. Throughout this text, we will always mean the spectrum relative

to $\mathscr{L}(\mathscr{H})$. As a result of the functional calculus and spectral representation theorems, the spectrum is frequently one of the most valuable tools available for characterizing operators.

The spectrum of a bounded linear operator is bounded as a subset of $\mathbb{C}$ and is closed.

The spectrum of a compact operator consists of a countable number of finite multiplicity generalized eigenvalues. The only accumulation point that is possible is 0, which occurs when $\mathscr{H}$ is infinite dimensional. The resolvent $(\boldsymbol{C} - \lambda\mathbb{I})^{-1}$, which is analytic off of the spectrum (by the Riesz functional calculus), has a pole at each point of the spectrum.

The spectrum of a compact symmetric operator, $\boldsymbol{C}$, is constrained to $\mathbb{R} \cap [-\|\boldsymbol{C}\|, \|\boldsymbol{C}\|] \subset \mathbb{C}$. The spectrum of a positive compact symmetric operator is constrained to $[0, \|\boldsymbol{C}\|]$.

Any compact symmetric operator (and so any state) has an orthonormal basis of eigenvectors. Thus, there exists a sequence of orthornormal eigenvectors $|\psi_k\rangle$ and eigenvalues $\lambda_k \in [-\|\boldsymbol{C}\|, \|\boldsymbol{C}\|]$ decreasing to zero such that

$$\boldsymbol{C} = \sum_k \lambda_k |\psi_k\rangle \langle\psi_k| \tag{2.3.1.21}$$

where the limit of finite numbers of terms in the sum converges to $\boldsymbol{C}$ uniformly. We will call this its spectral representation. For states, $\lambda_k \geq 0$ and $\sum_k \lambda_k = 1$, so this can also be read as saying that every state is a convex combination (of a countable number of pure states) that converges in trace norm.

We can also construct a much larger and more versatile functional calculus for a compact symmetric operator $\boldsymbol{C}$ and any bounded, complex-valued function $f : \sigma(\boldsymbol{C}) \to \mathbb{D}\,\|f\| \subset \mathbb{C}$ by the formula

$$f(\boldsymbol{C}) = \sum_k f(\lambda_k) |\psi_k\rangle \langle\psi_k| \tag{2.3.1.22}$$

Considerably more complex techniques are required to even describe the spectral structure and the representation of unbounded operators. [91] [131] However, although these are in general very important to quantum theories, we will make comparatively little use of them apart from a proof about approximate simultaneous position and momentum measurements and some results on semigroup generators. We will reference these technical results as needed, but it is mostly sufficient to note that they are similar in usage even though their intellectual content is quite different.

2.3.2 Operations and Effects in Quantum Statistical Mechanics

We are now in a position to explain the use of the trace and trace class operators in the representation of a measurement theory. The essential idea is that the trace functions as a method of calculating the quantum

statistical mechanical expectation value of an observable against a state. The suitability of this choice can be seen from the linearity (2.3.1.6) and boundedness (2.3.1.7) properties. Moreover, our duality results show that any linear functional on the compact or trace class operators can be represented as a trace against another bounded operator. This suggests that any functional that could serve as a viable candidate for an expectation must be equivalent to tracing against some bounded operator. Kraus and later authors take this line of argument to its axiomatic and philosophical extreme. [86] [16] We will satisfy ourselves with the statement that this is the best choice and it recreates the expectation values of determinative measurements in traditional quantum mechanics when it is applied to pure states.

Specifically, suppose our system is in a state $\boldsymbol{\rho}$ (conflating the terms in a now harmless way) and we are interested in the expectation value of a traditional quantum observable, $\boldsymbol{A}$, that is compact and symmetric. The traditional result of for a state vector ψ is that the detector reading we obtain if we average over many measurements is

$$a = \langle\psi| \boldsymbol{A} |\psi\rangle \tag{2.3.2.1}$$

Then for $\boldsymbol{\rho} = |\psi\rangle \langle\psi|$, we have by using a choice of basis for evaluating the trace that include ψ as one of the basis elements,

$$a = \langle\psi| \boldsymbol{A} |\psi\rangle = \langle\psi| \boldsymbol{A} |\psi\rangle \langle\psi| |\psi\rangle = \mathrm{Tr}\left[\boldsymbol{A} |\psi\rangle \langle\psi|\right] = \mathrm{Tr}\left[\boldsymbol{A}\boldsymbol{\rho}\right] \tag{2.3.2.2}$$

We can extrapolate from this (and experiment has confirmed for mixed states) that the same holds for general observables and general density matrices $\boldsymbol{\rho}$. We can build on this observation by defining projection operators $\boldsymbol{P}_k = |\psi_k\rangle \langle\psi_k|$ for the eigenspaces, where $\boldsymbol{A} |\psi_k\rangle = \lambda_k |\psi_k\rangle$ by way of the spectral representation. Then we obtain (by the fact that the uniform convergence of the spectral representation sum implies ultraweak convergence)

$$a = \mathrm{Tr}\left[\boldsymbol{A}\boldsymbol{\rho}\right] = \sum_k \lambda_k \mathrm{Tr}\left[\boldsymbol{P}_k\boldsymbol{\rho}\right] \tag{2.3.2.3}$$

where the $\mathrm{Tr}\left[\boldsymbol{P}_k\boldsymbol{\rho}\right]$ are interpreted as probabilities and the λ_k as measurements. This is identical to the interpretation of the spectral representation in traditional quantum mechanics. The difference here is that we can go a step further by using the properties of the trace and the fact that $\boldsymbol{P}_k = \boldsymbol{P}_k^*$ and $\boldsymbol{P}_k\boldsymbol{P}_k = \boldsymbol{P}_k$

$$\mathrm{Tr}\left[\boldsymbol{P}_k\boldsymbol{\rho}\right] = \mathrm{Tr}\left[\boldsymbol{P}_k^*\boldsymbol{P}_k\boldsymbol{\rho}\right] = \mathrm{Tr}\left[\boldsymbol{P}_k\boldsymbol{\rho}\boldsymbol{P}_k^*\right] \tag{2.3.2.4}$$

Based on this and more subtle arguments we arrive at the standard measurement model for traditional quantum systems. [86] The state of the system after a *single* selective measurement yielding the value λ_k

occurs is given by

$$\boldsymbol{\rho}' = \frac{\boldsymbol{P}_k \boldsymbol{\rho} \boldsymbol{P}_k^*}{\mathrm{Tr}\left[\boldsymbol{P}_k \boldsymbol{\rho}\right]} \tag{2.3.2.5}$$

This is a normalized state expressing the back-action of the measurement process for a known selective outcome. This is interesting in its own right and provides a more complete description of measurement processes than we had before. However, once we try to move beyond studying fancy Stern-Gerlach experiments, it becomes clear that this isn't rich enough to describe general non-ideal measurements. [16] In order to proceed, we need to introduce a general theory of *Operations* and *Effects* based on the theory of positive linear maps on the state space. The particular definitions that we will use in what follows come primarily from Davies [32]

Definition 2.3.5. *Operations*

Given a State Space $\mathscr{T}_{\mathrm{S}}(\mathscr{H})$, operations are defined as positive linear maps $\boldsymbol{T} : \mathscr{T}_{\mathrm{S}}(\mathscr{H}) \to \mathscr{T}_{\mathrm{S}}(\mathscr{H})$ such that $\forall \boldsymbol{\rho} \in \mathscr{T}_{+}(\mathscr{H})$, we have $\boldsymbol{T}\boldsymbol{\rho} \in \mathscr{T}_{+}(\mathscr{H})$ and

$$0 \leq \mathrm{Tr}\left[\boldsymbol{T}\boldsymbol{\rho}\right] \leq \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{2.3.2.6}$$

It is easy to show [121], that every operation is operator norm bounded and that quantity is equal to the supremum of the resulting trace functional over all states.

Operations are, in principle, sufficient for characterizing the result of a measurement. However, for technical reasons, it turns out to be very useful to introduce a notion of bounded linear operators that reproduce the transmission probability of the original operation. This produces a dual structure that is very useful for studying the convergence of approximations. From Davies [32], we have the following useful result (quoted more or less directly)

Proposition 2.3.6. *Existence of Operation Adjoints*

If $\boldsymbol{T} : \mathscr{T}_{\mathrm{S}}(\mathscr{H}) \to \mathscr{T}_{\mathrm{S}}(\mathscr{H})$ is a positive linear map then the adjoint $\boldsymbol{T}^* : \mathscr{L}_{\mathrm{S}}(\mathscr{H}) \to \mathscr{L}_{\mathrm{S}}(\mathscr{H})$ is a unique normal positive linear map. Moreover,

$$0 \leq \boldsymbol{T}^*(\mathbb{I}) \leq \mathbb{I} \tag{2.3.2.7}$$

if and only if

$$0 \leq \mathrm{Tr}\left[\boldsymbol{T}\boldsymbol{\rho}\right] \leq \mathrm{Tr}\left[\boldsymbol{\rho}\right] \ \forall \boldsymbol{\rho} \in \mathscr{T}_{+}(\mathscr{H}) \tag{2.3.2.8}$$

Every normal positive linear map $\boldsymbol{S} : \mathscr{L}_{\mathrm{S}}(\mathscr{H}) \to \mathscr{L}_{\mathrm{S}}(\mathscr{H})$ is the adjoint of a unique positive linear map $\boldsymbol{T} : \mathscr{T}_{\mathrm{S}}(\mathscr{H}) \to \mathscr{T}_{\mathrm{S}}(\mathscr{H})$

This result on the uniqueness of adjoints of maps on the state space is so useful because we can always view $\boldsymbol{T}(\boldsymbol{\rho}) = \boldsymbol{T}(\boldsymbol{\rho})\mathbb{I}_{\mathscr{H}}$ and so in the context of the trace as a kind of inner product we have

$$\mathrm{Tr}\left[\boldsymbol{T}(\boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{T}^{*}(\mathbb{I})\right] \tag{2.3.2.9}$$

The converse is of particular interest, because it implies that knowledge of the transition probability for every state is sufficient to specify an operation. This is in no way a priori obvious and will turn out to be very significant in how we construct the quantum stochastic process for reaction detection.

Definition 2.3.7. *Effects*

If an operation $\boldsymbol{T}$ is given such that following a measurement, a quantum system is found in the state

$$\boldsymbol{\rho}' = \frac{\boldsymbol{T}(\boldsymbol{\rho})}{\mathrm{Tr}\left[\boldsymbol{T}(\boldsymbol{\rho})\right]} \tag{2.3.2.10}$$

Then we associate to each such operation a unique effect $\boldsymbol{E} \in \mathscr{L}_{\mathrm{S}}(\mathscr{H})$ defined by

$$\boldsymbol{E} = \boldsymbol{T}^{*}(\mathbb{I}) \tag{2.3.2.11}$$

for which it is automatically true that

$$\mathrm{Tr}\left[\boldsymbol{T}(\boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{E}\right] \tag{2.3.2.12}$$

The set of all effects is a convex subset of $\mathscr{L}_{\mathrm{S}}(\mathscr{H})$

Since all projections on $\mathscr{H}$ are self-adjoint bounded operators and ubiquitous in the traditional quantum theory, it is useful to place them in their context as effects.

Proposition 2.3.8. *Projections as Extremal Effects*

Projections on $\mathscr{H}$ are the extreme points of the convex set of all effects.

This makes it clear that the projection operators play a deep role in characterizing the geometry of Operations, and by extension, the infinite dimensional geometry of measurements. With these definitions in mind, we immediately ask how general operations can be represented in terms of more familiar operators. Clearly, $\boldsymbol{T}(\boldsymbol{\rho}) = \boldsymbol{P}\boldsymbol{\rho}\boldsymbol{P}^{*}$ is a viable form, but how typical is this? For purity preserving operations, it turns out that this form is certainly typical. A purity preserving operation (or pure operation) is an operation that maps pure states to pure states. Pure operations are of particular interest because they will correspond to the evolutions on the free states of our transport theory. From Davies [32], we have the following representation

result for pure operations (and a few simple notes on his proof that make it easy to see why this should be true)

Theorem 2.3.9. *Representation of Purity Preserving Operations*

If $\boldsymbol{T} : \mathscr{T}_{\mathrm{S}}(\mathscr{H}) \to \mathscr{T}_{\mathrm{S}}(\mathscr{H})$ *is a positive linear map such that* $\forall\, |\psi_1\rangle\langle\psi_1| \in \mathscr{T}_{\mathrm{S}}(\mathscr{H})$, $\exists \psi_2 \in \mathscr{H}, \|\psi_2\| = 1$ *such that* $\boldsymbol{T}(|\psi_1\rangle\langle\psi_1|) = |\psi_2\rangle\langle\psi_2|$, *Then the map* $\boldsymbol{T}$ *is of one of the following forms*

$$\boldsymbol{T}(\boldsymbol{\rho}) = \boldsymbol{B}\boldsymbol{\rho}\boldsymbol{B}^{*},\ \boldsymbol{B} \in \mathscr{L}(\mathscr{H}, \mathscr{H}) \tag{2.3.2.13}$$

where $\boldsymbol{B}$ *is uniquely determined up to a complex coefficient of modulus 1 or*

$$\boldsymbol{T}(\boldsymbol{\rho}) = \boldsymbol{B}\boldsymbol{\rho}^{*}\boldsymbol{B}^{*} \tag{2.3.2.14}$$

where $\boldsymbol{B} : \mathscr{H} \to \mathscr{H}$ *is bounded and conjugate linear and is uniquely determined up to a complex coefficient of modulus 1 or*

$$\boldsymbol{T}(\boldsymbol{\rho}) = \mathrm{Tr}\left[\boldsymbol{B}\boldsymbol{\rho}\right]|\psi\rangle\langle\psi| \tag{2.3.2.15}$$

where $\boldsymbol{B} \in \mathscr{L}_{+}(\mathscr{H})$ *and* $|\psi\rangle \in \mathscr{H}$

If $\boldsymbol{T}$ *is trace preserving, then it is of the first type and the operators* $\boldsymbol{B}$ *are unitary.*

Proof. By considering finite dimensional subspaces and operations converging in the uniform norm, we can reduce the problem to holding for a finite dimensional version. Moreover, we can show that any contradiction to this set of alternatives must hold explicitly on some two dimensional subspace otherwise the existence of a well-defined extension precludes contradiction. In this way, the problem reduces to a simple argument on the representation of purity preserving maps between two-dimensional operators. This is easily converted into a problem about affine mappings between Bloch vectors (as the coordinates of the Pauli matrices and the Identity). From this perspective, the alternatives can be confirmed to be exhaustive using the classification of linear isometries on $\mathbb{R}^3$. □

This theorem is very useful for constructing representations of an operation in a particularly simple form. For the most part, we will only need to concern ourselves with operations of the first variety. This result is related to Stinespring's dilation theorem for completely positive maps between unital C^* algebras [121], which affords us a representation $\phi(\boldsymbol{\rho}) = \boldsymbol{V}^{*}\pi(\boldsymbol{\rho})\boldsymbol{V}$ through a larger Hilbert space by way of composition with a unital *-homomorphism π. This is also related to similar representation theorems due to Kadison, Haag, Varadarajan and Kraus from the late 1960s.

2.3.3 Observables in Quantum Statistical Mechanics

The notion of operations on its own only allows us to talk about extremely simple events. Namely, although operations allow for more general measurement types and mixing of pure states, a single operation only allows us describe the outcome of a single measurement with isolated eigenvalues. In and of itself, this isn't powerful enough to describe the kind of reaction volume counting events that we use in the classical Pál-Bell theory. In traditional quantum mechanics, moving beyond discrete observables meant introducing spectral measures and spectral integral representations. In the traditional theory, the events were realized as projections and it was entirely sufficient to work with projection operator-valued measures. Now that events can take the form of any positive map on the state space, we might have to deal with considerably more complex structures.

A simple observation grounds the following discussion: the same trace duality that exists for Operations and Effects carries over to their vector measure extensions, Instruments and Observables, respectively. From this point of view, an observable can be understood as a function on the sigma algebra of Borel sets, taking values in the convex set of effects. Practically speaking, it turns out to be more efficient to define the objects of the theory a little more broadly and then use our knowledge of operations and effects for special cases.

Definition 2.3.10. *Observables as Positive Operator-Valued Measures*

Let $\mathscr{F}$ be a sigma algebra on a locally compact Hausdorff (LCH) topological space Ω. Let $\mathscr{H}$ be a separable Hilbert space. A Positive Operator Valued Measure is a map $\boldsymbol{E} : \mathscr{F} \to \mathscr{L}_+(\mathscr{H})$ satisfying three properties analogous to the standard requirements for a projection operator valued measure:

$$\boldsymbol{E}(B) \geq \boldsymbol{E}(\emptyset) = 0 \; \forall B \in \mathscr{F} \tag{2.3.3.1}$$

$$\forall (B_n)_{n\in\mathbb{N}} \subset \mathscr{F} \text{ s.t. } B_i \cap B_j = \emptyset \; \forall i \neq j$$
$$\boldsymbol{E}\left(\cup_n B_n\right) = \mathrm{w} \lim_{N\to\infty} \sum_{n=1}^{N} \boldsymbol{E}(B_n) \tag{2.3.3.2}$$

This is called an Observable if

$$\boldsymbol{E}(\Omega) = \mathbb{I}_{\mathscr{H}} \tag{2.3.3.3}$$

The above definition can be extended to arbitrary measurable subsets of an arbitrary set. However, by constraining Ω to be LCH we can apply the theory of Radon measures. In practice, we will further constrain this set to be a compact polish space in every practical example. As is typical of spectral measures, we can

define a weakly convergent integral that facilitates the construction of a functional calculus. In this case, we can prove that the resulting correspondence between measures and integrals is bijective and so they can be used interchangeably.

Definition 2.3.11. *Observables as Bounded Operator-Valued Integrals*

The linear space of Positive Operator Valued Measures on a Compact Polish space Ω *can be mapped bijectively to positive linear maps* $\overline{\boldsymbol{E}} : C(\Omega, \mathbb{R}) \to \mathscr{L}_{\mathrm{s}}(\mathscr{H})$. *This bijective mapping is achieved by way of a well-defined integral that converges weakly*

$$\overline{\boldsymbol{E}}(f) = \int_{\Omega} f(\omega) \mathrm{d}\boldsymbol{E}(\omega) \tag{2.3.3.4}$$

where $\mathrm{d}\boldsymbol{E}(\omega)$ *is constructed by using the fact that* $B \to \langle \boldsymbol{E}(B)\phi, \psi \rangle$ *defines a finite, complex-valued Radon measure on the LCH space* Ω. *The integral is then uniquely defined on* $C(\Omega, \mathbb{R})$ *by virtue of Radon measure theory. Conversely, every such positive linear operator evaluated against an inner product* $\left\langle \overline{\boldsymbol{E}}(f)\phi, \psi \right\rangle$ *defines a radon measure by Riesz-Kakutani. [56] We can extend this to yield a unique operator* $\boldsymbol{E}$ *by the usual functional calculus for symmetric operators type arguments. [91] That is, a complex measure so defined for any vector pair* ϕ, ψ *is easily extended to a well-defined operator. It is trivial to show that the resulting operator is positive.*

The resulting map satisfies $\overline{\boldsymbol{E}}(1) = \mathbb{I}_{\mathscr{H}}$ *if and only if* $\boldsymbol{E}$ *is an observable.*

An observable $\boldsymbol{E}$ *is a projection operator valued measure if and only if the linear map* $\overline{\boldsymbol{E}}$ *is an algebra homomorphism. This is a standard result related to Naimark's representation theorem for positive operator valued measures. [121]*

The positive operator-valued measure is defined as being weakly countably additive. This generalization makes it relatively easy to prove that an object that we construct is an observable. However, it does not undercut desired convergence properties nearly so much as it first seems. This is thanks to another easy corollary of Stinespring's dilation theorem due to Naimark: any regular, positive $\mathscr{L}(\mathscr{H})$-valued measure is identical on all Borel sets to a projection operator valued measure transformed by bounded operators in the manner of 2.3.2.13. Specifically, we find that for every positive operator valued measure E, there exists a bounded operator $\boldsymbol{V}$ and a projection operator valued measure P such that $E(B) = \boldsymbol{V}^* P(B) \boldsymbol{V}$, where $E(B)$ is a positive operators and $P(B)$ is a projection operator for every Borel set B. The required regularity is easily satisfied on LCH spaces under the assumptions of any of the theorems that we will be dealing with. [121]

Naimark's result permits us to exploit the norm convergence of a Riemann-Stiltjes integral for a projection operator-valued measure when characterizing the convergence of the Riemann-Stiltjes integral for a positive

operator-valued measure on suitably partially ordered set in Ω. Although this does not mean that the splitting of domains (and so countable additivity) is norm convergent, it does give us a direct justification for the norm convergence of the integral itself which is important in studying limit interchange operations. This is a powerful bootstrapping of convergence results that can be performed almost without remark just by temporarily replacing the underlying Hilbert space with a larger one. We will use this to avoid some technical difficulties in the study of approximations to QSPs.

2.3.4 Instruments and Transformative Measurement of Continuous Fields

In this section, we will finally be able to introduce a powerful operational measurement idea that will ground the primary motivating heuristic of this paper. Just as we defined an equivalency between effects and operations when understood as operators and their adjoints, we can construct an adjoint object for observables that are strongly countably additive. Where observables are a kind of effect valued measure, we define an operation valued measure that we call an instrument. That is, an instrument describes transformations on the system state, conditional on particular detection measurement events.

This turns out to be a very important notion. It allows us to imagine partitioning the path space of a reaction-transport process based on classically observable events. This idea of event partitioning is essential to discussing the kind of branching paths that we did in the classical measurement chapter. As we did in the discussion of operations, we will employ the phrase "positive map" to distinguish positive operators on the state space from positive operators on the Hilbert space.

Definition 2.3.12. *Instruments as Positive Map Valued Measures*

Let $\mathscr{F}$ be a sigma algebra on a locally compact Hausdorff (LCH) topological space Ω. Let $\mathscr{H}$ be a separable Hilbert space. A Positive Map Valued Measure $\mathscr{E}$ is a map from Borel sets to positive linear operators on the state space. That is, $\mathscr{E} : \mathscr{F} \to \mathscr{L}_+(\mathscr{T}_+(\mathscr{H}))$ This map must satisfy properties analogous to the standard requirements for a projection operator valued measure:

$$\mathscr{E}(B) \geq \mathscr{E}(\emptyset) = 0 \; \forall B \in \mathscr{F} \tag{2.3.4.1}$$

$$\forall (B_n)_{n\in\mathbb{N}} \subset \mathscr{F} \text{ s.t. } B_i \cap B_j = \emptyset \; \forall i \neq j$$
$$\lim_{N\to\infty} \left\| \mathscr{E}\left(\cup_{n=1}^{N} B_n\right)\boldsymbol{\rho} - \sum_{n=1}^{N} \mathscr{E}(B_n)\boldsymbol{\rho} \right\|_{\mathrm{Tr}} = 0 \; \forall \boldsymbol{\rho} \in \mathscr{T}(\mathscr{H}) \tag{2.3.4.2}$$

This is called an Instrument if it is trace preserving for all states $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\mathrm{Tr}\left[\mathscr{E}(\Omega)\boldsymbol{\rho}\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{2.3.4.3}$$

Note the use of the strong limit in the convergence of the countable additivity requirement. This is more restrictive than the requirements placed on observables and we will find that while every Instrument has an equivalent Observable, we have no converse to this. [32]

Proposition 2.3.13. *Adjoint Observables*

For every instrument $\mathscr{E}$ *on a compact Polish space, there is a unique observable* $\boldsymbol{E}$ *that is adjoint to it in the sense that* $\forall B \in \mathscr{F}$

$$\mathrm{Tr}\left[\mathscr{E}(B)\boldsymbol{\rho}\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{E}(B)\right] \tag{2.3.4.4}$$

As with observables, we can define an equivalent integral construction for any instrument. This takes much the same form.

Definition 2.3.14. *Instruments as State-Valued Integrals*

The linear space of Positive Map Valued Measures on a Compact Polish space Ω *can be mapped bijectively to positive bilinear maps on* $C(\Omega, \mathbb{R}) \times \mathscr{T}_+(\mathscr{H})$ *that we will refer to as* $\overline{\mathscr{E}}$*. This bijective mapping is achieved by way of a well-defined integral that converges weakly (in the trace sense of* $\mathscr{E}(B)\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$ *as a linear functional on the compact operators)*

$$\overline{\mathscr{E}}(f, \boldsymbol{\rho}) = \int_\Omega f(\omega)\mathrm{d}\mathscr{E}(\omega)\boldsymbol{\rho} \tag{2.3.4.5}$$

where $\mathrm{d}\mathscr{E}(\omega)$ *is constructed by using the fact that* $B \to \mathrm{Tr}\left[\boldsymbol{A}\mathscr{E}(B)\boldsymbol{\rho}\right]$ *defines a finite, complex-valued Radon measure on the LCH space* Ω *and a linear functional on* $\boldsymbol{A} \in \mathscr{C}(\mathscr{H})$*. The integral is then uniquely defined on* $C(\Omega, \mathbb{R})$ *by virtue of Radon measure theory. Conversely, every such bilinear operator inner product* $\mathrm{Tr}\left[\overline{\mathscr{E}}(f, \boldsymbol{\rho})\boldsymbol{A}\right]$ *defines a radon measure by Riesz-Kakutani. [56] We can extend this to yield a unique positive map for each Borel set* $B \to \mathscr{E}(B)$ *by a generalization of the usual functional calculus type arguments. [91] That is, a complex measure so defined for any operator pair* $\boldsymbol{A}, \boldsymbol{\rho}$ *is easily extended to a well-defined positive map valued measure. It is trivial to show that the resulting operator is positive.*

The resulting map satisfies $\mathrm{Tr}\left[\overline{\mathscr{E}}(1, \boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right]$ *if and only if* $\mathscr{E}$ *is an instrument.*

It is worth taking a moment to unpack the instrument definition a little bit in the context of reaction events. Suppose, as we do in section 3.3.2, that the existence of reactions of a particular type occurring can

be understood as classically observable event. Then we claim that conditional on a particular reaction having occurred in a particular phase space volume and time interval, we can define an operator that transforms any prior state into a posterior state. This Bayesian language choice is not an accident. In some sense, this is an update of a representation of our knowledge using an observed piece of data. We can do this for real nuclear experiments and it is precisely what we are doing when we express out going states in terms of incoming state and potentials in scattering theory. The difference here is that the time interval under consideration is asymptotically small rather than asymptotically large. However, this is consistent with working in a transport setting rather than on a single scattering experiment. The greater point is that defining a local, conditional transformation based on our knowledge of a scattering model is well within the scope of existing theory for quantum collisions.[65] In order to express this appropriately for use in a transport model will take some extra work, but instruments are the right objects for representing individual collisions as measurement events.

Proposition 2.3.15. *Composition of Instruments*

For every pair of instruments, $\mathscr{E}^1$ on $\mathscr{B}(\Omega_1)$ and $\mathscr{E}^2$ on $\mathscr{B}(\Omega_2)$ (for Ω_1 and Ω_2 compact metric spaces), $\exists \mathscr{E}$ a unique composite instrument.

$\mathscr{E}$ is defined on the Borel product space $\mathscr{B}(\Omega_1 \times \Omega_2)$ and is equal to the composition of the two instruments on every rectangular set (i.e. every product of Borel sets). That is, $\forall E_1 \in \mathscr{B}(\Omega_1), E_2 \in \mathscr{B}(\Omega_2)$ and $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$,

$$\mathscr{E}(E_1 \times E_2)\boldsymbol{\rho} = \mathscr{E}^1(E_1)\mathscr{E}^2(E_2)\boldsymbol{\rho} \tag{2.3.4.6}$$

This last proposition appears in [32] for compact metric spaces. It can be generalized to the desired compact Hausdorff spaces by using some convex compact representation theory. (see Lax [91] Theorem 1 p. 133 for the representation result that uses metrisability in Davies) This can also be understood in terms of reaction events. If we use the above analogy, we imagine that both free propagation and collision are represented as instruments, where free propagation is conditioned on the detection of no reactions in a given interval and collision is conditioned on the detection of a single reaction in a given interval. Then the proposition says that there is a composite instrument for describing no reaction followed by a reaction. This straight line propagation followed by a localized collision can be thought of as an operator dictionary for describing transport processes. The fact that each can be analyzed as measurements in their own right and then combined into a unique composite object in our quantum measurement theory is a fact of the most fundamental importance and we can exploit it to construct a quantum analogue for the Backward Chapman-Kolmogorov equation for reaction-transport processes.

Chapter 3

Classical Measurement Theory of Neutron Fields

In section 2.1.2, we reviewed the classical theory of nuclear systems. This provides some useful context for what most approaches to neutron transport look like. However, even from a classical perspective, a significant amount of richness has already been sacrificed in the standard construction of a linear transport model. [20] As a theory, it makes no claim to being able to calculate even two particle densities of the kind normally studied in standard classical non-equilibrium field theories. [5] Moreover, it remains unclear what the significance of such a doublet density would be in the context of a neutron field theory that does not support a well-defined number operator. In spite of the commonly accepted path length summation definition, one might be excused for doubting that the neutron flux means anything at all when taken on its own.

Throughout this work we will suppose that, much as quantum wave functions only have meaning when evaluated against observables, the neutron field is only given a substantive experimental meaning in the context of reaction rate computations. This idea is made into a simple measurement analogy as follows: depending on the local concentration of fissile material, the medium has a higher effective multiplication rate and so amplifies the neutron flux signal differentially. This medium-as-detector analogy actually has a long history in the literature. This analogy is particularly significant in some discussions of the adjoint transport equation [92] and variational estimates to the reaction rate. However, it is easy to see why this point of view has been historically overlooked outside of stochastic neutron transport theories.

Measurement-centric thinking is not necessary to understand most practical computational methods for large neutron numbers. In the large number limit in a uniform reaction volume, we can safely replace the quantum theory with its purely classical, spatially dependent, branching process form and the measurement interpretation becomes a mere curiosity. However, for small or low-density systems, the measurement-centric framework is indispensable. Moreover, this perspective clarifies why methods of the theory of distributions and weakly convergent empirical processes (particle simulation) can be applied universally to transport models.

In this chapter, we will expand on our discussion from section 2.1.3 on the probabilistic foundations of

stochastic neutron transport using the work of Pál and Pazsit. [122] We will focus on the facets of the theory that are significant for understanding the Pall-Bell equation as a classical branching process under continuous monitoring for detection by particle absorption. We will discuss how certain formulas lend themselves to measurement theoretic interpretation and will allow us to understand the quantum PDPs of chapter 5 as a kind of quantized Pal-Bell formula.

3.1 Reaction Volumes and the Observables of a Transport Theory

Before jumping into the mathematical theory of generalized branching processes, we will examine what measurements can be meaningfully understood in terms of a classical transport theory. Every standard text on neutron physics outlines a wide variety of experimental measurements that ground our general understanding of the properties of the neutron. [19],[82] Although there are many variations, there are essentially two flavors of measurement that come up repeatedly in different guises: Interferometric (relative-phase) and repeated position detection (which-path). We argue that only repeated position detection can be studied with a transport theory.

Any measurement performed using a neutron interferometer, relies on the measurement of relative wave packet phases. Given that classical transport processes arise from PDP-like position detection chains, it is reasonable to assume that transport processes are a kind of continuous "which path" measurement of the neutron field. Such measurements would continually erase relative phase information as a result of the conjugacy of the path and phase observables. This conclusion can be understood as a generalization of comparing the double-slit experiment without path detection to the double-slit experiment with path detection. [67] We conclude that the correct quantization of a transport theory cannot be used to understand interferometric measurements as it describes a measurement process with path detection.

If we accept the medium-as-detector analogy at face value, we need to consider what kind of interactions actually pin down particle paths. A particle path is not specified by simultaneous approximate speed and location selection via choppers and blocks. A particle path is specified by repeated reactions with nuclei of the medium. Symmetry considerations and uncertainty obviously make it impossible to claim that we know exactly which neutron is participating in which path. However, we can say that the set of all reactions and time stamps provides us with a trace of the composite path history, like a Lichtenberg figure etched into phase space. Thus, in our detector analogy, the only direct continuous observation is the set of all reactions. In general, the positions, momenta, and timestamps of reactions must all conform to suitable uncertainty

relations. However, this is easily subsumed in the classical uncertainties that we will build into the wave functions.

Our observable should provide the probability distribution associated to the set of possible reaction counts observed in any given Borel volume of phase space in any finite amount of time. That is, we claim that our measurement theory provides a measure μ that is countably additive on the Borel field of $\mathbb{N} \times \mathbb{R}^6$. This is only true in a classical setting. More precisely, we can do this for any Borel subset of $\mathbb{R}^3$ or we can do it on any Heisenberg Uncertainty principle compatible Borel subset of $\mathbb{R}^6$ by way of a representation of the Weyl-Heisenberg group. The specific mathematical structure of the relevant quantum measurement object is a positive operator valued measure taking values in $\mathscr{L}_+(\mathscr{L}_2(\mathbb{R}^3))$, but we will come back to the precise construction of this observable later. Our goal in this high-level discussion was simply to identify the physical quantity being measured in a transport theory and its classical representation.

We will find that classical reaction rate observables account for all of the meaningful quantities that contribute to stochastic neutron transport processes and the double differential scattering amplitudes obtained from single scattering experiments. The relative phase dependent observables from a many-body scattering theory can only be included if we retain interference effects from the scattering process across multiple sites, which would preclude a classical transport approximation. [117] This is possible in the general open quantum theory, as we can allow non-classical (off-diagonal) outgoing states. However, if we choose to do this, we should not expect to recover a classical transport approximation but rather a kind of medium-interaction renormalized multiple scattering approximation like in the theory of Galitskii's integral equations. [52] The quantum theory that we are developing has neutron optics and neutron transport as two distinct facets, just as with Osborn and Yip's field theory of neutron interactions does. [114] However, for the remainder of this classical discussion we will focus on observables that can be related to the classical reaction rate (i.e. those that will remain meaningful in the classical transport scaling limit).

3.2 Two Simple Examples of Reactor Measurements

This research is built on the idea that every quantity required for modeling a neutron transport process can be incorporated into a reactive model of the medium as particle detection. This is a naturally quantum mechanical notion since quantum theory is fundamentally just a more logically robust and integrated theory of measurement. Classical mechanics takes as axiomatic that every system can be modeled using (at most) an uncertain prior state and some noisy external driver. However, the inclusion of randomness is characteristic of the incidental lack of information and there is no need to make the measurement process part of the core

definition of the system. Measurement can just be layered on top after we are done making predictions about the state of the system at measurement time. Modern quantum theory starts from the premise that every measurement is (a) approximate and (b) system altering. From this jumping off point, we find that it is possible to conceive of virtually every system ever studied as driven by the back-action of some measurement process. [86] Our invocation of these philosophical foundations of physics leans heavily on our conception of the reaction process itself as a protracted measurement. In order to make this feel a little more natural, it is worth introducing a couple characteristic examples from conventional nuclear power reactors.

3.2.1 An Embedded Proportional Counter Neutron Detector

It is well known that most neutron counting measurements are not just perturbative of the state, they involve the thermalization and absorption of actual neutrons. [82] Suppose that an array of such absorption based detectors is incorporated into a reactor core. Given the small size of the detectors it is possible to incorporate this array without significantly altering the criticality of the overall system. However, the absorption rate could be indirectly recorded by way of some manner of stimulated electron cascade in the secondary instrumentation or the time integrated damage could be measured by way of track dosimetry after removal. Regardless, the detector array itself can be represented as a region with a special absorption rate and the key feature is event counting in the reaction volumes of interest.

It is worth noting that while this seems to introduce a selective process into the system, that is an illusion as the measurement was always selective. Indeed, nuclei do not continue to reside in a superposition of transmuted and non-transmuted states for very long as a result of environmental decoherence. The dynamics of transmutation are so dramatic that they cross energy scales, immediately coupling into the atomic processes of the rest of the nearby medium (e.g. the atom displacement caused by a fission event) and inducing decoherence to a classically selected state. [67], [16] This is not to suggest that the species of every atom of the system is known at all times, simply that it is in some sense knowable. The very fact of the existence of that classical coupling forces the system into a classical meter state and cat states decay so rapidly that they are of no consequence to the quantum theory of our system. These quantum measurement technicalities are all to say that there is nothing wrong with treating the detector as a part of the medium undergoing state selecting reactions just like the rest of the reactor core.

3.2.2 Indirect Reaction Rate Estimation through Calorimetry

A second example of reaction measurement takes the form of an indirect measurement. [16] (If we want to be technical, both are indirect measurement as we are directly measuring secondary electrons within the

embedded detector.) However, there is a much more indirect system measurement that is useful when the system is operating at a slowly varying power level. Fission events generate excess kinetic energy in the fission products, which is then transferred to the vibrational modes of other atoms through the linear energy transfer along the ionized particle track. Since these tracks are fabulously short for even high energy fission products in condensed matter (due to the high charge of the fission products), it is easy to correlate the local energy deposition with the local fission rate. Therefore, any measurement of the thermal energy in the medium near that point provides a smoothed estimate to the local fission rate. [3]

Since a thermometer is generally made of materials with fairly small reaction cross sections, it can be inserted in the system with an even smaller perturbation on the system. However, this comes at the cost of measuring a quantity that is only coupled to the state of the original quantum system through multiple intermediary processes. Still, this can be thought of as an indirect, non-destructive measurement of the fission rate per unit time that introduces a negligibly small change to the definition of the medium in the form of small regions of modified reaction rate to represent thermal instrumentation. In this case, modeling the measurement output reduces to modeling the atomic heat transfer dynamics induced by the stopping of fission products.

3.3 The Integral Form of the Pál-Bell Equation and Reaction Counting

So far in this chapter, we have predominantly discussed which measurements can be represented as an explicit part of a reaction-transport system in a classical transport theory. However, the other part of this picture is understanding which quantities contribute to forming predictions about the evolution of such a system in time. We will show that only the standard reaction rate distributions as a function of space and time are required in order to update the distribution of any measurement that is represented by a linear operator acting on the space of measures on the neutron count in phase space.

This is to say, there exists a canonical set of reaction rates that govern the dynamics of the system. If we can model those canonical reaction processes at intervening times, we can predict the reaction rate associated to **any** reaction process in any reasonable phase space volume at the end of the evolution period. Moreover, we will show that apart from the reaction events and the linear attenuation that they induce, the system evolves by a classical free propagation pathwise. Thus, our Backward Chapman-Kolmogorov equation can be interpreted as interaction-representation type time integrals over chains of single-reaction event and zero-reaction event propagators. This nonlinear integral form of Pál-Bell provides the right classical structure

to quantize in order to obtain a usable quantum measurement theory for the study of reaction-transport systems.

This section draws heavily from the work of Pál and Pázsit as their particular construction of stochastic neutronics emphasizes the general theory of branching processes and casts the particular physical assumptions of neutron transport in the corresponding form. [122] Our main modifications result from reinterpreting their work through the lens of quantum measurement theory. Specifically, we will be examining their ideas in the context of using piecewise deterministic markov processes (PDMPs) to model the evolution of continuous measurement systems. This approach relies on both modern research in path simulation quantum optics [16], [6] as well as older theories of quantum detector fields [32]. However, in this section we will eschew the quantum theory of probability in favor of classical commutative stochastic processes and only study the classical PDMPs rather than their quantum analogue. The latter problem, and its application to nuclear systems, will be reserved for chapter 5.

3.3.1 Number Counting and Geographic Spaces

We will begin by introducing some assumptions, notation, and definitions that will be used to understand reaction-transport processes throughout this text. The most basic definitions characterize a classical phase space for our theory of neutron number distributions. This will include some assumptions about both the relevant transition functions and the admissible detector geometries in order to avoid concerning ourselves with technicalities of relativistic physics or re-entrant geometries.

There are numerous physical problems with allowing large momentum values, ranging from the breakdown of phenomenological models near $|p| = m_n c$ to the approximation of Minkowski space-time structures and their profoundly different group structure from Euclidean spaces. We will eventually assume that the initial distributions and scattered state distributions are both vanishingly small in the high momentum tail and so do not meaningfully impact the outcome of the theory with their magnificent wrongness. This allows us to work with a simpler phase space structure without further comment.

We will avoid any detector geometries that would force us to account for re-entrant boundary conditions. This is not so much a real limitation as it is a source of needless and uninformative complication in our current problem. Thus, we will assume we are modeling a closed convex bounded detector with a smooth boundary and a perfect absorber just outside of that boundary. In such a system, a particle is counted when it leaves the edge but is also unable to return to the detector volume. The resulting boundary conditions are simple enough to avoid having to develop complex analytical conditions for constraining how information from functions on the boundary propagate to the interior along characteristics. The convexity also allows us

to effectively equate this to a reaction detection system in a vacuum which is another common formulation of the standard problem.

It is worth noting that the two assumptions taken together give us a phase space domain that can easily be compactified. Specifically, the position space is a closed and totally bounded subset of $\mathscr{V}_D \subset \mathbb{R}^3$ and the momentum space is only applied to functions with a modulus that decays exponentially for large values and so it can be given a one-point compactification $\mathscr{O} = \mathbb{R}^3 \cup \{\infty\}$, as is done in constructing the Riemann Sphere. Thus, by Tychanoff, the product of the two $\mathscr{V}_D \times \mathscr{O}$ is also compact in the product topology. This point will be important later when we are discussing quantum stochastic processes.

With these facts in mind, we define the sigma algebra of the geographic phase space $\mathscr{B}(\mathscr{V}_D \times \mathscr{O}) = \mathscr{G}$ of the problem to be the collection of macroscopic reaction volumes that can be used in detecting neutrons. In probability theoretic language, the sets in $\mathscr{G} \times \mathscr{P}(\mathbb{N})$ are the events for counting neutrons. More explicitly, for every time t, there exists a measure μ_t such that for every Borel subset $U \in \mathscr{G}$ of the geographic phase space and every natural number n, $\mu_t(U, n) \in [0, 1]$ and is countably additive on disjoint unions of sets while $\mu_t(\mathscr{V}_D \times \mathscr{O} \times \mathbb{N}) = 1$. That is, for every reasonable reaction volume, we can assign a probability to each possible number of neutrons that could be observed and this probability measure conforms to the usual rules of probability theory.

We further claim that this time indexed family of measures μ_t is a Markov process. In order to make this notion precise we have to introduce the idea of a conditional transition probability that connects this family of measures between times. [16] First, we define a probability density under the assumption that the neutron counting distribution is absolutely continuous with respect to a Lebesgue measure. In order to incorporate a causal link between particle counts and reaction events, we need to extend the event space to to represent a multi-particle distribution. The introduction of a causal structure on the density forces us to accept a much more complex event space than is necessary for the detector-centric model given above. Namely, $\prod_{i=1}^{n_1} \mathscr{G}$ is the true n_1 particle Borel sigma algebra. This actually allows us to describe the presence of each particle in different reaction volumes if we see fit. This particular additional richness of description becomes critical when we attempt to model the evolution due to reactions. For now, we will stick with a simpler case to keep the discussion easier to digest. Given the sets $B_1, B_2 \in \mathscr{G}$ for every $n_1, n_2 \in \mathbb{N}$ we can construct product sets $B_1^{n_1} = \prod_{i=1}^{n_1} B_1$ and $B_2^{n_2} = \prod_{i=1}^{n_2} B_2$. These describe the product of a fixed number of identical reaction volumes. This will facilitate the application of the Radon-Nikodym theorem to represent the measure as integral against a density. For simplicity of notation, we will represent the geographic phase space using the symbols $u_1 = (\bar{x_1^i}, \bar{k_1^i})_{i=1}^{n_1}$ and $\prod_{i=1}^{n_1} \mathrm{d}u_1 = \mathrm{d}\bar{x}_1^i \mathrm{d}\bar{k}_1^i$ for the vector and volume measure respectively. Then the

probability of detecting n_1 neutrons all in the reaction volume B_1 is given by

$$\mu_{t_1}(B_1, n_1) = \mu_{t_1}(B_1^{n_1}) = \iiint_{B_1^{n_1}} \mathrm{d}u_1 p(u_1, t_1) \tag{3.3.1.1}$$

and a two-time joint probability measure can be represented under a similar assumption

$$\mu_{t_2,t_1}(B_2, n_2; B_1, n_1) = \mu_{t_2,t_1}(B_2^{n_2}; B_1^{n_1}) = \iiint_{B_2^{n_2}} \mathrm{d}u_2 \iiint_{B_1^{n_1}} \mathrm{d}u_1 \; p(u_2, t_2; u_1, t_1) \tag{3.3.1.2}$$

Here we have equated our original model with the extended event space (without changing the symbol for our measure) on suitably simple events. For the sake of simplicity of notation, we will forego the multiple integrals in the future and simply apply the correct number of integrals based on the set that is being integrated over. We can now introduce a conditional density that allows us to propagate between states,

$$p(u_2, t_2) = \sum_{n_1 \in \mathbb{N}} \int_{(\mathscr{V}_D \times \mathscr{O})^{n_1}} \mathrm{d}u_1 \; p(u_2, t_2 | u_1, t_1) p(u_1, t_1) \tag{3.3.1.3}$$

when conditioning on sets of finite measure, representable as an integral over the function

$$p(u_2, t_2 | u_1, t_1) = \frac{p(u_2, t_2; u_1, t_1)}{p(u_1, t_1)} \tag{3.3.1.4}$$

This is meant to convey a heuristic justification for the use of the density of the conditional expectation at an earlier time as a propagator. For a more detailed explanation of the existence of such measures on sigma algebras including sets of zero measure, consult Rao's text.[127] A propagator is generally defined as the integral operator $\mathscr{T}(t_2|t_1)$ such that

$$\int_{B_2^{n_2}} \mathrm{d}u_2 p(n_2, u_2, t_2) = \mathscr{T}(t_2|t_1)\mu_{t_1} = \int_{B_2^{n_2}} \mathrm{d}u_2 \sum_{n_1} \int_{(\mathscr{V}_D \times \mathscr{O})^{n_1}} \mathrm{d}u_1 \; T(u_2, t_2 | u_1, t_1) p(u_1, t_1) \tag{3.3.1.5}$$

holds for every $B_2^{n_2}$.

In continuous-time systems without a discrete state space, the Markov property corresponds to the assumption that the Chapman-Kolmogorov equation holds. [134] This equation can most easily be defined in terms of the propagators:

$$T(u_3, t_3 | u_1, t_1) = \sum_{n_2 \in \mathbb{N}} \int_{(\mathscr{V}_D \times \mathscr{O})^{n_2}} \mathrm{d}u_2 \; T(u_3, t_3 | u_2, t_2) T(u_2, t_2 | u_1, t_1) \tag{3.3.1.6}$$

holds for all intermediate times t_2. This is essentially an explicit version of the semigroup property enumer-

ated for evolutions on a space of measures.

This formula tells us that, under the assumption that our system has enough information included (i.e. is Markovian), we can split off a small, easy to understand evolution. We can then use that to formulate a functional equation for the general propagator that has a solution analogous to an operator exponent in the linear case. As we will explain in what follows, we cannot expect the result to be a linear evolution on the neutron count density. However, by conditioning on particular paths, we can employ a kind of single-particle linearity up to the first collision event. This will make use of the multi-particle event space and require a modification of the decomposition that focuses on lineages rather than total count densities. The generator function for the distribution is then used to meld these lineages together into an independent tree approximation. As with genuine linear operator semigroups, we will find that this leads us to a representation by a kind of second resolvent equation. The resulting nonlinear precursor to the Pál-Bell equation turns out to be the most natural starting point for second quantization as the nonlinearity is manifestly a result of reaction intensities.

In order to arrive at the desired propagator formula, we need to define a useful prior condition. Since we are following a branching history of each neutron, it is reasonable to take the prior condition to be perfect knowledge of the presence of a neutron at a point (much as in the construction of green's function representations of PDEs [44]). By equation 3.3.1.5, this can be seen as sufficient for calculating the evolution of an arbitrary distribution up to the first collision and thus sufficient for calculating the first collision distribution. We will invoke this single particle conditioning interpretation repeatedly throughout this discussion. From a physical standpoint, this has a very natural reaction event interpretation. We can imagine that a decay from a bound state is detected by the neutron field at t_0 into the classical state with position and momentum u_0. This measurement event becomes the starting point for our predictive analysis as our system has been prepared into an initial configuration by a measurement. Thinking of both the neutron field and the matter field as detectors in their own right is of considerable mathematical and physical significance and will be discussed at some length in chapter 4.

It is important to note that so far we have focused on neutron number counting as our primary endeavor. A cursor examination of any book on quantum field theory will reveal that the number operator plays a key role in both second quantization and in quantum theories of transport. [8],[115] However, this turns out to be a somewhat less useful notion in coping with resonance scattering coupled to a transport process. As such, by shifting the focus to reaction rates, we will end up avoiding the entire issue of the proper representation and role of the number operator in the theory. A careful examination of the Pál-Bell equation reveals that the number operator is less central to even the classical theory than it first appears. It is simply used to

give a semblance of particle simulation intuition to the formulation of the model.

3.3.2 Reaction Intensity and Partial Probabilities

So far, we have defined the event space of our theory in terms of neutron counting events (i.e. we can only talk about probabilities for things like there are 10 neutrons in detector cell X between times t_0 and t). In order to construct a model for the propagator, we will find that this event space is inadequate. This is where the link to reaction theory will make its appearance. We claim that the transport process is driven by reaction events. This is in direct analogy to the classical field theories of nonequilibrium dynamics, where the process driving operator is the collision integral. [5] Every other contribution to the evolution can be thought of in essentially deterministic terms. In order to construct a Chapman-Kolmogorov equation that is useful and interesting, we need a way to identify subsets of events where the evolution is simpler. The phase space and neutron number in a reaction volume cannot help us with this on their own. Thus, we enrich the state space of the theory by the addition of a marked point process for tracking event times and types. Specifically, we will find it useful to think of the first collision time and first collision type as events to condition on.

Using the fact that the collision count in the time interval $[t_1, t]$ forms disjoint sets, we split the propagator at the collision event time t into an evolution including one collision of type i at time t and n_2 subsequent decays back to randomly distributed free states at later times $\bar{t}' = (t'_j)_{j=1}^{n_2}$, given by $T_1^i(u_2, t, \bar{t}'|u_1, t_1)$ and any remaining full evolution past that point. Let $T_0(u_2, t_2|u_1, t_1)$ be the evolution of the system with no collisions from u_1, t_1 to u_2, t_2. By incorporating the first collision time and process duration as state parameters in purely heuristic manner, we obtain a Backward Chapman-Kolmogorov equation. As we did with the intermediate phase space coordinates, we will simplify these expressions by introducing a product integral notation for the decay times. There is a decay probability and permutation counting issue that we will ignore for now and make explicit in the detailed fission formulas. For now we will simply let the integration interval $[t, t_3]^{n_2}$ indicate that we are integrating over as many as n_2 delayed decay events occurring after the initial absorption time t.

$$T(u_3, t_3|n_1 = 1, u_1, t_1) = T_0(u_3, t_3|u_1, t_1)\delta_{n_3,1} + \sum_i \int_{t_1}^{t_3} \mathrm{d}t \sum_{n_2} \int_{[t,t_3]^{n_2}} \mathrm{d}t' \int_{(\mathscr{V}_D \times \mathscr{O})^{n_2}} \mathrm{d}u_2 \; T(u_3, t_3|u_2, \bar{t}') T_1^i(u_2, t, \bar{t}'|u_1, t_1) \quad (3.3.2.1)$$

We can put this in a form that is typical of PDMP theory by viewing collisions as a point process operating on an otherwise smooth flow on a manifold. Specifically, we can introduce a single step transition rate for

each transition type i, given by $W_i(u_3|u_2;t)$. Moreover, to enforce consistency constraints relating the flow to the reaction timestamp and location, we introduce delta distributions into our T_1 operator. Namely, with $u_2' = (x_2^j, k_2^j)_{j=1}^{n_2}$ and $u_1' = (x_2, k_1)$

$$T_1^i(u_2', t, \bar{t'}|u_1, t_1) = W_i(u_2'; \bar{t'}|u_1'; t) T_0(u_1', t|u_1, t_1) \delta\left(\bar{x_2} - \bar{x_1} - \frac{\bar{k_1}}{m_n}(t - t_1)\right) \tag{3.3.2.2}$$

We note further that the transition probability can be factored into a reaction intensity $Q_i(t, u_1')$ and a detector response operator $D_i(u_2, t, \bar{t'})$ (an independent neutron multiplication branching process) for reaction processes with $t' > t$ having non-zero probability. We will explain this in our discussion of compound processes in section 3.3.3. At this point, we have deviated in a mathematically important way from a typical PDMP and are implicitly dealing with a measure-valued branching process with finite lifetimes for quasi-bound states formed during the branching process. However, we will continue to analyze the problem using path integral type methods from the theory of PDMPs where equation 3.3.4.1 can be comfortably applied (up to the presence of a delay process). We will find that this PDMP way of looking at the problem is still justifiable with sufficient control of the event rate and the jump amplitude. Ultimately, we will prove that models of this form are mathematically meaningful by studying the fully quantized version and recovering this as a classical approximation. In the mean time, we obtain a formula reminiscent of the standard Pál-Bell precursor equation. With $u_2' = (\bar{x_1} + \bar{k_1}/m_n(t - t_1), \bar{k_2})$ and $u_1' = (\bar{x_1} + \bar{k_1}/m_n(t - t_1), \bar{k_1})$, and restricting to jumps that act on the k component only,

$$\begin{aligned}
T(n_3, u_3, t_3|u_1, t_1) &= T_0(u_3, t_3|u_1, t_1)\delta_{n_3,1} + \\
&\sum_i \int_{t_1}^{t_3} \mathrm{d}t \sum_{n_2} \int_{\mathscr{O}^{n_2}} \mathrm{d}k_2 \int_{[t,t_3]^{n_2}} \mathrm{d}t'\, T(u_3, t_3|u_2', \bar{t'}) T_1^i(u_2', t; \bar{t'}|u_1, t_1) && (3.3.2.3) \\
&= T_0(u_3, t_3|u_1, t_1)\delta_{n_3,1} + \\
&\sum_i \int_{t_1}^{t_3} \mathrm{d}t \sum_{n_2} \int_{\mathscr{O}^{n_2}} \mathrm{d}k_2 \int_{[t,t_3]^{n_2}} \mathrm{d}t'\, T(u_3, t_3|u_2', \bar{t'}) W_i(u_2'; \bar{t'}|u_1'; t) T_0(u_1', t|u_1, t_1) && (3.3.2.4) \\
&= T_0(u_3, t_3|u_1, t_1)\delta_{n_3,1} + \\
&\sum_{i,\text{direct}} \int_{t_1}^{t_3} \mathrm{d}t \int_{\mathscr{O}} \mathrm{d}k_2 \int_t^{t_3} \mathrm{d}t'\, T(u_3, t_3|u_2', t')\delta(t - t') W_i(u_2'; t'|u_1'; t) T_0(u_1', t|u_1, t_1) + \\
&\sum_{i,\text{compound}} \int_{t_1}^{t_3} \mathrm{d}t \sum_{n_2} \int_{\mathscr{O}^{n_2}} \mathrm{d}k_2 \int_{[t,t_3]^{n_2}} \mathrm{d}t'\, T(u_3, t_3|u_2', t') D_i(u_2', t, \bar{t'}) Q_i(t, u_1') T_0(u_1', t|u_1, t_1) && (3.3.2.5)
\end{aligned}$$

The delta distribution in this formula is really a notation for saying that the distribution of $t' > t$ is

concentrated on a set of extremely small measure such that for any overall interval $t_3 - t_1 >> \tau_{\text{direct}} = d_{\text{nuclear}}/v_{\text{thermal}}$, the interior integral can safely be discarded and $t' \sim t + \epsilon$ can approximated by t in the functional formulas. In this sense, the δ has its usual heuristic meaning and also conforms to the idea of a point measure, but does not actually agree with the delta distribution since this would require symmetry that is not present here.

This formula can describe a wide variety of branching processes driven by localized events that only induce transformations on the momentum and number space. However, to go further in characterizing this system as a measurement process for neutrons, we need to introduce specific reaction mechanisms and enforce consistency between the jump probability and the attenuation of free propagation. Contrary to classical convention, we use a right to left time ordering of operators. Although this theory is still commutative, we are starting with rigid ordering so that the analogy is clear when we do quantize.

3.3.3 Reaction Types

Our newly defined model, given by equation 3.3.2.5, includes a sum over unspecified reaction mechanisms. In order to make this meaningful, we need to introduce a finite set of explicit reaction processes. These processes must be specified at least by their boundedness and measure theoretic properties. In order to motivate the choice of these operator forms, we will discuss some typical reaction mechanisms observed in real nuclear systems.

In any standard text on nuclear reaction theory, it is possible to find a variety of classification systems for reaction types based on different models for reaction processes. [50], [59] However, for our purposes, one classification system is of particular interest. First, we identify a division of collisions into direct and compound processes.

Direct processes include a strong dependence on the incident momentum distribution but don't involve the formation of a quasi-bound state. This means that there is no potential for a time delay between the initial collision and the appearance of an outbound neutron. That is, the collision is instantaneous on transport time scales. There are direct neutron pickup reactions (e.g. $n \to 2n$), but in a practical sense the probability of direct multiplicative events below 100 MeV is virtually indistinguishable from zero. Thus, in a typical nuclear system, a direct reaction is always represented as potential scattering and is particle number conserving. In what follows, we will refer to this as a scattering reaction event.

Compound Processes involve the formation of a bound or quasi-bound state and they are ubiquitous at modest energies. Pre-compound reactions don't become significant for most power reactors and we will ignore them in this discussion. So, for our purposes, a compound reaction is modeled in two stages: absorption

and memoryless decay. If no decay neutron in a precursor state is created by the collision (i.e. a fully bound state is formed) then the reaction is counted as an absorption. On the other hand, if at least one precursor neutron is produced, then the process is some flavor of compound scattering or fission. A number of other mechanisms can also account for this kind of neutron production, such as the non-fission evaporation of neutrons from an excited nucleus. Again these events are mostly of significance well above the usual 2 MeV neighborhood for fast neutron production from fission. All of the neutrons generated as a mix of prompt and delayed emission processes will be rolled into a single fission reaction term. For example, compound elastic scattering will have a similar form with some accounting for doorway resonances, but we will allow the general fission term to stand in for both for now.

Therefore, in this decomposition, we will analyze three reaction types: Scattering ($\Delta t_{\text{rxn}} = 0$, $n = 1 \rightarrow n' = 1$), Absorption ($\Delta t_{\text{rxn}} >> t_3$, $n = 1 \rightarrow n' = 0$), and Fission ($\Delta t_{\text{rxn}} \geq 0$, $n = 1 \rightarrow n' > 0$). Again, strict accounting would require that we allow for fission events that have no emitted neutrons and compound non-fission events that preserve or increase number, but this is mostly a technicality for us since we can absorb those cases into the terms with the wrong name but the right form. Based on these considerations, we write down an explicit form of equation 3.3.2.5, which we will proceed to simplify term by term in sections 3.4 and 3.5.

$$
\begin{aligned}
T(n_3, u_3, t_3|u_1, t_1) = {} & T_0(u_3, t_3|u_1, t_1)\delta_{n_3,1} + \\
& \int_{t_1}^{t_3} \mathrm{d}t \int_{\mathscr{O}} \mathrm{d}k_2 \int_{t}^{t_3} \mathrm{d}t' \, T(u_3, t_3|n_2 = 1, u_2', t')\delta(t - t')W_{\text{scattering}}(n_2 = 1, u_2', t'|u_1'; t)T_0(u_1', t|u_1, t_1) + \\
& \int_{t_1}^{t_3} \mathrm{d}t \int_{\mathscr{O}} \mathrm{d}k_2 \int_{t}^{t_3} \mathrm{d}t' \, T(n_3, u_3, t_3|n_2 = 0, u_2', t')\delta(t_3 - t')D_{\text{absorption}}(n_2 = 0, u_2')Q_{\text{absorption}}(t, u_1')T_0(u_1', t|u_1, t_1) + \\
& \int_{t_1}^{t_3} \mathrm{d}t \sum_{n_2 > 0} \int_{\mathscr{O}^{n_2}} \mathrm{d}k_2 \int_{[t,t_3]^{n_2}} \mathrm{d}t' \, T(u_3, t_3|u_2', t')D_{\text{fission}}(u_2', u1', t, \bar{t}')Q_i(t, u_1')T_0(u_1', t|u_1, t_1) \quad (3.3.3.1)
\end{aligned}
$$

First, note that the D detector multiplication product and the final propagator in the pure absorption term will actually be delta functions for suppressing unnecessary integrals and sums. Next, note the $n_2 + 1$ time indexes in $D_{\text{fission}}(u_2', u_1', t, \bar{t}')$. This is present to encode the fact that fission is a time-delayed reaction process. So, a collection of neutrons will be instantaneously "created" during the initial collision at t but will only enter the reactive free neutron population at some distribution of later times $\bar{t}'$. Finally, it is also worth observing that throughout this and other sections, we suppress the number index because it is included in the integration domain representation and it is not worth writing that out every time. We only include it in, for example, $W_{\text{scattering}}(n_2 = 1, u_2', t'|u_1'; t)$ to contrast with the impact of the fission operator.

3.3.4 The Backward Chapman-Kolmogorov Equation and Evolution as Reaction Measurement

Before working out more detailed expressions for the specific reactions and the free propagator, we will introduce some simplifications that put the backward Chapman-Kolmogorov equation in a form that will easily be compared to the quantum reaction model that we develop in chapter 5. We will do this in two stages. First, we will introduce a rearrangement of the two time integrals. Second, we will operate with a linear functional and interpret the resulting formula.

We recall a simple calculation from the standard theory of time-ordered operators and the interaction representation. [7] When you have a normally convergent integral involving two integrals over a combined domain where one time is always larger than the other (as we do in equation 3.3.4.1 where $t' > t$) we can swap the order of integration with Fubini-Tonelli and the domains can be reorganized as below:

$$\int_{t_1}^{t_3} \mathrm{d}t \int_{t}^{t_3} \mathrm{d}t' \, f(t,t') = \int_{t_1}^{t_3} \mathrm{d}t \int_{t_1}^{t_3} \chi_{\{t' > t\}} \mathrm{d}t' \, f(t,t') = \int_{t_1}^{t_3} \mathrm{d}t' \int_{t_1}^{t'} \mathrm{d}t \, f(t,t')$$

Notice that we have introduced a right to left time ordering of the integrals that will make the comparison simpler later. We will use this one the scattering and fission terms and we will evaluate the integral of t' against the delta function in the absorption term. This is to highlight the fact that the second event in this case is never observed, so the second integral is superfluous. This leaves us with

$$\begin{aligned}
T(n_3,u_3,t_3|u_1,t_1) &= T_0(u_3,t_3|u_1,t_1)\delta_{n_3,1} + \\
&\int_{t_1}^{t_3} \mathrm{d}t' \int_{t_1}^{t'} \mathrm{d}t \int_{\mathscr{O}} \mathrm{d}k_2 \; T(n_3,u_3,t_3|n_2=1,u_2',t')\delta(t-t')W_{\text{scattering}}(n_2=1,u_2',t'|u_1';t)T_0(u_1',t|u_1,t_1) + \\
&\qquad \int_{t_1}^{t_3} \mathrm{d}t \int_{\mathscr{O}} \mathrm{d}k_2 \; D_{\text{absorption}}(n_2=0,u_2')Q_{\text{absorption}}(t,u_1')T_0(u_1',t|u_1,t_1) + \\
&\sum_{n_2>0} \sum_{n_2'<n_2} \int_{[t_1,t_3]^{n_2'}} \mathrm{d}t' \int_{t_1}^{t_1'} \mathrm{d}t \int_{\mathscr{O}^{n_2'}} \mathrm{d}k_2 \; T(n_3,u_3,t_3|n_2',u_2',t')D_{\text{fission}}(u_2',u_1',t,t')Q_{\text{fission}}(t,u_1')T_0(u_1',t|u_1,t_1)
\end{aligned} \tag{3.3.4.1}$$

where t_1' is the first decay time among time ordered integrals over the decay times and the residual $n_2 - n_2'$ neutrons do not contribute to the final free neutron count. Now that we have constructed the form that we will use in future discussions, we will introduce one last observation. Suppose that we have some linear functional ℓ_Q on the space of number measures at time t_3. Specifically, we will consider those linear functionals associated to the weak-* topology on the space of number counting measures. This topology is an important one for many reasons. However, the most physically compelling reason is that it is the topology in which approximation by empirical measures converges. That is, it is the sense in which

particle simulations yield meaningful results. By the theory of Radon measures and the Riesz-Kakutani representation theorem[56], all such functionals can be represented by multiplication by a complex valued function of $(u_3^j)_{j=1}^{n_3}$ followed by integration over u_3 and summation over $n_3 \in [0,N] \cap \mathbb{N}$, as this is an LCH space. Thus, by also multiplying by $p(u_1)$ and integrating over u_1, we obtain

$$\begin{aligned}
Q(t_3|t_1) = &\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_3\ f_Q(u_3,1) \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ T_0(u_3,t_3|u_1,t_1)p(u_1) \\
&+ \int_{t_1}^{t_3}\mathrm{d}t' \int_{t_1}^{t'}\mathrm{d}t \int_{\mathscr{O}}\mathrm{d}k_2 \sum_{n_3=0}^{N}\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,n_3) \\
&\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ T(n_3,u_3,t_3|n_2=1,u_2',t')\delta(t-t')W_{\text{scattering}}(n_2=1,u_2',t'|u_1';t)T_0(u_1',t|u_1,t_1)p(u_1) \\
+\int_{t_1}^{t_3}\mathrm{d}t \int_{\mathscr{O}}\mathrm{d}k_2 \sum_{n_3=0}^{N}\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} &\mathrm{d}u_3\ f_Q(u_3,n_3) \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ D_{\text{absorption}}(n_2=0,u_2')Q_{\text{absorption}}(t,u_1')T_0(u_1',t|u_1,t_1)p(u_1) \\
&+ \sum_{n_2>0}\sum_{n_2'<n_2}\int_{[t_1,t_3]^{n_2'}}\mathrm{d}t' \int_{t_1}^{t_1'}\mathrm{d}t \int_{\mathscr{O}^{n_2'}}\mathrm{d}k_2 \sum_{n_3=0}^{N}\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,n_3) \\
&\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ T(u_3,t_3|u_2',\bar{t}')D_{\text{fission}}(n_2',u_2',u_1',t,\bar{t}')Q_{\text{fission}}(t,u_1')T_0(u_1',t|u_1,t_1)p(u_1) \qquad (3.3.4.2)
\end{aligned}$$

by defining the total Q-reaction rate as

$$\begin{aligned}
\sum_{n_3=0}^{N}\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3) \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ T(u_3,t_3|u_1,t_1)p(u_1) &= \sum_{n_3=0}^{N}\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3)p(u_3) \\
\equiv Q(t_3|t_1) = \sum_{n_3} Q(n_3,t_3|t_1) = \sum_{n_3}\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1 &\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_3\ Q(n_3,u_3,t_3|u_1,t_1)p(u_1) \qquad (3.3.4.3)
\end{aligned}$$

where the Q-reaction propagator is understood as the Q-reaction density generated by an observed particle at a vector u_1. The relationship between this propagator and the source function for the neutrons is best understood as a product of 1-particle propagators that takes a simple from when contracted against a source that generates a vector of single particle distributions like D_{fission}. Thus there is no incongruity in viewing this as a propagation of reaction events in that it is connecting decay n_1-tuples with Q-reaction distributions.

$$Q(n_3,u_3,t_3|n_1,u_1,t_1) = \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3)T(u_3,t_3|n_1,u_1,t_1) \qquad (3.3.4.4)$$

then defining the uncollided Q-reaction rate as

$$\begin{aligned}
\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,1) \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ T_0(u_3,t_3|u_1,t_1)p(u_1) \\
= \int_{(\mathscr{V}_D\times\mathscr{O})^1} \mathrm{d}u_3\ f_Q(u_3,1)p_0(u_3,t_3,n=1) \equiv Q_0(t_3|t_1)
\end{aligned}$$

and by restoring our path delta function from earlier, we can define the Q-reaction rate induced by initially scattered neutrons as

$$\begin{aligned}
&\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,n_3)\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\ T(u_3,t_3|n_2=1,u_2,t')\\
&\quad \delta(t-t')\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ \delta\left(\bar{x_2}-\bar{x_1}-\frac{\bar{k_1}}{m_n}(t-t_1)\right) W_{\text{scattering}}(n_2=1,u_2,t'|u_1';t)T_0(u_1',t|u_1,t_1)p(u_1)\\
&\quad = \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\ Q(n_3,u_3,t_3|u_2,t')\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ Q_{\mathrm{s}}^1(u_2,t,t'|u_1,t_1)p(u_1)\\
&\quad = \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\ Q(u_3,t_3|u_2,t')Q_{\mathrm{s}}^1(u_2,t,t')\\
&\quad = \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,n_3)p_{\mathrm{s},1}(u_3,t_3;t|t_1) = Q_{\mathrm{s},1}(n_3,t_3;t,t'|t_1) \qquad (3.3.4.5)
\end{aligned}$$

where

$$Q_{\mathrm{s}}^1(u_2,t,t') = \delta(t-t')\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ \delta\left(\bar{x_2}-\bar{x_1}-\frac{\bar{k_1}}{m_n}(t-t_1)\right) W_{\text{scattering}}(n_2=1,u_2,t'|u_1';t)T_0(u_1',t|u_1,t_1)p(u_1) \qquad (3.3.4.6)$$

we can define the Q-reaction rate induced by initially absorbed neutrons as

$$\begin{aligned}
&\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(n_3=0)\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\ D_{\text{absorption}}(n_2=0,u_2)\\
&\qquad \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ \delta\left(\bar{x_2}-\bar{x_1}-\frac{\bar{k_1}}{m_n}(t-t_1)\right) Q_{\text{absorption}}(t,u_1')T_0(u_1',t|u_1,t_1)p(u_1)\\
&\qquad = f_Q(n_3=0)\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\ \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ Q_{\text{abs}}^1(u_2,t|u_1,t_1)p(u_1)\\
&\qquad \equiv FQ_{\text{abs},1}(t|t_1) \qquad (3.3.4.7)
\end{aligned}$$

where

$$\begin{aligned}
Q_{\text{abs}}^1(u_2,t|u_1,t_1) = &\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\ D_{\text{absorption}}(n_2=0,u_2)\\
&\int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ \delta\left(\bar{x_2}-\bar{x_1}-\frac{\bar{k_1}}{m_n}(t-t_1)\right) Q_{\text{absorption}}(t,u_1')T_0(u_1',t|u_1,t_1)p(u_1) \qquad (3.3.4.8)
\end{aligned}$$

and

$$F = f_Q(n_3=0) \qquad (3.3.4.9)$$

Finally, we can define the Q-reaction rate induced by initially fissioned neutrons generating n_2 neutrons and

n_2' decays in $[t_1, t_3]$ as

$$\begin{aligned}
&\int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,n_3) \int_{(\mathscr{V}_D\times\mathscr{O})^{n_2'}} \mathrm{d}u_2\ T(u_3,t_3|n_2',u_2,t') \\
&\quad \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ \delta\left(\bar{x_2} - \bar{x_1} - \frac{\bar{k_1}}{m_n}(t-t_1)\right) D_{\text{fission}}(n_2,n_2',u_2,u_1,t,\bar{t'}) Q_{\text{fission}}(t,u_1) T_0(u_1',t|u_1,t_1) p(u_1) \\
&= \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3 \int_{(\mathscr{V}_D\times\mathscr{O})^{n_2'}} \mathrm{d}u_2\ Q(n_3,u_3,t_3|n_2',u_2,\bar{t'}) \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ Q^1_{\text{fission}}(n_2,n_2',u_2,t,\bar{t'}|u_1,t_1) p(u_1) \\
&\qquad = \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3 \int_{(\mathscr{V}_D\times\mathscr{O})^{n_2'}} \mathrm{d}u_2\ Q(n_3,u_3,t_3|n_2',u_2,\bar{t'}) Q^1_{\text{fission}}(n_2',u_2,t,\bar{t'}|t_1) \\
&\quad = \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3\ f_Q(u_3,n_3) p_{\text{fission},1}(u_3,t_3;n_2,n_2';t,\bar{t'}|t_1) \equiv Q_{\text{fission},1}(n_3,t_3;n_2,n_2';t,\bar{t'}|t_1)
\end{aligned} \tag{3.3.4.10}$$

where

$$\begin{aligned}
&Q^1_{\text{fission}}(n_2,n_2',u_2,t,t'|t_1) \\
&\quad = \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_1\ \delta\left(\bar{x_2} - \bar{x_1} - \frac{\bar{k_1}}{m_n}(t-t_1)\right) D_{\text{fission}}(n_2,n_2',u_2,u_1,t,t') Q_{\text{fission}}(t,u_1) T_0(u_1',t|u_1,t_1) p(u_1)
\end{aligned} \tag{3.3.4.11}$$

note that per the discussion of the structure of the multi-particle source-propagator above, this expression is formed from a product of 1-particle decay distributions. Again, when contracted against the n_2' particle full propagator, it simplifies significantly.

Thus, we obtain the following formula,

$$\begin{aligned}
Q(t_3|t_1) = Q_0(t_3|t_1) &+ \int_{t_1}^{t_3} \mathrm{d}t' \int_{t_1}^{t'} \mathrm{d}t \sum_{n_3=0}^{N} Q_{\text{s},1}(n_3,t_3;t|t_1) + \int_{t_1}^{t_3} \mathrm{d}t\ F Q_{\text{abs},1}(t|t_1) \\
&+ \sum_{n_2>0} \sum_{n_2'<n_2} \int_{[t_1,t_3]^{n_2'}} \mathrm{d}t' \int_{t_1}^{t_1'} \mathrm{d}t \sum_{n_3=0}^{N} Q_{\text{fission},1}(n_3,n_2,n_2',u_2,t_3;t,\bar{t'}|t_1)
\end{aligned} \tag{3.3.4.12}$$

where this can be cast in terms of reaction evolutions as

$$
\begin{aligned}
Q(t_3|t_1;p) &= Q_0(t_3|t_1;p) \\
&\quad + \int_{t_1}^{t_3} \mathrm{d}t' \int_{t_1}^{t'} \mathrm{d}t \sum_{n_3=0}^{N} \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_3 \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\, Q(n_3,u_3,t_3|u_2,t')Q^1_{\mathrm{s}}(u_2,t,t';p) \\
&\qquad + \int_{t_1}^{t_3} \mathrm{d}t\, FQ_{\mathrm{abs},1}(t|t_1;p) \\
&\quad + \sum_{n_2>0} \sum_{n_2'<n_2} \int_{[t_1,t_3]^{n_2'}} \mathrm{d}t' \int_{t_1}^{t_1'} \mathrm{d}t \sum_{n_3=0}^{N} \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3 \ldots \\
&\qquad \int_{(\mathscr{V}_D\times\mathscr{O})^{n_2'}} \mathrm{d}u_2\, Q(n_3,u_3,t_3|n_2',u_2,\bar{t}')Q^1_{\mathrm{fission}}(n_2,n_2',u_2,t,\bar{t}'|t_1;p) \qquad (3.3.4.13)
\end{aligned}
$$

We will examine the fission operator more carefully in section 3.5. We have also simplified our references to the prior single-particle momentum distribution by including a $;p$ in the operators that would be integrated against the prior state at t_1.

The above expression involves some very messy operators that we are suppressing by expressing them in terms of initial event densities. We have also interchanged orders of integration repeatedly without really addressing the underlying boundedness of the functions. We will assume all of the functions to be continuous on a compact domain and therefore bounded. Moreover, as mentioned before, all functions of momentum will be assumed to decay exponentially to zero for large momenta. Finally, there is no pure probabilistic justification for this formula. Operator equivalencies that could be justified in simpler systems are difficult to support in the context of a branching measure-valued process. However, we will obtain a technical foundation for this theory by starting from a well-defined quantum theory that can be understood as a quantization of formula 3.3.4.13.

We now have a general model for the evolution of an important class of linear functionals in terms of the density of other canonical reaction processes along linear paths averaged over prior distributions. That is to say, suppose we know something about the number distribution at time t_1 because of some preparatory measurement like striking a target to generate a distribution of spallation neutrons that are then thermalized and allowed to enter our reaction volume along a beam line. (note that this preparatory process too is a reaction measurement) Then, we can predict the reaction rate signal obtained by some localized detector (what we have been calling the Q-reaction rate) just by knowing the other fission scattering and absorption reaction rates for the system. This gives us a formulation of the most general standard equation of stochastic neutron transport that supports our decision to build our quantum theory based on a reaction detection heuristic. Specifically, as long as we can express the free propagation in terms of information about the

reaction process, this justifies our decision to study the system dynamics only using reaction rate observables. This last condition is the subject of section 3.4.

3.4 Linear Attenuation, Semi-groups, and Scattering Cross Sections

The purpose of this section is to analyze the structure of the free single-particle propagator $T_0(u_1', t|u_1, t_1)$ and simultaneously draw a connection between the reaction intensities $W_i(n_2, u_2'; t'|u_1'; t)$ and the scattering cross sections of nuclear collision theory. This relationship is fundamental to both the definition of scattering measurements [65][125][59] and to the general theory of radiation attenuation and energy deposition [117] [142]. As such, the theory of this subject is incredibly well developed. For this reason, it is a basic conceptual building block of the theory of neutron transport. In fact, these results will also prove significant in characterizing one of the fundamental existence requirements of the general quantum theory of neutron transport.

The prototypical model for this process (given in section 2.1.2) is ubiquitous in nuclear engineering and radiation protection physics. Indeed, it is deeply intuitively appealing to view the geographic space divided into thin slabs oriented along a momentum direction, with each slab scattering a small number of particles off the prescribed momentum path in direct analogy to a mini scattering experiment. By connecting to scattering theory, it gives a justification for a particular choice of function for $\Sigma(v, x)$. Indeed, by carefully examining this analogy in the case of potential scattering it is possible to show that error estimates that result from ignoring atomic components of the scattering Hamiltonian are negligible. [117] Moreover, studying the beam averaged result of the scattering experiment provides a natural justification for the introduction of isotropic scattering approximations. These results are very helpful in directly calculating the approach to thermal equilibrium for the velocity distribution of the set of neutrons born from fission. [117] [19]

Unfortunately, the simplest version of this model becomes mathematically suspect in the presence of even the compound scattering events common at upper thermal energies for complex nuclei. Worse yet, the comparison to empirical reality doesn't hold up. Attempts to normalize the computed distributions to be consistent with reactor benchmarks are as ubiquitous as they are fraught. In particular, problems with inconsistencies in the system metrology have become increasingly vexing as data quality has improved. [116] The structure of differential measurement uncertainty (as expressed through covariance matrices among multiple simultaneous cross sections) is readily violated by classical adjustment procedures. Modern correction procedures can help produce stable and reasonably accurate estimates to integral reaction measures such as

the k_{eff} of benchmark reactors. However, this does not preserve the supposedly simple link between scattering cross sections and nuclear systems. We claim that this is not the result of an intrinsically faulty premise but rather a consequence of incomplete accounting of the stochastic neutron dynamics that contribute to the definition of macroscopic transport coefficients. Thus it is important to understand these models in a more general quantum context that incorporates not just the classical envelope [7] but the underlying quantum measurement dynamics in our transport model.

To this end, there is different but closely related justification for the form of the free propagator based on a standard argument from PDMP theory and stochastic neutronics [122] that is still essentially commutative but generalizes nicely to the quantized version of this theory [16]. We will examine the free propagator as the solution of a functional equation and then compare the result to general theories of linear operator semigroups. We begin with a simple observation: the free evolution $T_0(u_1', t|u_1, t_1)$ forms a semigroup in the time parameter.

$$T_0(u_2, t_3|u_1, t_1) = T_0(u_2, t_3|u_1', t_2)T_0(u_1', t_2|u_1, t_1) \tag{3.4.0.1}$$

where $u_1' = (\bar{x_1} + \bar{k_1}/m_n(t_2 - t_1), \bar{k_1})$ and $u_2 = (\bar{x_1} + \bar{k_1}/m_n(t_3 - t_1), \bar{k_1})$. This notation is a little bit overly verbose in order to make it connect with the earlier formula. Given the linear path condition between collisions, it actually suffices to specify $T_0(t_2|u_1, t_1)$ as the measure of the event that a single neutron at u_1 at time t_1 fails to have any collisions in the interval $[t_1, t_2]$. In this case, we can use the fact that the path constraining delta incorporates the path constraint as $t_2 \to t_1$ since

$$\lim_{t_2 \to t_1} \delta\left(\bar{x_2} - \bar{x_1} - \frac{\bar{k_1}}{m_n}(t_2 - t_1)\right)\delta(k_2 - k_1) = \delta(u_2 - u_1) \tag{3.4.0.2}$$

when δ are viewed as approximating measures with the limit representing a kind of weak-* convergence as measured against the space of continuous functions. This allows us to leave this out of the propagator normalization and conclude that this propagator must satisfy the simpler normalization condition

$$\lim_{t_2 \to t_1} T_0(u_2, t_3|u_1, t_1) = 1 \tag{3.4.0.3}$$

The resulting functional equation is well known as having a unique solution in the space of continuous functions given by the exponent of a function linear in the semigroup parameter. [129] Specifically, we claim that there is a reaction measure absolutely continuous with respect to a Lebesgue integral in time $\mathrm{d}t'$ and we represent this via a density function $f(t') = R(t', \bar{x_1} + \frac{\bar{k_1}}{m_n}(t' - t_1), \bar{k_1})$, where f is the RND given by the usual change of measure type theorem [56], but R can only be understood as a global function of (x, k)

evaluated along a path. Under the assumption of the existence of such a function, the free propagator is given by

$$T_0(u_2,t_3|u_1,t_1)=\exp\left(-\int_{t_1}^{t_3}\mathrm{d}t' R(t',\bar{x_1}+\frac{\bar{k_1}}{m_n}(t'-t_1),\bar{k_1})\right)=\exp\left(-\int_{x_1}^{x}\Sigma(v,x')\mathrm{d}x'\right) \tag{3.4.0.4}$$

Thus we conclude that as compared with the first approach to addressing this problem,

$$R(t',\bar{x_1}+\frac{\bar{k_1}}{m_n}(t'-t_1),\bar{k_1})=v\Sigma(v,\bar{x_1}+\frac{\bar{k_1}}{m_n}(t'-t_1)) \tag{3.4.0.5}$$

The existence of a function R must be justified by examining the consistency conditions for the continuity of the underlying field theory as a quantum stochastic process observed on a geographic space. We will perform this analysis in some detail in chapters 5 and 6. In the classical case, we will satisfy ourselves with a simplified version of this observation. We have asserted that in this model the rate of change in the free propagator (having already incorporated the path dependence) is driven entirely by reactions. Previously, we represented this by the formula 3.3.2.4. In order for both to be true, we find that R must correspond to an integral over all outgoing states for all double differential transition densities, integrated over the propagation interval and contracted over the outgoing one particle states

$$R(t,\bar{x_1}+\frac{\bar{k_1}}{m_n}(t-t_1),\bar{k_1})=\sum_i\sum_{n_2}\int_{\mathscr{O}^{n_2}}\mathrm{d}k_2\int_{[t,\infty)^{n_2}}\mathrm{d}t'\,W_i(n_2,u_2';\bar{t'}|\bar{x_1}+\frac{\bar{k_1}}{m_n}(t-t_1),\bar{k_1};t) \tag{3.4.0.6}$$

and so,

$$T_0(u_2,t_3|u_1,t_1)=\exp\left(-\int_{t_1}^{t_3}\mathrm{d}t\;\sum_i\sum_{n_2}\int_{[t,\infty)^{n_2}}\mathrm{d}t'\;\int_{\mathscr{O}^{n_2}}\mathrm{d}k_2\;W_i(n_2,u_2;t'|u_1';t)\right) \tag{3.4.0.7}$$

Although it is not overwhelmingly important to where an understanding of the quantized version, it is important to note that in all of these equations, these transition probabilities correspond to macroscopic reaction rates, which is to say that these are all functions of the neutron phase space density in general. This nonlinearity in the classical evolution equations can be understood as a consequence of approximating non-commutative single particle processes by commutative ones on a space of reduced dimensionality via a nonlinear kinetic equation. Deriving the detailed dependence of these expressions on the elements of the quantum theory is one of the goals of this work.

One final note of comparison is important. The exponential form of these free propagators is characteristic of the evolution induced by linear operators on infinite dimensional spaces. [91] [77] In particular, we are

interested in evolutions having the semigroup property, as they are important for characterizing Markovian systems. [36] A family of bounded linear operators $\boldsymbol{T}(t)$, defined on a Banach space B, is characterized as a semigroup if it has the following properties

$$\boldsymbol{T}(t+s) = \boldsymbol{T}(t)\boldsymbol{T}(s)\ \forall t, s \geq 0 \tag{3.4.0.8}$$

$$\boldsymbol{T}(0) = \boldsymbol{I} \tag{3.4.0.9}$$

A semigroup is said to be uniformly continuous in its semigroup parameter if

$$\lim_{t\to 0} \|\boldsymbol{T}(t) - \boldsymbol{I}\| = 0 \tag{3.4.0.10}$$

While it is said to be strongly continuous if

$$\lim_{t\to 0} \|\boldsymbol{T}(t)x - \boldsymbol{I}x\| = 0\ \forall x \in B \tag{3.4.0.11}$$

By standard results of functional analysis, we have that every uniformly continuous semigroup is generated by a bounded linear operator $\boldsymbol{G}$ and, conversely, bounded linear operator $\boldsymbol{G}$ generates a uniformly continuous semigroup. Specifically,

$$\boldsymbol{T}(t) = e^{t\boldsymbol{G}} = \sum_{n=0}^{\infty} \frac{t^n \boldsymbol{G}^n}{n!} \tag{3.4.0.12}$$

where the sum converges in the uniform norm. This is a direct result of the fact that $\boldsymbol{G}$ is uniformly bounded on B and we have a well-defined Riesz functional calculus for analytic functions (that can be applied to the exponential function) of bounded operators on a Banach space. The converse result is obtained by applying it to the natural logarithm. Thus, we have a complete characterization of uniformly bounded semigroups in terms of exponential functions of bounded operators. We can extend this to strongly continuous semigroups of contractive operators (by Hille-Yoshida) with a more subtle definition of what we mean by exponentiation. In this case, the generators are densely defined unbounded self-adjoint operators satisfying some nice decay properties for the resolvent ($\|\boldsymbol{R}(\lambda)\| \leq 1/\lambda$). [91] Such generators possess their own functional calculus with properties familiar from the standard theory of mathematical quantum mechanics on Hilbert spaces. [125]

The extension to strongly continuous semigroups on a Banach space is not a mere technicality. First, there are many important unbounded operators that we wish to use as generators of processes, like the position and momentum observables or the streaming transport operator. Semigroups with bounded generators can always be extended from a semigroup to a group and thereby inverted. Therefore, restricting our attention

to semigroups with bounded generators would prevent us from ever describing processes that are irreversible. For example, even a simple diffusion cannot be reversed but it can be represented as a strongly continuous semigroup with a laplacian generator. Second, the Hilbert space theory is actually inadequate for what we are about to attempt. In order to model quantum stochastic processes by linear operators we need to define the process on density matrices. This is a convex cone of positive trace class operators. Thus, a QSP can be modeled as a positivity preserving process on a space of bounded linear operators on a Hilbert space, $B(H)$. However, while $B(H)$ is a Banach space in the operator norm and the Trace class operators form a Banach space in the trace norm, neither is a Hilbert space and the restriction to the Hilbert-Schmidt space is too restrictive. As such, the analysis of evolution equations must be understood in terms of strongly continuous semigroups on Banach spaces. [91] [32]

The main point of this digression is that there are evolution operators for quantum theories that are a natural analogue for the commutative propagators that we described above. Moreover, an analysis of these propagators can be done in terms of their generators. This will allow us to prove certain quantum results that exhibit a deep explanation for the classical results presented heuristically in this section. For example, we will show that any representation of the free dynamics must include a representation of the reaction processes and these can be included explicitly as part of the generator. From here, it is only a small leap to imagine the Pál-Bell free propagators obtained from a result like Ehrenfest's Theorem applied to a suitable quantum reaction model.

3.5 Delayed Neutron Kinetics and Detector Sensitivity

The purpose of this section is to provide a detailed accounting of time delayed contributions to neutron physics. We have repeatedly made reference to delayed reactions or finite duration collisions or compound reactions. Loosely speaking, this means that $W_i(n_2, u_2'; \bar{t'}|u_1'; t) > 0$ for $t' - t > 0$ on a set of measure greater than 0. However, it is known that in a microscopic model, even direct potential scattering events will occur over a time interval greater than zero. So how do we make this distinction reasonably precise in reference to the very small nuclear transit time?

Supposing that no delta distribution like approximations have been made to the propagators yet, this can be understood in terms of the transition rates W_i, the thermal neutron speed, and the effective nuclear diameter. Specifically, we can introduce a measure on the set of transition intervals $t' - t$

$$\mu_{i,t}(\{t' - t \in E \subset \mathbb{R}_+\}) = \int_{\mathscr{O}} \mathrm{d}u_1' \sum_{n_2} \int_{\mathscr{O}^{n_2}} \mathrm{d}u_2 \; W_i(n_2, u_2; \bar{t'}|u_1'; t) \tag{3.5.0.1}$$

There is unimpeachable empirical evidence that for a large class of power reactor systems currently in operation, there is a set $E_{\text{delayed}} = \{t' - t | (t' - t)/\tau_{\text{direct}} = v_{\text{thermal}}(t' - t)/d_{\text{nuclear}} > 10\}$ such that

$$\mu_{\text{fission},t}(E_{\text{delayed}}) > 0.0064 \frac{\int_{\mathscr{O}} \mathrm{d}u_1 \; v_1 \sigma_{\text{fission}}(u_1)\psi(u_1;t)}{\int_{\mathscr{O}} \mathrm{d}u_1 \; \psi(u_1;t)} \tag{3.5.0.2}$$

where this quantity is large enough to substantively change the dynamics of the system. [3] [20] [137] Moreover, fission processes are not the only reactions that induce delayed transitions. In fact, any compound or resonance scattering process can yield a macroscopic time delay. This includes even processes as simple as compound elastic scattering and the formation of doorway resonances, as can be observed in neutron thermalization in the presence of complex nuclei. [59]

Given the success of potential scattering in explaining the results of neutron optical measurements, it is tempting to model these systems using the potential scattering framework. This turns out to be difficult for multiple reasons. First, the class of potentials required for inducing the formation of a quasi bound state are fantastically ill-behaved. In particular, such potentials cannot be compactly supported. This precludes the kind of support rescaling used in the Boltzmann-Grad limit of interacting particle systems. Second, by virtue of the fact that direct processes are defined by the action of an isometric linear operator of the form $S = \lim_{t\to\infty} \Omega_{-t}^* \Omega_t$, there is no notion of process duration, only an initiation time. Thus, we cannot think of their dynamics as taking place on a time scale compatible with the time scale of the geographic space of the transport process. In the usual construction of transport equations, this assumption is encoded by the statement that all collision processes are instantaneous. [20] However, this is incompatible with the idea that there exist processes with a finite duration.

Having ruled out inclusion of compound processes in the direct scattering term, our best option appears to be the introduction of a new type of reaction transition operator, corresponding to compound reaction processes. We have already been including these terms in our formulas with the index $i =$ fission. For example, $W_{\text{fission}}(n_2, u_2; t' | u_1'; t) = D_{\text{fission}}(n_2, u_2', u_1', t, t') Q_{\text{fission}}(t, u_1')$ has been used in the final and most complex term of most versions of the Pál-Bell equation that we have presented so far. This term actually is a place holder for all resonance or compound scattering processes.

In understanding the resonance reaction terms in the Pál-Bell theory, we will identify a multistage part process for a typical compound reaction that follows a framework common to modern theories of nuclear resonance analysis. [59] In particular, the reaction is understood in terms of

1. an absorption event where a quasi-bound or compound or precursor state is formed

2. a bound state evolution where the newly formed system irreversibly approaches an effectively quasi-

equilibrium distribution over the available bound states

3. a decay event where the once quasi-bound nucleus once again releases one or more particles into free states

This analysis is something of an oversimplification because the stages need not be neatly separated and quantum correlation effects can be retained during the evolution. However, for nuclear collisions, the time span of distortion where an incident particle transitions into a quasi-bound particle is far smaller than the time interval of free propagation or the expected life time of the quasi-bound state. Thus, the stage separation is less of an oversimplification for nuclear collisions than for electromagnetic ones where these time scales are comparable and mathematically technical renormalizations are essential to applying the apparatus of scattering theory. [125] Moreover, the large number of states available to transform through and the high degree of connectedness in a nuclear system can lead to the rapid loss of memory of the incoming state and a resulting factorization of the absorption and decay distributions for most shell-like models. [50] [148] [145] [102] For some very important processes and systems studied in recent years, this Fechbach-Hauser or statistical spectral theory type of reasoning does not hold up to scrutiny. [70] [17] [113] [61] However, traditional neutron transport theories do not account for the influence of these processes. Therefore, we will postpone this discussion until chapter 7.

In the classical neutron transport theory, the first stage of the reaction can be treated separately from the combined effect of the second and third stages. Namely, we view the reaction in terms of the population of bound states through an absorption event, followed by the collective decay. This computation can be done in many ways. The simplest is to use an optical potential for total absorption and then to model the reaction evolution process as immediately attaining an equilibrium bound state distribution (or fission product precursor distribution) and then exponential decay through transmission across a potential barrier. Although this is a bit reductive as compared to full fission models, the essential ideas about transition function factorization and representation hold up. The key observations that fall out of this are

1. The absorption process depends only on the incident momentum and the species of the reacting nucleus

2. The decay process is approximately independent of the state prior to absorption and can be expressed as a function of the decaying species only

3. For a given decaying species and source state, the temporal distribution is (like any radioactive decay) approximately exponential in time

In order to conform to the transport theoretic assumption that the reaction events are localized and instantaneous, we will simplify this model even further by assuming that all neutrons that will be produced

eventually are born at $t' = t$ in their bound states and then decay into a free state with an distribution obtained from $\mu_{i,\ell,t}$, where ℓ is a precursor index. That is, by conditioning the decay time distribution not just on the type of reaction i but on the outgoing excited state and species ℓ we can treat it as exponential with a fixed decay constant. In practice, ℓ is defined in a coarse sense and results from averaging over an equilibrium distribution of states for the same precursor compound nucleus. This averaged decay precursor analysis can be done using only data from a reactor experiment by observing the decay of flux distributions in pulsed reactors using the peeling method. [3] Regardless of how the effective bound precursor states are obtained, this analysis has been performed on many systems. Once we have these distributions and a reaction dependent yield fraction for each precursor group, we can form our compound reaction transport operator from a sum of weighted contributions using the usual finite additivity over a disjoint union of events argument. [56] [122]

This is given a relatively simple form in Pázsit and Pál as follows. [122] We begin by considering the instantaneous absorption and bound state population event. Informally, we imagine that there is a fluctuating field including M bound states available at every coordinate location $\bar{x} \in \mathscr{V}_D$. We can generalize this to facilitate the construction of a mathematically well-defined object by constructing a branching measure of bound states with an RND in direct analogy to the geographic space measure of the neutron number counting model. In this way, we will instead say that conditional on the detection of a fission reaction in a phase space volume E at the time t, there is a time indexed family of measures assigning a probability to observing a decay from a collection of M bound states. This measure is supported on the same volume E and (absent any prior fission collisions) is zero on sets outside of E. In the abstract theory that we outlined above, the absorption event is determined entirely by the quantity $Q_{\text{fission}}(t, u_1')$.

In order to describe the set of excitations that occur at time t as a result of this collision, we will define an M vector of integer valued random variables $(\nu_\ell)_{\ell=0}^{M}$. These random variables represent different numbers of neutrons born from fission at the time of the initial collision t. ν_0 neutrons are born to a free state and released promptly. Likewise, ν_ℓ neutrons are born to the ℓth bound state and then decay into a free state (and so appear in the free neutron field) with an exponential distribution of the delay interval length $t' - t$ having a single decay constant parameter λ_ℓ. The distribution of the number of neutrons born in each bound state is taken to be a function of the incident neutron energy and the bound state only. This discards any anisotropy to the bound state formation process, which is equivalent to a kind of orientation-beam averaging of the collision process. [117] We define the resulting distribution to be the function $f(\nu_\ell = n_\ell; \forall 0 \leq \ell \leq M | k_1)$ where k_1 is the neutron momentum at the collision time t. This provides the first factor that we use to construct the detector response function $D_{\text{fission}}(n_2, u_2', u_1', t, t')$. In particular,

it accounts for the full dependence on the prior momentum k_1.

Having characterized the bound neutron "creation" process, we need to model the independent decay process. In general, it is easy to see why the decay of individual neutrons would alter the state for subsequent decays, possibly even connecting previously distinct states by altering the internal nuclear potential by the removal of a particle. This quickly gets into very deep quantum field theory and is not the approach that we will take here. [38] Instead we will assume independent neutrons decaying by transmission through a temporally constant mean field potential (for each precursor). [107] [108] Thus, we assume that the decay events are independent exponential distributions where the decay parameter λ_ℓ is determined exclusively by the bound state in which the neutron was formed. Moreover, we assume that the momentum of the decay neutrons is such that they are independent and identically distributed random variables that are each given by the same one particle measure, which is absolutely continuous with respect to the decay momentum Lebesgue measure $\mathrm{d}k_2$. We define the resulting Radon-Nikodym density for the decay distribution of the ℓth bound state as $w^\ell_{\text{fission}}(k_2)$. Finally, we recognize that this can be combined with the independent decay claim to yield a product decay density for an n_ℓ particle system conditional on the assumption that exactly n'_ℓ particles decay in the interval $[t, t_3]$ and $n_\ell - n'_\ell$ fail to decay in the same interval.

$$\begin{aligned}
&\int_{[t,t_3]^{n'_\ell}} \mathrm{d}t' T(n_3, u_3, t_3 | n_2, u'_2, \bar{t}') D_{\text{fission}}(n_2, u'_2, u'_1, t, \bar{t}') \\
&\quad = \frac{n_\ell!}{n'_\ell!(n_\ell - n'_\ell)!} e^{-\lambda_\ell (n_\ell - n'_\ell)(t_3 - t)} \int_{[t,t_3]^{n'_\ell}} \mathrm{d}t' \prod_{i=1}^{n'_\ell} \left(T(n_3, u_3, t_3 | u'_{2,i}, \bar{t}') w^\ell_{\text{fission}}(k_{2,i}) \lambda_\ell e^{-\lambda_\ell (t'_i - t)} \right) \quad (3.5.0.3)
\end{aligned}$$

Where the product integral is time ordering in indexes. This formula is best read as a time ordered sequence of events from right to left. First, $n_\ell - n'_\ell$ are selected that fail to decay. There are $n_\ell!/(n'_\ell!(n_\ell - n'_\ell)!)$ combinations of neutrons that can be selected for non-decay (this factor has been pulled out side of the expression for clarity). Then n'_ℓ neutrons decay independently, each with a rate $\lambda_\ell e^{-\lambda_\ell (t' - t)}$. However, as these events certainly occur in the interval $[t, t_3]$ by our conditioning assumption, it suffices to integrate the decay rate over the interval to determine the measure of the event for each emitted neutron. This precise form is only possible because we are not interested in the order of decay. Finally, we presume that the neutrons decay into a small region of the product domain about $(k_{2,i})_{i=1}^{n'_\ell}$ and propagates via the full propagator from there. During the non-decay interval, the coordinate of the precursor does not evolve. This is something we can easily modify but in this model it remains static throughout the period prior to the decay. Finally, we sum this over possible precursor distributions weighted by the discrete density $f(\nu_\ell = n_\ell; \forall 0 \leq \ell \leq M | k_1)$.

This yields a relatively simple formula for the compound state formation and decay

$$C_\ell^{(m_\ell,m'_\ell)} \equiv \frac{m_\ell!}{m'_\ell!(m_\ell - m'_\ell)!} e^{-\lambda_\ell(m_\ell - m'_\ell)(t_3 - t)} \tag{3.5.0.4}$$

$$\begin{aligned}
&\int_{t_1}^{t_3} \mathrm{d}t \iiint_t^{t_3} \mathrm{d}t^{n_{2,'}} \iiint_{\mathscr{O}} \mathrm{d}\bar{k}_2^{n_2}\, T((u_3^l)_{l=1}^{n_3}, t_3 | (u_2^{j,'})_{j=1}^{n_2}, (t'_j)_{j=1}^{n_2}) \\
&\qquad D_{\text{fission}}((u_2^{j,'})_{j=1}^{n_2}, u'_1, t, (t'_j)_{j=1}^{n_2}) Q_{\text{fission}}(t, u'_1) T_0(u'_1, t | u_1, t_1) \\
&\quad = \int_{t_1}^{t_3} \mathrm{d}t \sum_{n_2=1}^{N} \sum_{\substack{(m_0,\ldots,m_\ell,\ldots,m_M) \\ m_0+\cdots+m_\ell+\cdots+m_M=n_2}} f((\nu_\ell)_\ell = (m_\ell)_\ell | k_1) Q_{\text{fission}}(t, u'_1) T_0(u'_1, t | u_1, t_1) \\
&\sum_{\substack{(n_{3,\ell})_1^M \\ \sum_i n_{3,\ell} = n_3}} \prod_{\ell=0}^{M} \sum_{m'_\ell=0}^{m_\ell} C_\ell^{(m_\ell,m'_\ell)} \sum_{\substack{(n_{\ell,i})_1^{m'_\ell} \\ \sum_i n_{\ell,i} = n_{3,\ell}}} \prod_{i=1}^{m'_\ell} \left(\int_t^{t_3} \mathrm{d}t'_i \int_{\mathscr{O}} \mathrm{d}k_{2,i}\, T(n_{\ell,i}, u_3, t_3 | u'_{2,i}, t'_i) w_{\text{fission}}^\ell(k_{2,i}) \lambda_\ell e^{-\lambda_\ell(t'_i - t)} \right)
\end{aligned} \tag{3.5.0.5}$$

The apparent complexity of the formula comes from three facts. First, we must account for every allocation to the bound states. Second, we must account for every possible decomposition of the contributions to the terminal state from the different decay particles. Finally, we must account for every possible number of decays occurring during the given interval (this is the sum over m'_ℓ). The two products are actually easily understood as the result of an overall tensor product representation among the newly created neutrons and their corresponding bound states. By splitting first on the bound states for a given allocation, we get a product over bound states. Then after separating out the different possible numbers of decays, we can split on the individual particle indexes so that the action of the many particle propagator can be made explicit in terms of contributions due to a product of subtrees of the branching process.

We should also take note of the interior integral over the $\prod_i \mathrm{d}k_{2,i}$ measures. These are all formally identical to $\mathrm{d}k_2$ and can be reduced to evaluated expectations. However, the integral over $\mathrm{d}k_2$ in the original abstract formulas that we presented (for example in equation 3.3.2.4), must be understood as part of the composite many particle evolution. This takes the form of a product measure when multiple particles are generated in the process of the reaction. This process is fundamentally a many particle dynamics that is tree-like and where the operators representing tree-like branching events stay well bounded and the reaction rate distribution is bounded by linear growth in time. This turns out to be characteristic of a large family of quantum stochastic models and we will use it to study the generalization of the classical measurement theory.

Returning to our earlier analogy of the medium as a detector, we find that it is a helpful way of thinking

about delayed neutron reactions. There is a measurement probability of the neutron by the detector and a subsequent amplification and delay process whereby the detected signal of a single neutron is converted into many bound neutrons. Part of the signal is transmitted instantaneously (prompt neutrons). However, some neutrons experience a delayed propagation where they are trapped in a bound state and then released as a kind of retarded signal. In this process, some fraction of the nuclei undergo a classically observable transmutation and the lattice structure gets disrupted by radiation damage, slowly altering the detector efficiency. Moreover, when the adjoint equations of neutron transport are viewed as a model of the sensitivity of the medium, we see that a model for the spatio-temporal dynamics of the field of bound neutrons and the classically well-defined species of nuclei after reactions provide a new generalized class of "adjoint" equations. Where the transport equations describe the evolution of the neutron density by way of reaction tracking, these secondary equations describe the evolution of the nuclear species density and the delayed neutron density (again via reaction rates) in a way that is relevant to a more general theory of nuclear systems.

The complementarity between the free and bound states can be understood in the same terms as the relationship between the neutron flux equations and the spatially dependent delayed neutron precursor population equations. [137] Any expression for the dynamic reactivity must include the effect of the precursor (bound state) dynamics in the variational representation of the reactivity. Consider, for example, how Stacey's formula for the reactivity includes terms for the decay process contributions. This analysis leads to a generalized adjoint solution that is obtained as the solution of the equations that result from the stationarity of the reactivity functional with respect to perturbations of the underlying variables.

The characterization that we have given in this section is sufficient for most problems of classical nuclear engineering. We will find that it is easy to model this process in the quantum stochastic measurement theory by treating the absorption and decay processes as observed jump transitions into and out of a collection of bound states that evolve collectively according to a simple Hamiltonian generated unitary group. This model becomes a natural generalization of the population of and decay from a collection of bound states that we described for the classical stochastic measurement model.

Chapter 4

Two-Instrument Heuristic for Reaction-Transport

In this chapter, we are going to build on the classical measurement theory interpretation that we obtained from the Pál-Bell theory of neutron transport in the last chapter. The goal now is to identify the essential properties of a reaction-transport system so that we can formulate the quantization on purely operational grounds. Realistically, it is neither possible nor desirable to remove all ambiguity from the quantization without reference to the particular system that we are modeling. However, we can demonstrate a conceptual justification for reducing the dimensionality of the model. This chapter constitutes the first stage in this process.

We will begin, in section 4.1, by identifying the most defining features from chapter 3. Second, in section 4.2, we will discuss the idea of an Instrument and what information is essential to making these features meaningful. Third, in section 4.3, we will propose a general heuristic picture of the evolution of information in a reaction-transport theory. Finally, in section 4.4, we will attempt to write down a set of necessary and sufficient conditions for applying this modeling framework to new systems.

4.1 Essential Approximations of Stochastic Neutronics

Throughout the chapter 3, we used measurement theoretic ideas to build a working theory of stochastic neutron transport. Some of these assumptions can be weakened without any harm to the basic integrity of the model. However, others are essential to viewing the stochastic process as a branching graph of collisions indexed on a geographic space. We enumerate the key assumptions below.

The main measurements of interest in characterizing a given neutron field are the reaction rate distributions for each reaction type at each time. The evolution of any reaction measurement, R, can be completely characterized as an operator-valued function of a standard exhaustive set of reaction rate densities. However, we can also model relationships between reaction events using information about the number of neutrons present in a volume. This allows us to perform a kind of path-wise linearization.

We define the sigma algebra of the geographic phase space $\mathscr{B}(\mathscr{V}_D \times \mathscr{O}) = \mathscr{G}$ of the problem to be the

collection of macroscopic reaction volumes that can be used in detecting neutrons. In probability theoretic language, the sets in $\mathscr{G} \times \mathscr{P}(\mathbb{N})$ are the events for counting neutrons. More explicitly, for every time t, there exists a measure μ_t such that for every Borel subset $U \in \mathscr{G}$ of the geographic phase space and for every natural number n, $\mu_t(U, n) \in [0, 1]$ and is countably additive on disjoint unions of sets while $\mu_t(\mathscr{V}_D \times \mathscr{O} \times \mathbb{N}) = 1$. That is, for every reasonable reaction volume, we can assign a probability to each possible number of neutrons that could be observed and this probability measure conforms to the usual rules of probability theory.

The reaction rate probability measure of the reaction count $n_{\text{rxn}} \in \mathbb{N}$ in a given detection volume U in the time interval $(t, t_2]$, conditional on the existence of a single neutron in that time interval, can be computed from a measure absolutely continuous with respect to the Lebesgue measure on the geographic space. The resulting reaction rate Radon-Nikodym density can be expressed as a reaction rate operator acting on a single neutron Radon-Nikodym density.

Building on this, we note that the reaction rate probability measure of the reaction count $n_{\text{rxn}} \in \mathbb{N}$ in a given detection volume U in the time interval $(t, t_2]$, conditional on the existence of a collection of n distinct neutrons each with a prior distribution $p_i(u_i)$, can be computed as a measure absolutely continuous with respect to the product Lebesgue measure of n copies of the geographic space. Moreover, the reaction counting Radon-Nikodym density can be factored into a sum of products of single particle reaction counting densities for the neutrons present in the system as a result of the different event chains. We will use the phrase *independent neutron tree factorization* to describe this assumption that n-particle event chaining is representable as a sum of products of single particle event-chains descending from the same parent neutron.

The independent neutron tree factorization is implicit in every term of the Chapman-Kolmogorov equation, but can be seen most explicitly in the formula 3.5.0.5. This factorization is only possible for a static medium or in some kind of propagation of chaos limit. [83] Although this is not strictly needed to formulate a useable theory, it dramatically simplifies numerous practical aspects of the application of the theory. The potency of this assumption is apparent even a classical context by virtue of the fact that this assumption makes it possible for the standard form of the Pál-Bell equation to be obtained in terms of generator functions from the Chapman-Kolmogorov equation that we derived earlier. We will examine some of the consequences of not making this simplification in chapter 6. The version of this theory with a non-static medium would still lead to a nonlinear kinetic equation, it just won't be of the familiar type because the indirect correlation of the single particle fields relative to the geographic space will not be negligible.

The path averaging representation amounts to a kind of path integral over the space of possible reaction event sequences that would yield a given reaction count in the detection volume U. The probability associated to a given reaction space event (which we will discuss in detail in section 4.2) can be determined from the

distribution of individual branching neutron paths and their corresponding reaction measures. In particular, temporally isolated reaction events are linked into chains by free evolutions. So, the reaction measure can be given a representation in terms of a conditional expectation taken over time-ordered products of absorptions, scattering events, decays, and free propagations. We found this construct implicitly in the second resolvent type form for reaction measurements in the equation 3.3.4.13. We also see it with more explicit chaining of free and interaction operators in the equation 3.3.4.1.

Our next observation relates to the analysis done in section 3.5. There is a de facto time localization of branching collisions by generating new neutrons in a bound state at the time of the initial collision and giving their decay process a finite extent in time. The branching rate and the time dependence of the decay process are the functions of significance for modeling the effect of compound reaction event on the macroscopic free neutron field. These functions bear a complex dependence on the nucleus with which the neutron reacted and the energy at which the reaction occurred. This suggests that we need to specify an empirically characterizable set of quasi-bound states for neutrons corresponding to compound nuclear states or fission precursors. In the current classical model, the two become conflated as a single compound decay event. This limitation can be circumvented by adding more bound states and introducing classical decay rates between different internal states. Regardless of the internal mechanics (which will need to be more complex in the quantum theory either way), the main assumption here is that there is a field of bound states in the medium that are indexed against the geographic space. This reaction time dependence is in direct analogy to the processes modeled in zero point reactor kinetics [3] but occurring with different initiation and decay times and counts on each Borel subset of the geographic space.

The population of these bound states and their decay back into the free neutron field is the essential mechanism for modeling the contribution of time-extended collisions to the transport process. The transition mechanics of this process are explicit in formula 3.5.0.5 and explained in the paragraphs following it. Just as the neutron field can be understood as a geographic space subset dependent measure on the free neutron count. The space of bound states can be viewed as a complimentary field to the free neutron field that encodes a geographic space subset dependent measure on the bound neutron count.

Finally, we assume the free evolutions follow linear trajectories and reactions only modify momentum and induce branching in the number space. There is no jump process in coordinate space. Thus, a free propagation over the interval $[t_0, t_1)$ takes $u_0 \to u_1$ where $u_0 = (\bar{x_0}, k_0)$ and $u_1 = (\bar{x_0} + \bar{k_0}/m_n(t_1 - t_0), \bar{k_0})$. A subsequent reaction at t_1 would yield some distribution over $n_2 \in \mathbb{N}$ and $k_2 \in \mathscr{O}$ with $u_2^i = (\bar{x_0} + \bar{k_0}/m_n(t_1 - t_0), \bar{k_2}^i)\ \forall i \in n_2$. Reaction events only involve one neutron and can be localized to a single point in time even though multiple neutrons can decay in the same Borel set, in the same time interval. This precludes

the need to account for multi-particle collisions. In general, we can examine both of these assumptions by using the quantum theory and examining the quality of the approximations produced by the substitution of the simpler model. This is to say that these don't materially constrain the quantum theory in its basic construction and can be examined as explicit approximations for different neutron densities and collision detection operators. However, we will always use these assumptions before passing to a fully classical limit.

4.2 Operational Ideas in Neutron Detection

In this section, we will apply the basic operational ideas from quantum measurement theory to the detection of particles in phase space. These ideas will be used to describe collections of reaction events as time indexed neutron detection measurements that produce a phase space localization of the neutron that is detected. The operational ideas that we develop here will be used in section 4.3 to loosely describe a quantum stochastic process that satisfies the properties outlined in section 4.1. This idea will then be made technically precise in chapter 5.

4.2.1 Approximate Phase Space Observables

Using the definitions from section 2.3, we can introduce a theory of approximate position and momentum observables. We know from traditional quantum theory that ideal position or momentum observables can be conditioned on finite volume subsets and, in principle, we can have also partial knowledge of the conjugate variable without violating Heisenberg's uncertainty principle.[125] However, traditional quantum theories do not include a framework for representing the operators that enable the possession of such partial knowledge of non-commuting variables. It is relatively easy to show that there is no joint classical probability distribution for the general ideal non-commuting observables $\boldsymbol{Q}$ and $\boldsymbol{P}$, and this requirement has been tested empirically using Bell Inequalities. [24] However, by introducing an ambiguity function we will show that there is a notion of a joint distribution that is relevant. In particular, we can construct an Observable that has approximate position and momentum as Marginal Observables.

Definition 4.2.1. *Marginal Observables*

Given an Observable $\boldsymbol{E}$ *on* $\Omega_1 \times \Omega_2$ *then* $\forall B_i \in \mathscr{F}$ *the sigma algebra on* Ω_i*, we define the marginal observable*

$$\boldsymbol{E_1}(B_1) = \boldsymbol{E}(B_1 \times \Omega_2) \tag{4.2.1.1}$$

and

$$\boldsymbol{E_2}(B_2) = \boldsymbol{E}(\Omega_1 \times B_2) \tag{4.2.1.2}$$

What we will describe below is a fairly general theory of non-ideal observables that facilitates the representation of simultaneous incomplete information about noncommuting observables. This section is a generalization of a theory of joint observables originally developed by Davies and later expanded by Ford and Lewis for use in constructing quantum stochastic processes. [57] We will use this generalization to develop a significant result in section 4.2.2.

As a brief aside, the analysis in this section relates closely to the Wigner function and the theory of quantum mechanics on phase space. [28] [112] [55] We will discuss the significance of representing the free non-interacting propagator in terms of a product of Weyl-Heisenberg groups in the phase space quantization in section 7.2.3. This has profound implications for constructing semiclassical approximations and transport scaling limits. However, the existence and uniqueness results that dominate this text are independent of this choice. For now it is sufficient to note that Wigner Transform facilitates the unitary equivalence of the phase space quantization to the canonical quantization. [35]

We begin by defining a position observable that incorporates an apparatus uncertainty function. In general, such a quantity depends on the method of measurement being used. However, since this will be characterizing absorption and decay events, for us this will be a representation of imperfect knowledge due to condensed matter uncertainty in the location of the nucleus and its total interaction rate with a beam of incident neutrons. Thus, the α in what follows can be taken as function derived from scattering theory by averaging over relative orientations, nuclear center-of-mass positions, and nuclear center-of-mass momenta due to random oscillations within the atom. Although these random effects can be incorporated explicitly into the system state ρ, the individual nuclear center-of-mass states are nearly independent to a first approximation. This approach neglects many important dynamical processes involving phonons and lattice disruptions due to the slowing down of fission fragments. However, this difference would only appear as a more complex dependence on the matter field parameters of α in the definition of the global QSP.

Definition 4.2.2. *Approximate Position Observable*

We define a norm convergent integral representation for any $g \in C(\mathbb{R}, \mathbb{C})$ using the spectral integral based functional calculus for functions of an ideal position observable $\boldsymbol{Q}$, $\mathrm{d}\boldsymbol{Q}$ is a Projection Operator Valued Measure

$$g(\boldsymbol{Q}) = \int_{\mathbb{R}^3} g(x)\, \mathrm{d}\boldsymbol{Q}(x)$$

Based on this, we can choose g to be convolution of a characteristic function $\chi_{_E}$ on a set $E \in \mathscr{B}(\mathbb{R}^3)$ with

a non-negative measurable function $f \in L_1$ having unit norm. We have that, by [56] proposition 8.8,

$$g = \int_{\mathbb{R}^3} f(y)\chi_{_E}(x-y)\mathrm{d}y = f * \chi_{_E}(x) \tag{4.2.1.3}$$

is a bounded and uniformly continuous function. Therefore, the functional calculus applies and

$$\boldsymbol{Q_f}(E) = \int_{\mathbb{R}^3} f * \chi_{_E}(x)\ \mathrm{d}\boldsymbol{Q}(x) \tag{4.2.1.4}$$

is an observable since $f * \chi_{_{\mathbb{R}^3}}(x) = 1$ and $\boldsymbol{Q_f}(E) = \overline{\boldsymbol{Q_f}}(\chi_{_E})$ and then approximating by simple functions we can obtain a positive linear map on $C(\mathbb{R}^3)$ which is an observable by the Bounded Operator-Valued Integral form of an observable.

We recall the definition of mean and variance in a quantum context

Definition 4.2.3. *Approximate Position Expectation Value*

$$\mathbb{E}[\boldsymbol{\rho}, \boldsymbol{Q_f}] = \int_{\mathbb{R}^3} x\ \mathrm{Tr}\left[\mathrm{d}\boldsymbol{Q_f}(x)\boldsymbol{\rho}\right] \tag{4.2.1.5}$$

Definition 4.2.4. *Approximate Position Variance*

$$\mathrm{var}[\boldsymbol{\rho}, \boldsymbol{Q_f}] = \int_{\mathbb{R}^3} (x \cdot x)\mathrm{Tr}\left[\mathrm{d}\boldsymbol{Q_f}(x)\boldsymbol{\rho}\right] - \left(\int_{\mathbb{R}^3} x\mathrm{Tr}\left[\mathrm{d}\boldsymbol{Q_f}(x)\boldsymbol{\rho}\right]\right)^2 \tag{4.2.1.6}$$

The Approximate Momentum Observable can be defined identically, relative to the $\boldsymbol{P}$ projection operator valued measure on $\sigma(\boldsymbol{P}) = \mathbb{R}^3$

Definition 4.2.5. *Approximate Momentum Observable*

We define a norm convergent integral representation for any $g \in C(\mathbb{R}, \mathbb{C})$ using the spectral integral based functional calculus for functions of an ideal momentum observable $\boldsymbol{P}$, $\mathrm{d}\boldsymbol{P}$ is a Projection Operator Valued Measure

$$g(\boldsymbol{P}) = \int_{\mathbb{R}^3} g(x)\ \mathrm{d}\boldsymbol{P}(x)$$

Based on this, we can choose g to be convolution of a characteristic function $\chi_{_E}$ on a set $E \in \mathscr{B}(\mathbb{R}^3)$ with a non-negative measurable function $f \in \mathscr{L}_1$ having unit norm. The functional calculus applies and

$$\boldsymbol{P_f}(E) = \int_{\mathbb{R}^3} f * \chi_{_E}(x)\ \mathrm{d}\boldsymbol{P}(x) \tag{4.2.1.7}$$

is an observable by the Bounded Operator-Valued Integral form of an observable.

The mean and variance for the momentum variable is defined identically to that for the position operators

Definition 4.2.6. *Approximate Momentum Expectation Value*

$$\mathbb{E}[\boldsymbol{\rho}, \boldsymbol{P_f}] = \int_{\mathbb{R}^3} x \ \mathrm{Tr}\left[\mathrm{d}\boldsymbol{P_f}(x)\boldsymbol{\rho}\right] \tag{4.2.1.8}$$

Definition 4.2.7. *Approximate Momentum Variance*

$$\mathrm{var}[\boldsymbol{\rho}, \boldsymbol{P_f}] = \int_{\mathbb{R}^3} (x \cdot x)\mathrm{Tr}\left[\mathrm{d}\boldsymbol{P_f}(x)\boldsymbol{\rho}\right] - \left(\int_{\mathbb{R}^3} x\mathrm{Tr}\left[\mathrm{d}\boldsymbol{P_f}(x)\boldsymbol{\rho}\right]\right)^2 \tag{4.2.1.9}$$

We note that the somewhat awkward notation $\mathrm{Tr}\left[\mathrm{d}\boldsymbol{Q_f}(x)\boldsymbol{\rho}\right]$ is really an indication of using the $\mathrm{Tr}\left[\boldsymbol{Q_f}(E)\boldsymbol{\rho}\right]$ as the measure of a set $E \in \prod_{i=1}^{3} \mathscr{B}(\mathbb{R})$ for use in approximation of integrals for the three separate components of the momentum each having a spectrum constrained to $\mathbb{R}$. Strictly speaking, the original $\boldsymbol{Q}$ integrals are constructed from Riemann-Stiltjes integrals. So, they are expressed as projection operator differences on the individual spectra. In this way, the POVM $\boldsymbol{Q}$ factors component-wise in order to arrive at the claimed norm convergence of the integral. Explicit expressions for this can be found in many books on mathematical quantum mechanics and this works only because the component operators are pairwise commuting. [125] Regardless, we can also think of the trace evaluated measure $\mathrm{Tr}\left[\boldsymbol{Q_f}(E)\boldsymbol{\rho}\right]$ as a complex Radon measure on $\mathbb{R}^3$ as an LCH space. The usual simple function theory of integration applies, but we only obtain weak convergence, which is fine for the expectations of the first and second moments.

It is easy to show using the L_2 representation and a direct computation that the mean and the variance of the approximate position and momentum variables can be expressed as the sum of the quantum uncertainty and the classical variance in the apparatus function f.

$$\mathbb{E}[\boldsymbol{\rho}, \boldsymbol{P_f}] = \mathbb{E}[\boldsymbol{\rho}, \boldsymbol{P}] + \mathbb{E}[f] \tag{4.2.1.10}$$

$$\mathbb{E}[\boldsymbol{\rho}, \boldsymbol{Q_f}] = \mathbb{E}[\boldsymbol{\rho}, \boldsymbol{Q}] + \mathbb{E}[f] \tag{4.2.1.11}$$

and

$$\mathrm{var}[\boldsymbol{\rho}, \boldsymbol{P_f}] = \mathrm{var}[\boldsymbol{\rho}, \boldsymbol{P}] + \mathrm{var}[f] \tag{4.2.1.12}$$

$$\mathrm{var}[\boldsymbol{\rho}, \boldsymbol{P_f}] = \mathrm{var}[\boldsymbol{\rho}, \boldsymbol{Q}] + \mathrm{var}[f] \tag{4.2.1.13}$$

We can use this and the identical form of the definitions to anticipate the correct definition of a joint approximate position and momentum observable. The following results are presented in a one dimensional

form in Davies without the representation theory and using slightly different Fourier transform arguments. [32] The approach used here makes the results easier to generalize to other families of similarly related observables.

Remark The proofs that follow rely on a collection of mathematical results that are often bundled under the name "the canonical quantization". This is essentially a shared L_2 representation of $\boldsymbol{P}$ and $\boldsymbol{Q}$ where these obey the Weyl form of the Heisenberg commutation relation: let $\boldsymbol{U}(s)$ be the unitary group generated by $i\boldsymbol{P}$, then $\boldsymbol{U}(s)\boldsymbol{Q}\boldsymbol{U}(-s) = \boldsymbol{Q} - s\boldsymbol{I}$. When this commutation relation holds, we can construct an L_2 representation of $\mathscr{H}$ such that $\forall \phi \in D(\boldsymbol{P}) \cap D(\boldsymbol{Q}) \subset \mathscr{H}$

$$\boldsymbol{P}\phi = i\nabla_{\bar{x}}\phi(\bar{x}) \tag{4.2.1.14}$$

$$\boldsymbol{Q}\phi = \bar{x}\phi(\bar{x}) \tag{4.2.1.15}$$

A nice proof of this that plays off of the work of Sinai on the Translation Representation in a clever way can be found in Lax chapter 35.[91] At any rate, this representation is technically sound for a suitable choice of L_2 space and we will use it along with standard results from Fourier theory on L_2 [56] to prove the existence of a joint observable.

Proposition 4.2.8. *Existence of Joint Approximate Phase Space Measurement Observable*

For $\boldsymbol{Q}$ acting on $\mathscr{H}$ with multiplicity 1 in each coordinate, we can represent $\mathscr{H}$ by $L_2(\mathbb{R}^3, \mathbb{R}; m)$ for m the Lebesgue measure on $\mathbb{R}^3$ and $\boldsymbol{P}$ and $\boldsymbol{Q}$ as in the remark above. Then $\exists \boldsymbol{A}$ an Observable on $\Omega = \mathbb{R}^3 \times \mathbb{R}^3$ such that it has marginal observables $\boldsymbol{A_1} = \boldsymbol{Q}$ and $\boldsymbol{A_2} = \boldsymbol{P}$.

In particular, for any $\alpha \in D(\boldsymbol{P}) \cap D(\boldsymbol{Q}) \cap L_2(\mathbb{R}^3, \mathbb{R}; m) \cap L_1(\mathbb{R}^3, \mathbb{R}; m)$ such that $\alpha(-\bar{q}) = \alpha(\bar{q})$ and

$$\int (-i)\nabla_{\bar{q}}\alpha(\bar{q})\alpha(\bar{q})^* = \langle \boldsymbol{P}\alpha, \alpha\rangle = 0 = \langle \boldsymbol{Q}\alpha, \alpha\rangle = \int \bar{q}\alpha(\bar{q})\alpha(\bar{q})^* \tag{4.2.1.16}$$

and $\|\alpha\|_2 = 1$, typified by the gaussian distribution, we can define a vector $\alpha_{x,k}$ (hereafter referred to as the apparatus function), that is given in the relevant L_2 representation as

$$\alpha_{x,k}(\bar{q}) = e^{i\bar{k}\cdot\bar{q}}\alpha(\bar{q} - \bar{x}) \tag{4.2.1.17}$$

then $\boldsymbol{A}$ takes the form of a weakly convergent integral:

$$\boldsymbol{A}(E) = \frac{1}{(2\pi)^3}\int_E |\alpha_{x,k}\rangle \langle \alpha_{x,k}| \, \mathrm{d}^3x \, \mathrm{d}^3k \tag{4.2.1.18}$$

where $\mathrm{d}^3x\,\mathrm{d}^3k$ *is the product of the Lebesgue measure on* $\mathbb{R}^3 \times \mathbb{R}^3$

Proof.

Let $\alpha \in L_2(\mathbb{R}^3, \mathbb{R})$ that satisfies the equations 4.2.1.16. Then we can define a function $\alpha_{x,k} \in L_2(\mathbb{R}^3, \mathbb{R})$ by 4.2.1.17 and we find that for an unbounded domain

$$\begin{aligned}
\langle \boldsymbol{P}\alpha_{x,k}, \alpha_{x,k}\rangle &= -i \int \mathrm{d}^3q \nabla_{\bar{q}}(\alpha(\bar{q}-\bar{x})e^{i\bar{k}\cdot\bar{q}})\alpha(\bar{q}-\bar{x})e^{-i\bar{k}\cdot\bar{q}} \\
&= \int \mathrm{d}^3q\ \bar{k}\alpha(\bar{q}-\bar{x})\alpha(\bar{q}-\bar{x})^* + \langle \boldsymbol{P}\alpha, \alpha\rangle \\
&= \bar{k}\left\|\alpha\right\|_2^2 + 0 \\
&= \bar{k}
\end{aligned} \tag{4.2.1.19}$$

again using the translation invariance of the Lebesgue measure

$$\begin{aligned}
\langle \boldsymbol{Q}\alpha_{x,k}, \alpha_{x,k}\rangle &= \int \mathrm{d}^3q\bar{q}(\alpha(\bar{q}-\bar{x})e^{i\bar{k}\cdot\bar{q}})\alpha(\bar{q}-\bar{x})e^{-i\bar{k}\cdot\bar{q}} \\
&= \int \mathrm{d}^3(q-x)\ (\bar{q}-\bar{x})\alpha(\bar{q}-\bar{x})\alpha(\bar{q}-\bar{x}) + \bar{x}\int \mathrm{d}^3(q-x)\ \alpha(\bar{q}-\bar{x})\alpha(\bar{q}-\bar{x}) \\
&= \langle \boldsymbol{Q}\alpha, \alpha\rangle + \bar{x}\left\|\alpha\right\|_2^2 \\
&= \bar{x}
\end{aligned} \tag{4.2.1.20}$$

Thus, $\alpha_{x,k}$ represents a rapidly decaying distribution about the phase space point $(\bar{x}, \bar{k})$.

Since $\alpha_{x,k} \in L_2(\mathbb{R}^3, \mathbb{C})$, it is clearly a representation of an element of the complex Hilbert space $\mathscr{H}$. Thus, for any state $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$ it is definitionally true that

$$\rho(\bar{x}, \bar{k}) \equiv \frac{1}{(2\pi)^3}\langle \boldsymbol{\rho}\alpha_{x,k}, \alpha_{x,k}\rangle \geq 0 \tag{4.2.1.21}$$

Moreover, by $\langle \boldsymbol{\rho}\alpha_{x,k}, \alpha_{x,k}\rangle \leq \left\|\boldsymbol{\rho}\right\|\left\|\alpha\right\|_2 < \infty$, we also know that $\rho(\bar{x}, \bar{k}) \leq \left\|\boldsymbol{\rho}\right\|\left\|\alpha\right\|_2 \leq 1$ is a uniform bound in phase space. However, we need to establish integrability properties in order to be able to use this as a probability distribution that can induce a positive operator valued measure. Specifically, we need to prove that $\int \mathrm{d}^3x\ \mathrm{d}^3k\rho(\bar{x}, \bar{k}) = 1$. In order to achieve this, it is useful to perform a rescaling in order to avoid the tedious business of tracking 2π's. Specifically, using $\bar{k}_1 = \bar{k}/2\pi$ we can define

$$\rho'(\bar{x}, \bar{k}) \equiv \langle \boldsymbol{\rho}\alpha_{x,2\pi k}, \alpha_{x,2\pi k}\rangle$$

then

$$\int \mathrm{d}^3x\ \mathrm{d}^3k\rho(\bar{x},\bar{k}) = (2\pi)^3 \int \mathrm{d}^3x\ \mathrm{d}^3k_1\rho(\bar{x},2\pi\bar{k}_1) = \int \mathrm{d}^3x\ \mathrm{d}^3k_1\rho'(\bar{x},\bar{k}_1)$$

Since the left hand side is equal to 1 if and only if the right hand side is, it suffices to prove the integral normalization for $\rho'(\bar{x},\bar{k})$. For convenience, we will use the notation $\alpha'_{x,k} = \alpha_{x,2\pi k}$. This simple change of variables makes Fourier transforms $\mathscr{F}$ operate much more cleanly in the absence of derivatives and so our work becomes less error prone.

By the spectral representation of positive trace class operators, every $\boldsymbol{\rho}$ is a norm convergent convex sum of pure states. Thus, in order to study the integral $\int \mathrm{d}^3x\ \mathrm{d}^3k\rho'(\bar{x},\bar{k})$ it suffices to apply the monotone convergence theorem to the sum of positive functions $\boldsymbol{\rho} = \sum_i \lambda_i |\psi_i\rangle \langle\psi_i|$. Thus, it suffices to prove that for any $\boldsymbol{\rho} = |\psi\rangle \langle\psi|$ such that $\|\psi\|_2 = 1$, we have $\int \mathrm{d}^3x\ \mathrm{d}^3k\rho'(\bar{x},\bar{k}) = 1$. If this relation holds, then by Lidskii and the fact that all states have a unit trace,

$$\begin{aligned}\int \mathrm{d}^3x\ \mathrm{d}^3k\rho'(\bar{x},\bar{k}) = \int \mathrm{d}^3x\ \mathrm{d}^3k \sum_i \lambda_i \left\langle |\psi_i\rangle \langle\psi_i|\, \alpha'_{x,k}, \alpha'_{x,k}\right\rangle \\ = \sum_i \lambda_i \int \mathrm{d}^3x\ \mathrm{d}^3k \boldsymbol{\rho}'_{\psi_i}(\bar{x},\bar{k}) = \sum_i \lambda_i = 1 \quad (4.2.1.22)\end{aligned}$$

where the exchange of the summation limit with the integral was affected by the monotone convergence theorem. We can now prove the simpler result to complete the argument that $\rho'(\bar{x},\bar{k})$ is a phase space probability density function. This argument depends on some Fourier theory on $\mathbb{R}^n$. We begin by simplifying the expression using the pure state assumption

$$\rho'(\bar{x},\bar{k}) = \left\langle \boldsymbol{\rho}\alpha'_{x,k}, \alpha'_{x,k}\right\rangle = \left\langle \psi \left\langle \alpha'_{x,k}, \psi\right\rangle, \alpha'_{x,k}\right\rangle = |\left\langle \alpha'_{x,k}, \psi\right\rangle|^2$$

Then, using the exact form of the apparatus function, we can represent the inner product as a convolution

$$\left\langle \psi, \alpha'_{x,k}\right\rangle = \int \mathrm{d}^3q\psi(q)e^{-i2\pi\bar{k}\cdot\bar{q}}\alpha(\bar{q}-\bar{x}) = e^{-i2\pi\bar{k}\cdot\bar{x}} \int \mathrm{d}^3q\psi(q)\alpha(-(\bar{x}-\bar{q}))e^{i2\pi\bar{k}\cdot(\bar{x}-\bar{q})} = e^{-i2\pi\bar{k}\cdot\bar{x}}\psi * \alpha'_k(\bar{x})$$

where $\alpha'_k(q) = e^{i2\pi\bar{k}\cdot(\bar{q})}\alpha(-\bar{q})$

$$\int \mathrm{d}^3x\rho'(\bar{x},\bar{k}) = \int \mathrm{d}^3x(\psi * \alpha'_k(\bar{x}))^*(\psi * \alpha'_k(\bar{x}))$$

but this can be seen as an inner product of two functions, each of which is the convolution of two functions in L_2. So $\psi * \alpha'_k \in L_2$ by a variation on Cauchy-Schwartz. By the generalized Young's inequality [56] and

the fact that the apparatus function is integrable $\alpha \in L_1$, the convolution is again integrable, $\psi * \alpha'_k \in L_1$. Thus, since $\psi * \alpha'_k \in L_1 \cap L_2$, we can apply Plancharel's theorem to the L_2 inner product of convolutions and know that the Fourier transform of each convolution will still be in L_2 and the inner product will still make sense. Thus,

$$\int \mathrm{d}^3x\rho'(\bar{x},\bar{k}) = \int \mathrm{d}^3\xi \mathscr{F}(\psi * \alpha'_k)^*(\xi)\mathscr{F}(\psi * \alpha'_k)(\xi)$$

However, by the standard convolution theorem combined with the fact that we know a Fourier inverse exists for the convolved product, we have

$$\mathscr{F}(\psi * \alpha'_k)^*(\xi)\mathscr{F}(\psi * \alpha'_k)(\xi) = \mathscr{F}(\psi)(\bar{\xi})^*\mathscr{F}(\psi)(\bar{\xi})\mathscr{F}(\alpha'_k)(-\bar{\xi})^*\mathscr{F}(\alpha'_k)(-\bar{\xi})$$

Finally, using $\mathscr{F}(e^{i2\pi\bar{k}\cdot(\bar{q})}f(\bar{q})) = \mathscr{F}(f)(\bar{\xi}-\bar{k})$, we have (using translation and reflection invariance of the measure and finally Plancharel again)

$$\begin{aligned}
\int \mathrm{d}^3k \int \mathrm{d}^3x\rho'(\bar{x},\bar{k}) &= \int \mathrm{d}^3k \int \mathrm{d}^3\xi \mathscr{F}(\psi)(\bar{\xi})^*\mathscr{F}(\psi)(\bar{\xi})\mathscr{F}(\alpha)(-\bar{k}-\bar{\xi})^*\mathscr{F}(\alpha)(-\bar{k}-\bar{\xi}) \\
&= \int \mathrm{d}^3\xi \mathscr{F}(\psi)(\bar{\xi})^*\mathscr{F}(\psi)(\bar{\xi}) \int \mathrm{d}^3k \mathscr{F}(\alpha)(-\bar{k}-\bar{\xi})^*\mathscr{F}(\alpha)(-\bar{k}-\bar{\xi}) \\
&= \int \mathrm{d}^3\xi \mathscr{F}(\psi)(\bar{\xi})^*\mathscr{F}(\psi)(\bar{\xi}) \int \mathrm{d}^3k \mathscr{F}(\alpha')(\bar{k})^*\mathscr{F}(\alpha)(\bar{k}) \\
&= \|\psi\|_2 \|\alpha\|_2 \\
&= 1
\end{aligned}$$

We are now in a position to define a positive operator valued measure using the phase space density operator. Indeed, by applying the spectral representation argument above to an arbitrary $\boldsymbol{\rho}$, we get that $\forall E \in \mathscr{B}(\mathbb{R}^3 \times \mathbb{R}^3)$

$$\ell_E(\boldsymbol{\rho}) \equiv \int_E \mathrm{d}^6(x,k)\rho(\bar{x},\bar{k}) = \int_E \mathrm{d}^6(x,k)\rho'(\bar{x},\bar{k}) = \sum_i \lambda_i \int_E \mathrm{d}^6(x,k)\boldsymbol{\rho}'_{\psi_i}(\bar{x},\bar{k}) \leq \sum_i \lambda_i = \mathrm{Tr}\left[\boldsymbol{\rho}\right] \quad (4.2.1.23)$$

while $\rho(\bar{x},\bar{k}) \geq 0 \forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$, which together imply that ℓ_E is a positive bounded linear functional. Therefore, by the duality theory for trace class operators, we have that $\forall E \in \mathscr{B}(\mathbb{R}^3 \times \mathbb{R}^3) \exists \boldsymbol{A}(E) \in \mathscr{L}_+(\mathscr{H})$ such that

$$\ell_E(\boldsymbol{\rho}) = \mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{A}(E)\right] \quad (4.2.1.24)$$

Moreover, for fixed $\boldsymbol{\rho}$, by virtue of $\rho(\bar{x},\bar{k})$ a norm convergent sum of uniformly continuous (again Young's

inequality) functions, we can define a unique finite positive Radon measure μ

$$\mu_{\boldsymbol{\rho}}(E) = \ell_E(\boldsymbol{\rho}) \tag{4.2.1.25}$$

this justifies the claim that $\boldsymbol{A}$ is an observable since it guarantees weak countable additivity. We further note that, since $\alpha_{x,k}$ is a normalized vector, for $\boldsymbol{\rho} = |\psi\rangle\langle\psi|$,

$$\begin{aligned}
\mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{A}(E)\right] &= \int_E \mathrm{d}^6(x,k)\rho(\bar{x},\bar{k}) \\
&= \int_E \mathrm{d}^6(x,k)\frac{1}{(2\pi)^3}\left\langle \boldsymbol{\rho}\alpha_{x,k}, \alpha_{x,k}\right\rangle \\
&= \int_E \mathrm{d}^6(x,k)\frac{1}{(2\pi)^3}\left\langle \psi, \alpha_{x,k}\right\rangle\left\langle \alpha_{x,k}, \psi\right\rangle \\
&= \int_E \mathrm{d}^6(x,k)\frac{1}{(2\pi)^3}\mathrm{Tr}\left[\boldsymbol{\rho}\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|\right]
\end{aligned}$$

Thus, we can extend to any state by the trace convergence of the spectral representation to arrive at an expression for $\boldsymbol{A}(E)$ that converges ultraweakly in $\mathscr{L}_+$

$$\mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{A}(E)\right] = \int_E \mathrm{d}^6(x,k)\mathrm{Tr}\left[\boldsymbol{\rho}\frac{1}{(2\pi)^3}\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|\right] \tag{4.2.1.26}$$

and by $\mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{A}(\Omega)\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right]$ we have

$$\int_\Omega \mathrm{d}^6(x,k)\frac{1}{(2\pi)^3}\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right| = \boldsymbol{I} \tag{4.2.1.27}$$

This is already quite clearly a potent tool for representing phase space distributions associated to states using observables and indeed it is a kind of mollification of the Wigner Function itself. However, we can also prove that this is precisely the observable that has the approximate position and momentum variables as its marginal observables. We will prove this by direct computation of the marginals on arbitrary pure states ψ.

Specifically, using the definition of the Fourier transform and Plancharel again

$$\begin{aligned}
\langle \boldsymbol{A}_1(E)\psi,\psi\rangle &= \mathrm{Tr}\left[\boldsymbol{A}(E\times\mathbb{R}^3)\left|\psi\right\rangle\left\langle\psi\right|\right] \\
&= \int_{E\times\mathbb{R}^3} \mathrm{d}^6(x,k)\mathrm{Tr}\left[\left|\psi\right\rangle\left\langle\psi\right|\frac{1}{(2\pi)^3}\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|\right] \\
&= \int_{E\times\mathbb{R}^3} \mathrm{d}^6(x,k)\mathrm{Tr}\left[\left|\psi\right\rangle\left\langle\psi\right|\left|\alpha'_{x,k}\right\rangle\left\langle\alpha'_{x,k}\right|\right] \\
&= \int_{E\times\mathbb{R}^3} \mathrm{d}^6(x,k)\mathscr{F}_{q\to k}(\psi(\bar{q})\alpha(\bar{q}-\bar{x}))^*\mathscr{F}_{q\to k}(\psi(\bar{q})\alpha(\bar{q}-\bar{x})) \\
&= \int \mathrm{d}^3x\chi_{_E}\int \mathrm{d}^3k\mathscr{F}_{q\to k}(\psi(\bar{q})\alpha(\bar{q}-\bar{x}))^*\mathscr{F}_{q\to k}(\psi(\bar{q})\alpha(\bar{q}-\bar{x})) \\
&= \int \mathrm{d}^3x\chi_{_E}\int \mathrm{d}^3q(\psi(\bar{q})\alpha(\bar{q}-\bar{x}))^*\psi(\bar{q})\alpha(\bar{q}-\bar{x}) \\
&= \int \mathrm{d}^3q|\psi(\bar{q})|^2\int \mathrm{d}^3x\chi_{_E}(\bar{x})|\alpha(\bar{q}-\bar{x})|^2 \\
&= \int \mathrm{d}^3q|\psi(\bar{q})|^2(\chi_{_E}*|\alpha|^2)(\bar{q})
\end{aligned}$$

Thus,

$$\boldsymbol{A}_1(E) = \int_{\mathbb{R}^3}(\chi_{_E}*|\alpha|^2)(\bar{q})\mathrm{d}\boldsymbol{Q}(x) = \boldsymbol{Q}_{|\alpha|^2}(E) \tag{4.2.1.28}$$

Similarly, we can prove the corresponding result for the momentum observable by using the computation we did for the original proof of normalization (also using a reflection symmetry of α)

$$\begin{aligned}
\langle \boldsymbol{A}_2(E)\psi,\psi\rangle &= \mathrm{Tr}\left[\boldsymbol{A}(\mathbb{R}^3\times E)\left|\psi\right\rangle\left\langle\psi\right|\right] \\
&= \int_{\mathbb{R}^3\times E} \mathrm{d}^6(x,k)\mathrm{Tr}\left[\left|\psi\right\rangle\left\langle\psi\right|\left|\alpha'_{x,k}\right\rangle\left\langle\alpha'_{x,k}\right|\right] \\
&= \int_{\mathbb{R}^3\times E} \mathrm{d}^6(x,k)(\psi*\alpha'_k(\bar{x}))^*(\psi*\alpha'_k(\bar{x})) \\
&= \int \mathrm{d}^3k\chi_{_E}(\bar{k})\int \mathrm{d}^3x(\psi*\alpha'_k(\bar{x}))^*(\psi*\alpha'_k(\bar{x})) \\
&= \int \mathrm{d}^3k\chi_{_E}(\bar{k})\int \mathrm{d}^3\xi\mathscr{F}(\psi)(\bar{\xi})^*\mathscr{F}(\psi)(\bar{\xi})\mathscr{F}(\alpha)(-\bar{k}+\bar{\xi})^*\mathscr{F}(\alpha)(-\bar{k}+\bar{\xi}) \\
&= \int \mathrm{d}^3\xi\mathscr{F}(\psi)(\bar{\xi})^*\mathscr{F}(\psi)(\bar{\xi})\int \mathrm{d}^3k\chi_{_E}(\bar{k})|\mathscr{F}(\alpha)(\bar{\xi}-\bar{k})|^2 \\
&= \int \mathrm{d}^3\xi|\mathscr{F}(\psi)(\bar{\xi})|^2\chi_{_E}*|\mathscr{F}(\alpha)|^2(\bar{\xi})
\end{aligned}$$

Thus,

$$\boldsymbol{A}_2(E) = \int_{\mathbb{R}^3}(\chi_{_E}*|\mathscr{F}(\alpha)|^2)(\bar{p})\mathrm{d}\boldsymbol{P}(p) = \boldsymbol{P}_{|\mathscr{F}(\alpha)|^2}(E) \tag{4.2.1.29}$$

This completes the proof. □

Some additional comments on this joint approximate Observable are warranted as this will be a basic tool of our later theory.

Remark

First, we use the domain of $\mathbb{R}^3 \times \mathbb{R}^3$ extensively and the translation invariance of the Lebegue measure. Absent these properties, it becomes much harder to recreate an observable like this. Probably the easiest way to get around the fact that our geographic space is a compact convex subset is to extend it to all of $\mathbb{R}^3 \times \mathbb{R}^3$ but only consider functions that decay rapidly outside of a compact convex subset and then compactify both the position and momentum domains by addition of a closure point at infinity. The decision to only consider rapidly decaying functions is well justified on both physical and mathematical grounds. We will need to examine system conditions for enforcing this in more detail once we have a fully defined model in chapter 5.

Remark

Second, we can relate the observable $\boldsymbol{A}$ directly to the Wigner distribution theory of phase space quantization. This is accomplished by studying the fourier transform of the phase space density function $\rho(\bar{x}, \bar{k})$, which we know to belong to $L_1(\mathbb{R}^3 \times \mathbb{R}^3)$. This turns out to be representable in terms of the product of two functions of the Weyl operator as we elaborate in proposition 4.2.9. This makes a very clean connection with phase space quantization theory and indicates that propagating subsystems by way of the Moyal bracket introduces no substantive technical hurdles as any such propagator can be transformed back into an expression in terms of the approximate phase space observables.

Remark

Third, the form of the observable $\boldsymbol{A}$ is very significant in and of itself. There is an obvious parallel to the usual formal expressions for position and momentum observables. Any quick perusal of an elementary graduate text in quantum mechanics will reveal a prolific use of expressions commonly called resolutions of identity. [133] Inserting operators that look like $\boldsymbol{I} = \int |p\rangle \langle p| \, \mathrm{d}p$ in clever places allows for fast and practical asymptotic approximations. Of course, in a technical sense, this is more appropriately understood as the introduction of L_2 representations and spectral integral representations. However, this style of argument is a potent source of physical intuition even when it does not come with formal proofs for the meaning of these limiting objects. By establishing that phase space measurements have a compatible representation, we open up the option of using quantum phase space constructs in the same way we normally would position of momentum exclusively. Moreover, when understood in the proper technical sense (that we introduced above), we can easily prove by direct computation that $\boldsymbol{A}$ automatically enforces Heisenberg uncertainty relations.

Remark

Naturally, all of this power comes at a cost, but one that it turns out we can pay with equanimity. Where the Wigner function is only a quasi-probability measure (having sub-Heisenberg volumes of negative mass), our phase space density function $\rho(\bar{x}, \bar{k})$ is a true probability distribution on $\mathbb{R}^6$ and a nice one at that. One is inclined to balk at this as a quantum impossibility. However, we have introduced an arbitrary function α for smearing out our position and momentum information in a consistent way. This choice has no a priori universality. There is no reason to prefer one over another across all experiments. However, upon choosing one appropriate to our problem, we find enormous simplification. Analogously to choosing the right mother wavelet for representing a particular signal or the right coherent state for introducing a semi-classical approximation[1], the right choice here will make our entire problem much simpler. Moreover, we will find that there are clear measurement theoretic motivations for basing our choice on the condensed matter structure of our system. Regardless of our theoretical viewpoint, given that part of the goal of this work is a functional parametrization of the theory, we are free to treat this as an infinite dimensional parameter to fit to experimental data.

Proposition 4.2.9. *The Weyl operator can be used to construct a transform of the density matrix, such that the classical two dimensional Fourier transform of the approximate density matrix is equal to the product of the Wigner function times the Weyl operator averaged against the apparatus function. This says that the approximate phase space measurement can be understood as the Wigner distribution convolved with the apparatus function.*

4.2.2 Approximate Phase Space Instruments

We are finally in a position to prove an essential result for the construction of the reaction-transport quantum stochastic process. We claim that there exists an approximate phase space instrument such that its adjoint is the approximate phase space observable (defined in proposition 4.2.8) and has an integral form compatible with the developed theory for transition processes. This result is motivated by the theory of covariant instruments developed for finite dimensional models.

Proposition 4.2.10. *Existence of Approximate Phase Space Instruments*

For $\boldsymbol{A}$ an Observable on $\Omega = \mathbb{R}^3 \times \mathbb{R}^3$ defined as in proposition 4.2.8 such that it has marginal observables $\boldsymbol{A_1} = \boldsymbol{Q}$ and $\boldsymbol{A_2} = \boldsymbol{P}$. We can define an approximate phase space Instrument $\mathscr{E}_\alpha$ on the phase space $\Omega = \mathbb{R}^3 \times \mathbb{R}^3$ adjoint to $\boldsymbol{A}$.

In particular, for any $\alpha \in D(\boldsymbol{P}) \cap D(\boldsymbol{Q}) \cap L_2(\mathbb{R}^3, \mathbb{R}; m) \cap L_1(\mathbb{R}^3, \mathbb{R}; m)$ *such that* $\alpha(-\bar{q}) = \alpha(\bar{q})$ *and*

$$\int (-i)\nabla_{\bar{q}}\alpha(\bar{q})\alpha(\bar{q})^* = \langle \boldsymbol{P}\alpha, \alpha\rangle = 0 = \langle \boldsymbol{Q}\alpha, \alpha\rangle = \int \bar{q}\alpha(\bar{q})\alpha(\bar{q})^* \tag{4.2.2.1}$$

and $\|\alpha\|_2 = 1$*, typified by the gaussian distribution, we can define a vector* $\alpha_{x,k}$ *(hereafter referred to as the apparatus function), that is given in the relevant* L_2 *representation as*

$$\alpha_{x,k}(\bar{q}) = e^{i\bar{k}\cdot\bar{q}}\alpha(\bar{q} - \bar{x}) \tag{4.2.2.2}$$

then $\mathscr{E}_\alpha$ *takes the form of a trace norm convergent integral:*

$$\mathscr{E}_\alpha(E, \boldsymbol{\rho}) = \frac{1}{(2\pi)^3}\int_E \mathrm{d}^3x\ \mathrm{d}^3k\, |\alpha_{x,k}\rangle \langle \alpha_{x,k}|\, \boldsymbol{\rho}\, |\alpha_{x,k}\rangle \langle \alpha_{x,k}| \tag{4.2.2.3}$$

where $\mathrm{d}^3x\ \mathrm{d}^3k$ *is the product of the Lebesgue measure on* $\mathbb{R}^3 \times \mathbb{R}^3$

Proof. With the properties established in proposition 4.2.8, this is a remarkably easy proof. Indeed, we begin by simplifying the instrument

$$\mathscr{E}_\alpha(E, \boldsymbol{\rho}) = \int_E \mathrm{d}^3x\ \mathrm{d}^3k\rho(\bar{x}, \bar{k})\, |\alpha_{x,k}\rangle \langle \alpha_{x,k}| \tag{4.2.2.4}$$

but $\mathrm{Tr}\left[|\alpha_{x,k}\rangle \langle \alpha_{x,k}|\right] = \|\alpha\|_2 = 1$, thus

$$\mathrm{Tr}\left[\mathscr{E}_\alpha(E, \boldsymbol{\rho})\right] \leq \int_E \mathrm{d}^3x\ \mathrm{d}^3k\rho(\bar{x}, \bar{k})\mathrm{Tr}\left[|\alpha_{x,k}\rangle \langle \alpha_{x,k}|\right] \leq \int_E \mathrm{d}^3x\ \mathrm{d}^3k\rho(\bar{x}, \bar{k}) \leq \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{4.2.2.5}$$

This establishes the strong convergence and boundedness. Strong additivity follows from the countable additivity of $\int_E \mathrm{d}^3x\ \mathrm{d}^3k\rho(\bar{x}, \bar{k})$ since this guarantees that a countable sum of integrals over disjoint subsets remains norm bounded, while for every finite collection equality clearly holds by the definition of the integral. Moreover, this also gives us that $\mathscr{E}_\alpha(\emptyset) = 0$. For every positive simple function $f(\bar{x}, \bar{k}) = \sum_i \chi_{E_i} a_i$,

$$\int_E \mathrm{d}^3x\ \mathrm{d}^3k f(\bar{x}, \bar{k})\, |\alpha_{x,k}\rangle \langle \alpha_{x,k}| = \sum_i a_i \int_{E\cap E_i} \mathrm{d}^3x\ \mathrm{d}^3k\, |\alpha_{x,k}\rangle \langle \alpha_{x,k}| = \sum_i a_i \boldsymbol{A}(E \cap E_i) \geq 0 \tag{4.2.2.6}$$

thus by the density of simple functions in L_1, it follows that $\mathscr{E}_\alpha(E, \cdot) \geq 0$. This establishes that $\mathscr{E}_\alpha(E)$ is a

positive map valued measure. Moreover, for $\boldsymbol{\rho} = |\psi\rangle\langle\psi|$, we can use Parseval and the fact that $\left\|\alpha'_{x,k}\right\|_2 = 1$

$$\begin{aligned}
\mathrm{Tr}\left[\mathscr{E}_\alpha(\Omega, \boldsymbol{\rho})\right] &= \int \mathrm{d}^3x\ \mathrm{d}^3k \sum_i \left\langle \psi_i, \left|\alpha'_{x,k}\right\rangle \left\langle\alpha'_{x,k}\right| \psi\right\rangle \left\langle \left|\alpha'_{x,k}\right\rangle \left\langle\alpha'_{x,k}\right| \psi, \psi_i\right\rangle \\
&= \int \mathrm{d}^3x\ \mathrm{d}^3k \left\langle \left|\alpha'_{x,k}\right\rangle \left\langle\alpha'_{x,k}\right| \psi, \left|\alpha'_{x,k}\right\rangle \left\langle\alpha'_{x,k}\right| \psi\right\rangle \\
&= \int \mathrm{d}^3x\ \mathrm{d}^3k \left\langle \alpha'_{x,k}, \alpha'_{x,k}\right\rangle \rho(\bar{x}, \bar{k}) = 1
\end{aligned}$$

Which can be combined with the spectral representation and the trace convergence of this integral to obtain

$$\mathrm{Tr}\left[\mathscr{E}_\alpha(\Omega, \boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{4.2.2.7}$$

proving that this is in fact an instrument. It remains to be proven that this instrument is adjoint to $\boldsymbol{A}$. However, by the above calculation for proving that $\mathscr{E}_\alpha$ is an instrument, we have that

$$\mathrm{Tr}\left[\mathscr{E}_\alpha(E, \boldsymbol{\rho})\right] = \int_E \mathrm{d}^6(x,k)\rho(\bar{x}, \bar{k}) = \mathrm{Tr}\left[\boldsymbol{\rho}\boldsymbol{A}(E)\right] \tag{4.2.2.8}$$

which completes the proof. □

Remark

Although conceptually similar to a result in Davies [32] about approximate position instruments, as far as this author knows, this is a genuinely new result. Ford and Lewis did further work in 1974 on the relation between an approximate position observable and the phase space observable but it appears that this remained unpublished. A consequence of their research appears in their 1986 critique of macroscopic and microscopic views of quantum stochastic processes [57] where they demonstrate that a QSP built on position measurements at different times can be Fourier transformed into a product of measurement operators evaluated against quantum correlation due to multi-time non-commutativity and a kind of generalized Wigner function for an n-particle system. Ford and Lewis proved that the contributions due to measurement and innate dynamics factor under a Fourier transform. This is significant in understanding correlation formation in systems where position is approximately observed. In some sense, it indicates that the essential dynamics are not unanalyzable for imperfect choices of the apparatus function. There may be an analogous version of this result for the transform objects somewhere in the large body of Wigner function theory as applied to multi-particle semi-classical dynamics. However, this for our purposes, this form is more useful.

Remark

Proposition 4.2.10 implies that phase space measurements can be cast in an approximate form that is fully compatible with transition processes.(confer [32] chapter 6) These processes are special among quantum stochastic processes, because it is relatively easy to study the approach to equilibrium. Other systems can be studied in long time limits using concentration inequalities and classical approximations. [83] However, the technical features of these theories are quickly overwhelming and they offer little in the way of easy intuition. Transition processes offer a comfortable middle ground with additional noncommutative structure but relatively simple definitions of convergence to equilibrium.

Remark

Using our theory of purity preserving operations from before, we can generalize this result a little bit. Let $\boldsymbol{U}_{x,k}, \boldsymbol{V}_{x,k}$ be a strongly continuous family of unitary operators on $\mathscr{H}$. Then, without doing harm to the claim that this is an instrument or the attendant properties, we can form a new instrument

$$\mathscr{E}_{\alpha,\boldsymbol{U},\boldsymbol{V}}(E,\boldsymbol{\rho}) = \frac{1}{(2\pi)^3}\int_E \mathrm{d}^3x\ \mathrm{d}^3k \boldsymbol{U}_{\boldsymbol{x},\boldsymbol{k}} \left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right| \boldsymbol{V}_{x,k}\boldsymbol{\rho}\boldsymbol{V}_{x,k}^* \left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right| \boldsymbol{U}_{x,k}^* \tag{4.2.2.9}$$

We will find the more general version useful in studying systems with different representations in different subspaces. Moreover, by using Sz.Nagy's Dilation theorem, any contraction can be represented as a unitary on a larger Hilbert space. [121] So, for a very large class of phase space sampling measurements, we can construct instruments that have nice analytic processes. Moreover, the dilation considerations are not even necessary if we are content with $\mathscr{E}_{\alpha,\boldsymbol{U},\boldsymbol{V}}$ being a more general positive map valued measure.

4.2.3 Quantum Stochastic Processes and Continuous-Time Measurement Systems for Reaction Counting

Now that we have a well-defined theory of instruments for describing instantaneous measurements, we can discuss what a finite duration quantum measurement process is structured like. In general, a measurement process that is extended in time is simply a time indexed family of positive-map valued measures. However, this family must conform to certain consistency constraints. Chief among these is a kind of strong continuity in the sense that this measurement process is also a propagator for the state of the system. In addition, given the connection to probabilities, the sum over all events must be trace preserving. Finally, these measurement propagators must exhibit a Markov-like property that is directly analogous to the Chapman-Kolmogorov equation but defined on an operator algebra. Ultimately, these properties will conspire to give our theory a structure that is profoundly reminiscent of a classical piecewise deterministic process. We will need to do

some more work to make this into a reaction-transport theory but the building blocks are intrinsic in the definitions that we will present in this section.

We will begin by describing the classical measurement space that will be used for describing the outcomes of instruments. A more abstract approach has proven useful in applying the theory of PDPs to general quantum measurement systems. However, this works counter to our goal of developing a quantization for reaction-transport models. Instead, we will introduce a specific event space relevant to reaction transport. We will assume that every reaction is classically measurable in the sense that information about the event does not have a self-interfering structure. Even if it is practically impossible to detect every reaction, the associated system states cannot persist in Schroedinger's Cat states and will be quickly collapsed by interactions with the environment. [67] Thus, all uncertainty about the occurrence of individual collisions is a kind of classical uncertainty, while the particle dynamics of the reaction itself can be represented as a quantum measurement process.

With this in mind we will define the sample space constructively in terms of finite integer numbers of reactions, at times and phase space coordinates. This approach can be seen as agnostic to which particle participated in the reaction, just that a particle did. Thus it lends itself to symmetrization and knowledge of the occurrence of the collision event with respect to a particular particle is purely a result of the distinguishability of the particles through phase space localization. Ultimately, the decision to represent the collisions as distinguishable by particle or not will impact the system statistics in a meaningful way as it does for Bosons and Fermions. We will return to this problem later. For now we will treat it as a particle independent definition.

We imagine the system as a single detector that records the position, momentum, reaction type and timestamp for each collision. Thus, we specify a finite set of reaction types T and a geographic phase space $G = \mathscr{V}_D \times \mathscr{O}$, and a time domain consisting of the positive real line $\mathbb{R}_+ = [0, \infty)$. We further define the sigma algebra of the typed geographic phase space $\mathscr{P}(T) \times \mathscr{B}(\mathscr{V}_D \times \mathscr{O}) = \mathscr{G}$ to be the collection of macroscopic reaction volumes that can be used in detecting neutron reaction events. In the models we will introduce in this paper, we will generally only consider events of fixed reaction type so that $\mathscr{G} = \cup_{\ell \in T} \mathscr{B}(\mathscr{V}_D \times \mathscr{O}) \times \{\ell\}$. By the usual measurability results on compact subsets of $\mathbb{R}^n$, we can exclusively worry about sets of the form $\mathscr{B}(\mathscr{V}_D) \times \mathscr{B}(\mathscr{O}) \times \{\ell\}$ when studying event measures and integral properties. [56]

We now can define the sample space (here we mean a topological space, not a vector space and not a sigma algebra of sets) X_t for a given fixed time interval $[0, t]$ in terms of all possible reaction event sequences that could occur in that interval. [32] We can define a countable collection of sets A_t^n defined to be the subset of X_t having exactly n events. We will define the composite sigma algebra in terms of the union

over these and we will address their individual measurability and measure properties. Therefore, we adopt the definition $X_t = \cup_{n=0}^{\infty} A_t^n$. The union over finite numbers of events is sufficient because we assume that the allowed sets of reaction events have no temporal cluster points. This can be thought of physically as an infinitesimal detector saturation following each event. As a technical point, we also exclude the possibility of reaction events at the left endpoint of the time interval associated to the sample space. This makes it possible to construct compositions of time intervals without risking event collisions at the endpoint. Since $[0, t]$ is a compact set, for every temporal radius of separation ϵ, there is a maximum number of events that can be included while maintaining the proposed separation. In order to account for every possible $\epsilon > 0$ we must account for any finite number of events. However, it is sufficient to only consider the A_t^n with finite n individually when analyzing the measurement topology (and by extension the Borel sets). Based on this same temporal isolation assumption, we exclude any sequence of the form $\{(x_1, t_1), (x_2, t_1), \dots\}$.

In order to represent the event with no reactions $n = 0$, we introduce a sample point z. Thus, we have $A_t^0 = \{z\}$. The set with only one event can also be understood simply. It consists of all possible typed geographic phase space points and all times in the admissible interval $(x, p, \ell, t_1) \in \mathscr{V}_D \times \mathscr{O} \times T \times (0, t]$. Since there is no issue with ordering or time isolation, we have $A_t^1 = \mathscr{V}_D \times \mathscr{O} \times T \times (0, t]$. For any finite number $n > 1$ we then admit any time ordered sequence $0 < t_1 < \cdots < t_n \leq t$ and any typed geographic phase space point sequence $((x_i, p_i, \ell_i, t_i))_{i=1}^n$, as a valid point in the sample subspace of fixed reaction count A_t^n. The union of all such time-ordered finite reaction count subspaces will be called $\tilde{X}_t$.

In order to construct a topology on this set, we will first construct a topology on a superset that includes all time orderings and non-isolated points and then apply it to $\tilde{X}_t$ using the relative topology. (This is an alternative to constructing the topology on the superset and then quotienting out the alternate time orderings as is done in the direct construction of tensor products.) We begin by considering the finite reaction count superspace with the product topology on $\prod_{i=1}^n \mathscr{V}_D \times \mathscr{O} \times T \times (0, t]$. Here we use the one point compactification of $\mathbb{R}^3$ as the topology on each copy of $\mathscr{V}_D$, we use the one-point compactification of $\mathbb{R}^3$ as the topology on each copy of $\mathscr{O}$, we use the discrete topology on each copy of T (making every one of the reaction types to be its own closed/open set), and we use the relative topology on $(0, t] \subset \mathbb{R} \cap [0, t + \epsilon]$. Then we combine the fixed reaction count subspace topologies using the topology induced by a disjoint union metric [37] on reaction count. The advantage of this approach is that it gives use an easy proof of local compactness on each fixed reaction count subspace (Tychanoff) since compactness is hereditary. An easy proof of second countability follows as well, as it too is hereditary. We also get Hausdorff again virtually for free. We refer to the resulting topological space with a subspace topology as X_t.

Proposition 4.2.11.

The full sample space X_t is Locally Compact Hausdorff and second countable.

The typed geographic space $G \times T$ is a compact metric space and the single event sample space A_t^1 is a relatively compact metric space.

The full sample space X_t is not complete but it is representable as a $G_{\delta\sigma}$ in a Polish Space.

Proof.

For the first claim, it suffices to show that every point has a compact neighborhood and we can identify a countable dense subset. Given a point $((x_i, p_i, \ell_i, t_i))_{i=1}^n$, we can construct a closed ball of radius ϵ in both $\mathscr{V}_D$ and $\mathscr{O}$ which we will denote by $\overline{B_{\mathscr{V}_D}}(\epsilon)$ and $\overline{B_{\mathscr{O}}}(\epsilon)$ respectively. Then the set $(x_i + \overline{B_{\mathscr{V}_D}}(\epsilon)) \times (p_i + \overline{B_{\mathscr{O}}}(\epsilon)) \times \{\ell_i\}$ is a compact neighborhood of the typed geographic point (x_i, p_i, ℓ_i) in the given topology excluding the temporal component. This is possible because $\mathscr{V}_D$ and $\mathscr{O}$ are both compact spaces. Since every point in the sample space has a minimum time gap between all reaction detection times in the sample point, we can choose a $\tau > 0$ such that $\forall 1 \leq i < j \leq n$, $t_j - t_i > \tau$, $t_1 > \tau$, and $t - t_n > \tau$, then we can construct a neighborhood

$$\prod_{i=1}^{n} (x_i + \overline{B_{\mathscr{V}_D}}(\epsilon)) \times (p_i + \overline{B_{\mathscr{O}}}(\epsilon)) \times \{\ell_i\} \times [t_i - \frac{\tau}{3}, t_i + \frac{\tau}{3}] \tag{4.2.3.1}$$

The interior is non-empty and still includes the point by virtue of excluding the endpoints and overlapping events. If the right end point is part of the event, then the last term in the product can be included in the compact set $[t - \frac{\tau}{3}, t]$. This is a neighborhood of the point because, in the relative topology on $(0, t]$, $(t - \epsilon, t]$ is an open set since it is of the form $(t - \epsilon, t + \epsilon) \cap (0, t]$.

By Tychanoff, this neighborhood constructed above is compact in the given product topology. The Hausdorff property follows from the fact that two points in the sequence space are only different if they differ on some dimension for some reaction count. It suffices to check for the existence of separating sets in each component (position, momentum, type) so that it can be verified for at least one point. This last condition is trivial to confirm since the topology is inherited from obviously Hausdroff topologies. Second countability is similarly obvious using the second countability of $\mathbb{R}^n$ and the preservation of countable cardinality under finite products.

$G = \mathscr{V}_D \times \mathscr{O} \times T$ and $A_t^1 = \mathscr{V}_D \times \mathscr{O} \times T \times (0, t]$ since there are no cluster points to exclude. The one point compactification of $\mathbb{R}^3$ comes with the topology of a three sphere. Therefore, each subspace in the product is metric. Furthermore, the product topology on a countable family of metric spaces can be realized using the metric $d(x, y) = \sum_n 2^{-n} d_n(x_n, y_n)$. This is easy to see by recognizing that any open set contains an

intersection of open balls in the subspaces and conversely. Therefore, both of these spaces are metric spaces. Relative compactness is obvious by Tychanoff.

Completeness of X_t is easily contradicted by choosing a sequence of otherwise converging points in $n > 1$ such that $t_2 \to t_1$, which is clearly not a point in the sample space. Let $\overline{X}_t$ be the full superspace that we use to assign a topology to the finite reaction number subspaces of $\tilde{X}_t$ using the relative topology. The finite particles number subspaces of $\overline{X}_t$ are easily shown to be complete since they are each a finite product of complete spaces. By construction, $\overline{X}_t$ is a countable disjoint union of such subspaces isolated by the disjoint union metric. Therefore, the full superspace is a Polish space. It suffices now to characterize subset $\tilde{X}_t \subset \overline{X}_t$. This can be done using a decomposition that we will develop in proposition 5.7.3 for analyzing measurability. Specifically,

$$A_t^n = \bigcup_{m=n}^{\infty} \bigcup_{a \in F_m^n} \lambda(E_{a,1} \times E_{a,2} \times \cdots \times E_{a,m}) \tag{4.2.3.2}$$

where each element of the double union are copies of z or $A_{t/m}^1$. Each A_t^1 is a countable union over finite products of G_δ sets (in order to produce the half open time interval). This in turn can be restructured as a countable union of G_δ sets. Moreover, X_t is a countable union of A_t^n sets. Therefore, X_t is a $G_{\delta\sigma}$ set in $\overline{X}_t$.

□

Remark LCH v. Compact Polish

Although many of the quantum measurement theorems developed above have referred to compact Polish spaces, we will find that the absence of completeness causes us no real problems going forward. Indeed, in proving the existence and uniqueness of QSP we will only need to apply these results directly to the typed geographic phase space, which is compact. For example, some convexity arguments for the composition of instruments do really require compactness, but we will only apply this to instruments acting directly on the typed geographic spaces. Moreover, by the standard theory of Radon measures (including Riesz-Kakutani), LCH is good enough for unique representation of linear functionals on the space of continuous functions, which is all that we need for many measure representation applications. So, situations that will need to make direct reference to the sample space of the QSP are not without tools. Moreover, as we proved in the theorem, the underlying geographic typed space is a compact metric space (i.e. a compact Polish space).

The limitations around metrisability in the relative topology is a serious deficit. Indeed, many hard problems around Borel topologies are substantially simplified if we have a complete metric space to work with. Many complex events and approximation schemes can be easily shown to be constructed from Borel sets by using one-to-one measurable maps between complete metric spaces and Kuratowski's theorem. [118] Still, as the

known results around LCH spaces and functional calculuses demonstrate, we can make a lot of progress without having incredibly nice properties on the domain so long as the range is a C^* algebra.

This reaction counting sample space makes it possible to study the kind of counting events discussed in the chapter on classical neutron transport measurement theory. However, it makes it easy to exclude precisely the kinds of divergent reaction clustering events that would cause grievous technical problems for any PDP type representation, while also retaining the most critical topological features. We will finally define a composition map for points belonging to temporal subintervals of a sample space: $\lambda : X_s \times X_t \to X_{s+t}$. This map is defined by

$$\lambda(((x_i, p_i, \ell_i, t_i))_{i=1}^{n_1}, ((y_j, q_j, \ell_j, t_j))_{j=1}^{n_2}) = \\ ((x_1, p_1, \ell_1, t_1), \ldots, (x_{n_1}, p_{n_1}, \ell_{n_1}, t_{n_1}), (y_1, q_1, \ell_1, t_1 + s), \ldots, (y_{n_2}, q_{n_2}, \ell_{n_2}, t_{n_2} + s)) \quad (4.2.3.3)$$

This can be extended to multiple products through composition, $\lambda_3 : X_s \times X_t \times X_u \to X_{s+t+u}$, $\forall a \in X_s, b \in X_t, c \in X_u$

$$\lambda_3(a, b, c) = \lambda(\lambda(a, b), c) \quad (4.2.3.4)$$

going forward we will suppress the composition index as the properties of the function are the same regardless of the number of products.

Proposition 4.2.12.

$\lambda : X_s \times X_t \to X_{s+t}$, *defined by*

$$\lambda(((x_i, p_i, \ell_i, t_i))_{i=1}^{n_1}, ((y_j, q_j, \ell_j, t_j))_{j=1}^{n_2}) = \\ ((x_1, p_1, \ell_1, t_1), \ldots, (x_{n_1}, p_{n_1}, \ell_{n_1}, t_{n_1}), (y_1, q_1, \ell_1, t_1 + s), \ldots, (y_{n_2}, q_{n_2}, \ell_{n_2}, t_{n_2} + s)) \quad (4.2.3.5)$$

is a continuous and bijective function from $X_s \times X_t$ in the product topology into X_{s+t} in the subspace topology.

Proof.

Since X_{s+t} has a topology that separates subspaces of different reaction count numbers, it suffices to prove continuity on a subspace with a fixed reaction count, say n. If the splitting time s is excluded as an event location from the range, the pre-image of every point in the range is a single, well-defined point in the product space. Moreover, every open set U_{t+s} can be split into two parts using $O^n_{u<s}$ and $O^n_{u>s}$, the open sets consisting of the union over all particle number subspaces less than n and including all time stamps less than s or greater than s. It is easy to show that these are open sets by using the finite reaction count product

topology to reduce the representation of open sets to finite intersections of pre-images of single-reaction open sets (i.e. in a typed geographic space cartesian product with $(0, s)$). So,

$$U^n_{t+s} = (U^n_{t+s} \cap O^n_{u<s}) \cup (U^n_{t+s} \cap O^n_{u>s}) = \bigcup_{n_1+n_2=n} (U^n_{t+s} \cap O^n_{u<s} \cap A^{n_1}_s) \cup (U^n_{t+s} \cap O^n_{u>s} \cap A^{n_2}_t)$$

This is a finite union of sets (each of which is open) the preimage under λ commutes with all of these operations when they are finite in number and open sets are preserved under finite unions and intersections. Therefore, it suffices to check that $\lambda^1(U^n_{t+s} \cap O^n_{u<s} \cap A^{n_1}_s)$ is open and $\lambda^1(U^n_{t+s} \cap O^n_{u>s} \cap A^{n_2}_t)$ is open for any U^n_{t+s} open in $X_{t+s}/\{(x, p, \ell, s) \in \mathscr{V}_D \times \mathscr{O} \times T \times \{s\}\}$. However, on sets constrained to a fixed particle number range and one of the two disjoint time domains $(0, s)$ or $(s, s + t)$, we know that λ acts like an identity map. Thus, since open sets are defined the same way in both systems, we have that λ is continuous.

If we look at sets that include a reaction at the splitting time s, we simply need to modify the decomposition to include $O^n_{u\leq s}$ rather than $O^n_{u<s}$ and use the fact that in on the first component sub space of the preimage, the temporal topology is the relative topology obtained from $\mathbb{R} \cap (0, s]$. By accounting for the fact that events at the time s are always assigned to the first factor, we obtain the conclusion that λ is also surjective onto X_{s+t}. □

Remark

We define a Borel sigma algebra on X_t to be the sigma algebra containing all open subsets of X_t in the topology defined above.

We define a sigma algebra $\mathscr{X}_t$ extending the Borel sigma algebra on X_t to be any sigma algebra on X_t that includes the Borel sigma algebra as a sub algebra. We can define all further mathematical objects on any such sigma sub algebra, since most of our approximations only require the countable unions, intersections, and complements of open subsets. Every finite Borel measure on an LCH space is Radon and so has all of the desired approximation properties from the classical Lebesgue theory (Lusin, integration of LSC functions as increasing limits). Thus, we will generally not concern ourselves with what has been included in the sigma algebras $\mathscr{X}_t$ beyond the sub sigma algebra consisting of all Borel sets.

It is worth noting that when we apply λ to sequences of temporally constrained subspaces, the inclusion of a zero event time segment has no impact on the target space. So, $\lambda_3 : X_{t_1} \times X_{t_2} \times X_{t_3} \to X_{t_1+t_2+t_3}$ and $\lambda : X_{t_1+t_2} \times X_{t_3} \to X_{t_1+t_2+t_3}$ has the following interesting comparison for $E_1 \in X_{t_1}$, $E_3 \in X_{t_3}$, and $\tilde{E}_1 \in X_{t_1+t_2}$ such that $\tilde{E}_1|_{t_1} = E_1$ we have

$$\lambda_3(E_1, z, E_3) = \lambda(\tilde{E}_1, E_3) \tag{4.2.3.6}$$

likewise, up to any indication of the time intervals involved

$$\lambda_3(z,z,z) = \lambda(z,z) = z \tag{4.2.3.7}$$

we will use these observations without remark in the future.

Having defined a classical reaction counting sample space and a rule for composing events, we can now define precisely what we mean by a Quantum Stochastic Process.

Definition 4.2.13. *Quantum Stochastic Process for Reaction Counting*

A Quantum Stochastic Process (QSP) for reaction counting consists of: a sigma algebra $\mathscr{X}_t$ generated by the reaction counting sample space X_t, a continuous composition map $\lambda : X_s \times X_t \to X_{s+t}$, and a family of positive map valued measures $\mathscr{E}_t : \mathscr{X}_t \to \mathscr{L}_+(\mathscr{T}_+(\mathscr{H}))$

$$\mathscr{E}_t(B) \geq \mathscr{E}_t(\emptyset) = 0 \; \forall B \in \mathscr{X}_t \tag{4.2.3.8}$$

$$\forall (B_n)_{n\in\mathbb{N}} \subset \mathscr{X}_t \text{ s.t. } B_i \cap B_j = \emptyset \; \forall i \neq j$$
$$\mathscr{E}_t\left(\cup_n B_n\right) = \mathrm{s}\lim_{N\to\infty} \sum_{n=1}^{N} \mathscr{E}_t(B_n) \tag{4.2.3.9}$$

This positive map valued measure evaluated on the full sample space X_t must be trace preserving for all states $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\mathrm{Tr}\left[\mathscr{E}_t(X_t, \boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{4.2.3.10}$$

This positive map valued measure evaluated on the full sample space X_t must be strongly continuous in time for all states $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\mathrm{s}\lim_{t\to 0} \mathscr{E}_t(X_t, \boldsymbol{\rho}) = \boldsymbol{\rho} \tag{4.2.3.11}$$

For all states $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$, $\forall s,t \geq 0$, and $\forall E \in \mathscr{X}_s,\ F \in \mathscr{X}_t$,

$$\mathscr{E}_t(F, \mathscr{E}_s(E, \boldsymbol{\rho})) = \mathscr{E}_{s+t}(\lambda(E \times F), \boldsymbol{\rho}) \tag{4.2.3.12}$$

which is well-defined because continuous maps are always measurable functions.

This definition has numerous significant implications. The most obvious is that conditioning on the full space is probability preserving and therefore the most closely analogous to the evolutions of traditional

quantum mechanics. The second is that the special structure of the QSP evaluated on no event or one event has a particularly simple structure that can be used to produce easy to understand events, where as general Borel sets for $n > 1$ events can be fairly opaque. Finally, the last requirement in the definition 4.2.13 of a QSP can be understood as a quantum analogue for the Chapman-Kolmogorov equation itself. [32] Indeed, this says that the set of reaction events contains enough information to determine future reaction probabilities when combined with a prior state. We can treat the outcome of a composition of events the same way that we can treat the outcome of the evolution conditioned on one set of events and then iterated evolution conditioned on another set of events translated in time without regard for any outside information. That is, the requirement 4.2.3.12 is directly analogous to the Markov property.

4.3 A Heuristic Description of Reaction-Transport Systems

Unlike in other common approaches to quantization, this work does not rely on a functional calculus applied to the canonical quantization for an L_2 representation. The approach to quantization that we will be adopting in this text is grounded in an operational measurement model. Bohr insisted on a correspondence principle in the early constructions of quantum mechanics to limit the set of possible quantized models to those that would recreate classical measurements. This has continued to be a guiding light in studying ever more complex systems. Examples of this classical consistency idea range from the preservation of gauge invariance in electrodynamic field equations[123] to the existence of exponential envelopes for decay processes[7]. We too will rely on consistency with a well-established classical measurement theory to focus our attention on practicable models.

Nearly all approaches to transport quantization to date have relied on consistency with classical particle number counting, while collision operators constitute supplementary data used to configure a model for the propagator of the quasi-particle number state. [8] [126] [38] [18] [76] Our approach will break from this conventional vision of transport, which has proven to be mostly applicable to particle conserving and non-resonance processes. Instead, we will rely on a point of view employed by mathematical quantum optics: reaction detection counting consistency. Unlike in other quantum transport theories, absorption and decay events are of central importance in quantum optics.[16] This is not to say that number operators are not important. Number operators are useful in representing complex many-body correlations in quantum fields and in studying the relationship to classical branching models. They just are not the primary observable that motivates the quantization model. This quantization model is developed to study the evolution of reaction rates from a quantum measurement perspective.

We have already presented a classical reaction rate theory in chapter 3. The primary features of the classical theory that constrain our quantum theory in a meaningful way have already been identified in section 4.1. Now, using this and a quantum theory of reaction counting (whose components we defined in section 4.2), we will arrive at a conceptual model for a fully quantized reaction-transport model. This model will be given an explicit form in chapter 5. The resulting theory includes multiple undetermined functional "parameters" that can be understood in terms of scattering experiments and macroscopic system symmetries. We will examine these more closely in chapter 6.

4.3.1 Free and Bound Spaces

Although many authors have associated the neutron transport equation to a linearization of the classical Boltzmann dynamics [21], this claim is far from a meaningful characterization of the foundations of neutron transport. In particular, this assertion suggests that the dynamics of neutrons can be understood as a perturbative result of single species gas dynamics. Such systems can be well understood in terms of the existing interacting particle systems theory for hard spheres. [83] [110] The problem that we are studying diverges radically from the linearized Boltzmann physics, even though the superficial form of the classical average number density equation is similar. Indeed, collisions of interest are not interactions between neutrons at all, but coupling to a second field. If one were to draw a classical IPS analogy for this problem it would likely be the Lorentz Gas. [66] This is not really a productive analogy either because of the centrality of resonance scattering and branching dynamics to the study of nuclear systems. Thus, on the one hand, a reaction-transport model should explicitly include quantum resonance dynamics as part of the system model. At the same time, a reaction-transport model must permit neutrons to undergo successive collisions with different nuclei.

With these facts in mind, we can look back at our characterization of a classical neutron measurement theory in section 4.1, and how time-delayed neutron kinetics are handled. There, we introduced bound states that could be populated by collisions with absorption. These populated bound states could decay exponentially back into the continuum to continue the transport and branching process. Thus, in order to be consistent with the classical neutron transport observations, there should be some family of absorbed or otherwise excited particles that subsequently decay with an exponential envelope. This brings us to our first observation: the quantum dynamics can only account for the standard transport experiments if we allow for neutrons to exist in either free or bound states.

Free states must populate bound states via a mechanism that induces spatially exponential absorption rates for single particle states averaged over a suitable path distribution. Conversely, bound states decay

back into free states with a distribution in time that has an exponential envelope. As a result, the transitions between free and bound states are individually instantaneous but the bound state can be populated for a finite duration on transport time scales. For such distributions, probability of both absorption and decay is differentiable in the duration of the considered time interval (i.e. it looks linear in time for small time intervals).

We suppose that this model can take the form of a reaction counting QSP. All reactions transfer neutrons between free and bound states. We count different reactions as separate types. The nuclei to which the neutrons bind following an absorption are distinguishable and therefore provide a kind of dynamic coordinate system for tracking neutrons. Given that we have chosen to model the reactions as classical measurement events, for any individual point in our event space and a set of particles that began in either pure free or bound states, we will (up to multi-particle wavefunction overlap with the same nucleus) be able to determine the pure free or bound state of every particle in the system at a later time. This implies a (conditional) purity preserving form to the transition events themselves. This is not true for more general sets of the sample space sigma algebra.

4.3.2 0-Instruments and Collisionless Propagation Semigroups

With a quantum stochastic process for reaction counting in mind we will introduce two kinds of components for describing our theory. The first of these is the zero event evolution or 0-Instrument. This can be technically understood as a Quantum Stochastic Process evaluated against the $n = 0$ reaction count sequence represented by z, thus it is a positive map valued measure on a singleton set $\{z\}$. That is, the propagator $S_t\boldsymbol{\rho} = \mathscr{E}_t(z, \boldsymbol{\rho})$. We will prove in chapter 5 that this is in fact a strongly continuous semi-group for cases of interest to us. This propagator acts on both the bound and the free spaces at the same time, evolving the system according to a suitable subsystem dynamics.

In general, these evolutions can be very complicated in their own right. However, for our free space we will assume this is dispersive evolution by a laplacian generator over an interval small enough to comfortably be approximated by translation. This particularly simple propagation on the free space is what communicates information between different nuclei. Viewed conversely, nuclear and transmutation states hold information that allows a kind of effective communication between neutrons.

The bound state part of the zero event evolution can be very complicated (even a QSP in its own right for cases that we won't explicitly cover [70]). However, the simplest way to think of it is as a shell model embedded in a continuum of free states. [113][59] The shell model dynamics can be reliably dilated to a unitary evolution and then the open part is handled by absorptions and decays.

4.3.3 1-Instruments and Jump Operators

The second component that is of interest to us is the quantum stochastic process conditioned on the occurrence of a single collision in a vanishingly small time interval. This jump operator represents the infinitesimal contribution due to the possibility that a jump occurs at a time t, normalized to the duration. We will prove that such an instrument exists in chapter 5. However, for now, we will satisfy ourselves with the idea that this assigns an operation to every possible reaction location in phase space and reaction type. This operation describes the transformation of a state as a result of the "measurement". Here the measurement is an instantaneous reaction transforming a free state into a bound state or a bound state into a free state.

These jumps operators come in two broad types: absorptions and decays. We assert (as we did above) that both events are instantaneous in and of themselves but exponentially distributed. Absorptions and decays don't need to be exactly inverses of one another. Indeed, it is possible to have nuclear states that absorb directly but that do not decay back into the continuum at the same rate. An example of this would be stable compound states. However, many practical models of neutron thermalization neglect these kinds of quasi-bound states because they violate the principle of microscopic balance. [117] In general, if we do have a perfect symmetry between absorptions and decays, we can prove much stronger results about convergence to equilibrium. Although we can be specific about the types of absorptions as part of the reaction index $i \in T$, this has some odd implications for interference of decay mechanisms. We will use an approximation of this kind in describing our model of neutron thermalization. However, it generally suffices to characterize the system as having just the two basic kinds of transitions.

4.3.4 The Two-Instrument Model of Reaction-Transport

The essential idea of this quantization technique is as follows: the relationship between the evolution of states of the neutron field and reaction counting events can be understood as a neutronic system being transformed by the back action of the continuous detection of reaction events. The neutrons of the neutron field can exist in two dominant subspaces: free states and bound states. Any transition between the two states is always registered as a reaction count. More precisely, the detection of a reaction event leads to a transition between the free and bound subspaces. Although this seems backwards to anyone who works with particle simulations, the two perspectives are equivalent in a quantum measurement framework where the transition is a selective measurement.

We can make this idea a little bit more intuitive by assigning some measure of agency. We can imagine a field of free neutrons and a field of accessible bound states in direct analogy with the particle-hole dichotomy

of electrons in a Fermi gas. [53] Then, instead of trying to classify energy states and assign a Gibbs measure, we imagine a non-equilibrium process where one spatially distributed field measures the spatial distribution of the other. In particular, as a neutron passes a nucleus in coordinate space, there is an integral over a temporally continuous (in particular exponential) probability density that gives the total probability of detection of the neutron by the nucleus. The derivative of this detection probability can be thought of as the jump rate from a free to a bound state. Conditional on the detection of a jump, the neutron is no longer in a free state and the nucleus has transitioned from a quiescent to an excited state. This construct has a direct analogy in theory of QSPs that we will examine carefully in chapter 5.

Conversely, we can imagine nuclei that have absorbed neutrons and are now in an excited state are continually monitored by the vacuum state of the free neutron field. Given the nature of the quantum decay process, this vacuum state detection is bounded by an exponential function in time. This process for the decay of excited atoms is studied extensively in quantum optics for laser pumping. [16] When a neutron is detected by the local vacuum state of the free neutron field, the nucleus transitions to a lower energy state and the neutron free field has a neutron added to it in a momentum cone with a probability consistent with the relevant decay energy distribution. The resulting single neutron coordinate space distribution is coextensive with the range of probable positions of the nucleus in the atom, while the momentum space distribution is consistent with at least the atomic excitation uncertainty about a point in the nuclear momentum decay distribution.

The composite of these two continuous measurement processes is a phase space dependent, type-indexed reaction counting QSP that directly connects to quantum resonance scattering models through a time dependent excitation and decay process and accounts for uncertainty in the medium through radar ambiguity functions incorporated into the definition of the absorption and decay detection instruments. The name that we have given to this model is based on the fact that the model is predominantly defined by an instrument for absorption event detection and an instrument for decay event detection. Once these are defined, along with a bound state dynamics, much the rest of the quantized reaction-transport model follows by necessity. In this sense, it is unequivocally a transport model defined in terms of nuclear reaction dynamics.

We can extend this model by tracking additional decay and absorption types that lead to the formation of different nuclear species. This adds a component of evolution to the medium itself that makes it possible to directly describe burn-up of fuel or formation of poisons. In this sense, the bound space can also be understood as a kind of correlation field. It enables communication of information between neutrons over time. This leads to the slow formation of macroscopic patterns in the multi-time correlation among reactions. Information otherwise does not propagate between neutrons or between nuclei as they are energetically and

spatially isolated from one another to such a degree that they are effectively Bosonic relative to their own kind.

4.4 Axiomatic Requirements of a Quantized Reaction-Transport Theory

This last section is not critical to the validity of the dissertation as it is applied to nuclear engineering. However, this work is motivated by the idea that the origin of the transport equation is not in particular approximations to poisson brackets or in nuclear potential-specific scaling limits. Rather, the transport equation is grounded in the modeling of continuous and suitably bounded reaction rate measurements along trajectories. In this way, the underlying measurement theory can be applied across a wide range of scientific endeavors from mathematical epidemiology and systems biology [105][103][109] to geospatial statistical models for community development economics [130][27][110]. Fundamentally, we are interested in characterizing strongly correlated many-agent systems in the presence of seven important simplifications.

- The particles can be classified into two groups that we will call the free field and the correlation field.
- The free field interacts with the correlation field but the particles of the free field do not interact with one another.
- The correlation field has internal structure to each particle. This internal structure is generally quiescent but can be excited by interaction with a component of the free field.
- The particles of the free field propagate (parametrically as a function of a classical momentum state) between elements of the correlation field, thereby creating the potential for correlations between the internal states of separate particles of the correlation field and (conversely) creating the potential for indirect correlations between particles of the free field.
- The coupling between the two fields can be expressed as discrete integral events (reaction transitions) but the interaction probability for a single pair transition can be expressed as a continuous function of time that to second order takes the form of a square modular overlap of the vector representations of the individual particles.
- the reaction transitions can remove particles from the free field or add them to it but there is some finite maximum number of particles that can be free at a given time. In a conservative process like thermalization, this is the starting free population.

- Decays into the free field from the correlation field can be measured by probing any excited correlation particles with a free field vacuum state.

The essential idea of this framework is that such a system can be represented as a QSP tracking the transitions between the two systems as a function of the distribution of bound and free states. These transitions can be divided into four non-overlapping subsets: free to bound transitions, bound to free transitions, free to free transitions, and bound to bound transitions. In this work we will only consider the first three kinds. The free to bound transitions can be understood as the free field being measured by an instrument form of the correlation field. The bound to free transitions can be understood as the correlation field being measured by an instrument form of the free field. Their coupled evolutions are just the back action of the respective quantum measurements combined with a kind of independent non-interacting evolution on their localized subspaces.

Chapter 5

Reaction-Transport Quantum Stochastic Processes

This chapter introduces the technical mathematical results for representing quantum stochastic processes relevant to problems of stochastic neutron transport. We will develop an abstract theory for mapping reaction models to transport QSPs and we will prove that this mapping is unique up to particular set of physically meaningful modeling choices. The process of deriving this equivalence will yield all of the technical results that we require to justify the use of this theory for modeling in nuclear engineering.

The essential idea for the particle simulation analogy and its relation to measurements that inspired this section is a result of the work of Belavkin and Barchielli. [6] This perspective has since been developed and is espoused in tremendous detail in modern texts on quantum optics. [16] [67] [147] The uniqueness theory in this section is derived from an abstract collection of theorems due to Davies on the direct detection of quasi-particles in quantum fields. [32] The comparison to the classical theory in terms of approximate phase space measurements draws on the work of Ford and Lewis. [57] In order to obtain a transport theory of the form 3.3.4.13, we have equated phase space localized reactions with classical events. Therefore, it is also apparent that the conclusions reached in this section can also be related to the uniqueness results obtained for event enhanced quantum theory. [74]

5.1 Quantum Stochastic Reaction-Transport Processes

In this chapter, we will develop a fairly general theory of quantum stochastic processes for reaction-transport. We begin by re-expressing the heuristic assumptions outlined in section 4.3 in terms of explicit mathematical assumptions that every theory describing a reaction-transport system must satisfy. We draw an explicit connection to scattering theory and to the elements of the classical Pál-Bell theory of neutron transport. Then, by mapping elements of our heuristic model to concrete components in a quantum stochastic process theory due to Davies, we will build an explicit bridge from models of individual reaction events to mesoscale transport dynamics. This construction will include a specialization of the theory to the phase space localizing measurements that are characteristic of a mesoscale transport process. Finally, we will use Davies' theory for

general continuous quantum measurement processes to establish the uniqueness of this bridge from nuclear reaction to transport theories.

To set some expectations, we will indicate some notation and describe what a successful theory would look like. Following the arc of section 4.3, we assume the existence of a state $\boldsymbol{\rho}$ with projections onto bound and free subspaces: $\boldsymbol{\rho}_B = \Pi_B \boldsymbol{\rho} \Pi_B$ and $\boldsymbol{\rho}_F = \Pi_F \boldsymbol{\rho} \Pi_F$. Conditional on having a state consisting of pure bound and pure free states for all particles at $t = 0$ and an explicit knowledge of the set of all reactions that have taken place in the interval $[0, t_1]$, the state at the end of the interval t_1 should be block diagonal in the bound and free subspaces. Moreover, the bound states of different bound particles should not be able to interfere with one another and so can be represented as a classical tensor product of states of the individual bound particles.

The overall evolution of the system should be able to be represented by a quantum stochastic process $\mathscr{E}_t$. The 0-reaction evolutions on the bound and free spaces should be independent and purity preserving. We will represent a non-collision evolution as a semi-group $\boldsymbol{S}_t \boldsymbol{\rho} = \mathscr{E}_t(z, \boldsymbol{\rho})$.

Finally, we introduce a single jump event localized in phase space and time such that $\mathscr{J}$ is a positive-map valued measure on phase space. This is to say, $\mathscr{J}$ gives the phase space distribution associated to an event occurring in an infinitesimal time interval (i.e. a scattering event or a jump between free and bound subspaces). We further associate to $\mathscr{J}$ an observable $\boldsymbol{R}$ for the phase space localized reaction rate. With this in mind, a successful theory would give a unique way of associating to these inputs a unique QSP such that we can assign a probability to each sequence of reaction events (having finite detection volumes in phase space). In particular, we would arrive at an effective path space measure with a Chapman-Kolmogorov form for a quantum piecewise deterministic process.

Specifically, we seek to prove that any viable Reaction-Transport model can be represented as follows: $\forall E \in \mathscr{X}_t$ of the product Borel form, $t_i \leq r_{i+1}$, $E = \{(x_i, p_i, \ell_i, s_i)_{i=1}^m : r_i < s_i \leq t_i, (x_i, p_i, \ell_i) \in E_i\}$, and $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\mathscr{E}_t(E, \boldsymbol{\rho}) = \prod_{i=1}^{m} \int_{(r_i, t_i]} \mathrm{d}s_i \boldsymbol{S}_{t-s_m} \mathscr{J}(E_m) \boldsymbol{S}_{s_m - s_{m-1}} \mathscr{J}(E_{m-1}) \dots \mathscr{J}(E_1) \boldsymbol{S}_{s_1} \boldsymbol{\rho} \tag{5.1.0.1}$$

This formula can be read in much the same way as the reaction-centric Backward Chapman-Kolmogorov equation of classical neutron reaction counting theory 3.3.4.13. From right to left we start from a prior state and successively apply measurement events that also transform. This leads to a composite measure on any chain of events that can be broken into free propagations joined by reactions. We will refer to this kind of path measure as a PDP model. The goal of obtaining such an intuitive path measure will ground the

development of the theory in the rest of this section.

There are two general comments to make on the content of this chapter. First, the definitions relating to multi-particle states given in sections 5.2 and 5.3 are fairly technical and both less transparent and less general than they could be. However, given any finite initial particle number, for the problems we will discuss in the rest of this text, all of the sums relating to particle number and reaction type are finite. As a result, the existence and uniqueness results as well as the transitions between the bound and free spaces can most easily be understood by focusing on the single particle case. Under these circumstances, the approximate phase space instrument described in section 4.2.2 is fully sufficient to the task at hand. Moreover, for the single particle case, the transformations back and forth between the two spaces can be thought of as block rotations in a (Bound, Free) vector space.

Second, the most important observation in this comes down to a representation problem. We are constructing an equivalence that will make it possible to draw a direct connection to the classical stochastic neutron theory. Essentially, we are proving in this chapter that any quantum stochastic process we might want to use to study a reaction transport system can be expressed as a quantum piecewise deterministic process (PDP). Conversely, any quantum piecewise deterministic process that could be viably used for estimating transport-like processes (while enforcing consistency with linear attenuation) is generated by a correspondingly well-behaved quantum stochastic process. A more general version of this idea has been developed for application to other classes of quantum fields. However, the concrete particle simulation version that we develop here makes it easy to apply quantum measurement theory to modeling nuclear systems.

5.2 Free and Bound Fock Subspaces

We will introduce two subspaces to our underlying Hilbert space and constrain the set of states correspondingly. The assumptions presented in this section should be compared to the heuristic discussion in section 4.3.1. We begin by observing that at any given instant, there are some number of neutrons in free states and some number in bound states. However, given that the set of all absorption and decay events are classically detectable, it is reasonable to suppose that no single particle is in a mixture of free and bound states. Based on this, we introduce a simplification by splitting the Hilbert space into a tensor product of the two distinguishable subspaces $\mathscr{H} = \mathscr{H}_F \otimes \mathscr{H}_B$. Then each of these subspaces is treated as a Fock space of single particle states having a maximum total number of particles N. This is no real restriction on the physics as there is no way to have more neutrons free or bound than we have nucleons in the total reaction volume. In practice, the maximum is much smaller than that. At any rate, our dynamics will need to be consistent

with this limit. The Fock spaces each include a cemetery state c_F or c_B containing no particles. The Fock space is then taken to be the closure of the linear span of all of the finite particle number subspaces with the cemetery state.

$$\mathscr{H}_F = \bigoplus_{n=1}^{N} \bigotimes_{i=1}^{n} \mathscr{H}_F^1 \bigoplus c_F \tag{5.2.0.1}$$

The single free particle Hilbert space is of the form $\mathscr{H}_F^1 = L_2(\mathbb{R}^3, \mathbb{C}) \otimes \mathbb{C}^{k_F} \otimes e_F$ having a phase space distribution function (represented in whatever way is convenient, say an L_2 coordinate space representation or a phase space quantized $\mathbb{R}^6$ distribution) and a k_F vector for indicating a kind of species index. The e_F vector is a labeling vector indicating the fact that the particle is in the free subspace and it can be used to select off subsets of particles belonging to the free subspace. In this text, we will almost always use $k_F = 1$ so that the free states are just phase space distributions. Likewise,

$$\mathscr{H}_B = \bigoplus_{n=1}^{N} \bigotimes_{i=1}^{n} \mathscr{H}_B^1 \bigoplus c_B \tag{5.2.0.2}$$

The single free particle Hilbert space is of the form $\mathscr{H}_B^1 = L_2(\mathbb{R}^3, \mathbb{C}) \otimes \mathbb{C}^{k_B} \otimes e_B$ having a phase space distribution function (represented as an L_2 momentum space representation) and a k_B vector for indicating a kind of species index. The e_B vector is a labeling vector indicating the fact that the particle is in the bound subspace and it can be used to select off subsets of particles belonging to the bound subspace. In practice, we will almost always use $k_B = |T|/2$ so that there is a phase space distribution and a collection of bound state subspaces each having an absorption and a decay transition connecting it to the free space. We will return to this point later.

Although valid elements of $\mathscr{T}_+(\mathscr{H}_F \otimes \mathscr{H}_B)$ can include mixed states, we will generally be interested in convex sums of pure states with regard to bound and free particle number. This is a way of saying that the distribution over the number of particles in bound and free states will only exhibit classical uncertainty rather than quantum uncertainty. We will define all of our free evolutions and transitions to preserve pure number states. It is also worth noting that there is a kind of independent particle approximation at work here since we are not anti-symmetrizing and our operators will be independent of the number of particles in a given subspace. Finally, we comment that this Hilbert space includes no tracking of ongoing transmutation information about the medium. This is possible using the same methods but we will not address this topic until chapter 6.

The states in this theory are not symmetrized over particles because the single particle states are assumed to be a priori distinguishable by mean phase coordinates. However, in reformulating this in a symmetrized form, we would simply need to modify the operator definitions below in order to guarantee that once the

detection and absorption/decay operators had acted on the same particle, the result was formed into a symmetric vector. The basic structure of the operators is compatible with this kind of operation. We have chosen not to address this for simplicity.

5.3 Pure-State Preserving Collisionless Propagator Model For Mesoscopic Streaming

We will now introduce the first of three major features common to all reaction transport theories: the existence of particle streaming in the absence of collisions. The assumptions and results in this section should be compared to the heuristic model outlined in section 4.3.2. We will refer to the collisionless propagator by the symbol $\boldsymbol{S}_t$. This is the simplest part of the transport process and the easiest component to quantize. Indeed, as we have already discussed in section 3.4, streaming can easily be understood as propagation of a beamlet along a fixed momentum path. Up to the existence of classical momenta, this is essentially a translation operator. In a quantum context this translation can be understood to act on a single particle phase space density function $\rho_1(\bar{x}, \bar{p})$. There are a few different approximations to this operator that agree to within a small error on the class of initial states that are of interest to us. We will begin by building an abstract model and we will demonstrate some concrete alternatives in later sections.

In order for a time-indexed operator family $\boldsymbol{S}_t$ to represent the process that would become streaming in a mesoscopic system, the propagator must satisfy three abstract requirements. First, $\boldsymbol{S}_t$ must be a strongly continuous operator semigroup on the Banach space of states $\mathscr{T}(\mathscr{H})$. Second, $\boldsymbol{S}_t$ must transform pure states into other pure states. Third, any valid streaming propagator $\boldsymbol{S}_t$ must leave the number of particles in the bound and free subspaces invariant for any state without a mixed number representation. More specifically, collsionless evolutions on the subspaces of separate particles will typically be left unmixed if they were not initially mixed in order to facilitate the independent branching approximation. Beyond this, we note that for $\boldsymbol{S}_t$ to be incorporated naturally in piecewise deterministic process representations, it has to include both the collisionless evolution of the free single particle state and the bound single particle states. This means that while $\boldsymbol{S}_t$ acts like mesoscopic streaming on the free states, it must act like quasi-bound oscillation on the bound states. Finally, in order for this to be integrated into a single framework with a reaction process, the collisionless evolution probability must be consistent with the reaction probability over every finite interval. We discuss this self consistency in more detail in section 5.4. For now, it suffices to note that we must allow $\boldsymbol{S}_t$ to be contractive rather than trace preserving. We will proceed by examining these requirements one at a time.

We begin by evaluating the requirement that $\boldsymbol{S}_t$ be a strongly continuous operator semigroup. The semigroup property is an operatorial form of the Markov property that we have established as a requirement of the free propagator in the classical case. In a quantum stochastic process, we find that the strongly continuous semigroup property for collisionless evolution

$$\mathscr{E}_{t+s}(z,\cdot) = \mathscr{E}_t(z,\mathscr{E}_s(z,\cdot))$$
$$\lim_{t\to 0} \|\mathscr{E}_t(z,\boldsymbol{\rho}) - \boldsymbol{\rho}\|_{\mathrm{Tr}} = 0$$

follows from the assumption of a bounded reaction rate. (we will prove this in a later section) However, more generally we will need to assume it to be the case. As we have discussed, strongly continuous semigroups have densely defined, closed infinitesimal generators that uniquely determine the semigroup. Generators provide a useful tool for classifying and analyzing operator semigroups and we will use the properties of the generator for $\boldsymbol{S}_t$ extensively. In order to constrain the form of the generator of $\boldsymbol{S}_t$ we will need to establish additional properties that follow from our additional constraints.

Next, we claim that the free evolution should preserve pure states. Specifically, $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$ This is primarily because particles should not become entangled as a result of free translation or evolution in separate nuclei. This is a result of what we called the independent neutron tree hypothesis in section 4.1. This assumption allows us to only worry about the quantum correlated evolution of children of the same parent neutron. In general, only when multiple particles are absorbed by the same nucleus is there a reason to expect the formation of an entangled state and this event is sufficiently improbable for most systems that neglecting it does not harm a neutron transport theory. However, this same consideration does not apply to neutrons born from a multiplication process. When this happens, we can model them as being born entangled and the mixed state being preserved by the "off-diagonal" pairings of the collisionless evolution.

However, the presence of other particles in a bound state does not influence the evolution of a given particle. This is essentially a bosonic independent particle approximation. (This also provides an argument for symmetrizing the bound states Fock space) That is, particles in bound states evolve independently of each other in some kind of modified mean field and each of their evolutions can be modeled by a contractive operator (exponential decay) on the quasibound state. This line of argument can be compared to the simple decay model in Baym or doorway resonances in Lipperheide. [7],[59] Both translation of individual free particles and exponential decay of bound states can be mostly understood as a Hamiltonian evolution plus a complex reaction operator to account for jumps. In order to allow for a more substantive modification of the nuclear dynamics, we would need to allow for a composition of two QSPs with one in the bound state

and one connecting the bound and free states. The current theory has not yet been extended to that case.

Finally, we come to the decomposition of the free evolution onto subspaces. We will construct this in two stages. First, recognizing that $\boldsymbol{S}_t$ must be of the form $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$, we initially focus on the way that a pure state transforms by decomposing $\boldsymbol{B}_t$. In particular, we suppose that for every *single-particle* vector ψ, its free evolution can be simplified to $\boldsymbol{B}_t|\psi\rangle = \Pi_{1,0}\Pi_F^1\boldsymbol{B}_t^1\Pi_F^1\Pi_{1,0}|\psi\rangle + \Pi_{0,1}\Pi_B^1\boldsymbol{B}_t^1\Pi_B^1\Pi_{0,1}|\psi\rangle$. We then suppose that $\boldsymbol{B}_t$ decomposes into fixed numbers of particles in the bound and free subspaces

$$\boldsymbol{B}_t = \sum_{n+m\leq N}\Pi_{n,m}\bigotimes_{i=1}^{n}\Pi_{F,i}^1\boldsymbol{B}_t^1\Pi_{F,i}^1 \otimes \bigotimes_{j=1}^{m}\Pi_{B,j}^1\boldsymbol{B}_t^1\Pi_{B,j}^1\Pi_{n,m} \tag{5.3.0.1}$$

Where $\Pi_{n,m}$ projects onto the subspace with n free and m bound particles, while $\Pi_{B,j}^1$ maps the jth single particle bound state to a single particle state and $\Pi_{F,i}^1$ maps the ith single particle free state to a single particle state. Moreover, $\boldsymbol{B}_t^1$ is a strongly continuous single particle free evolution This can be further decomposed into a denumerable sequence of bound subspaces where bound state mixing is only permitted on restricted subspaces of $\mathbb{C}^{k_B}$. In this case, we repeat the splitting procedure for $\Pi_{B,j}^1\boldsymbol{B}_t\Pi_{B,j}^1 = \sum_{\ell'\in T/G}\Pi_{B,j,\ell'}^1\boldsymbol{B}_t^1\Pi_{B,j,\ell'}^1$. Now, as a direct result of this form

$$\boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^* = \sum_{n+m\leq N}\sum_{n'+m'\leq N}(\Pi_{n,m}\Pi_F^n\boldsymbol{B}_t\Pi_F^n \otimes \Pi_B^m\boldsymbol{B}_t\Pi_B^m\Pi_{n,m})\boldsymbol{\rho}(\Pi_{n',m'}\Pi_F^{n'}\boldsymbol{B}_t\Pi_F^{n'} \otimes \Pi_B^{m'}\boldsymbol{B}_t\Pi_B^{m'}\Pi_{n',m'})^* \tag{5.3.0.2}$$

where $\Pi_F^n\boldsymbol{B}_t\Pi_F^n = \bigotimes_{i=1}^n\Pi_{F,i}^1\boldsymbol{B}_t^1\Pi_{F,i}^1$. Thus any definite bound and free number state is left with the same number of bound and free neutrons as a result of a collisionless evolution since only one term in the sum will be retained and that term will act on each particle individually in its respective bound or free space. This is important for discussions of quantum trajectories and classical pathwise approximation. It is worth noting that persistence of a priori mixed states is left intact as a result of the off diagonal number terms. However, for a system that starts with particles in classically defined states (e.g. an incident beam) the only way for particles to end up entangled is through a jump that creates an entangled state. At any rate, we are now in a position to state the key definition for quantum models of mesoscopic streaming.

Definition 5.3.1. *Collisionless Reaction-Transport Propagator*

A Collisionless Reaction-Transport Propagator is defined as a strongly continuous pure state preserving semigroup on $\mathscr{T}(\mathscr{H})$ *such that* $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$ *with* $\|\boldsymbol{B}_t\| \leq 1$, $\boldsymbol{B}_t$ *having a generator* $\boldsymbol{Y}$ *and*

$$\begin{aligned}\boldsymbol{S}_t\boldsymbol{\rho} &= \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^* \\ &= \sum_{n+m\leq N}\sum_{n'+m'\leq N}(\Pi_{n,m}\Pi_F^n\boldsymbol{B}_t\Pi_F^n \otimes \Pi_B^m\boldsymbol{B}_t\Pi_B^m\Pi_{n,m})\boldsymbol{\rho}(\Pi_{n',m'}\Pi_F^{n'}\boldsymbol{B}_t\Pi_F^{n'} \otimes \Pi_B^{m'}\boldsymbol{B}_t\Pi_B^{m'}\Pi_{n',m'})^* \quad (5.3.0.3)\end{aligned}$$

where $\Pi_F^n\boldsymbol{B}_t\Pi_F^n = \bigotimes_{i=1}^n \Pi_{F,i}^1\boldsymbol{B}_t^1\Pi_{F,i}^1$ *and* $\Pi_B^m\boldsymbol{B}_t^1\Pi_B^m = \bigotimes_{i=1}^m \Pi_{B,i}^1\boldsymbol{B}_t\Pi_{B,i}^1$ *with* $\Pi_F^1\boldsymbol{B}_t^1\Pi_F^1$ *a strongly continuous semigroup on a single free particle space having a generator* $\boldsymbol{Y}_F^1$ *and* $\Pi_B^1\boldsymbol{B}_t^1\Pi_B^1$ *is a strongly continuous semigroup on a single bound particle space having a generator* $\boldsymbol{Y}_B^1$.

We observe that the constraint $\|\boldsymbol{B}_t\| \leq 1$, is part of a consistency consideration. Namely, any probability mass lost from the streaming field must be accounted for in the total jump probability over the same interval. This consistency issue is of critical importance and appears to be quite complex, but is actually surprisingly easy to enforce. Moreover, this is already a requirement from classical neutron transport theory so it does not exclude any viable theories. We will return to this point in section 5.4.

5.4 Bounded Reaction Rate Model For Mesoscopic Reaction Rates

We now introduce the second of three major features common to all quantum reaction-transport theories: the existence of bounded mesoscopic reaction rates. The assumptions and results in this section should be compared to the heuristic model outlined in section 4.3.3 and the classical attenuation theory of section 3.4. We will approach the question of defining a bounded reaction rate from two different perspectives. First, we will examine the requirement that the detectable event count remains bounded by a linear function of t in every finite time interval $[0, t]$. Second, we will assume that we have a collisionless reaction transport propagator $\boldsymbol{S}_t$ and a transition PMV measure on phase space $\mathscr{J}$ (and the attendant reaction rate observable $\boldsymbol{R}$) as in 5.1.0.1 and characterize the existence of a reaction rate in terms of its role in a self-consistent linear attenuation formula. These two versions of the notion of a bounded reaction rate turn out to have a complex inter-relationship and both are important to understanding reaction-transport systems.

The essential idea of a bounded reaction rate can best be understood in contrast to a Brownian motion process. Whereas a diffusion equation describes a random process that evolves in response to an

asymptotically large number of asymptotically weak collisions, a transport process involves sparse collisions with dramatic consequences. [106] Traditionally, when describing conservative systems without resonances, stochastic processes that evolve according to a diffusion equation are described by Brownian motion processes. General reaction-transport processes can be described by a class of stochastic processes known as Continuous-Time Random Walks (CTRWs) that include classical diffusions and anomalous super-diffusion-like Levy flights. The classification of CTRWs provides an intuition for what an appropriate constraint on the reaction count distribution would look like. [106],[16] Indeed, in order for a Levy flight to be well-defined, the reaction rate must be almost surely bounded at all times. If the reaction rate diverged on a set of non-zero measure, then the defining asymptotic approximations of a transport process would fail. To illustrate what that would look like, sample paths of a Brownian motion are almost surely everywhere non-differentiable. This is to say, every interval in time can be understood as a cluster point for collisions. Thus, for a reaction rate to be a meaningful notion, we need to exclude these kinds of events. This means classically excluding diffusion processes in favor of processes with an expected mean free path length greater than 0.

Quantum mechanically, we can formulate this first version of a bounded reaction rate most clearly for a quantum stochastic process. Specifically,

Definition 5.4.1. *Bounded Reaction Rate for a QSP*

A quantum stochastic process $\mathscr{E}_t$ on $\mathscr{X}_t$ (the sigma algebra generated by X_t), with the non-interaction event z is said to have a Bounded Reaction Rate if it satisfies a trace differentiability requirement on the set containing at least one event: $\exists K_\tau > 0$ s.t. $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$ and $\forall t \in (0, \tau]$

$$\mathrm{Tr}\left[\mathscr{E}_t(X_t \backslash \{z\}, \boldsymbol{\rho})\right] \leq K_\tau t \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.4.0.1}$$

In order to understand this requirement more clearly, we note that for any QSP used to model a reaction transport process, the collisionless propagator is given by $\mathscr{E}_t(z, \boldsymbol{\rho}) = \boldsymbol{S}_t \boldsymbol{\rho}$. Thus, we can break the set of all events into the collisionless propagator and the part with a linearly bounded growth in time. Both parts are Banach space-valued functions that are differentiable in time. Moreover, we will find that when we combine the Bounded Reaction Rate and Collisionless Reaction-Transport Propagator assumptions, something wonderful happens to simplify the QSP into a manageable quantum process.

We will now move on to the second version of the bounded reaction rate requirement. This is imposed by how reaction rates are used in classical reaction-transport theories. A reaction rate must be consistent with a effect it has on the particle distribution. In classical transport theories, this idea is formulated as particle conservation. In the stochastic neutronics formulation, this is presented as a kind of conservation

of probability that forces as constraint on the free propagator in section 3.4. Regardless of your preferred justification, if you are modeling reaction rates and you wish the probability distribution to be interpreted in the frequentist sense, then there is a classical compatibility requirement that must be satisfied. We will begin our justification of this by using an easily interpreted form. We have introduced a collisionless reaction-transport propagator $\boldsymbol{S}_t$, a transition PMV measure $\mathscr{J}$, and an operator $\boldsymbol{R}$ that allows us to calculate the total instantaneous reaction rate in the system. Then if $\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right]$ is the total uncollided flux (or fraction of the population having not experienced a reaction) and $\mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{S}_t\boldsymbol{\rho}\right]$ is the instantaneous reaction rate, then standard linear attenuation arguments yield the following formula

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] = -\mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{S}_t\boldsymbol{\rho}\right] \tag{5.4.0.2}$$

Using the generator $\boldsymbol{Y}$ of $\boldsymbol{B}_t$, we can easily convert this to a form that we will find to be easier to use in establishing validity.

Definition 5.4.2. *Mesoscopic Reaction Rate*

Suppose $\boldsymbol{S}_t$ is a collisionless reaction-transport propagator $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$ with $\boldsymbol{Y}$ the generator of $\boldsymbol{B}_t$. A PMV measure $\mathscr{J}$ on the typed geographic phase space G defines a mesoscopic reaction rate if and only if $\forall\,|\psi\rangle \in D(\boldsymbol{Y})$

$$\mathrm{Tr}\left[\mathscr{J}\left(G, |\psi\rangle\langle\psi|\right)\right] = -(\langle\boldsymbol{Y}\psi,\psi\rangle + \langle\psi,\boldsymbol{Y}\psi\rangle) \tag{5.4.0.3}$$

It is worth noting that for a collisionless evolution that is meant to be Hamiltonian apart from the transition events, this requirement is satisfied for a particularly simple form of $\boldsymbol{Y}$. Namely,

$$\boldsymbol{Y} = -i\boldsymbol{H} - \frac{1}{2}\boldsymbol{R} \tag{5.4.0.4}$$

we will take advantage of this to construct simple models in the applications chapter.

5.5 The Approximate Phase Space Instrument As a Single Reaction Event Measurement

We now introduce the last of three major features common to all reaction transport theories: the existence of mesoscopic phase space correlated reaction processes. The assumptions and results in this section should be compared to the heuristic model outlined in section 4.3.3. In this section, we will define the family of jump PMV measures $\mathscr{J}$ that will be used throughout the remainder of the text. Although a very large

class of models fall into the scope of this family of PMV measures, it is considerably more specific than the general theory for which the main result of this chapter holds. (cf. Davies chapter 4) Our hope is that the balance struck is appropriate to covering a wide variety of cases while illuminating the most critical path simulation approximations and the selection of model components. The PMV measures introduced in this section are a close relative of the phase space approximation measures that we developed in section 4.2.2. As such, the corresponding reaction rate operator $\boldsymbol{R}$ is many-body, vector version of the phase space observable evaluated over the whole space and contracted against a detection potential. We will examine and interpret simplified versions of this operator in more detail in chapter 6.

We begin by defining two classes of operators that in their simplest form are simply matrices with a 1 somewhere in the top row and zero elsewhere. That is, these are operators that rotate neutrons between free and bound states. We have had to make some modifications to this simple premise to account for typed transitions and general (Bound, Free) Fock spaces consisting of multiple particles in both the bound and free spaces.

Definition 5.5.1. *Absorption Operator*

An absorption operator $\boldsymbol{e}^{j}_{a,\ell}$ is a map between a fixed particle number apparatus state in the free subspace and a fixed particle number apparatus state in the bound subspace. That is, given $|\psi_1\rangle \in \mathscr{H}_F, |\phi_1\rangle \in \mathscr{H}_B$, where

$$|\psi_1\rangle = \left|\psi_1^1\right\rangle \otimes \cdots \otimes \left|\alpha_{x_j,k_j}\right\rangle \otimes \cdots \otimes \left|\psi_1^{n_1}\right\rangle$$
$$|\phi_1\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle$$

, $\exists\, |\psi_2\rangle \in \mathscr{H}_F, |\phi_2\rangle \in \mathscr{H}_B$, where

$$|\psi_2\rangle = \bigotimes_{i=1}^{j-i} \left|\psi_1^i\right\rangle \otimes \bigotimes_{i=j+i}^{n_1} \left|\psi_1^i\right\rangle$$
$$|\phi_2\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle \otimes \gamma_\ell(\left|\alpha_{x_j,k_j}\right\rangle)$$

and γ_ℓ maps one apparatus state to a tensor product of some fixed number of apparatus states with each particle unitarily transformed by an operator $\hat{\boldsymbol{U}}_\ell$ and

$$\boldsymbol{e}^{j}_{a,\ell} |\psi_1\rangle \otimes |\phi_1\rangle = |\psi_2\rangle \otimes |\phi_2\rangle \tag{5.5.0.1}$$

Note that this projects on to only states of the appropriate initial particle numbers in the free and bound

states.

Remark

For a single particle system, an absorption operator can be understood as a rotation from a free to a bound subspace combined with unitary re-representation in the bound space.

Definition 5.5.2. *Decay Operator*

A decay operator is a map $\boldsymbol{e}^{j}_{d,\ell}$ *between a fixed particle number apparatus state in the bound subspace and a fixed particle number apparatus state in the free subspace. That is, given* $|\psi_1\rangle \in \mathscr{H}_B, |\phi_1\rangle \in \mathscr{H}_F$*, where*

$$|\psi_1\rangle = \left|\psi_1^1\right\rangle \otimes \cdots \otimes \left|\alpha_{x_j,k_j}\right\rangle \otimes \cdots \otimes |\psi_1^{n_1}\rangle$$
$$|\phi_1\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle$$

, $\exists\, |\psi_2\rangle \in \mathscr{H}_B, |\phi_2\rangle \in \mathscr{H}_F$*, where*

$$|\psi_2\rangle = \bigotimes_{i=1}^{j-i} \left|\psi_1^i\right\rangle \otimes \bigotimes_{i=j+i}^{n_1} \left|\psi_1^i\right\rangle$$
$$|\phi_2\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle \otimes \gamma_\ell(\left|\alpha_{x_j,k_j}\right\rangle)$$

and γ_ℓ *maps one apparatus state to a tensor product of some fixed number of apparatus states, each particle unitarily transformed by an operator* $\hat{\boldsymbol{U}}_\ell$ *and*

$$\boldsymbol{e}^{j}_{d,\ell}\, |\psi_1\rangle \otimes |\phi_1\rangle = |\psi_2\rangle \otimes |\phi_2\rangle \tag{5.5.0.2}$$

Note that this projects on to only states of the appropriate initial particle numbers in the free and bound states.

Remark

For a single particle system, a decay operator can be understood as a rotation from a bound to a free subspace combined with unitary re-representation in the free space.

We are now able to define the primary tool of our theory by extending the approximate phase space instrument of section 4.2.2:

Definition 5.5.3. *Reaction-Transport Transition PMV*

For $\mathscr{G}$ the sigma algebra on a typed geographic phase space, we define a map $\mathscr{J} : \mathscr{G} \times \mathscr{T}_+(\mathscr{H}) \to \mathscr{T}_+(\mathscr{H})$ to be a Reaction-Transport Transition PMV if for every $E = F \times T_E \in \mathscr{G}$ and every state $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$,

$$\mathscr{J}(E, \boldsymbol{\rho}) = \frac{1}{(2\pi)^3} \int_F \mathrm{d}^3x \, \mathrm{d}^3k \sum_{\ell \in T_E} \boldsymbol{U_\ell} \left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right| \boldsymbol{V}_{x,k,\ell} \boldsymbol{\rho} \boldsymbol{V}^*_{x,k,\ell} \left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right| \boldsymbol{U}^*_\ell \tag{5.5.0.3}$$

Here T is a countable set.

A detection operator, $\left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right| \boldsymbol{V}_{x,k,\ell}$ is to be understood as being applied to each particle of a free or bound state Fock space separately with the remaining particles being transformed by identity operators. Each detection operator only applies to either the free subspace or the bound subspace, not both. $\boldsymbol{U_\ell}$ is an absorption operator or a decay operator acting between fixed particle number subspaces for each $\ell \in T$ and so the composition yields a sum over j index for removal, so that an absorption takes the form

$$\sum_{j=1}^{n} \boldsymbol{e}^j_{a,\ell} \left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right|_j \boldsymbol{V}^j_{x,k,\ell} \tag{5.5.0.4}$$

where the existing bound states are injectively mapped into the higher particle number bound space. While a decay, takes the form

$$\sum_{j=1}^{m} \boldsymbol{e}^j_{d,\ell} \left|\alpha_{x,k}\right\rangle \left\langle\alpha_{x,k}\right|_j \boldsymbol{V}^j_{x,k,\ell} \tag{5.5.0.5}$$

where the existing free states are injectively mapped into the higher particle number free space. Taken together, this defines the form of the operator acting on a multi-particle vector.

We can define a phase space operator function as a sum over weights on reduced particle number spaces for any convex combination of pure states with definite bound and free particle numbers

$$\boldsymbol{\rho}_{V,\ell}(\bar{x}, \bar{k}) = \sum_j \frac{1}{(2\pi)^3} \left\langle \boldsymbol{V}^*_{x,k,\ell} \alpha_{x,k}, \boldsymbol{\rho}_j \boldsymbol{V}^*_{x,k,\ell} \alpha_{x,k} \right\rangle \boldsymbol{\rho}_{i \neq j} = \sum_j \rho_{j,V,\ell}(\bar{x}, \bar{k}) \boldsymbol{\rho}_{i \neq j} \tag{5.5.0.6}$$

In order for $\mathscr{J}$ to be a Reaction-Transport Transition PMV, we additionally require that $\exists c > 0$ s.t. $\forall \ell \in T$

$$\|\boldsymbol{U}_\ell\| \leq c \tag{5.5.0.7}$$

and that the phase space operator function satisfies

$$\mathrm{Tr}\left[\sum_\ell \boldsymbol{\rho}_{V,\ell}(\bar{x}, \bar{k})\right] \leq K \sum_j \rho_j(\bar{x}, \bar{k}) \tag{5.5.0.8}$$

where $\rho_j(\bar{x}, \bar{k})$ is the single particle phase space density function as defined in section 4.2.2, applied to the jth single particle pure state.

Proposition 5.5.4.

Every Reaction-Transport Transition PMV $\mathscr{J}$ is a Positive Map Valued Measure.

$\mathrm{Tr}\left[\mathscr{J}(G, \boldsymbol{\rho})\right] \leq K \mathrm{Tr}\left[\boldsymbol{\rho}\right]$

Proof.

All of our estimates that involve convergence for the approximate phase space instrument rely on the fact that of the density function $\rho(\bar{x}, \bar{k})$ is well bounded. If this holds on each particle for the multiparticle operation, we can employ a nearly identical argument to the theory developed in section 4.2.2 to prove strong countable additivity. Meanwhile, positivity follows from the sum over integrals of bounded, strongly continuous, purity preserving operators: $\sum_\ell \sum_j \int \mathrm{d}x A_x^{j,\ell} \boldsymbol{\rho} (A_x^{j,\ell})^*$. The positivity computation from the original proof in section 4.2.2 remains essentially valid since a sum of positive operators is also positive, likewise for a composition of positive operators.

Trace boundedness follows immediately from approximate phase space instrument theory of 4.2.2 and the reaction sum boundedness constraint.

□

Remark

For all applications to neutron thermalization, it suffices for the absorptions and decays to involve single particle rotations which makes $|T| < \infty$ easy to accomplish. This does require a bound on the maximum number of particles generated through multiplication, but this is perfectly acceptable for medium energy neutron physics in the absence of a thermodynamic limit. Moreover, the summability constraint 5.5.0.8 is automatically satisfied if the reaction type set T is finite, which will be the case for all of the models that we study in this paper.

Remark

In studying many macroscopic applications we can comfortably work with non-symmetrized subspaces because we are studying branching trees as independent from one another. In dealing with systems where interference of multi-particle states is an important consideration, more care is required.

Remark

Since multiparticle subspaces are still tensor normalized in a Fock space and the individual operations are between fixed particle number spaces, $\|\boldsymbol{U}_\ell\| \leq c$ can be understood as a bound on the nuclear excitation energy of particles added to the nucleus by an absorption process. For a conservative process, $\boldsymbol{U}_\ell$ should be represented by a partial isometry.

Remark

Arguably, the external phase space integral should include, for each particle, a pair of integration variables and a $(2\pi)^3$ normalization factor. The interior operators should include a tensor product of independent phase space projections as well as a tensor product of $\boldsymbol{V}_{x,k,\ell}$ and $\boldsymbol{U}_{\boldsymbol{\ell}}$ operators where $\boldsymbol{V}_{x,k,\ell} = \boldsymbol{U}_{\boldsymbol{\ell}} = \boldsymbol{I}$ on all but one. This would indicate a nonselective phase space localization measurement occurring on every particle at the time of the detected jump. It would have implications for the relationship between reaction rates and number operators. However, for all but one particle, we have replaced this by a tensor product with identity operators for $\boldsymbol{V}_{x,k,\ell}$ and $\boldsymbol{U}_{\boldsymbol{\ell}}$ and the phase space projectors and no addition phase space integrals without altering a classical transition probability. This follows from the ultraweak formula 4.2.1.27.

Remark

The summability constraint could be be satisfied for a countable reaction type set for potentials $\boldsymbol{V}_{x,k,\ell} = V(\bar{x} - \bar{x}_\ell, \bar{k})$ that are contractive and where the potential decreases quickly enough to preserve summability with increasing ℓ. This kind of construction could be used when studying a field of detectors with independent bound spaces separated by significant distance relative to the decay scale of α. The LCH character of the typed geographic sequence space would remain intact with a countable number of types. However, some results relating to classical limits would become much harder. At any rate, we will not examine such models in this text.

Remark

There is an item of interest for the use of this theory in the construction of scaling limits. By the proof in section 4.2.2, this PVM approaches an instrument as $\boldsymbol{V} \to \boldsymbol{I}$. This suggests that under the right scaling conditions for our model of the bound states, we obtain a particle conservative continuum representation of the medium as a limit of well defined objects.

Remark

Finally, we note that by using the V, ℓ dependent density matrix, we can express the PVM in a simpler form for $\boldsymbol{\rho} = \boldsymbol{\rho}_F^n \otimes \boldsymbol{\rho}_B^m$:

$$\mathscr{J}(E, \boldsymbol{\rho}) = \mathscr{J}_{\mathscr{A}}(E, \boldsymbol{\rho}) + \mathscr{J}_{\mathscr{D}}(E, \boldsymbol{\rho}) \tag{5.5.0.9}$$

$$\mathscr{J}_{\mathscr{A}}(E, \boldsymbol{\rho}) = \int_E \mathrm{d}^3x\, \mathrm{d}^3k \sum_{\ell \in T_d} \sum_j \rho_{j,V,\ell}(\bar{x}, \bar{k}) \boldsymbol{\rho}_{F,j}^{n-1} \otimes \boldsymbol{\rho}_B^m \otimes |\boldsymbol{e}_{a,\ell}\alpha_{x,k}\rangle \langle \boldsymbol{e}_{a,\ell}\alpha_{x,k}| \tag{5.5.0.10}$$

$$\mathscr{J}_{\mathscr{D}}(E, \boldsymbol{\rho}) = \int_E \mathrm{d}^3x\, \mathrm{d}^3k \sum_{\ell \in T_a} \sum_j \rho_{j,V,\ell}(\bar{x}, \bar{k}) \boldsymbol{\rho}_F^n \otimes |\boldsymbol{e}_{d,\ell}\alpha_{x,k}\rangle \langle \boldsymbol{e}_{d,\ell}\alpha_{x,k}| \otimes \boldsymbol{\rho}_{B,j}^{m-1} \tag{5.5.0.11}$$

Again, for neutron thermalization this will always be a single particle generated in the conjugate space. However, it can, in principle, be more than one so long as we have nice convergence properties with respect to the sum over types.

For a single particle, this reduces to

$$\mathscr{J}(E, \boldsymbol{\rho}) = \mathscr{J}_{\mathscr{A}}(E, \boldsymbol{\rho}) + \mathscr{J}_{\mathscr{D}}(E, \boldsymbol{\rho}) \tag{5.5.0.12}$$

$$\mathscr{J}_{\mathscr{A}}(E, \boldsymbol{\rho}) = \int_E \mathrm{d}^3x\, \mathrm{d}^3k \sum_{\ell \in T_d} \rho_{V,\ell}(\bar{x}, \bar{k}) |\boldsymbol{e}_{a,\ell}\alpha_{x,k}\rangle \langle \boldsymbol{e}_{a,\ell}\alpha_{x,k}| \tag{5.5.0.13}$$

$$\mathscr{J}_{\mathscr{D}}(E, \boldsymbol{\rho}) = \int_E \mathrm{d}^3x\, \mathrm{d}^3k \sum_{\ell \in T_a} \rho_{V,\ell}(\bar{x}, \bar{k}) |\boldsymbol{e}_{d,\ell}\alpha_{x,k}\rangle \langle \boldsymbol{e}_{d,\ell}\alpha_{x,k}| \tag{5.5.0.14}$$

This formula is considerably easier to imagine. There is a weighted rotation between bound and free spaces that transforms a single particle phase space distribution in one into a single particle phase space distribution in the other.

For the remainder of section 5, we will refer to the structure of these measures by calling them Reaction-Transport PMVs. However, we will only need to use the fact that they are positive map valued measures for our proofs and so we will always represent them as $\mathscr{J}$ or at most $\mathscr{J}_\ell$ when we use subsets of the typed geographic phase space that have a single type only and we wish to distinguish.

5.6 Reaction-Transport PDPs

A direct quantization of the reaction-centric Backward Chapman-Kolmogorov equation of classical neutron reaction counting theory, equation 3.3.4.13, would take the form of equation 5.1.0.1 for $\mathscr{J}$ a Reaction-Transport PMV and $\boldsymbol{S}_t$ a Collisionless Reaction-Transport Propagator. As such, we will proceed by defining an operator valued measure on a rectangular subalgebra that generates the full sample space sigma algebra

$\mathscr{X}_t$ using this formula and attempt to identify the class of quantum stochastic processes that are representable in this way.

Definition 5.6.1. *Rectangular Product Family*

The Rectangular Product Family $R \subset \mathscr{X}_t$ consists of all sets E of the product Borel form, $t_i \leq r_{i+1}$, $E = \{(x_i, p_i, \ell_i, s_i)_{i=1}^m : r_i < s_i \leq t_i, (x_i, p_i, \ell_i) \in E_i\}$ where $E_i \in \mathscr{G}$ and $m \in \mathbb{N}$.

We will refer to sets in this family as rectangular sets.

Proposition 5.6.2.

The collection of all countable unions of sets in the Rectangular Product Family forms an Algebra of sets.

Proof.

$\emptyset \in R$ since $\emptyset \in \mathscr{G}$

Given $E^1, E^2 \in R$, we need to show that $E^1 \cap E^2 \in R$. If they consist of a different number of reactions, then the intersection is empty. If they consist of the same number of reactions and the temporal boundary points r_i, t_i are identical then $E^1 \cap E^2 = \prod_i E_i^1 \cap E_i^2 \times (r_i, t_i] \in R$. If the temporal end points don't match up, we can choose a common temporal mesh refinement and apply the the same argument to produce a disjoint union of combinations of possible intersections. For example, let $E^1 = (E_1^1 \times (t_1, t_3]) \times (E_2^1 \times (t_3, t_5]) \times (E_3^1 \times (t_5, t_6])$ and $E^2 = (E_1^2 \times (t_1, t_2]) \times (E_2^2 \times (t_2, t_4]) \times (E_3^2 \times (t_4, t_6])$ Then we can define $E_1 = E_1^1 \cap E_1^2, E_2 = E_1^1 \cap E_2^2, E_3 = E_2^1 \cap E_2^2, E_4 = E_2^1 \cap E_3^2, E_5 = E_3^1 \cap E_3^2$ and we find that since three events must occur and (in order to be in both sets) an event must occur in each proscribed time interval for both sequences, some of these intersections are incompatible with the time overlap requirements. So,

$$E^1 \cap E^2 = (E_1 \times (t_1, t_2]) \times (E_3 \times (t_3, t_4]) \times (E_5 \times (t_5, t_6]) \in R \tag{5.6.0.1}$$

A similar argument can be applied to any mismatched time sequence to reduce it to either a disjoint union of sequence subintervals times intersections of Borel sets or to an empty set. Indeed, if the pair of rectangular sets is such that two intervals at the same point in the reaction sequence have no overlap then the intersection is empty. Similarly, if more than one event of one sequence is included in a single temporal region of another sequence, the result will be an empty intersection because there are no compatible sequences.

The complement of any rectangular set in X_t consists of a countable union of the other possible numbers of reaction counts. Moreover, we will show in proposition 5.7.3 that every A_t^n is measurable using a decomposition into a countable union of rectangular sets and therefore $A_t^n \in R, \forall t, n$. This allows us to represent

the complemented time intervals where there were no events by a finite disjoint union over relevant $A^n_{\Delta t}$ sets λ-composed with complemented $\mathscr{G}$-Borel sets.

We have proven that R is an elementary family, so by a standard result of basic measure theory [56], the fact that this set is closed under countable unions means that this is also an algebra. □

Remark

The fact that we have expanded this to include countable unions is not a major limitation as countable unions of measurable sets for a finite measure can be replaced by countable disjoint unions and used to expand the measure as a sum of elementary terms. This idea is how we will use the rectangular sets of product Borel form to analyze more complex events in the space of time ordered sequences in the typed geographic phase space.

Remark

Since the open sets of $\mathscr{X}_t$ are a union of sets of definite reaction count (i.e. sequence length), it generally suffices to characterize the properties of $\mathscr{X}_t$ and R working on a fixed reaction count subspace.

Remark

Recall that the topology that we defined on A^n_t is given by a product topology over n reactions. Since the product topology involves finite intersections of preimages of open sets in the individual topologies, the open sets of the product topology have the rectangular sets as a topology base. Thus, the sigma algebra generated by R includes the Borel sigma algebra generated by X_t. As such, we will generally take $\mathscr{X}_t$ to be the sigma algebra generated by R going forward.

Definition 5.6.3. *Reaction-Transport PDP*

We define a Reaction-Transport Piecewise Deterministic Process or Reaction-Transport PDP to be an Operator Valued Measure $\mathscr{E}_t$ on the rectangular product family R, such that $\forall E \in R$ and $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\mathscr{E}_t(E, \boldsymbol{\rho}) = \prod_{i=1}^{m} \int_{(r_i, t_i]} \mathrm{d}s_i \boldsymbol{S}_{t-s_m} \mathscr{J}(E_m) \boldsymbol{S}_{s_m - s_{m-1}} \mathscr{J}(E_{m-1}) \dots \mathscr{J}(E_1) \boldsymbol{S}_{s_1} \boldsymbol{\rho} \tag{5.6.0.2}$$

Here $\mathscr{J}$ is a Reaction-Transport Transition PMV on the typed geographic phase space G and $\boldsymbol{S}_t$ is a Collisionless Reaction-Transport Propagator.

Together, $\mathscr{J}$ and $\boldsymbol{S}_t$ must define a mesoscopic reaction rate through a trace compatibility constraint as in the definition 5.4.2.

In order to fully understand the motivation for this definition, we will need to construct a comparison between this definition and the classical equation 3.3.4.13. (which we reproduce here for quick reference)

$$
\begin{aligned}
Q(t_3|t_1;p) = Q_0(t_3|t_1;p) \\
&+ \int_{t_1}^{t_3} \mathrm{d}t' \int_{t_1}^{t'} \mathrm{d}t \sum_{n_3=0}^{N} \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_3 \int_{\mathscr{V}_D\times\mathscr{O}} \mathrm{d}u_2\, Q(n_3,u_3,t_3|u_2,t')Q^1_{\mathrm{s}}(u_2,t,t';p) \\
&\qquad + \int_{t_1}^{t_3} \mathrm{d}t\, FQ_{\mathrm{abs},1}(t|t_1;p) \\
&+ \sum_{n_2>0} \sum_{n_2'<n_2} \int_{[t_1,t_3]^{n_2'}} \mathrm{d}t' \int_{t_1}^{t_1'} \mathrm{d}t \sum_{n_3=0}^{N} \int_{(\mathscr{V}_D\times\mathscr{O})^{n_3}} \mathrm{d}u_3 \ldots \\
&\qquad \int_{(\mathscr{V}_D\times\mathscr{O})^{n_2'}} \mathrm{d}u_2\, Q(n_3,u_3,t_3|n_2',u_2,\bar{t'})Q^1_{\mathrm{fission}}(n_2,n_2',u_2,t,\bar{t'}|t_1;p) \qquad (5.6.0.3)
\end{aligned}
$$

First, we abstract this a little by rewriting it with a reaction type index and an operator abstraction more like equation 3.3.2.4, but interpreting the absorption and decay as a two collision term and suppressing multi-particle considerations. The operator form used here suggests a linearity that is purely illusory in the classical case. However, it makes it easier to understand the motivation for the quantum model.

$$
Q(t|t_0)p = Q_0(t|t_0)p + \sum_{\ell\in T} \int_{t_1}^{t_3} \mathrm{d}s\, Q(t_3|s)Q_\ell(s)Q_0(s|t_0)p \qquad (5.6.0.4)
$$

Second, we recognize that f_Q allows for evaluating the reaction probability for any kind of phase space constraint on a reaction volume at a fixed time. We can leverage the fact that the individual reaction types of the propagator are observable for any fixed time in this way to define a path space measure on the set of reactions. This is accomplished by subdividing the full interval into subintervals where we repeatedly apply the disjoint single reaction alternatives and take the resulting distribution to be the new classical distributional state of the system. Thus, we will take p to be the analog for a single particle $\boldsymbol{\rho}$ and focus on evaluating the probability associated to a rectangular set $\forall E \in \mathscr{R}_{t-t_0}$, where E is of the product Borel form, $t_i \leq r_{i+1}$, $E = \{(x_i,p_i,\ell_i,s_i)_{i=1}^m : r_i < s_i \leq t_i, (x_i,p_i,\ell_i) \in E_i\}$. With this kind of set in mind we define a measure over an extended interval $Q_E(t|t_0;p)$ as only measuring the subset of paths passing through a series of event state gates encoded in the rectangular set E. This same notion has been invoked in the construction of Weiner measures from finite product distributions. [56] [139] This notion has also been discussed in general path space integration theory in terms of time slicing. [80] [150]

Then we can approximate $Q_E(t|t_0;p)$ using a kind of finite iterative construction. In particular, we consider the information encoded in the set E: we know that no reaction happen prior to r_1 then $Q_E(r_1|t_1)p =$

$Q_0(r_1|t_0)p$. Taking this as the new initial state, $p_1 = Q_0(r_1|t_0)p$. Then, from the specification of E we know that a reaction of type ℓ_1 occurs in the interval $r_1 < s_1 \leq t_1$. However, all of the evolution operators except

$$\int_{r_1}^{t_1} \mathrm{d}s; Q(t_1|s)Q_{\ell_1}(s)Q_0(s|r_1)p_1$$

transform the distribution through a path space complementary to this event. Thus, the only set contributing to the measure of E can be described by

$$Q_E(t_1|t_0)p = \int_{r_1}^{t_1} \mathrm{d}s; Q(t_1|s)Q_{\ell_1}(E_1, s)Q_0(s|r_1)Q_0(r_1|t_0)p \tag{5.6.0.5}$$

where, again suppressing particle number considerations we can make the phase space integration over an interaction subdomain explicit

$$Q_\ell(E_1, s)Q_0(s|t_0)p = \int_{E_1} \mathrm{d}u_1 \; Q_{\ell_1}(u_1', u_1, s)Q_0(u_1, s|t_0)p \tag{5.6.0.6}$$

using the analysis of section 3.4, we find that the free propagator can be understood as an exponentially decaying semigroup satisfying equation 3.4.0.4,

$$Q_0(t_2|t_1) = Q^0_{(t_1 - t_2)} \tag{5.6.0.7}$$

iterating in this manner, we arrive at the equation

$$Q_E(t|t_0)p = \prod_{i=1}^{m} \int_{(r_i, t_i]} \mathrm{d}s_i Q^0_{(t-s_m)} Q_{\ell_m}(E_m, s_m) Q^0_{(s_m - s_{m-1})} Q_{\ell_{m-1}}(E_{m-1}, s_{m-1}) \dots Q_{\ell_1}(E_1, s_1) Q^0_{(s_1 - t_0)} p \tag{5.6.0.8}$$

This is a classical form that allows us to understand the single particle Quantum Reaction-Transport PDP model, given by 5.1.0.1 for a free propagator satisfying 5.4.0.2 and a reaction operator given by 5.5.0.12, as a kind of path integral quantization. It is worth noting that in both the classical and the quantum cases, attempting to obtain the non-selective propagator by summing arbitrarily over such paths will lead to meaningful divergence problems. This is sometimes called the Path Integral Representation of the Propagator and is used extensively in direct calculation of asymptotic approximations and in renormalizations of quantum field theory. [16] Although very useful for algorithmically constructing approximations by way of diagram summations [52], the infinite sum formula is not generally convergent, even in a weak sense. Thus,

although it is an interesting way to look at the physics of the problem, we will avoid it for now. We have an altogether different route for constructing more general propagators. Specifically, we will show below that any Reaction-Transport PDP model uniquely corresponds to a QSP.

5.7 The Propagators of a QSP with Bounded Reaction Rate

In order to follow through on our promise to build an extension theory for Reaction-Transport PDP models, we need to introduce some additional constraints on the class of QSPs for reaction counting. These constraints will be motivated by the physics discussed in sections 5.3, 5.4, and 5.5. Let $\mathscr{E}_t$ be a QSP on the sigma algebra $\mathscr{X}_t$ generated by the full sample space X_t(cf. definition 4.2.13). We will begin by supposing that $\mathscr{E}_t$ has a bounded reaction rate (cf. definition 5.4.1). As discussed in section 5.4, this assumption is well grounded in physical requirements of the classical theory and it dramatically reduces the complexity of the possible QSPs.

In particular, following the main sequence of lemmas from Davies' classification theory [32] we find that for an QSP with a bounded reaction rate it is possible to define a fully non-selective propagator $\boldsymbol{T}_t$ and decompose it into $\boldsymbol{S}_t$ and $t\mathscr{J}$ parts to first order in t. This idea will be developed carefully and will lead us to general definition of the class of QSPs relevant to the modeling of quantum reaction-transport systems. In this section, we are largely following the line of reasoning used by Davies in the construction of his classification theorem, but with some added interpretations and technical results.

Definition 5.7.1. *Non-Selective Propagator*

For each QSP for reaction counting on the sample space X_t, we can define a positive operator family $\boldsymbol{T}_t : \mathscr{T}_+(\mathscr{H}) \to \mathscr{T}_+(\mathscr{H})$ by the formula, $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\boldsymbol{T}_t\boldsymbol{\rho} = \mathscr{E}_t(X_t, \boldsymbol{\rho}) \tag{5.7.0.1}$$

By the composition law for QSPs for reaction counting $\lambda(X_t, X_s) = X_{t+s}$ and

$$\boldsymbol{T}_{t+s}\boldsymbol{\rho} = \mathscr{E}_{t+s}(\lambda(X_t, X_s), \boldsymbol{\rho}) = \mathscr{E}_t(X_t, \mathscr{E}_s(X_s, \boldsymbol{\rho})) = \boldsymbol{T}_t\boldsymbol{T}_s\boldsymbol{\rho} \tag{5.7.0.2}$$

By the strong continuity of $\mathscr{E}_t$ and trace conservation of $\mathscr{E}(X_t, \cdot)$,

$$\lim_{t\to 0} \|\boldsymbol{T}_t\boldsymbol{\rho} - \boldsymbol{\rho}\|_{\mathrm{Tr}} = 0 \tag{5.7.0.3}$$

Thus, it follows that $\boldsymbol{T}_t$ is a strongly continuous semigroup on $\mathscr{T}(\mathscr{H})$.

This semigroup defines a mixing evolution (some pure states are transformed to mixed states) that incorporates contributions from all possible numbers of jumps in the given interval. By evaluating the QSP on the set of all possible sequences of jumps in the interval, this semigroup corresponds to a maximally non-selective evolution. Recalling the definition of a quantum stochastic process, this is the evolution that is required to be trace preserving. Moreover, by the positivity and strong countable additivity of $\mathscr{E}_t(\cdot, \boldsymbol{\rho})$, we have that $\forall E \in \mathscr{X}_t$, $\exists (E_n)_{n=1}^{\infty}$ each consisting of sets with a fixed number of reactions n, such that $E = \cup_n E_n$ and

$$\mathscr{E}_t(\cup_{n=1}^{\infty} E_n, \boldsymbol{\rho}) = \lim_{N\to\infty} \sum_{n=1}^{N} \mathscr{E}_t(E_n, \boldsymbol{\rho}) \tag{5.7.0.4}$$

Where the limit converges in the trace norm for each $\boldsymbol{\rho}$ and so the sum of positive terms has a uniform trace bound

$$\lim_{N\to\infty} \sum_{n=1}^{N} \mathrm{Tr}\left[\mathscr{E}_t(E_n, \boldsymbol{\rho})\right] \leq \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.7.0.5}$$

This allows us to apply the bounded reaction rate to each term of our decomposition of the space of possible reaction event sequences. It follows that any reaction count based decomposition that we can construct for $\boldsymbol{T}_t$ automatically has nice convergence properties. We will use this fact to prove that $\boldsymbol{S}_t$ and $\mathscr{J}$ are well-defined mathematical objects for any QSP with a bounded reaction rate. We will now describe some of the sets used in Davies to prove a sharper bound on multiple reaction sets.

Definition 5.7.2. A_t^n

A_t^n is the set of points in X_t with exactly n reactions in the time interval $(0, t]$.

Proposition 5.7.3.

A_t^n is a measurable set for any sigma algebra $\mathscr{X}_t$ that extends the Borel sigma algebra for the topology on the sample space given in section 4.2.3.

Proof.

In the disjoint union topology over reaction number introduced in section 4.2.3, it is clear that A_t^n is the intersection of the open subset of the larger product space containing exactly n reactions with the subspace $\tilde{X}_t$. Therefore, in the relative topology, A_t^n is an open set and so it is measurable. □

There is another more interesting proof that illustrates a decomposition idea that we will use repeatedly.

Proof.

$A_t^0 = \{z\}$ and $A_t^1 = G \times T \times [0,t]$ are obvious enough. For $n > 1$, we proceed as in analogy to the construction in the sample space LCH proof. For every m we can define a partition of t into m half closed intervals of length t/m. Then, we can let F_m^n be the collection of all subsets $a \in \mathscr{P}(\{1,\ldots,m\})$ such that $|a| = n$. Every, $a \in F_m^n$ can be thought of as a representation of an indicator function on the set of intervals in our partition. For every such a, there is a valid allocation of n reactions into the set of m subintervals. Then let $E_{a,r} = z(1-\chi_{a}(r)) + A^1_{t/m}\chi_{a}(r)$ defines a function on the index set mapping to an element in $\mathscr{X}_{t/m}$, using this and the λ sample space set composition map (extended to an arbitrary finite number of sets), we can define a decomposition of A_t^n

$$A_t^n = \bigcup_{m=n}^{\infty} \bigcup_{a \in F_m^n} \lambda(E_{a,1}, E_{a,2}, \ldots, E_{a,m}) \tag{5.7.0.6}$$

The equality holds because by the isolation of reaction events, every element of A_t^n must be in one of the compositions for some m, while conversely every element of the union is isolated and includes exactly n reaction events. This is clearly a measurable set for any sigma algebra that extends the Borel sigma algebra for the topology on the sample space given in section 4.2.3. Indeed, one can see this for each element of the double union in the product topology since the half open intervals in time are Borel sets in time whereas the rest of the products are copies of z or $A^1_{t/m}$. □

Definition 5.7.4. B_t^n

B_t^n is the set of points in X_t with n or more reactions in the time interval $(0,t]$.

$$B_t^n = \bigcup_{i=n}^{\infty} A_t^i \tag{5.7.0.7}$$

Proposition 5.7.5.

B_t^n is a measurable set. Specifically,

$$B_t^n = \bigcup_{m=n}^{\infty} \bigcup_{a \in F_m^n} \lambda(C_{a,1} \times C_{a,2} \times \cdots \times C_{a,m}) = \bigcup_{m=n}^{\infty} D_{t,m}^n \tag{5.7.0.8}$$

where $C_{a,r} = X_{t/m}(1-\chi_{a}(r)) + B^1_{t/m}\chi_{a}(r)$ and

$$D_{t,m}^n = \bigcup_{a \in F_m^n} \lambda(C_{a,1} \times C_{a,2} \times \cdots \times C_{a,m}) \tag{5.7.0.9}$$

Moreover $\forall \mu_{\rho,A}$ *such that* $\mu_{\rho,A}(E) = \mathrm{Tr}\left[\boldsymbol{A}\mathscr{E}(E,\boldsymbol{\rho})\right]$*, then as* $m \to \infty$

$$\chi_{D^n_{t,m}} \nearrow \chi_{B^n_t} \tag{5.7.0.10}$$

holds $\mu_{\rho,A}$ *almost surely.*

Proof.

This can be proven in a manner similar to the argument for the representation A^n_t but using $X_{t/m}$ copies instead of z. The last convergence result follows directly from the properties of finite measures of infinite unions of increasing sets. □

We can use the set decompositions described above, in conjunction with the simplicity of the individual $D^n_{t,m}$ and the integral representation of PMV measures (cf. definition 2.3.14) to prove sharper bounds on the contribution of terms with n or more jumps.

Proposition 5.7.6. *Trace Bounding of n-Reaction Events*

Every Bounded Reaction Rate QSP $\mathscr{E}_t$ *satisfies an exponential bound controlled by the minimum number of reaction events in a measurable set. Specifically,*

$$\mathrm{Tr}\left[\mathscr{E}(B^n_t,\boldsymbol{\rho})\right] \leq \frac{K^n t^n \mathrm{Tr}\left[\boldsymbol{\rho}\right]}{n!} \tag{5.7.0.11}$$

Proof.

Using the integral representation of PMV measures we have $\forall E \in \mathscr{X}_t$

$$\mathrm{Tr}\left[\mathscr{E}_t(E,\boldsymbol{\rho})\right] = \mathrm{Tr}\left[\overline{\mathscr{E}}_t(\chi_{_E},\boldsymbol{\rho})\right] = \int_{X_t} \chi_{_E}(\omega)\mathrm{dTr}\left[\mathscr{E}_t(\omega,\boldsymbol{\rho})\right] \tag{5.7.0.12}$$

Then we can apply proposition 5.7.5 and Fatou for $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$ to obtain

$$\mathrm{Tr}\left[\mathscr{E}_t(B^n_t,\boldsymbol{\rho})\right] = \int_{X_t} \lim_{m\to\infty} \chi_{D^n_{t,m}}(\omega)\mathrm{dTr}\left[\mathscr{E}_t(\omega,\boldsymbol{\rho})\right] \leq \lim_{m\to\infty} \mathrm{Tr}\left[\mathscr{E}_t(D^n_{t,m},\boldsymbol{\rho})\right] \tag{5.7.0.13}$$

Therefore it suffices to obtain a bound on $\mathrm{Tr}\left[\mathscr{E}_t(D^n_{t,m},\boldsymbol{\rho})\right]$, which is relatively simple due to its explicit product form and the union over different allocations of n. Indeed, consider any fixed $a \in F^n_m$ Then by the

markov type property for QSP composition and the bounded reaction rate applied to $B_t^1 = X_t/\{z\}$

$$\begin{aligned}\mathrm{Tr}\left[\mathscr{E}_t(\lambda(C_{a,1}\times\cdots\times C_{a,m}),\boldsymbol{\rho})\right] &= \mathrm{Tr}\left[\mathscr{E}_{t/m}(C_{a,m},\mathscr{E}_{t(m-1)/m}(\lambda(C_{a,1}\times\cdots\times C_{a,m-1}),\boldsymbol{\rho}))\right]\\ &\leq (1(1-\chi_{_a}(m))+K\frac{t}{m}\chi_{_a}(m))\mathrm{Tr}\left[\mathscr{E}_{t(m-1)/m}(\lambda(C_{a,1}\times\cdots\times C_{a,m-1}),\boldsymbol{\rho})\right]\end{aligned}$$

arguing inductively and using the fact that regardless of the particular choice of a there are exactly n terms with $\chi_{_a}(r)=1$, we obtain

$$\mathrm{Tr}\left[\mathscr{E}_t(\lambda(C_{a,1}\times\cdots\times C_{a,m}),\boldsymbol{\rho})\right]\leq\left(\frac{Kt}{m}\right)^n\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.7.0.14}$$

Since there are m choose n vectors in F_m^n, $|F_m^n| = m!/((m-n)!n!)$. Thus, using subadditivity over the union with disregard for any overlap, we obtain the upper bound,

$$\mathrm{Tr}\left[\mathscr{E}_t(D_{t,m}^n,\boldsymbol{\rho})\right]\leq\frac{m!(Kt)^n}{m^n(m-n)!n!}\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.7.0.15}$$

Now it suffices to control this function as $m\to\infty$. But indeed,

$$\begin{aligned}(m-n)!m^n &= (m-n)!\times((m-n+1)+(n-1))\times((m-n+2)+(n-2))\times\cdots\times(m+0)\\ &= (m-n)!\times\prod_{j=1}^{n}(m-n+j)\times(1+\frac{(n-2)}{(m-n+2)})\times\cdots\times 1\\ &= m!+\mathscr{O}\left((m-1)!\right)\end{aligned}$$

it follows that $m!/((m-n)!m^n)\to 1$ and so our conclusion is obtained. □

This is a powerful conclusion and facilitates the construction of a reaction event infinitesimal generator. Indeed, summing over all possible reaction counts provide an exponential upper bound to the growth rate of the trace in time.

$$\sum_{n=1}^{\infty}\mathrm{Tr}\left[\mathscr{E}(B_t^n,\boldsymbol{\rho})\right]\leq e^{Kt}\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.7.0.16}$$

This implies a very strong kind of trace convergent control over the total reaction count in any finite interval. A similar proof gives us that collisionless operators $\boldsymbol{S}_t\boldsymbol{\rho}=\mathscr{E}_t(z,\boldsymbol{\rho})$ have an exponentially decaying lower bound.

Proposition 5.7.7. $\boldsymbol{S}_t$ *are Bounded Below*

If $\boldsymbol{S}_t\boldsymbol{\rho} = \mathscr{E}_t(z, \boldsymbol{\rho})$ *for* $\mathscr{E}_t$ *a QSP with bounded reaction rate, then*

$$\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] \geq e^{-Kt}\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.7.0.17}$$

Proof.

Indeed, as per the usual measurable set decomposition argument for finite positive measures

$$\mathrm{Tr}\left[\mathscr{E}_t(X_t, \boldsymbol{\rho}) - \mathscr{E}_t(z, \boldsymbol{\rho})\right] = \mathrm{Tr}\left[\mathscr{E}_t(X_t/\{z\}, \boldsymbol{\rho})\right] \leq Kt\mathrm{Tr}\left[\boldsymbol{\rho}\right]$$

thus since $\mathrm{Tr}\left[\mathscr{E}(X_t, \boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right]$,

$$\mathrm{Tr}\left[\mathscr{E}_t(z, \boldsymbol{\rho})\right] \geq (1 - Kt)\mathrm{Tr}\left[\boldsymbol{\rho}\right]$$

by iterating in this manner using the fact that $z_t \in X_t$ satisfies $z_t = \lambda(z_{t/m}, \ldots, z_{t/m})$ and the composition factorization argument from the previous proof, we obtain the result

$$\left(1 - \frac{Kt}{m}\right)^m \mathrm{Tr}\left[\boldsymbol{\rho}\right] \leq \mathrm{Tr}\left[\mathscr{E}_t(z, \boldsymbol{\rho})\right] \tag{5.7.0.18}$$

and the result follows as $m \to \infty$ □

Using the fact that $\boldsymbol{S}_t$ is trace bounded below by a quantity growing to $\mathrm{Tr}\left[\boldsymbol{\rho}\right]$ as $t \to 0$, and that it is also bounded above by $\mathrm{Tr}\left[\boldsymbol{\rho}\right]$, we can easily prove that $\boldsymbol{S}_t$ is a strongly continuous semi-group on the trace class operators.

Proposition 5.7.8. $\boldsymbol{S}_t$ *are Strongly Continuous Semigroups*

If $\boldsymbol{S}_t\boldsymbol{\rho} = \mathscr{E}_t(z, \boldsymbol{\rho})$ *for* $\mathscr{E}_t$ *a QSP with bounded reaction rate, then*

$$\lim_{t \to 0} \left\|\boldsymbol{S}_t\boldsymbol{\rho} - \boldsymbol{\rho}\right\|_{\mathrm{Tr}} = 0 \tag{5.7.0.19}$$

and $\boldsymbol{S}_{t+s}\boldsymbol{\rho} = \boldsymbol{S}_s\boldsymbol{S}_t\boldsymbol{\rho}$

By this result, we know the every QSP with a bounded reaction rate has a collisionless propagator $\boldsymbol{S}_t$ that is a strongly continuous semigroup. At this point, we will further assume that $\boldsymbol{S}_t$ has the required purity and subspace preserving structure to be a Collisionless Reaction Transport Propagator. Building on this, we will prove that any QSP with a bounded reaction rate and a Collisionless Reaction Transport Propagator

for the zero event propagator has a well defined single event PMV measure. This fact is instrumental in constructing a useful definition of a Reaction-Transport QSP.

5.8 The Single Reaction PMV of a QSP with Bounded Reaction Rate and Collisionless Reaction Transport Propagator

We will now outline the main arguments that lead to the definition of a single reaction PMV measure for a QSP. We continue to follow Davies' system of definitions and proofs for the classification of QSPs for measurement of quantum fields, but with some added interpretations and technical details. [32] We begin by introducing a finite duration version of the reaction generator PMV measure.

Definition 5.8.1. *Finite-Duration Single-Reaction PMV*

For any set $E_t \in \mathscr{X}_t$ such that $E_t \subset A_t^1 = \{(x,p,\ell,t_1) \in \mathscr{V}_D \times \mathscr{O} \times T \times [0,t]\}$, let $\Pi_G : A_t^1 \to G$ be the projection of a single reaction event set onto the typed geographic phase space $G = \mathscr{V}_D \times \mathscr{O} \times T$ by $\Pi_G((x,p,\ell,t_1)) = (x,p,\ell)$. Then, for any set $E \subset G$ we can define the single particle pre-image in A_t^1 as $\Pi_G^{-1}(E) = \{(x,p,\ell,t_1) : (x,p,\ell) \in E, t_1 \in (0,t]\}$

We define the Finite-Duration Single-Reaction PMV measure on the Borel sigma algebra $\mathscr{G}$ of the typed geographic phase space G as,

$$\mathscr{J}_t(E,\cdot) = \frac{1}{t}\mathscr{E}_t(\Pi_G^{-1}(E),\cdot), \forall E \subset G \text{ s.t.} E \in \mathscr{G} \tag{5.8.0.1}$$

For any bounded reaction rate QSP, the Finite-Duration Single-Reaction PMV is a trace continuous, positive map valued measure. Indeed, by the bounded reaction rate and the fact that $\mathscr{J}_t(G,\boldsymbol{\rho}) = t^{-1}\mathscr{E}_t(A_t^1,\boldsymbol{\rho})$ and $A_t^1 \subset B_t^1 = X_t/\{z\}$, we have

$$0 \leq \mathrm{Tr}\left[\mathscr{J}_t(G,\boldsymbol{\rho})\right] \leq \frac{1}{t}\mathrm{Tr}\left[\mathscr{E}_t(B_t^1,\boldsymbol{\rho})\right] \leq K\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.8.0.2}$$

while the countable additivity flows directly from that of $\mathscr{E}_t$.

We recall that the construction of the Chapman-Kolmogorov equation was formulated in terms of integrals over a phase space copy corresponding to an intermediate system state. QSPs seem like an incongruous tool for representing such a structure. Indeed, prior to this section, it didn't even seem like we could make use of the compactness that we have forced on the typed geographic phase space since the sample space we constructed based off of it was merely LCH. The Finite-Duration Single-Reaction PMV brings us a step

closer to the classical world we seemed to have left behind when constructing QSPs. Here we have a measure (albeit an operator valued one) defined on the geographic phase space. The possibility of constructing such a unique measure on just the typed geographic phase space (i.e. without any kind of time order structure) stems from the fact that a single reaction subspace has no special time-ordering properties. This is precisely what makes it an ideal building block for decomposing QSPs.

We can identify our next step in one of two different ways. Reasoning analytically, we can note that there is an explicit time dependence on the interval analogous to the time dependence inherent in a finite difference formula. In order to choose a building block that is scale independent, it would be nice to eliminate this time dependence by taking the limit as $t \to 0$ much as we would when constructing a derivative. Physically, we can recognize that for any finite interval subset $E_t \subset A_t^1$ can have temporal correlations that are lost under projection followed by pre-image. Thus, this is not a good model for measurable structures over any finite interval. However, the information lost in a finite energy system gets smaller and smaller as this time window goes to zero (confer the Heisenberg uncertainty principle of time-energy form). Thus, if we want a physically reliable representation, it makes sense to try to find the limiting PMV measure and use that to construct approximations.

Before we address the problem of existence for limiting measures, we are going to show that the finite-duration single-reaction PMV is precisely the kind of infinitesimal generator of jumps that we have argued it to be heuristically.

Proposition 5.8.2. *Non-selective Propagators Decompositions*

The non-selective propagator for a bounded reaction rate QSP can be expanded in powers of t, such that the zeroth order term is a Collisionless Propagator and the first order term is the finite-duration single-reaction PMV with a residual error bounded by terms of second order in t. Specifically, asymptotically in t,

$$\boldsymbol{T}_t\boldsymbol{\rho} = \boldsymbol{S}_t\boldsymbol{\rho} + t\,\mathscr{J}_t(G, \boldsymbol{\rho}) + \mathscr{O}(t^2) \tag{5.8.0.3}$$

Proof.

We begin by noting a simple decomposition in measurable sets:

$$\boldsymbol{T}_t(\boldsymbol{\rho}) = \mathscr{E}_t(X_t, \boldsymbol{\rho}) = \mathscr{E}_t(z \cup B_t^1, \boldsymbol{\rho}) = \mathscr{E}_t(z, \boldsymbol{\rho}) + \mathscr{E}(\bigcup_{i=1}^{\infty} A_t^i, \boldsymbol{\rho}) = \boldsymbol{S}_t\boldsymbol{\rho} + \mathscr{E}_t(A_t^1, \boldsymbol{\rho}) + \mathscr{E}_t(B_t^2, \boldsymbol{\rho}) \tag{5.8.0.4}$$

then using the definition of the finite-duration single-reaction PMV, we find

$$\boldsymbol{T}_t(\boldsymbol{\rho}) = \boldsymbol{S}_t\boldsymbol{\rho} + t\,\mathscr{J}_t(G,\boldsymbol{\rho}) + \mathscr{E}_t(B_t^2,\boldsymbol{\rho}) \tag{5.8.0.5}$$

However, we know that these are all positive operators and $\mathscr{E}_t(B_t^2,\boldsymbol{\rho})$ has a trace norm bound by proposition 5.7.6

$$\mathrm{Tr}\left[\mathscr{E}_t(B_t^2,\boldsymbol{\rho})\right] \leq \frac{K^2}{2}\mathrm{Tr}\left[\boldsymbol{\rho}\right]t^2$$

Since this is a trace class operator that is positive and has trace converging to zero as $t \to 0$ the dyadic sequence of decreasing time durations converges to a positive trace class operator with only zero eigenvalues (i.e. the zero operator) as t^2. This is precisely the substance of the claim. □

This asymptotic expansion provides both the interpretation we asserted and facilitates a technical proof of the existence of a limiting operator. The general idea here is that a derivative is defined by first order terms in the expansion parameter. As such, we can reorganize the expansion into "time differentiable functions" on one side and $t\,\mathscr{J}_t$ on the other (plus some second order or higher terms. It follows from the validity of the equality for every finite t that there is a limiting $\mathscr{J}$. This kind of proof of differentiability is pretty common in classical analysis. Here we have a variety of non-commutative technicalities to contend with, but the spirit of the proof remains the same. Before proceeding we will introduce a lemma that resolves the aforementioned technicalities.

Definition 5.8.3. *Strongly Continuous Semigroup Generators and Domains*

Let $\boldsymbol{Z}_t$ be a strongly continuous semigroup of operators from a Banach Space $\mathscr{T}(\mathscr{H})$ into itself. Then the Domain $D(\boldsymbol{W}) \subset \mathscr{T}(\mathscr{H})$ of its generator $\boldsymbol{W}$ is the set of elements of the Banach Space for which the following limit is defined

$$\boldsymbol{W}\boldsymbol{\rho} = \lim_{t\to 0}\frac{\boldsymbol{Z}_t\boldsymbol{\rho} - \boldsymbol{\rho}}{t} \tag{5.8.0.6}$$

and convergence of the limit in the strong topology (i.e. the trace norm for each $\boldsymbol{\rho} \in D(\boldsymbol{W})$)

Lemma 5.8.4. *WOT Convergent sequences belong to the Generator Domain*

$\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$ and all $\forall \boldsymbol{S}_t$ Collisionless Reaction Transport Propagator with generator $\boldsymbol{W}$, If $\exists (t_n)_{n\in\mathbb{N}}$ such that $t_n \to 0$, and

$$\frac{\boldsymbol{S}_{t_n}\boldsymbol{\rho} - \boldsymbol{\rho}}{t_n} \to \boldsymbol{\rho}' \in \mathscr{T}_+(\mathscr{H}) \tag{5.8.0.7}$$

converging in the Weak Operator Topology, Then $\boldsymbol{\rho} \in D(\boldsymbol{W})$

Remark

This is not in general obvious and the proof here relies on the particular purity preserving from of the Collisionless Reaction Transport Propagator $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$.

A full proof of this technical result appears in [32] as Lemma 3.1 p.73 and there is nothing materially to add to it other than to remark that it only depends on the form of $\boldsymbol{S}_t$.

Lemma 5.8.5. *Equality of Generator Domains and Trace Norm Convergence of $\mathscr{J}_t$*

For every bounded reaction rate QSP $\mathscr{E}_t$ with a Collisionless Reaction Transport Propagator $\boldsymbol{S}_t$ having a densely defined generator $\boldsymbol{W}$, and a non-selective propagator $\boldsymbol{T}_t$ having a densely defined generator $\boldsymbol{Z}$, we have the following:

(1) $D(\boldsymbol{Z}) = D(\boldsymbol{W})$

(2) $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H}), \exists \boldsymbol{\rho}' \in \mathscr{T}_+(\mathscr{H})$ *such that* $\lim_{t\to 0} \| \mathscr{J}_t(G, \boldsymbol{\rho}) - \boldsymbol{\rho}' \|_{\mathrm{Tr}} = 0$

Proof.

This follows from the previous lemma using the fact that any sequence $\mathscr{J}_{t_n}(G, \boldsymbol{\rho})$ is uniformly bounded and so by the equivalence of the weak and ultra weak topologies on operator norm bounded sets, and the weak* compactness of the unit ball in the ultra weak topology by Alaoglu, there is a convergent subsequence in the weak operator topology. Then using the relation

$$\frac{\boldsymbol{T}_{t_n}\boldsymbol{\rho} - \boldsymbol{\rho}}{t_n} - \frac{\boldsymbol{S}_{t_n}\boldsymbol{\rho} - \boldsymbol{\rho}}{t_n} = \mathscr{J}_{t_n}(G, \boldsymbol{\rho}) + \mathscr{O}(t)$$

and the previous lemma, any such sequence is also convergent in the trace norm. (extending from the common domain of definition of the generators by density) □

From these properties, we can establish that $\mathscr{J}_t$ converges to a PMV measure as $t \to 0$.

Proposition 5.8.6. *Existence and Uniqueness of $\mathscr{J}$*

For every bounded reaction rate QSP $\mathscr{E}_t$ with a Collisionless Reaction Transport Propagator $\boldsymbol{S}_t$ such that the Finite-Duration Single-Reaction PMV has a trace that is absolutely continuous with respect to a product Lebesgue measure on the typed geographic phase space (with a sum over types), $\exists (t_n = 2^{-m_n}), m_n \to \infty$ and $\exists \mathscr{J}$ a unique PMV measure, such that in the integral representation form of a PMV measure as a positive bilinear map $\mathscr{J} : C(G, \mathbb{R}) \times \mathscr{T}_+(\mathscr{H}) \to \mathscr{T}_+(\mathscr{H})$ converges as $\forall \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H}), f \in C(G, \mathbb{R})$

$$\| \mathscr{J}(f, \boldsymbol{\rho}) - \mathscr{J}_{t_n}(f, \boldsymbol{\rho}) \|_{\mathrm{Tr}} \to 0 \tag{5.8.0.8}$$

$\mathrm{Tr}\left[\mathscr{J}(G,\boldsymbol{\rho})\right]$ *being a positive linear functional on* $\mathscr{T}(\mathscr{H})$, $\exists \boldsymbol{R} \in L_+(\mathscr{H})$ *such that*

$$\mathrm{Tr}\left[\mathscr{J}(G,\boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{\rho}\right] \tag{5.8.0.9}$$

We call this positive linear operator "the total reaction rate".

Proof.

Again by compactness in the weak operator topology, the limit $\mathscr{J}$ exists. Specifically, we begin by choosing a countable dense subset $\{f_k\} \subset C(G,\mathbb{R})$ (which can be obtained using Stone-Weierstrass on the algebra of products of rational coordinate and variance gaussians on the position and momentum subspaces respectively and doing this for each type of reaction). Then we choose a countable dense subset $\{\boldsymbol{\rho}_k\} \subset \mathscr{T}(\mathscr{H})$ using the separability of $\mathscr{H}$ and the density of the finite rank operators belonging to $D(\boldsymbol{W})$. Then, we find that we can choose the (t_n) sequence uniformly for any finite collection of pairs $\{(f_k,\boldsymbol{\rho}_k)\}$ by obtaining a cluster point $\mathscr{J}(f_k,\boldsymbol{\rho}_k)$ for each weakly convergent sub sequence $\mathscr{J}_{t_n}(f_k,\boldsymbol{\rho}_k)$. Next we bound the trace norm of the bilinear function by

$$\left\|\mathscr{J}_{t_n}(f_k,\boldsymbol{\rho}_k)\right\|_{\mathrm{Tr}} \leq \|f\|_{\sup}\left\|\mathscr{J}_t(G,\boldsymbol{\rho}_k)\right\|_{\mathrm{Tr}} \tag{5.8.0.10}$$

to extend the convergence from any finite subset to the full countable dense subset $\{(f_k,\boldsymbol{\rho}_k)\} \subset C(G,\mathbb{R}) \times \mathscr{T}(\mathscr{H})$ for a single choice of dyadic subsequence. If this were not possible, then we could contradict the uniform t convergence bounding argument from lemma 5.8.5 on the domain of the generators.

Using the lemma 5.8.5, we can prove that $\mathrm{Tr}\left[\mathscr{J}(f,\boldsymbol{\rho}) - \mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] \to 0$ for all $f,\boldsymbol{\rho}$. Specifically, every symmetric trace class operator and every continuous function has a decomposition into positive and negative parts. Thus, by the linearity of the trace, it suffices to prove the desired equality for f and $\boldsymbol{\rho}$ both positive. If this is so, by compactness of G, $\exists c > 0$ such that $0 \leq f \leq c1$. We begin by noting that by Riesz-Kakutani

$$\mathrm{Tr}\left[\mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] = \int_G f(g)\mathrm{d}\mu_{t_n,\boldsymbol{\rho}}(g) \tag{5.8.0.11}$$

$$\mu_{t_n,\boldsymbol{\rho}}(E) = \mathrm{Tr}\left[\mathscr{J}_{t_n}(E,\boldsymbol{\rho})\right] \tag{5.8.0.12}$$

with μ a radon measure. Then by Radon-Nikodym applied by the assumption of absolute continuity with respect to the product Lebesgue measure on the geographic phase space,

$$\mathrm{Tr}\left[\mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] = \int_G f(g)\frac{\mathrm{d}\mu_{t_n,\boldsymbol{\rho}}}{\mathrm{d}g}\mathrm{d}g \tag{5.8.0.13}$$

and since the measure and the functions are both positive, Fatou applies and we have

$$\int_G \liminf_{n\to\infty} f(g)\frac{\mathrm{d}\mu_{t_n,\boldsymbol{\rho}}}{\mathrm{d}g}\mathrm{d}g \leq \liminf_{n\to\infty}\int_G f(g)\frac{\mathrm{d}\mu_{t_n,\boldsymbol{\rho}}}{\mathrm{d}g}\mathrm{d}g \tag{5.8.0.14}$$

and so using the trace convergence of lemma 5.8.5 to make the left hand side of the above inequality converge to $\mathscr{J}$, we have

$$\mathrm{Tr}\left[\mathscr{J}(f,\boldsymbol{\rho})\right] \leq \liminf_{n\to\infty}\mathrm{Tr}\left[\mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] \leq K\mathrm{Tr}\left[\boldsymbol{\rho}\right]\|f\|_u < \infty \tag{5.8.0.15}$$

Then, we can use a value trapping argument to prove the equality of the traces,

$$\begin{aligned}
\mathrm{Tr}\left[\mathscr{J}(c1,\boldsymbol{\rho})\right] &= \mathrm{Tr}\left[\mathscr{J}(c1-f,\boldsymbol{\rho})\right] + \mathrm{Tr}\left[\mathscr{J}(f,\boldsymbol{\rho})\right] \\
&\leq \liminf_{n\to\infty}\mathrm{Tr}\left[\mathscr{J}_{t_n}(c1-f,\boldsymbol{\rho})\right] + \liminf_{n\to\infty}\mathrm{Tr}\left[\mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] \\
&\leq \liminf_{n\to\infty}\mathrm{Tr}\left[\mathscr{J}_{t_n}(1c,\boldsymbol{\rho})\right] \\
&= \mathrm{Tr}\left[\mathscr{J}(1c,\boldsymbol{\rho})\right]
\end{aligned}$$

The last equality follows directly from reinterpreting the integral form and using lemma 5.8.5. Now we note that in the above sequence of bounds, we have established,

$$\liminf_{n\to\infty}\mathrm{Tr}\left[\mathscr{J}_{t_n}(c1-f,\boldsymbol{\rho})\right] + \liminf_{n\to\infty}\mathrm{Tr}\left[\mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] = \mathrm{Tr}\left[\mathscr{J}(c1-f,\boldsymbol{\rho})\right] + \mathrm{Tr}\left[\mathscr{J}(f,\boldsymbol{\rho})\right] \tag{5.8.0.16}$$

however both terms are positive and satisfy 5.8.0.15 so if either of the two terms in the LHS sum is strictly less than the RHS partner term, the whole formula would fail. Thus we conclude that $\mathrm{Tr}\left[\mathscr{J}(f,\boldsymbol{\rho}) - \mathscr{J}_{t_n}(f,\boldsymbol{\rho})\right] \to 0$ for all $f, \boldsymbol{\rho}$. The result then follows from a standard result for convergence of sequences uniformly bounded in trace norm. □

Remark

This proof differs from the one presented for the analogous result in Davies. Here we remove the metrisability constraint on the geographic phase space and replace it with the arguments relating to the specific topology. We also arrive at the lim inf bound by relying on the absolute continuity of $\mathrm{Tr}\left[\mathscr{J}_{t_n}\right]$. This is entirely reasonable given the kind of spatially distributed measurements that we wish to introduce in the general model and the fact that we intend to obtain point reactions as a scaling limit. It also gets around the metrisability constraint and allows us to use a weaker topology.

Proposition 5.8.7.

Every bounded reaction rate QSP $\mathscr{E}_t$ with a Collisionless Reaction Transport Propagator $\boldsymbol{S}_t$, has a total reaction rate operator $\boldsymbol{R}$ that satisfies the consistency requirements for a mesoscopic reaction rate.

Proof.

If $\boldsymbol{S}_t$ is a Collisionless Reaction Transport Propagator, then $\exists \boldsymbol{B}_t$ a strongly continuous semigroup on $\mathscr{H}$ with a densely defined generator $\boldsymbol{Y}$ such that $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$. So, if $|\psi\rangle \in D(\boldsymbol{Y}) \subset \mathscr{H}$, then

$$\begin{aligned}\lim_{t\to 0} t^{-1}(\boldsymbol{S}_t |\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|) &= \lim_{t\to 0} t^{-1}(|\boldsymbol{B}_t\psi\rangle\langle\boldsymbol{B}_t\psi| - |\psi\rangle\langle\psi| + |\boldsymbol{B}_t\psi\rangle\langle\psi| - |\boldsymbol{B}_t\psi\rangle\langle\psi|)\\ &= \lim_{t\to 0} t^{-1}(|\boldsymbol{B}_t\psi\rangle\langle\boldsymbol{B}_t\psi| - |\boldsymbol{B}_t\psi\rangle\langle\psi|) + \lim_{t\to 0} t^{-1}(|\boldsymbol{B}_t\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|)\\ &= |\boldsymbol{Y}\psi\rangle\langle\psi| + |\psi\rangle\langle\boldsymbol{Y}\psi|\end{aligned}$$

which proves that $|\psi\rangle\langle\psi| \in D(\boldsymbol{W})$ where $\boldsymbol{W}$ is the Generator of $\boldsymbol{S}_t$ as a strongly continuous semigroup on $\mathscr{T}(\mathscr{H})$.

With this fact in hand, we can apply the approximation method of the lemma 5.8.5, we have

$$\lim_{t\to 0} \mathrm{Tr}\left[\frac{\boldsymbol{S}_t |\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|}{t}\right] = \lim_{t\to 0} \mathrm{Tr}\left[\frac{\boldsymbol{T}_t |\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|}{t}\right] - \lim_{t\to 0} \mathrm{Tr}\left[\mathscr{J}_t(G, |\psi\rangle\langle\psi|)\right] \tag{5.8.0.17}$$

and since $\mathrm{Tr}\left[\boldsymbol{T}_t\boldsymbol{\rho} - \boldsymbol{\rho}\right] = 0$ for all states, it follows from the above calculation and the trace convergence of $\mathscr{J}_t \to \mathscr{J}$ that

$$\mathrm{Tr}\left[|\boldsymbol{Y}\psi\rangle\langle\psi| + |\psi\rangle\langle\boldsymbol{Y}\psi|\right] + \mathrm{Tr}\left[\mathscr{J}(G, |\psi\rangle\langle\psi|)\right] = 0 \tag{5.8.0.18}$$

Therefore, we have our conclusion $\forall \boldsymbol{\rho} \in \mathrm{span}(\{|\psi\rangle\langle\psi| : |\psi\rangle \in D(\boldsymbol{Y})\})$ but by the dense domain of $D(\boldsymbol{Y}) \subset \mathscr{H}$ and the spectral representation which gives all states as a convex combination of pure states converging in trace norm, we have that the conclusion holds on a dense subset of states. We extend to the closure by using a trace continuous integral form of the mesoscopic reaction rate formula, which is obtained by viewing formula 5.8.0.17 as a differentiable function of time and replacing $|\psi\rangle\langle\psi|$ with $\boldsymbol{S}_s\left(|\langle\rangle\langle(|\,\psi)\right)$

$$\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] - \mathrm{Tr}\left[\boldsymbol{\rho}\right] = -\int_0^t \mathrm{d}s\ \mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{S}_s\boldsymbol{\rho}\right] \tag{5.8.0.19}$$

□

Remark

By the Lebesgue differentiation theorem, we can obtain a second form of the mesoscopic reaction rate formula that motivated the definition

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] = -\mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{S}_t\boldsymbol{\rho}\right] \tag{5.8.0.20}$$

This lemma fundamentally asserts that bounded reaction rate QSP with $\boldsymbol{S}_t$ a Collisionless Reaction Transport Propagator automatically has a well-defined mesoscopic reaction rate. This is a significant clue that bounded reaction rate QSPs are in fact the right mathematical objects for modeling quantized Pál-Bell processes.

Finally, we are able to define the following PMV measure uniquely associated to each QSP of interest

Definition 5.8.8. *Single-Reaction Generator PMV*

For every bounded reaction rate QSP $\mathscr{E}_t$ with a Collisionless Reaction Transport Propagator $\boldsymbol{S}_t$, we define the Single-Reaction Generator PMV measure, $\forall E \subset G, \boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$

$$\mathscr{J}(E, \boldsymbol{\rho}) = \lim_{t\to 0} t^{-1}\mathscr{E}_t(\Pi_G^{-1}(E), \boldsymbol{\rho}) \tag{5.8.0.21}$$

where convergence is in the trace norm as per proposition 5.8.6.

Lemma 5.8.9.

For every bounded reaction rate QSP $\mathscr{E}_t$ that is trace absolutely continuous with respect to the product Lebesgue measure on the typed geographic space has a Collisionless Reaction Transport Propagator $\boldsymbol{S}_t$, $\mathscr{J}_t$ converges uniformly in time to $\mathscr{J}$.

Every such $\mathscr{J}_t$ has an integral representation such that for each $E \in \mathscr{G}$

$$t\,\mathscr{J}_t(E, \boldsymbol{\rho}) = \int_0^t \mathrm{d}s \boldsymbol{S}_{t-s}\mathscr{J}(E, \boldsymbol{S}_s\boldsymbol{\rho}) \tag{5.8.0.22}$$

$\mathscr{J}$ so defined is unique.

Proof.

We begin by approximating t from below by the closest dyadic rational that can be obtained as the product of an integer and the number 2^{-m}. This is accomplished using a floor function that drops the fractional part of a real number which we will symbolize as $\lfloor\cdot\rfloor$. In particular, the best such dyadic approximant is given by $2^{-m}\lfloor 2^m t\rfloor$. Thus, the interval $(0, t]$ can be approximated arbitrarily well from below by $(0, 2^{-m}\lfloor 2^m t\rfloor]$ for m

sufficiently large. This interval can be broken into a disjoint union of subintervals of the form $(2^{-m}k, 2^{-m}(k+1)]$ where $k \in \mathbb{N}$ and $0 \leq k \leq \lfloor 2^m t \rfloor]$. For a suitable subsequence of $m \in \mathbb{N}$, we have by proposition 5.8.6 that each $s \in (0,t)$ is approximated by a decreasing dyadic sequence such that in a sequence of local interval about s, $\mathscr{J}_{2^{-m}}(f, \boldsymbol{S}_{\frac{r-1}{2^m}}\boldsymbol{\rho}) \to \mathscr{J}(f, \boldsymbol{S}_s\boldsymbol{\rho})$ in trace norm. Building on this in the obvious way $\boldsymbol{S}_{2^{-m}(\lfloor 2^m t \rfloor - r)}\mathscr{J}_{2^{-m}}(f, \boldsymbol{S}_{\frac{r-1}{2^m}}\boldsymbol{\rho}) \to \boldsymbol{S}_{t-s}\mathscr{J}(f, \boldsymbol{S}_s\boldsymbol{\rho})$.

Now, having analyzed the integrand, we can construct a direct approximation of the PMV measure $\mathscr{J}_{2^{-m}(\lfloor 2^m t \rfloor)}$. We do this in two steps. First, we use the definition of $t\mathscr{J}_t$ to obtain from the integral representation bilinear function form of $\mathscr{E}_t(\Pi_G^{-1}(\cdot), \cdot)$

$$2^{-m}(\lfloor 2^m t \rfloor)\mathscr{J}_{2^{-m}(\lfloor 2^m t \rfloor)} = \mathscr{E}_{2^{-m}(\lfloor 2^m t \rfloor)}(f, \boldsymbol{\rho}) = \int_{\Pi_G^{-1}(G)} f(g)\mathrm{d}\mathscr{E}(g \times s, \boldsymbol{\rho}) \tag{5.8.0.23}$$

We can simplify this further by decomposing $\Pi_G^{-1}(E) \subset A^1_{2^{-m}\lfloor 2^m t \rfloor}$ using the trick from our second measurability proof. Let $E_{k,r} = z(1 - \chi_{_k}(r)) + \Pi_G^{-1}(E) \cap A^1_{2^{-m}}\chi_{_k}(r)$ defines a function on the index set mapping to an element in $\mathscr{X}_{2^{-m}}$, using this and the λ sample space set composition map extended to an arbitrary finite number of sets, we can define a decomposition of any set in $A^1_{2^{-m}\lfloor 2^m t \rfloor}$ but, in particular, we can approximate $\Pi_G^{-1}E$ with an error trace bounded by 2^{-m}. Thus, using the disjoint union

$$\Pi_G^{-1}(E) = \bigcup_{k=1}^{\lfloor 2^m t \rfloor} \lambda(E_{k,1}, E_{k,2}, \ldots, E_{k,\lfloor 2^m t \rfloor}) \tag{5.8.0.24}$$

we have established a combination of terms that account for all possible events in the approximate interval. Finally, we can use the measure decomposition to split over the terms of the disjoint union an obtain

$$\int_{\Pi_G^{-1}(E)} f(g)\mathrm{d}\mathscr{E}(g \times s, \boldsymbol{\rho}) = \sum_{k=1}^{\lfloor 2^m t \rfloor} \int_{\lambda(E_{k,1} \times E_{k,2} \times \cdots \times E_{k,\lfloor 2^m t \rfloor})} f(g)\mathrm{d}\mathscr{E}(g \times s, \boldsymbol{\rho}) \tag{5.8.0.25}$$

Now, we note that f is independent of the time parameter, so we can use this to simplify the problem on factorizable sets. In particular, for any $E \in \mathscr{G}$ we have by virtue of $\mathscr{E}_{2^{-m}}(z, \boldsymbol{\rho}) = \boldsymbol{S}_{2^{-m}}\boldsymbol{\rho}$

$$\mathscr{E}(\lambda(E_{k,1} \times E_{k,2} \times \cdots \times E_{k,\lfloor 2^m t \rfloor}), \boldsymbol{\rho}) = \mathscr{E}(E_{k,\lfloor 2^m t \rfloor}, \mathscr{E}(E_{k,\lfloor 2^m t \rfloor - 1}, \ldots \mathscr{E}(E_{k,1}, \boldsymbol{\rho}) \ldots)) \tag{5.8.0.26}$$

$$= \boldsymbol{S}_{2^{-m}(\lfloor 2^m t \rfloor - k)}\mathscr{E}_{2^{-m}}(\Pi_G^{-1}(E), \boldsymbol{S}_{\frac{k-1}{2^m}}\boldsymbol{\rho}) \tag{5.8.0.27}$$

By virtue of the norm convergence of the Riemann sum that defines the integral form of $\mathscr{E}_t$ and the strong convergence of $\boldsymbol{S}_t$, we can exchange the integral of f with the outer $\boldsymbol{S}_t$ to obtain (again using the definition

of $\mathscr{J}_t$ the finite-duration single reaction PMV measure in terms of $\mathscr{E}_t$)

$$2^{-m}(\lfloor 2^m t\rfloor)\mathscr{J}_{2^{-m}(\lfloor 2^m t\rfloor)} = \sum_{k=1}^{\lfloor 2^m t\rfloor} \boldsymbol{S}_{2^{-m}(\lfloor 2^m t\rfloor - k)} \left(\frac{1}{2^m} \int_{E\times(\frac{k-1}{2^m},\frac{k}{2^m}]} f(g)\mathrm{d}\mathscr{E}(g\times s, \boldsymbol{S}_{\frac{k-1}{2^m}}\boldsymbol{\rho}) \right) \tag{5.8.0.28}$$

By our earlier argument about the convergence of the PMVs on the dyadic time mesh and a simple measure theoretic argument about the convergence of the sum of 2^{-m} weighted terms to an integral over the time parameter, we have

$$t\,\mathscr{J}_t(f,\boldsymbol{\rho}) = \int_0^t \mathrm{d}s \boldsymbol{S}_{t-s}\mathscr{J}(f,\boldsymbol{S}_s\boldsymbol{\rho}) \tag{5.8.0.29}$$

Using definition 2.3.14, we obtain the desired PMV measure defined in the usual way.

Uniform convergence over sequences in time converging to zero follows in the trace norm by the Lebesgue differentiation theorem.

Uniqueness is now an easy result of supposing there exist two cluster points $\mathscr{J}_1$ and $\mathscr{J}_2$ for different subsequences converging to zero and using the uniform convergence to show that they are identical in the topology induced by the trace norm. □

It is useful to think of this representation as a kind of fundamental theorem of calculus for QSPs. It allows us to break arbitrary single reaction events into integrals over compositions of zero-reaction events and single reaction generator PMVs. This has an intuitive physical interpretation that connects back to the classical theory. If we know that an event occurred in a given interval we can represent this as a path integral over free evolutions with exponentially decaying mass with a single reaction event at an arbitrary time. When we introduced the time integral in the Pál-Bell theory, it used a heuristic inspired by the same decomposition over subsets. This is the technically precise version of equation 3.3.2.2 for quantum stochastic processes. We will use this extensively below to show that every bounded reaction rate QSP of interest can be represented in a piecewise deterministic Markov process form.

5.9 Reaction-Transport QSPs

In the previous sections, we established that every QSP with a bounded reaction rate has a strongly continuous zero-reaction semigroup. If we further assume that this semi-group is a Collisionless Reaction Transport Propagator, then we proved that the QSP has a unique PMV measure $\mathscr{J}$ corresponding to a single reaction in an interval $[0,t]$ as $t\to 0$. Now we are in a position to define the class of QSPs that could plausibly be used for modeling reaction-transport systems.

Definition 5.9.1. *Reaction-Transport QSP*

A Reaction-Transport QSP is defined to be a QSPs $\mathscr{E}_t$ over a typed geographic space G, with a sigma algebra $\mathscr{X}_t$ that contains the Borel sigma algebra generated by the reaction sample space X_t with a single reaction space consisting of a typed geographic space G having a sigma algebra $\mathscr{G}$. Furthermore, this QSP must satisfy three requirements:

(1) It must have a bounded reaction rate

$$\mathrm{Tr}\left[\mathscr{E}_t(X_t\{z\},\boldsymbol{\rho})\right] \leq Kt\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.9.0.1}$$

(2) It must have $\boldsymbol{S}_t\boldsymbol{\rho} = \mathscr{E}_t(z,\boldsymbol{\rho})$ a collisionless reaction-transport propagator.

(3) It must have a Single-Reaction Generator PMV $\mathscr{J}(E,\boldsymbol{\rho}) = \lim_{t\to 0} t^{-1}\mathscr{E}_t(\Pi_G^{-1}(E),\boldsymbol{\rho}), \forall E \in \mathscr{G}$ that is a Reaction-Transport Transition PMV measure. Moreover, $\mathrm{Tr}\left[\mathscr{E}_t(\Pi_G^{-1}(E),\boldsymbol{\rho})\right] = \mu_{t,\boldsymbol{\rho}}$ satisfies $\mu_{t,\boldsymbol{\rho}} << g$ where g is a Lebesgue product measure on the geographic phase space.

5.10 RT PDP Representation of Reaction-Transport QSPs

In this section, we prove that every Reaction-Transport PDP is generated by a Reaction-Transport QSP and conversely every Reaction-Transport QSP is uniquely determined by its PDP formula. This uniqueness and existence relationship establishes that Reaction-Transport QSPs are the correct quantization of the Pál-Bell equation. Davies develops a classification theory of bounded reaction rate QSPs that hinges on a similar class of QSPs being uniquely determined by their $\mathscr{J}$ PMV measure and their free propagator $\boldsymbol{S}_t$. Along the way he uses an approximation scheme on Borel product sets to prove necessity and sufficiency of knowledge of $\mathscr{J}$ and $\boldsymbol{S}_t$ for specifying a QSP. For our purposes, it is this approximation scheme that is the most important part of the theory and we will restructure the arguments to emphasize this. For the original theory of quantum field particle detection see [32] Theorems 3.5 and 3.6 pages 75-79.

Theorem 5.10.1. *RT QSP = RT PDP*

An operator valued measure is a Reaction-Transport QSP if and only if it can be evaluated on the subalgebra R of a sigma algebra X_t by a Reaction-Transport PDP

Proof.

We begin with a simplifying observation about the algebra R. As noted in proposition 5.6.2 and the remarks following it, $\mathscr{X}_t$ can be taken to be the sigma algebra generated by R. As such, we can prove results on the

rectangular sets and then extend them to the algebra R. By standard extension theorems from a premeasure to a measure, this line of argument is sufficient to uniquely determine a QSP on $\mathscr{X}_t$ from a representation on the rectangular sets. We will use this simplification throughout the rest of this proof to simplify the kinds of sets that we need to contemplate. In particular, we will use an arbitrary rectangular set E of the product Borel form, $t_i \leq r_{i+1}$, $E = \{(x_i, p_i, \ell_i, s_i)_{i=1}^m : r_i < s_i \leq t_i, (x_i, p_i, \ell_i) \in E_i\}$ where $E_i \in \mathscr{G}$ and $m \in \mathbb{N}$. That is $E = \prod_{i=1}^m (E_i \times (r_i, t_i])$.

We will proceed by addressing the forward direction of the proof. We will suppose that we have a Reaction-Transport QSP and then prove that it is representable on the rectangular product family R by a Reaction-Transport PDP.

First we note that from the definition of a Reaction-Transport QSP, there is a unique well-defined Single-Reaction Generator PMV $\mathscr{J}$ that is a Reaction-Transport PMV on the typed geographic phase space G and there is a zero reaction propagator $\mathscr{E}_t(z, \boldsymbol{\rho}) = \boldsymbol{S}_t$ given by a Collisionless Reaction-Transport Propagator. We also know that together, $\mathscr{J}$ and $\boldsymbol{S}_t$ define a mesoscopic reaction rate through a trace compatibility constraint as in the definition 5.4.2. This is a direct result of proposition 5.8.7. Thus, it suffices to show that on the rectangular sets, equation 5.6.0.2 is a valid formula for $\mathscr{E}_t(E, \boldsymbol{\rho})$.

In order to achieve the PDP representation on a general rectangular set E, we will begin by introducing an integral representation of a Finite-Duration Single-Reaction PMV in terms of a Single-Reaction Generator PMV and a zero-reaction propagator. One can think of this as a reaction-transport QSP analogue for the fundamental theorem of calculus. The desired result was proven in lemma 5.8.9.

$$t\,\mathscr{J}_t(E, \boldsymbol{\rho}) = \int_0^t \mathrm{d}s \boldsymbol{S}_{t-s}\,\mathscr{J}(E_1, \boldsymbol{S}_s\boldsymbol{\rho})$$

We build on this by extending it to an arbitrary rectangular set. The premise of the decomposition is essentially the same, however convergence is now guaranteed by lemma 5.8.9. Indeed, for any set E as defined earlier in the proof, we can simplify the problem in two steps. First, we notice that in the intervals $t_i \leq r_{i+1}$ there can be no events otherwise we are on a different reaction count subspace than the one specified by E. Thus, we can use the obvious decomposition (using a notation $z \times (0, r_1]$ which is obviously silly but useful for keeping track of the temporal interval subspaces)

$$E = \lambda(z \times (0, r_1], E_1 \times (r_1, t_1], z \times (t_1, r_2], E_2 \times (r_2, t_2], \ldots, E_m \times (r_m, t_m], z \times (t_m, t]) \tag{5.10.0.1}$$

whereby

$$\mathscr{E}_t(E,\boldsymbol{\rho}) = \mathscr{E}_{t-t_m}(z, \mathscr{E}_{t_m-r_m}(E_m \times (r_m,t_m], \mathscr{E}_{r_m-t_{m-1}}(z, \dots \mathscr{E}_{t_1-r_1}(E_1 \times (r_1,t_1], \mathscr{E}_{r_1}(z,\boldsymbol{\rho}))\dots))) \quad (5.10.0.2)$$

$$= \boldsymbol{S}_{t-t_m}\mathscr{E}_{t_m-r_m}(\Pi_G^{-1}(E_m), \boldsymbol{S}_{r_m-t_{m-1}}\dots\mathscr{E}_{t_1-r_1}(\Pi_G^{-1}(E_1), \boldsymbol{S}_{r_1}\boldsymbol{\rho})\dots) \quad (5.10.0.3)$$

$$= \boldsymbol{S}_{t-t_m}(t_m-r_m)\mathscr{J}_{t_m-r_m}(E_m, \boldsymbol{S}_{r_m-t_{m-1}}\dots(t_1-r_1)\mathscr{J}_{t_1-r_1}(E_1, \boldsymbol{S}_{r_1}\boldsymbol{\rho})\dots) \quad (5.10.0.4)$$

Now, applying our single event integral representation on each $E_k \times (r_k, t_k]$ event, we can obtain the desired form by using the semigroup property to combine the collisionless propagators. Specifically, we have (with an operator notation $\mathscr{J}(E_m)\boldsymbol{\rho} = \mathscr{J}(E_m,\boldsymbol{\rho})$ to avoid the iterated parentheses)

$$\mathscr{E}_t(E,\boldsymbol{\rho}) = \prod_{i=1}^{m}\int_{(r_i,t_i]} \mathrm{d}s_i \boldsymbol{S}_{t-t_m}\boldsymbol{S}_{t_m-s_m}\mathscr{J}(E_m)\boldsymbol{S}_{s_m-r_m}\boldsymbol{S}_{r_m-t_{m-1}}\boldsymbol{S}_{t_{m-1}-s_{m-1}}\mathscr{J}(E_{m-1})\dots\mathscr{J}(E_1)\boldsymbol{S}_{s_1-r_1}\boldsymbol{S}_{r_1}\boldsymbol{\rho} \quad (5.10.0.5)$$

which reduces to the desired form

$$\mathscr{E}_t(E,\boldsymbol{\rho}) = \prod_{i=1}^{m}\int_{(r_i,t_i]} \mathrm{d}s_i \boldsymbol{S}_{t-s_m}\mathscr{J}(E_m)\boldsymbol{S}_{s_m-s_{m-1}}\mathscr{J}(E_{m-1})\dots\mathscr{J}(E_1)\boldsymbol{S}_{s_1}\boldsymbol{\rho} \quad (5.10.0.6)$$

This completes the forward direction of the proof.

Now we will prove the converse: that any Reaction-Transport PDP specifies a $\mathscr{J}$ and $\boldsymbol{S}_t$ such that a unique Reaction-Transport QSP can be constructed on the full sigma algebra X_t in a way that extends the PDP formula. Moreover, this Reaction-Transport QSP will have $\mathscr{J}$ as its Single-Reaction Generator PMV and $\boldsymbol{S}_t$ as its zero reaction propagator.

This proof is comparatively simple as it suffices to show that if the PDP formula, equation 5.6.0.2, is valid on rectangular sets of the generating algebra R, then there is a well-defined PMV measure family (with the properties of a QSP) on each fixed reaction number subspace. We could base this directly off of a decomposition of elements in R into sums over disjoint rectangular sets. However, we will use another approximation scheme that will enable us to extend our Reaction-Transport PDP computations to reaction sets with overlap. We are still relying on the $\mathscr{X}_t$ generating property of R in that we are not allowing a more general time dependence in the sets of geographic typed space sets for our formula. As such, we can recognize that a measure theoretic extension argument of the kind already discussed must be invoked behind the scenes. In what follows, $\mathscr{E}_t$ is a new operator valued measure that we are defining from the given $\mathscr{J}$ and $\boldsymbol{S}_t$ of a reaction-transport PDP.

We begin with the zero reaction subspace. Here we define $\mathscr{E}_t$ using the collisionless reaction-transport

propagator.

$$\mathscr{E}_t(z, \boldsymbol{\rho}) = \boldsymbol{S}_t \boldsymbol{\rho} \tag{5.10.0.7}$$

In order to understand this as a PMV measure, we need to recognize that the restriction of the sigma algebra to this subspace consists of $\{z, \emptyset\} \equiv \mathscr{Z}$. Strong countable additivity is trivial. Positivity is part of the definition of a collisionless reaction-transport propagator. If this extends to a QSP on R then we have established that the zero reaction propagator agrees with $\boldsymbol{S}_t$ by definition.

Now we will extend this to a bounded reaction rate PMV measure on R in two steps. First, we define a PMV measure on $\mathscr{Z} \times \prod_{i=1}^{m} (\mathscr{G} \times \{t_i\} \times \mathscr{Z})$. Then, we extend it to R using time-ordered integrals over all of the time parameters in the original PMV measure. To address the first step, we define a new operator valued measure by

$$\mathscr{J}(\prod_{i=1}^{m} E_i \times s_i, \boldsymbol{\rho}) = \boldsymbol{S}_{t-s_m} \mathscr{J}(E_m) \boldsymbol{S}_{s_m - s_{m-1}} \mathscr{J}(E_{m-1}) \dots \mathscr{J}(E_1) \boldsymbol{S}_{s_1} \boldsymbol{\rho} \tag{5.10.0.8}$$

We can use proposition 2.3.15 to prove by induction that a finite composition of PMV measures $\mathscr{J}$ on $\mathscr{G}$ and $\boldsymbol{S}_{\Delta t}$ on $\mathscr{Z}$ yields a unique PMV measure on the product space.

Now, in order to perform the extension to the time-dependent space, note that the time dependence is only present in the strongly continuous semigroup $\boldsymbol{S}_t$. It it a standard result of the theory for semigroups on a Banach space (see for example [91] Theorem 4 p.421), that $\forall \boldsymbol{\rho} \in \mathscr{T}(\mathscr{H})$

$$\int_0^t \mathrm{d}s \boldsymbol{S}_s \boldsymbol{\rho} \in D(\boldsymbol{W}) \tag{5.10.0.9}$$

and moreover this operator function is everywhere strongly differentiable. That is, by integrating in time as a limit of Riemann sums, we obtain an operator family with even better properties than the original semigroup. Thus, it follows that we can define a time ordered integral that conforms to the time-ordered subspace $\mathscr{X}_t$

$$\iiint\limits_{0<s_1<s_2<\dots<s_m\leq t} f \equiv \int_0^t \mathrm{d}s_m \int_0^{s_m} \mathrm{d}s_{m-1} \dots \int_0^{s_3} \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 f \tag{5.10.0.10}$$

and a domain constraint operator $D_t = \prod_{i=1}^{m} (r_i, t_i]$

$$\chi_{D_t}(s_m, \dots, s_1) = \prod_{i=1}^{m} \chi_{(r_i, t_i]}(s_i) \tag{5.10.0.11}$$

so that any interval product constrained and (obviously) time ordered set of R, say $E_t^m = \prod_{i=1}^{m} (E_i \times (r_i, t_i]) \cap$

X_t where $E_t^m \subset A_t^m$, can be given a value under the operator valued measure by the definition

$$\mathscr{E}_t(E_t^m, \boldsymbol{\rho}) = \iiint\limits_{0<s_1<s_2<\cdots<s_m\leq t} \chi_{D_t}(s_m, \ldots, s_1)\, \mathscr{J}(\prod_{i=1}^{m} E_i \times s_i, \boldsymbol{\rho}) \tag{5.10.0.12}$$

now by decomposing any set $E \in R$ into its fixed reaction number subspaces $E \cap A_t^n$ we can directly compute the measure for any $\boldsymbol{\rho} \in \mathscr{T}(\mathscr{H})$ and the resulting measure is trace countably additive and positive by the above arguments regarding the integrand $\mathscr{J}(\prod_{i=1}^{m} E_i \times s_i, \boldsymbol{\rho})$ and the strongly (in trace norm) convergent behavior of each finite time integral. We conclude that this is in fact a PMV measure on the algebra generated by R and so also on $\mathscr{X}_t$. Now in order to complete the proof, we note that it suffices to prove that the resulting PMV measure is a bounded reaction rate QSP with $\mathscr{J}$ as its Single-Reaction Generator PMV.

Before proceeding with the rest of the proof we will quickly note that because these integrals are trace norm convergent Riemann sums over a bounded time mesh and the $\mathscr{J}$ and $\boldsymbol{S}_t$ operators are trace norm continuous and linear, we can commute the integrals with any finite number of operators that are independent of the time index that the integral is over. This property will be essential to establishing the Chapman-Kolmogorov type property of our newly defined PMV measure $\mathscr{E}$.

Now, we recall that for a PMV measure to be a QSP, it must satisfy three properties:

(i) trace preserving on the full sample space

$$\mathrm{Tr}\left[\mathscr{E}_t(X_t, \boldsymbol{\rho})\right] = \mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.10.0.13}$$

(ii) trace continuity on the full sample space

$$\mathrm{s}\lim_{t\to 0} \mathscr{E}_t(X_t, \boldsymbol{\rho}) = \boldsymbol{\rho} \tag{5.10.0.14}$$

(iii) Chapman-Kolmogorov property For all states $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$, $\forall s, t \geq 0$, and $\forall E \in \mathscr{X}_s,\ F \in \mathscr{X}_t$,

$$\mathscr{E}_t(F, \mathscr{E}_s(E, \boldsymbol{\rho})) = \mathscr{E}_{s+t}(\lambda(E \times F), \boldsymbol{\rho}) \tag{5.10.0.15}$$

We will start with the last of these. Using our limit switch observation about integrals from above, we can prove the Chapman-Kolmogorov property. We let the rectangular subalgebra of X_s be referred to as R_s and its restriction to an n_1 event subspace as $R_s^{n_1}$. For the given PMV, we can extend this to all time ordered events (not necessarily restricted to non-overlapping time intervals) with time-independent Borel subsets of

the typed geographic phase space associated to each reaction counted and we call this $\overline{R}_s^{n_1}$. Now, by our usual fixed reaction number subspace decomposition argument, it suffices to consider $E \in \overline{R}_s^{n_1}, F \in \overline{R}_t^{n_2}$. Then $\lambda(E,F) \in \overline{R}_{s+t}^{n_1+n_2}$ and has a definition point of non-overlap of the temporal subsets (namely s). Thus, we can factor the characteristic function into the first n_1 components and the next n_2 components,

$$\chi_{D_{t+s}}(s_{n_1+n_2},\ldots,s_1) = \prod_{i=1}^{n_1} \chi_{(r_i,t_i]}(s_i) \times \prod_{i=n_1+1}^{n_1+n_2} \chi_{(r_i,t_i]}(s_i) = \chi_{D_s}(s_{n_1},\ldots,s_1)\chi_{D_t}(s_{n_1+n_2},\ldots,s_{n_1+1})$$

and we can break the time ordered integral into two subsets of integrals (where we have used a known property of the composition function to exclude any overlap between the $(0,s]$ and $(s,s+t]$ domains)

$$\begin{aligned}
\iiint\limits_{\substack{(s_i)_{i=1}^{n_1},(s_j)_{j=n_1+1}^{n_1+n_2} \\ s_i<s_j \forall i<j \\ s_{n_1}<s<s_{n_1+1} \\ s_{n_1+n_2}<s+t}} f &= \int_s^{t+s} \mathrm{d}s_{n_1+n_2} \int_s^{s_{n_1+n_2}} \mathrm{d}s_{n_1+n_2-1} \ldots \int_0^{s_2} \mathrm{d}s_1 f \\
&= \int_s^{t+s} \mathrm{d}s_{n_1+n_2} \int_s^{s_{n_1+n_2}} \mathrm{d}s_{n_1+n_2-1} \ldots \int_s^{s_{n_1+2}} \mathrm{d}s_{n_1+1} \int_0^{s} \mathrm{d}s_{n_1} \ldots \int_0^{s_2} \mathrm{d}s_1 f \\
&= \iiint\limits_{s<s_{n_1+1}<s_{n_1+n_2}\leq t} \iiint\limits_{0<s_1<s_2<\cdots<s_{n_1}\leq s} f
\end{aligned}$$

finally, we note that the integrand PMV measure factorizes naturally

$$\mathscr{J}(\prod_{i=1}^{n_1+n_2} E_i \times s_i, \boldsymbol{\rho}) = \mathscr{J}(\prod_{i=n_1+1}^{n_1+n_2} E_i \times s_i, \mathscr{J}(\prod_{i=1}^{n_1} E_i \times s_i, \boldsymbol{\rho}))$$

thus, applying the our limit interchanging result, we have

$$\begin{aligned}
\mathscr{E}_{s+t}(\lambda(E,F),\boldsymbol{\rho}) = & \iiint\limits_{s<s_{n_1+1}<s_{n_1+n_2}\leq t} \chi_{D_t}(s_{n_1+n_2},\ldots,s_{n_1+1}) \\
& \mathscr{J}\left(\prod_{i=n_1+1}^{n_1+n_2} E_i \times s_i, \iiint\limits_{0<s_1<s_2<\cdots<s_{n_1}\leq s} \chi_{D_s}(s_{n_1},\ldots,s_1)\mathscr{J}(\prod_{i=1}^{n_1} E_i \times s_i, \boldsymbol{\rho})\right) \qquad (5.10.0.16)
\end{aligned}$$

Thus, on any fixed reaction count subspace,

$$\mathscr{E}_{s+t}(\lambda(E\times F),\boldsymbol{\rho}) = \mathscr{E}_t(F,\mathscr{E}_s(E,\boldsymbol{\rho})) \qquad (5.10.0.17)$$

as required.

The remaining two requirements will be established with the help of the bounded reaction rate that

follows directly the from the assumed form of $\mathscr{E}_t$. Indeed, it is easily proven by direct computation that

$$\iiint\limits_{0<s_1<s_2<\cdots<s_n\leq t} 1 = \frac{t^n}{n!} \tag{5.10.0.18}$$

Now, again using the Trace convergence of the integrals,

$$\mathrm{Tr}\left[\mathscr{E}_t(A_t^n, \boldsymbol{\rho})\right] \leq \iiint\limits_{0<s_1<s_2<\cdots<s_n\leq t} \mathrm{Tr}\left[\mathscr{J}(\prod_{i=1}^{n_1} G\times s_i, \boldsymbol{\rho})\right] \tag{5.10.0.19}$$

Since the integrand PMV measure is a positive operator on every subset, its evaluation is increasing for increasing set inclusions. Moreover, on the full space for any fixed sequence of time indexes ($z \times \prod_{i=1}^{n}(G\times\{t_i\}\times z)$) and for every positive trace class operator ($\boldsymbol{\rho}$), the integrand is trace bounded by the fact that $\mathscr{J}$ is a Reaction-Transport transition PMV and proposition 5.5.4. Indeed, this guarantees us that $\mathrm{Tr}\left[\mathscr{J}(G,\boldsymbol{\rho})\right] \leq K\mathrm{Tr}\left[\boldsymbol{\rho}\right]$. On the other hand, we also know that $\boldsymbol{S}_t$ a Collisionless Reaction Transport Propagator means that $\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] \leq \mathrm{Tr}\left[\boldsymbol{\rho}\right]$, thus by successively bounding each term in the product integrand, we have

$$\mathrm{Tr}\left[\mathscr{J}(\prod_{i=1}^{n_1} G\times s_i, \boldsymbol{\rho})\right] \leq K^n\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.10.0.20}$$

so, we have proven that the full PMV measure has a bounded reaction rate, since by combining our estimates, we have

$$\mathrm{Tr}\left[\mathscr{E}_t(A_t^n, \boldsymbol{\rho})\right] \leq \frac{K^n t^n}{n!}\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.10.0.21}$$

and so by summing over subspaces of fixed reaction number n

$$\mathrm{Tr}\left[\mathscr{E}_t(X_t, \boldsymbol{\rho})\right] \leq e^{Kt}\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.10.0.22}$$

With this upper bound established, we can extend our proof of the Chapman-Kolmogorov property (iii) to any countable combination of reaction count subspaces, which is sufficient for the general result by using the decomposition $\lambda(E,F) = \lambda(\cup_{n_1}(E\cap A_s^{n_1}), \cup_{n_2}(F\cap A_t^{n_2})) = \cup_{n_1,n_2}\lambda((E\cap A_s^{n_1}, (F\cap A_t^{n_2}))$ where all of the unions are disjoint.

Furthermore, on any fixed interval $(0,\tau], \exists K_\tau > 0$ s.t. $\forall\boldsymbol{\rho}\in\mathscr{T}(\mathscr{H}), \forall t\in(0,\tau]$

$$\mathrm{Tr}\left[\mathscr{E}_t(B_t^1, \boldsymbol{\rho})\right] \leq K_\tau t\mathrm{Tr}\left[\boldsymbol{\rho}\right] \tag{5.10.0.23}$$

which proves that the PMV measure $\mathscr{E}$ has a bounded reaction rate.

Now, we can complete the proof that $\mathscr{E}_t$ is a QSP by performing a simple decomposition analysis of $\boldsymbol{T}_t\boldsymbol{\rho} = \mathscr{E}_t(X_t, \boldsymbol{\rho})$ based on our representation and reaction rate estimates and the assumption of consistency of mesoscopic reaction rates. Indeed, using $X_t = z \cup A_t^1 \cup_{i>1} A_t^i$, we have

$$\mathscr{E}_t(X_t, \boldsymbol{\rho}) = \mathscr{E}_t(z, \boldsymbol{\rho}) + \mathscr{E}_t(A_t^1, \boldsymbol{\rho}) + \sum_{i=2}^{\infty} \mathscr{E}_t(A_t^i, \boldsymbol{\rho}) \tag{5.10.0.24}$$

but using our reaction count trace bound 5.10.0.21, the final summation can be trace bounded by t^2 times a constant times $\mathrm{Tr}\left[\boldsymbol{\rho}\right]$, while the other terms are easily interpreted in terms of simple formulas

$$\boldsymbol{T}_t\boldsymbol{\rho} = \boldsymbol{S}_t\boldsymbol{\rho} + \int_0^t \mathrm{d}s \boldsymbol{S}_{t-s} \mathscr{J}(G, \boldsymbol{S}_s\boldsymbol{\rho}) + \mathscr{O}(t^2) \tag{5.10.0.25}$$

but since $\lim_{t\to 0} \boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{\rho}$ in trace norm and the other terms vanish in trace norm, we have

$$\lim_{t\to 0} \left\|\boldsymbol{T}_t\boldsymbol{\rho} - \boldsymbol{\rho}\right\|_{\mathrm{Tr}} = 0 \tag{5.10.0.26}$$

which proves property (ii).

Finally, we need to prove the probability conservation property. This follows directly from the fact that every Reaction-Transport PDP has a well defined Mesoscopic Reaction Rate. We will use the differential form of the assumption derived in proposition 5.8.7 (the equivalence proven there only depends on the decomposition, not on the origin being a QSP),

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] = -\mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{S}_t\boldsymbol{\rho}\right] \tag{5.10.0.27}$$

but by the above decomposition, we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{T}_t\boldsymbol{\rho}\right] = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] + \mathrm{Tr}\left[\mathscr{J}(G, \boldsymbol{\rho})\right] \tag{5.10.0.28}$$

and so by the fact that $\boldsymbol{R}$ is the trace adjoint of $\mathscr{J}(G, \cdot)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{T}_t\boldsymbol{\rho}\right] = 0 \tag{5.10.0.29}$$

which since it holds uniformly in time gives us property (i) of a QSP.

Finally, we note that the decomposition also gives us trivially that the single-reaction generator PVM of the QSP is given by $\mathscr{J}$ from the reaction transport PDP. This completes the proof.

□

Remark

One way of looking at this (that relates it back to Davies' theory) is that the Collisionless Reaction Transport Propagator and the Reaction-Transport Transition PMV measure themselves are sufficient to uniquely specify both a QSP and a PDP formula. Therefore, since we can get them both from either the Reaction-Transport QSP or the Reaction-Transport PDP, there is sufficient information to create a bijective map between the two spaces of models. Since Davies' theory does not apply precisely as it is stated for the full range of LCH topologies that we might need to use, we have introduced a significant number of small modifications and additional calculations to justify its use. However, the principle of the mapping remains intact and this is a useful way of thinking about it.

Remark

Over the course of these proofs we have established a number of useful approximation procedures and simplified formulas for studying nuclear systems. For example, we have shown that we can approximate the action of the QSP on any state by taking a convex sum over pure states. Due to the form of the reaction-transport transition PMV and collisionless propagators, this can be understood in terms of the action of a stochastic simulation on vectors such as we encounter in Quantum Monte Carlo.

Remark

We have introduced a set of functions α, and operators $\boldsymbol{U}_\ell, \boldsymbol{V}_{x,k,\ell}, \boldsymbol{B}_F, \boldsymbol{B}_B$ that are sufficient for fully characterizing a reaction-transport process. These can be modeled individually based on the nuclear reaction absorption and decay dynamics involved, the streaming model, and the phase space detection model. Once they have been individually studied using a combination of theory and fitting to data, they can be synthesized into a complete reaction-transport model. This full modeling process is the primary long term goal of this work. The proofs completed in this chapter establish a number of constraining criteria on the structure of these operators. As long as we conform to these constraints, we will always be able to use the methods of this chapter to synthesize a reaction transport QSP with the necessary properties and approximation options. This yields a framework for constructing an infinite dimensional model selection problem.

Chapter 6

Application of Reaction-Transport QSPs

The objective proposed in the introduction was to derive a quantum neutron transport theory directly from a practical nuclear reaction model that can support resonance dynamics. Prior to this, no quantum transport models existed that were compatible with any nuclear reaction models that are used for nuclear data evaluation. This deficiency has had real but subtle consequences for the development of nuclear science and we set out to correct it. In order to accomplish this, we built a theory of quantum measurement in three stages.

First, we reformulated the classical stochastic theory into a more easily quantized form in chapter 3. Second, in chapter 4, we identified the most important features of this modified classical theory and formulated an analogy to quantum measurement theory. Finally, in chapter 5, we completed the mathematical foundation of this theory by establishing an equivalence between reaction-transport PDPs and reaction-transport QSPs. This result proved that a variety of powerful approximation techniques that are common in quantum optics can also be applied to the study of quantized neutron transport theories. However, the last chapter left open the question of how to apply these tools to the practical modeling of nuclear systems.

The purpose of the current chapter is to provide a simple physical interpretation for the mathematically precise, quantized reaction-transport theory that we developed in the last chapter. A quick inspection of the main definitions of the previous chapter shows that we have already used quantum measurement arguments to reduce the full space of operator-valued measures (on a reaction sample space) to a small collection of functional model parameters for specifying a bounded reaction rate QSP. Specifically, we have shown that a reaction-transport process can be completely defined simply by specifying a detector scale function α, an $\ell \in T$ indexed family of reaction operators $\boldsymbol{U}_\ell, \boldsymbol{V}_{x,k,\ell}$, and a pair of collisionless evolution generating operators $\boldsymbol{B}_F, \boldsymbol{B}_B$ for the free and bound subspaces respectively. Among these, $\boldsymbol{U}_\ell, \boldsymbol{V}_{x,k,\ell}$, and $\boldsymbol{B}_B$ constitute a nuclear reaction model compatible with a variety of standard tools from nuclear physics. Meanwhile, α defines a condensed matter scale function, and $\boldsymbol{B}_F$ defines a neutron streaming model. Although we have already proven a great deal about the necessary properties of these functional parameters, we have only made a few passing remarks about their meaning or how one would go about modeling them. By expanding on the

statistical modeling aspects of the theory, we will show that this technique represents a significant advance in the mathematical technology for modeling the assimilation of differential and integral cross section data.

6.1 The Quantum PDP Formula and Statistical Data Assimilation for Functional Transport Data

The neutron transport equation is well accepted as a classical tool for studying the mean space-time dynamics of a nuclear system. We recall a somewhat nonstandard integral form,

$$\begin{aligned}
\psi(\bar{x}+\bar{v}\Delta t,\bar{v},t+\Delta t)\Delta V_{\mathrm{xCell}}\Delta V_{\mathrm{vCell}} = \\
\exp\left(-\int_0^{\Delta t}\Sigma(\bar{v},\bar{x}+\bar{v}\tau)v\mathrm{d}\tau\right)\psi(\bar{x},\bar{v},t)\Delta V_{\mathrm{xCell}}\Delta V_{\mathrm{vCell}}+ \\
\int_0^{\Delta t}\exp\left(-\int_{\tau'}^{\Delta t}\Sigma(\bar{v},\bar{x}+\bar{v}\tau)v\mathrm{d}\tau\right)\ldots \\
\int_{\mathbb{R}^3} v'\Sigma_{\mathrm{ES}}(\bar{v'}\to\bar{v},\bar{x}+\bar{v}\tau',\bar{v'},t+\tau')\mathrm{d}^3v'\mathrm{d}\tau'\Delta V_{\mathrm{xCell}}\Delta V_{\mathrm{vCell}}+ \\
\int_0^{\Delta t}\exp\left(-\int_{\tau'}^{\Delta t}\Sigma(\bar{v},\bar{x}+\bar{v}\tau)v\mathrm{d}\tau\right)\ldots \\
(1-\beta)\frac{\chi(E)}{4\pi}\int_{\mathbb{R}^3}\nu(E')\Sigma_{\mathrm{fission}}(\bar{v'},\bar{x}+\bar{v}\tau')v'\psi(\bar{x}+\bar{v}\tau',\bar{v'},t+\tau')\mathrm{d}^3v'\mathrm{d}\tau'\Delta V_{\mathrm{xCell}}\Delta V_{\mathrm{vCell}}+ \\
\int_0^{\Delta t}\exp\left(-\int_{\tau'}^{\Delta t}\Sigma(\bar{v},\bar{x}+\bar{v}\tau)v\mathrm{d}\tau\right)\ldots \\
\frac{1}{4\pi}\int_{\mathbb{R}^3}\Sigma_{\mathrm{IS}}(\bar{v'}\to E,\bar{x}+\bar{v}\tau')v'\psi(\bar{x}+\bar{v}\tau',\bar{v'},t+\tau')\mathrm{d}^3v'\mathrm{d}\tau'\Delta V_{\mathrm{xCell}}\Delta V_{\mathrm{vCell}}+ \\
\int_0^{\Delta t}\exp\left(-\int_{\tau'}^{\Delta t}\Sigma(\bar{v},\bar{x}+\bar{v}\tau)v\mathrm{d}\tau\right)\ldots \\
\sum_i\lambda_i(\bar{x}+\bar{v}\tau')\chi_i(\bar{x}+\bar{v}\tau',E)C_i(\bar{x}+\bar{v}\tau',t+\tau')\mathrm{d}\tau'\Delta V_{\mathrm{xCell}}\Delta V_{\mathrm{vCell}} \quad (6.1.0.1)
\end{aligned}$$

In the language of time series analysis, this formula has been used to tremendous effect in modeling both filtering and prediction of detector signals in fission reactors. However, the neutron transport equation depends strongly on the family of functions $\Sigma_i(\bar{v},\bar{x})$. For a poor choice of these functions, it is relatively easy to construct a transport equation without solutions or without unique solutions. Indeed, Dautry and Lions analyze the integro-differential form without multiplication acting by weak differentiation in a Sobolev space. [30], [31] Their work shows that, in spite of its utility and intuitive appeal, this class of equations does not have the resiliency of diffusion operators. Even modest deviations from standard S-wave scattering

function momentum space cross sections can have disastrous consequences for the unwary.

At the same time, practical experience shows that for a wide variety of path simulation techniques [136] [89] as well as for iterative integral equation approximations [93], it is possible to obtain useful tools for performing statistical analysis of reactor detector signals. In these contexts, it appears that strictly positive, differentiable, and slowly-varying macroscopic cross sections are sufficient to obtain useful results. In particular, most analyses use the transport equation as an evolution equation for linear prediction, with construction of the macroscopic cross section as a statistical model selection problem. Analyzing the specific details of how this model selection problem is solved will help to both clarify the physical content of our new quantum reaction-transport model and to justify its significance.

6.1.1 Nuclear Data Evaluation for Application to Nuclear Systems

Two perspectives on the origin of cross sections will prove useful in the discussion that follows. First, macroscopic cross sections can be viewed as generic functions to fit based on benchmark reactor experiment data. We will refer to them as regression coefficient cross sections when they are obtained in this way. Second, macroscopic cross sections can be viewed as functional parameters derived from scattering theoretic models applied to scattering experiments. Scattering experiments are generally performed (as much as is possible) on isotopically pure samples. Thus a knowledge of prior measurements of the species composition of the nuclear system as a function of position is used to approximately combine the derived scattering functions into macroscopic cross section as a point-wise average (by percent composition) of the individual functional parameters by species. We will refer to these functions as scattering-derived cross sections when they are obtained in this way.

The scattering-derived cross section perspective is more fundamental from a statistical mechanical perspective. Space-time correlations can certainly be used to compute approximately optimal regression coefficient cross sections for a transport evolution model and a given spatially-indexed time series of detector outputs. However, the resulting fit does not necessarily incorporate the substantive constraints imposed by the microscopic physics. By contrast, scattering theory is a distillation of these principles as they apply to spatially and temporally isolated collisions.

Fitting a functionally parametrized resonance reaction model (a generalized scattering derived model) can be achieved by using a parametric optical model and fitting optimal parameters for a collected detector time series. [9] Alternatively, the techniques of nuclear statistical spectroscopy can be used to fit a scattering distribution consistent with a Hauser-Feshbach type model. [148] [85] Regardless of the specific method, this constructive approach yields a properly constrained subspace of cross section functions to optimize, which

can then be used to derive a mesoscopic cross section as a suitable average.

The essential idea is common enough but Parks offers a simple quantum mechanical justification in the context of resonance-free neutron thermalization. [117] This kind of synthetic technique for building macroscopic dynamics out of microscopic dynamics is typical of mathematical statistical mechanics generally. [79] [53] Moreover, the particular choice to use microscopic scattering cross sections as the basis of macroscopic cross sections is not arbitrary, but rather is grounded in the fundamental theory of kinetic equations. [5] [124]

6.1.2 Statistical Data Assimilation for Functional Transport Data

In spite of an obvious theoretical preference for the scattering-derived cross sections, there is a fundamental issue related to the consistency between the two. Namely, the neutron transport equation with macroscopic cross-sections furnished by a context-independent average over the classical output of a family of scattering models isn't a universally optimal model. The dynamics of a real reactor may deviate materially from this. Therefore, even a transport model with ideal scattering-derived cross sections may benefit from incorporating data taken from integral experiments.

There is an existing statistical methodology for incorporating data across related models called "data assimilation". [90] It is motivated by discrete Bayesian techniques for updating a model distribution that have long been common to nuclear data evaluation efforts. [100] However, the general problem requires the use of additional machinery for dealing with multiple models associated to different data sets and noisy continuous-time measurements. In this context, variations on the Kalman Filter have proven to be an effective approach to melding complex data sets. [138] In particular, a technique that couples an iterative Kalman filter based update scheme for the nuclear parameter covariance matrix to the EMPIRE nuclear reaction code was developed as an improvement to traditional adjustment methodologies. [116] However, this methodology exhibited a strong sensitivity to the initial choice of parameter uncertainties (as one would expect for a highly nonlinear Bayesian update scheme).

The nuclear data community made recourse to this type of unstable (but very clever) assimilation scheme for coupling macroscopic and microscopic measurements because the models and data sets for transport and scattering fundamentally don't describe the same thing in their conventional form. In 2012, there did not exist a scale bridging quantum reaction-transport model that could connect microscopic reaction dynamics explicitly with macroscopic neutron density distributions as phase space dependent time series. The only viable approach to data assimilation was to effectively ignore the latent relationship between the reaction and transport models in the mathematical formalism and to cope with it by making subtle choices about

which data sets to include in the analysis. The challenges of using this methodology can be understood by analogy to the collinearity bias problem in geographically weighted regressions. By making a methodology that incorporates the coupled nature of the data sets, we would produce an analysis is less sensitive to technical judgement and makes it easier to include a wider variety of data sources.

The experimental objective of the current text was to produce a mesoscopic quantum reaction-transport model that could bridge the two data sets. Indeed, the reaction-transport QSP was derived explicitly as an operationalized quantization of the Pál-Bell equation for neutron transport. Consequently, it is apparent that it is appropriate for modeling a transport system. It remains for us to show that the individual functional parameters of the resulting model can be modeled using scattering experiments. In fact, the PDP formula itself can be understood as a chain of scattering experiments carried out at different sites in the nuclear system.

6.1.3 The Full Reaction-Transport PDP

In order to understand physical content of the representation theorem 5.10.1 in the context of nuclear data analysis, we will start from the most general formula that we obtained for the PDP representation of the reaction transport QSP and systematically reduce it a case that represents a conventional scattering experiment. We will assemble all of the contributing definitions in one place for easy comparison

Any interval product constrained and (obviously) time ordered set of R, say $E_t^m = \prod_{i=1}^m (E_i \times (r_i, t_i]) \cap X_t$ where $E_t^m \subset A_t^m$, can be given a value under the operator valued measure by the definition

$$\mathscr{E}_t(E_t^m, \boldsymbol{\rho}) = \iiint\limits_{0<s_1<s_2<\cdots<s_m\leq t} \chi_{D_t}(s_m, \ldots, s_1)\, \mathscr{J}(\prod_{i=1}^m E_i \times s_i, \boldsymbol{\rho}) \tag{6.1.3.1}$$

where

$$\iiint\limits_{0<s_1<s_2<\cdots<s_m\leq t} f \equiv \int_0^t \mathrm{d}s_m \int_0^{s_m} \mathrm{d}s_{m-1} \ldots \int_0^{s_3} \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 f$$

is a time ordered integral.

$$\chi_{D_t}(s_m, \ldots, s_1) = \prod_{i=1}^m \chi_{(r_i,\, t_i]}(s_i)$$

is a product characteristic function on the time intervals for each reaction.

$$\mathscr{J}(\prod_{i=1}^m E_i \times s_i, \boldsymbol{\rho}) = \boldsymbol{S}_{t-s_m} \mathscr{J}(E_m) \boldsymbol{S}_{s_m - s_{m-1}} \mathscr{J}(E_{m-1}) \ldots \mathscr{J}(E_1) \boldsymbol{S}_{s_1} \boldsymbol{\rho}$$

is the Reaction-Transport Transition PMV measure iteratively composed with fixed duration Collisionless

Reaction Transport Propagators to cover m reaction events in the typed geographic phase space Borel sets (E_i) at times (s_i). Specifically, $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$ with $\|\boldsymbol{B}_t\| \leq 1$, $\boldsymbol{B}_t$ having a generator $\boldsymbol{Y}$ and

$$\begin{aligned}\boldsymbol{S}_t\boldsymbol{\rho} &= \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^* \\ &= \sum_{n+m\leq N}\sum_{n'+m'\leq N}(\Pi_{n,m}\Pi_F^n\boldsymbol{B}_t\Pi_F^n \otimes \Pi_B^m\boldsymbol{B}_t\Pi_B^m\Pi_{n,m})\boldsymbol{\rho}(\Pi_{n',m'}\Pi_F^{n'}\boldsymbol{B}_t\Pi_F^{n'} \otimes \Pi_B^{m'}\boldsymbol{B}_t\Pi_B^{m'}\Pi_{n',m'})^*\end{aligned}$$

where $\Pi_F^n\boldsymbol{B}_t\Pi_F^n = \bigotimes_{i=1}^n \Pi_{F,i}^1\boldsymbol{B}_t^1\Pi_{F,i}^1$ and $\Pi_B^m\boldsymbol{B}_t^1\Pi_B^m = \bigotimes_{i=1}^m \Pi_{B,i}^1\boldsymbol{B}_t\Pi_{B,i}^1$ with $\Pi_F^1\boldsymbol{B}_t^1\Pi_F^1$ a strongly continuous semigroup on a single free particle space having a generator $\boldsymbol{Y}_F^1$ and $\Pi_B^1\boldsymbol{B}_t^1\Pi_B^1$ is a strongly continuous semigroup on a single bound particle space having a generator $\boldsymbol{Y}_B^1$. While, for $E_i = F_i \times T_i \in \mathscr{G}$

$$\mathscr{J}(E_i)\boldsymbol{\rho} = \frac{1}{(2\pi)^3}\int_{F_i} \mathrm{d}^3x\ \mathrm{d}^3k \sum_{\ell\in T_i} \boldsymbol{U}_{\boldsymbol{\ell}}\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|\boldsymbol{V}_{x,k,\ell}\boldsymbol{\rho}\boldsymbol{V}_{x,k,\ell}^*\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|\boldsymbol{U}_\ell^*$$

Where a detection operator, $\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|\boldsymbol{V}_{x,k,\ell}$ is to be understood as being applied to each particle of a free or bound state Fock space separately with the remaining particles being transformed by identity operators. Each detection operator only applies to either the free subspace or the bound subspace, not both. $\boldsymbol{U}_{\boldsymbol{\ell}}$ is an absorption operator or a decay operator acting between fixed particle number subspaces for each $\ell \in T$ and so the composition yields a sum over j index for removal, so that an absorption takes the form

$$\sum_{j=1}^n \boldsymbol{e}_{a,\ell}^j\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|_j\boldsymbol{V}_{x,k,\ell}^j$$

where the existing bound states are injectively mapped into the higher particle number bound space. While a decay, takes the form

$$\sum_{j=1}^m \boldsymbol{e}_{d,\ell}^j\left|\alpha_{x,k}\right\rangle\left\langle\alpha_{x,k}\right|_j\boldsymbol{V}_{x,k,\ell}^j$$

where the existing free states are injectively mapped into the higher particle number free space.

Finally, we note that for any $\alpha \in D(\boldsymbol{P}) \cap D(\boldsymbol{Q}) \cap L_2(\mathbb{R}^3,\mathbb{R};m) \cap L_1(\mathbb{R}^3,\mathbb{R};m)$ such that $\alpha(-\bar{q}) = \alpha(\bar{q})$ and

$$\int(-i)\nabla_{\bar{q}}\alpha(\bar{q})\alpha(\bar{q})^* = \langle\boldsymbol{P}\alpha,\alpha\rangle = 0 = \langle\boldsymbol{Q}\alpha,\alpha\rangle = \int\bar{q}\alpha(\bar{q})\alpha(\bar{q})^* \tag{6.1.3.2}$$

and $\|\alpha\|_2 = 1$, typified by the gaussian distribution, we can define a vector $\alpha_{x,k}$ (hereafter referred to as the apparatus function), that is given in the relevant L_2 representation as

$$\alpha_{x,k}(\bar{q}) = e^{i\bar{k}\cdot\bar{q}}\alpha(\bar{q}-\bar{x})$$

then the following trace norm convergent integral is an instrument adjoint to the joint phase space observable defined in terms of a kind of "apparatus state basis",

$$\mathscr{A}(E,\cdot) = \frac{1}{(2\pi)^3}\int_E \mathrm{d}^3x\ \mathrm{d}^3k\, |\alpha_{x,k}\rangle\langle\alpha_{x,k}| \cdot |\alpha_{x,k}\rangle\langle\alpha_{x,k}|$$

where $\mathrm{d}^3x\ \mathrm{d}^3k$ is the product of the Lebesgue measure on $\mathbb{R}^3 \times \mathbb{R}^3$. This fact is what allows us to define the detection operators, decay operators, and absorption operators in terms of apparatus states.

This entire construction applies to $\boldsymbol{\rho} \in \mathscr{T}_+(\mathscr{H})$ which by the spectral representation theorem can be expressed as $\boldsymbol{\rho} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ such that $\sum_i \lambda_i = 1$ and $\lambda_i \geq 0$ and $\{|\psi_i\rangle\}$ is an orthonormal basis in $\mathscr{H} = \mathscr{H}_F \otimes \mathscr{H}_B$. We can further decompose the

$$\mathscr{H}_F = \bigoplus_{n=1}^{N} \bigotimes_{i=1}^{n} \mathscr{H}_F^1 \bigoplus c_F$$

The single free particle Hilbert space is of the form $\mathscr{H}_F^1 = L_2(\mathbb{R}^3, \mathbb{C}) \otimes \mathbb{C}^{k_F}$ having a phase space distribution function (represented in whatever way is convenient, say an L_2 coordinate space representation or a phase space quantized $\mathbb{R}^6$ distribution) and a k_F vector for indicating a kind of species index. In practice, we will almost always use $k_F = 1$ so that the free states are just phase space distributions. Likewise,

$$\mathscr{H}_B = \bigoplus_{n=1}^{N} \bigotimes_{i=1}^{n} \mathscr{H}_B^1 \bigoplus c_b$$

The single free particle Hilbert space is of the form $\mathscr{H}_B^1 = L_2(\mathbb{R}^3, \mathbb{C}) \otimes \mathbb{C}^{k_B}$ having a phase space distribution function (represented in whatever way is convenient, say an L_2 momentum space representation) and a k_B vector for indicating a kind of species index. In this representation we have left off the e_F and e_B vectors tensored to each particle to indicate whether they belong to the free or bound subspace. This would mostly serve an obscuring function in the formulas that we present below so we take it to be implicit.

In our free and bound space we have allowed for both a phase space distribution and a species representation. We have ignored an important physical issue up until now. We have not provided a mechanism for modeling transmutation of the medium. In a nuclear reactor, this would be a burn-up model. As a result, we do not yet have a model that can fully capture our vision for how correlations are communicated between neutrons by changes that occur in the medium during collisions. Moreover, such a mechanism can be used to constrain the maximum number of multiparticle decays into the medium (and so the total number of particles). The decision of how to represent this depends on how the reaction types are used to couple free and bound states. In the examples that follow, we will see two different approaches to this issue that come

with different limitations.

To begin with, we can always append an additional collection of classical states to the bound subspace that only transform under bound collisionless evolutions or absorption and decay events. This can be thought of as a supply of quiescent neutrons that can be activated or decay into the medium during nuclear transmutations. The accounting of this by reaction type is a very specific nuclear decay chain modeling exercise that is common to the analysis of nuclear systems. In general, we can represent this by extending the Hilbert space by forming a tensor product with a Hilbert subspace for the medium $\mathscr{H}_{\text{medium},\ell}$ as a fixed product of finite dimensional subspaces

$$\mathscr{H} = \mathscr{H}_F \otimes \mathscr{H}_B \otimes \bigotimes_{\ell=1}^{k_T} \mathscr{H}_{\text{medium},\ell}$$

then we can modify the collisionless evolution to have independent evolutions of the neutrons and the state of the medium (leaving off the (n, m) particle count subspace projectors as implicit)

$$\begin{aligned}
&\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^* \\
&= \sum_{n+m\leq N} \sum_{n'+m'\leq N} (\Pi_F^n \boldsymbol{B}_t \Pi_F^n \otimes \Pi_B^m \boldsymbol{B}_t \Pi_B^m \otimes \Pi_{\text{med}} \boldsymbol{B}_t \Pi_{\text{med}}) \boldsymbol{\rho} (\Pi_F^{n'} \boldsymbol{B}_t \Pi_F^{n'} \otimes \Pi_B^{m'} \boldsymbol{B}_t \Pi_B^{m'} \otimes \Pi_{\text{med}} \boldsymbol{B}_t \Pi_{\text{med}})^*
\end{aligned}$$

We can modify the jump operators to incorporate correlated transformations on the prior state of the medium that requires available absorption states

$$\boldsymbol{e}_{a,\ell}^j |\alpha_{x,k}\rangle \langle\alpha_{x,k}|_j \boldsymbol{V}_{x,k,\ell}^j |\psi\rangle = 0 \; \forall \Pi_{\text{med},\ell} |\psi\rangle = v \text{ s.t.} v_i = 0 \forall i < k_f^\ell \tag{6.1.3.3}$$

This zero condition will only be realized when bound neutrons absorbed at an index have displaced all of the quiescent neutrons into a higher energy state. In this case the site ℓ is "full". We also requires more than some minimum number of quiescent neutrons available to be freed into the medium for a decay to occur

$$\boldsymbol{e}_{d,\ell}^j |\alpha_{x,k}\rangle \langle\alpha_{x,k}|_j \boldsymbol{V}_{x,k,\ell}^j |\psi\rangle = 0 \; \forall \Pi_{\text{med},\ell} |\psi\rangle = v \text{ s.t.} v_i = 0 \forall i > k_{\min,\ell} \tag{6.1.3.4}$$

This zero condition will only be realized when decays have already emitted all neutrons available to be freed out of the medium.

That is, if too many neutrons are already bound to the nuclear site more cannot be absorbed. If the nucleus has been transmuted into a state that cannot effectively release neutrons at the given collision energy then more cannot decay. At the same time, when a jump does occur we need to account for how the medium

is transformed in a manner that is quantum correlated with the change in the distribution of free and bound neutrons. Thus, we redefine the absorption and decay operators as follows

Definition 6.1.1. *Correlation Encoding Absorption Operator*

An absorption operator $\boldsymbol{e}^{j}_{a,\ell}$ *is a map between a fixed particle number apparatus state in the free subspace and a fixed particle number apparatus state in the bound subspace. That is, given* $|\psi_1\rangle \in \mathscr{H}_F, |\phi_1\rangle \in \mathscr{H}_B, \bar{v}_1 \in \mathbb{C}^{k_{T,\ell}}$, *where*

$$|\psi_1\rangle = \left|\psi_1^1\right\rangle \otimes \cdots \otimes \left|\alpha_{x_j,k_j}\right\rangle \otimes \cdots \otimes |\psi_1^{n_1}\rangle$$
$$|\phi_1\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle$$
$$\bar{v}_1 = \sum_{i=1}^{k_{T,\ell}} c_i \bar{e}_i$$

, $\exists\, |\psi_2\rangle \in \mathscr{H}_F, |\phi_2\rangle \in \mathscr{H}_B, \bar{v}_2 \in \mathbb{C}^{k_{T,\ell}}$, *where*

$$|\psi_2\rangle = \bigotimes_{i=1}^{j-i} \left|\psi_1^i\right\rangle \otimes \bigotimes_{i=j+i}^{n_1} \left|\psi_1^i\right\rangle$$
$$|\phi_2\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle \otimes \gamma_\ell(\left|\alpha_{x_j,k_j}\right\rangle)$$
$$\bar{v}_2 = \sum_{i=2}^{k_{T,\ell}} c_{i-1} \bar{e}_i$$

and γ_ℓ *maps one apparatus state to a tensor product of some fixed number of apparatus states with each particle unitarily transformed by an operator* $\hat{\boldsymbol{U}}_\ell$ *and*

$$\boldsymbol{e}^{j}_{a,\ell} |\psi_1\rangle \otimes |\phi_1\rangle \otimes \bar{v}_1 = |\psi_2\rangle \otimes |\phi_2\rangle \otimes \bar{v}_2 \tag{6.1.3.5}$$

Note that this projects on to only states of the appropriate initial particle numbers in the free and bound states.

Remark

We have chosen a basis such that the absorption functions like a shift operator. The result is a partial isometry that maps some vectors to zero. This is meant to mimic the structure of Fermionic quantizations by creation operators. In practice, we will need to be a little more subtle in our treatment of transmutations in the medium but this is a schematic model.

Definition 6.1.2. *Correlation Encoding Decay Operator*

A decay operator is a map $\boldsymbol{e}^{j}_{d,\ell}$ *between a fixed particle number apparatus state in the bound subspace and a fixed particle number apparatus state in the free subspace. That is, given* $|\psi_1\rangle \in \mathscr{H}_B, |\phi_1\rangle \in \mathscr{H}_F, \bar{v}_1 \in \mathbb{C}^{k_{T,\ell}}$*, where*

$$|\psi_1\rangle = \left|\psi_1^1\right\rangle \otimes \cdots \otimes \left|\alpha_{x_j,k_j}\right\rangle \otimes \cdots \otimes |\psi_1^{n_1}\rangle$$
$$|\phi_1\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle$$
$$\bar{v}_1 = \sum_{i=1}^{k_{T,\ell}} c_i \bar{e}_i$$

, $\exists\, |\psi_2\rangle \in \mathscr{H}_B, |\phi_2\rangle \in \mathscr{H}_F, \bar{v}_2 \in \mathbb{C}^{k_{T,\ell}}$*, where*

$$|\psi_2\rangle = \bigotimes_{i=1}^{j-i} \left|\psi_1^i\right\rangle \otimes \bigotimes_{i=j+i}^{n_1} \left|\psi_1^i\right\rangle$$
$$|\phi_2\rangle = \bigotimes_{i=1}^{m_1} \left|\phi_1^i\right\rangle \otimes \gamma_\ell(\left|\alpha_{x_j,k_j}\right\rangle)$$
$$\bar{v}_2 = \sum_{i=1}^{k_{T,\ell}-r} c_{i+r} \bar{e}_i$$

and γ_ℓ^r *maps one apparatus state to a tensor product of* r *apparatus states, each particle unitarily transformed by an operator* $\hat{\boldsymbol{U}}_\ell$ *and*

$$\boldsymbol{e}^{j}_{d,\ell} |\psi_1\rangle \otimes |\phi_1\rangle \otimes \bar{v}_1 = |\psi_2\rangle \otimes |\phi_2\rangle \otimes \bar{v}_2 \tag{6.1.3.6}$$

Note that this projects on to only states of the appropriate initial particle numbers in the free and bound states.

If we allow more than one value of r*, we should include* r *sub ranges in our sums over* $\ell \in T$

Remark

We have chosen a basis such that the decay functions like an adjoint shift operator applied r times. The result is a partial isometry that maps some vectors to zero. This is meant to mimic the structure of Fermionic quantizations by annihilation operators. In practice, we will need to be a little more subtle in our treatment of transmutations in the medium but this is a schematic model.

This is a crude classical accounting kind of representation for the medium, but it conveys the essential idea. In general, some transitions are forbidden and corresponding gain in particle number is impossible.

In order to make this scheme work it will prove necessary to constrain the neutron number and medium transmutation state to be entangled in a way the conserves total particle number. We can always argue that the combined system decoheres into a product classical state generally. With this argument in mind we will typically consider states $\boldsymbol{\rho}$ and collisionless evolutions that are suitably diagonal in particle number. At this point, we have laid out a fairly general model that is too complex to make sense of all at once. In order to analyze the physics of this system we will introduce a series of simplifications that are fully compatible with modeling the jump operators that the QSP is assembled from.

6.1.4 The Single-Particle, Single-Collision Reaction-Transport PDP

By the spectral representation, we can develop a sound understanding of this problem by looking at a pure state $\boldsymbol{\rho} = |\psi\rangle\langle\psi|$ for $|\psi\rangle \in \mathscr{H}$. Moreover, since our system is built out of single reaction chains of the form $\boldsymbol{S}_{t-s_1}\mathscr{J}(E_1)\boldsymbol{S}_{s_1}$, we don't sacrifice anything by building our understanding up from the examination of a single reaction. We can easily add in a constraint on the time interval in which we allow the event to occur. However, this adds nothing interesting when we are looking as a single reaction. Instead, we consider a simpler rectangular set on which to evaluate the reaction-transport QSP's PDP formula, $E = E_1 \times (0,t] \subset A_t^1$ where $E_1 \in \mathscr{G}$

Now we have the simplified expression,

$$\begin{aligned}
\mathscr{E}_t(E,\boldsymbol{\rho}) &= \int_0^t \mathrm{d}s_1 \boldsymbol{S}_{t-s_1}\mathscr{J}(E_1)\boldsymbol{S}_{s_1}\boldsymbol{\rho} \\
&= \int_0^t \mathrm{d}s_1 \boldsymbol{B}_{t-s_1}\mathscr{J}\left(E_1, \boldsymbol{B}_{s_1}|\psi\rangle\langle\psi|\boldsymbol{B}_{s_1}^*\right)\boldsymbol{B}_{t-s_1}^* \\
&= \int_0^t \mathrm{d}s_1 \boldsymbol{B}_{t-s_1}\mathscr{J}\left(E_1, |\boldsymbol{B}_{s_1}\psi\rangle\langle\boldsymbol{B}_{s_1}\psi|\right)\boldsymbol{B}_{t-s_1}^*
\end{aligned}$$

Even for this simplified construction, if we were to evaluate the full $\mathscr{J}$ on an arbitrary number of particles and set of reaction types, the result would be a sum of reaction types and particle index. To focus on the individual neutron dynamics, we can focus on the single particle case. Although a particle must be explicitly in the bound or free subspace, lets gloss over this point for a moment an focus instead on the general form of the reaction term. The collisionless evolution does not connect spaces with different numbers of bound and free particles. Thus, regardless of what subspace the single particle wave function $|\psi_1\rangle\langle\psi_1|$ belongs to at $s = 0$, we will find that $|\boldsymbol{B}_{s_1}\psi_1\rangle\langle\boldsymbol{B}_{s_1}\psi_1| = |\psi_1(s_1)\rangle\langle\psi_1(s_1)|$ is in the same subspace. Therefore we can focus on the restriction of the jump operator to an incoming bound or free subspace with impunity

$\mathscr{J}(E_1, |\psi_1(s_1)\rangle \langle\psi_1(s_1)|) = \mathscr{J}(E_1, \Pi_{B/F} |\psi_1(s_1)\rangle \langle\psi_1(s_1)| \Pi_{B/F})$. Thus, focusing on a single reaction ℓ, we arrive at the form

$$\mathscr{E}_t(E, \boldsymbol{\rho}) = \int_0^t \mathrm{d}s_1 \boldsymbol{B}_{t-s_1} \frac{1}{(2\pi)^3} \int_{E_1} \mathrm{d}^3x \; \mathrm{d}^3k \boldsymbol{U}_{\boldsymbol{\ell}} |\alpha_{x,k}\rangle \langle\alpha_{x,k}| \boldsymbol{V}_{x,k,\ell} |\boldsymbol{B}_{s_1}\psi\rangle \langle\boldsymbol{B}_{s_1}\psi| \boldsymbol{V}^*_{x,k,\ell} |\alpha_{x,k}\rangle \langle\alpha_{x,k}| \boldsymbol{U}^*_{\ell} \boldsymbol{B}^*_{t-s_1} \tag{6.1.4.1}$$

$$= \int_0^t \mathrm{d}s_1 \frac{1}{(2\pi)^3} \int_{E_1} \mathrm{d}^3x \; \mathrm{d}^3k |\langle\alpha_{x,k}| \boldsymbol{V}_{x,k,\ell} |\boldsymbol{B}_{s_1}\psi\rangle|^2 \; |\boldsymbol{B}_{t-s_1}\boldsymbol{U}_{\boldsymbol{\ell}}\alpha_{x,k}\rangle \langle\boldsymbol{B}_{t-s_1}\boldsymbol{U}_{\boldsymbol{\ell}}\alpha_{x,k}| \tag{6.1.4.2}$$

Here we have brought the operators inside the vectors to indicate that they can be evaluated as acting on the single particle component in the L_2 representation of the relevant subspace with some other rotation-like transformation between subspaces happening apart from this and a shift happening in the medium. In order to understand the transformation between subspaces we will need to assume an initial configuration of the particle and medium. However, before we get into those subspace coupling details, we can comment further on the interpretation of the above single particle reaction formula in terms of conventional quantum mechanical perturbation theory.

The function $|\langle\alpha_{x,k}| \boldsymbol{V}_{x,k,\ell} |\boldsymbol{B}_{s_1}\psi\rangle|^2$ constitutes an ℓ reaction channel coupling probability density in the neighborhood of $\bar{x}, \bar{k}$ where the scale of the neighborhood is determined by the function α. Here the indexed operator family $\boldsymbol{V}_{x,k,\ell}$ can take a variety of forms but the intent of the notation is to evoke perturbation theoretic transition rates (such as in Fermi's Golden Rule) for some potential operator as an interaction hamiltonian. Indeed, both scattering models and condensed matter state transitions in the presence of a perturbing force conform to this structure. From this point of view, the transformation $|\langle\alpha_{x,k}| \boldsymbol{V}_{x,k,\ell} |\boldsymbol{B}_{s_1}\psi\rangle|^2 |\alpha_{x,k}\rangle \langle\alpha_{x,k}|$ corresponds to the preparation of a well defined "incoming" state weighted by the probability of its formation. This should be thought of as a detection process and relates to the condensed matter localization for free states or nuclear localization for bound states. These incoming states are not the generalized vectors common to Fourier analysis methods in informal scattering theory. Instead, they are more akin to a wavelet basis with a finite minimum scale. In order to proceed, we will need to look at a further simplified subset E_1 and examine the special cases of absorption and decay reactions separately.

Suppose $E_1 = B_{\bar{x},r} \times S_{\bar{k},\delta\theta,\delta k} \times \{\ell_1\} \in \mathscr{G}$. $B_{\bar{x},r}$ is a position space ball centered at $\bar{x}$ of radius r. $S_{\bar{k},\delta\theta,\delta k}$ is a momentum space shell segment centered at $\bar{k}$ with an angular extent (in polar angle relative to $\bar{k}$) of $\delta\theta$ and a radial thickness of δk. Using this, we can make the computation more explicit and more familiar from balance equation construction of neutron transport formulas. Moreover, in the models that we will discuss and at the energies and densities common to practical nuclear systems, we can use this phase space window

to differentiate individual neutron beamlets and reaction modes. Therefore, we can view this choice of phase space volume as a means of justifying the simplification to a single neutron beamlet and a single reaction type. So, instead of an approximation, we can view the resulting formula as evaluation on a measurement set chosen to simplify the expression. Specifically, by evaluating the QSP on this measurement set, we end up with a local evaluation that is equivalent to a single nuclear reaction experiment.

$$\mathscr{E}_t(E,\boldsymbol{\rho}) = \int_0^t \mathrm{d}s_1 \frac{1}{(2\pi)^3} \int_{B_{\bar{x},r}} \mathrm{d}^3x \int_{S_{\bar{k},\delta\theta,\delta k}} \mathrm{d}^3k |\langle \alpha_{x,k}| \boldsymbol{V}_{x,k,\ell} |\boldsymbol{B}_{s_1}\psi\rangle|^2 \ |\boldsymbol{B}_{t-s_1}\boldsymbol{U}_{\boldsymbol{\ell}}\alpha_{x,k}\rangle \langle \boldsymbol{B}_{t-s_1}\boldsymbol{U}_{\boldsymbol{\ell}}\alpha_{x,k}| \tag{6.1.4.3}$$

Absorption Process for Single Free Neutron

Although the above observations are interesting, we can gain a great deal more insight be viewing the reaction event as specifically an absorption or a decay. We will begin by considering the absorption of a free particle. Let's suppose that our phase space window isolates a single free neutron (that is not entangled with any other neutrons) and no bound neutrons. Moreover, suppose that the local medium is in a quiescent state. Specifically, for the only viable reaction $\ell \in T$, $\bar{v}^\ell = 1\bar{e}_1$. Then we can trace over all other particles in the system to obtain a model for the reduced density matrix including no decay reactions as none are possible using the correlation encoding decay operator. Written as a state, the density matrix takes a simplified form within the measurement window that is isomorphic to a single particle density matrix,

$$\boldsymbol{\rho}_1 = |\psi \otimes c_B \otimes 1\bar{e}_1\rangle \langle \psi \otimes c_B \otimes 1\bar{e}_1| \tag{6.1.4.4}$$

Now when we apply the evolution, we can define a single particle collisionless evolution on a single particle free space as $\boldsymbol{B}_{F,t}$ and a single particle evolution on the bound space as $\boldsymbol{B}_{B,t}$. Then we can represent the single reaction PDP as

$$\mathscr{E}_t(E,\boldsymbol{\rho}_1) = \int_0^t \mathrm{d}s_1 \frac{1}{(2\pi)^3} \int_{B_{\bar{x},r}} \mathrm{d}^3x \int_{S_{\bar{k},\delta\theta,\delta k}} \mathrm{d}^3k |\langle \alpha_{x,k}| \boldsymbol{V}_{x,k,\ell,a} |\boldsymbol{B}_{F,s_1}\psi\rangle|^2$$
$$|c_F \otimes \boldsymbol{B}_{B,t-s_1}\boldsymbol{U}_{\ell,a}\alpha_{x,k} \otimes 1\bar{e}_2\rangle \langle c_F \otimes \boldsymbol{B}_{B,t-s_1}\boldsymbol{U}_{\ell,a}\alpha_{x,k} \otimes 1\bar{e}_2| \tag{6.1.4.5}$$

Now, $|\langle \alpha_{x,k}| \boldsymbol{V}_{x,k,\ell,a} |\boldsymbol{B}_{F,s_1}\psi\rangle|^2$ can be understood as a macroscopic detection probability of the neutron beamlet being sampled in a scattering state $|\alpha_{x,k}\rangle \langle \alpha_{x,k}|$. Then $\boldsymbol{U}_{\ell,a}$ would be the contracting Moller wave operator that connects the scattering state to a reaction channel. We have performed the subspace rotation

explicitly in our pure state representation but used the same symbol for $\boldsymbol{U}_{\ell,a}$ even though in this case it is only the representation transformation unitary. Finally, we note that $\boldsymbol{B}_{B,t-s_1}$ is the quasi-bound state "hamiltonian" evolution. In this case, $\boldsymbol{B}_{B,t-s_1}$ is actually contractive (rather than unitary) due to conservation of probability accounting for decays back into the free neutron field. This is characteristic of evolutions driven by generalized optical potentials. [59]

Before dealing with the decay case, it is worth taking a moment to think about a matter of scale. Fundamentally, $\boldsymbol{B}_{B,t-s_1}$ describes an internal nuclear process that occurs at nuclear spatial and energy scales. On the other hand, in spite of describing neutrons, $\boldsymbol{B}_{F,s_1}$ transforms distributions with predominantly atomic scales. The reason for this is that, when a nucleus decays, there is an atomic scale uncertainty in the position of the nucleus within the atom resulting from thermal oscillations within the condensed matter lattice. How do we transform between these scales? Fundamentally, for a given absorption-decay pair, we have 4 operator families ($\boldsymbol{U}_{\ell,a}, \boldsymbol{V}_{x,k,\ell,a}, \boldsymbol{U}_{\ell,d}, \boldsymbol{V}_{x,k,\ell,d}$) and an apparatus function α. These can be chosen consistently to guarantee that the scale is captured correctly by the dispersion in any wavefunction produced by intial free beamlet gaussians at atomic scales. In fact, this can be done for every choice of α. So, a question arises as to whether there is a natural form and scale for the apparatus function. It seems like the apparatus function is a natural candidate for simplifying the form of the other operators and possibly enforcing useful symmetries locally. Moreover, it may be a convenient tool for introducing a scaling argument as we pass to a continuum limit in the classical case. For these reasons, we developed a theory in chapter 5 that does not demand a particular prior form or scale, even though it seems that an atomic scale gaussian is a physically natural choice for describing the free states.

Decay Process for Single Bound Neutron

We will now consider the decay of a bound particle. Let's suppose that our phase space window isolates a single bound neutron (that we treat approximately as not being entangled with any other neutrons) and no free neutrons. Moreover, suppose that the local medium is in a singly excited state. Specifically, for the only viable reaction $\ell \in T$, $\bar{v}^{\ell} = 1\bar{e}_2$. Then we can trace over all other particles in the system to obtain a model for the reduced density matrix including a single neutron decay reaction as no other reaction is possible using the correlation encoding decay operator. Written as a state, this takes a simplified form (isomorphic to single particle density amtrix) within the measurement window,

$$\boldsymbol{\rho}_2 = |c_F \otimes \phi \otimes 1\bar{e}_2\rangle \langle c_F \otimes \phi \otimes 1\bar{e}_2| \tag{6.1.4.6}$$

Now when we apply the evolution, we can define a single particle collisionless evolution on a single particle free space as $\boldsymbol{B}_{F,t}$ and a single particle evolution on the bound space as $\boldsymbol{B}_{B,t}$. Then we can represent the single reaction PDP as

$$\mathscr{E}_t(E,\boldsymbol{\rho}_2) = \int_0^t \mathrm{d}s_1 \frac{1}{(2\pi)^3} \int_{B_{\bar{x},r}} \mathrm{d}^3x \int_{S_{\bar{k},\delta\theta,\delta k}} \mathrm{d}^3k |\langle \alpha_{x,k}| \boldsymbol{V}_{x,k,\ell,d} |\boldsymbol{B}_{B,s_1}\phi\rangle|^2 \\ |\boldsymbol{B}_{F,t-s_1}\boldsymbol{U}_{\ell,d}\alpha_{x,k} \otimes c_B \otimes 1\bar{e}_1\rangle \langle \boldsymbol{B}_{F,t-s_1}\boldsymbol{U}_{\ell,d}\alpha_{x,k} \otimes c_B \otimes 1\bar{e}_1| \quad (6.1.4.7)$$

Now, $|\langle \alpha_{x,k}| \boldsymbol{V}_{x,k,\ell,d} |\boldsymbol{B}_{B,s_1}\psi\rangle|^2$ can be understood as a microscopic escape probability of the bound excited neutron decaying in an unbound continuum state $|\alpha_{x,k}\rangle \langle \alpha_{x,k}|$. Then $\boldsymbol{U}_{\ell,d}$ would be the dilating Moller wave operator that connects a continuum channel to a free beamlet state. We have performed the subspace rotation explicitly in our pure state representation but used the same symbol for $\boldsymbol{U}_{\ell,d}$ even though in this case it is only the representation transformation unitary. Finally, we note that $\boldsymbol{B}_{B,s_1}$ is the quasi-bound state "hamiltonian" evolution. In this case, $\boldsymbol{B}_{B,s_1}$ is actually contractive (rather than unitary) due to conservation of probability accounting for decays back into the free neutron field. This is characteristic of evolutions driven by generalized optical potentials. [59]

6.1.5 The Single-Particle, Two-Collision Reaction-Transport PDP

Now we are in a position to combine these events into an absorption followed by a decay that models compound elastic (or inelastic) scattering via a generalized optical potential. In order to achieve this, we will start from the prior state of the single absorption case. Let's suppose that our phase space window isolates a single free (non-entangled) neutron and no bound neutrons. Moreover, suppose that the local medium is in a quiescent state. Specifically, for the only viable reaction $\ell \in T$, $\bar{v}^\ell = 1\bar{e}_1$. Thus, no decay reactions are possible using the correlation encoding decay operator. Written as a state, the reduced density matrix is isomorphic to a simplified single particle density matrix within the absorption measurement window,

$$\boldsymbol{\rho}_1 = |\psi \otimes c_B \otimes 1\bar{e}_1\rangle \langle \psi \otimes c_B \otimes 1\bar{e}_1| \quad (6.1.5.1)$$

Now, we will use the two-reaction version of the PDP for an absorption in $E_1 = B_{\bar{x_1},r_1} \times S_{\bar{k_1},\delta\theta_1,\delta k_1} \times \{\ell_1\} = B_1 \times S_1 \times \{\ell, a\}$ followed by a decay into $E_2 = B_{\bar{x_2},r_2} \times S_{\bar{k_2},\delta\theta_2,\delta k_2} \times \{\ell_2\} = B_2 \times S_2 \times \{\ell, d\}$. Moreover, we will suppose that both happen in the interval $(0,t]$ but we will not further constrain their respective time domains. We haven't as yet had a need for a notation that supports arbitrary time ordered events in known typed geographic phase space domains. For simplicity, we will use $E_1 \times E_2$ to indicate all time ordered

sequences of events in E_1 followed by E_2.

$$\begin{aligned}
\mathscr{E}_t(E_1 \times E_2, \boldsymbol{\rho}_1) &= \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 \boldsymbol{S}_{t-s_2} \mathscr{J}(E_2) \mathrm{d}s_1 \boldsymbol{S}_{s_2-s_1} \mathscr{J}(E_1) \boldsymbol{S}_{s_1} \boldsymbol{\rho}_1 \\
&= \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 \boldsymbol{B}_{t-s_2} \mathscr{J}\left(E_2, \boldsymbol{B}_{s_2-s_1} \mathscr{J}\left(E_1, \boldsymbol{B}_{s_1} |\psi\rangle \langle\psi| \boldsymbol{B}_{s_1}^*\right) \boldsymbol{B}_{s_2-s_1}^*\right) \boldsymbol{B}_{t-s_2}^* \\
&= \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 \boldsymbol{B}_{t-s_2} \mathscr{J}\left(E_2, \boldsymbol{B}_{s_2-s_1} \mathscr{J}\left(E_1, |\boldsymbol{B}_{s_1}\psi\rangle \langle \boldsymbol{B}_{s_1}\psi|\right) \boldsymbol{B}_{s_2-s_1}^*\right) \boldsymbol{B}_{t-s_2}^*
\end{aligned}$$

Now, to proceed further, we will repeat the single reaction type reduction. This of course is a point where we could introduce a sub-summation over reaction types compatible with the same channel but that would obscure the formula in a way that is unhelpful at the moment.

$$\begin{aligned}
&\mathscr{E}_t(E_1 \times E_2, \boldsymbol{\rho}_1) = \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 \boldsymbol{B}_{t-s_2} \\
&\mathscr{J}\left(E_2, \frac{1}{(2\pi)^3} \int_{B_1} \mathrm{d}^3 x_1 \int_{S_1} \mathrm{d}^3 k_1 |\langle \alpha_{x_1,k_1}| \boldsymbol{V}_{x_1,k_1,\ell,a} |\boldsymbol{B}_{F,s_1}\psi\rangle|^2 \ |\boldsymbol{B}_{B,s_2-s_1} \boldsymbol{U}_{\ell,a} \alpha_{x_1,k_1}\rangle \langle \boldsymbol{B}_{B,s_2-s_1} \boldsymbol{U}_{\ell,a} \alpha_{x_1,k_1}|\right) \boldsymbol{B}_{t-s_2}^* \\
&= \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_1 \frac{1}{(2\pi)^3} \int_{B_2} \mathrm{d}^3 x_2 \int_{S_2} \mathrm{d}^3 k_2 |\boldsymbol{B}_{F,t-s_2} \boldsymbol{U}_{\ell,d} \alpha_{x_2,k_2}\rangle \langle \boldsymbol{B}_{F,t-s_2} \boldsymbol{U}_{\ell,d} \alpha_{x_2,k_2}| \\
&\frac{1}{(2\pi)^3} \int_{B_1} \mathrm{d}^3 x_1 \int_{S_1} \mathrm{d}^3 k_1 |\langle \alpha_{x_1,k_1}| \boldsymbol{V}_{x_1,k_1,\ell,a} |\boldsymbol{B}_{F,s_1}\psi\rangle|^2 \ |\langle \alpha_{x_2,k_2}| \boldsymbol{V}_{x_2,k_2,\ell,d} |\boldsymbol{B}_{B,s_2-s_1} \boldsymbol{U}_{\ell,a} \alpha_{x_1,k_1}\rangle|^2
\end{aligned}$$

Note that in the second equality we used the trace norm convergence of the integral (and thus its weak convergence) to apply the inner product (due to the second application of $\mathscr{J}$) inside the absorption integral.

The form that we have derived lends itself to direct evaluation for a given model. Moreover, it gives a form that is easily interpreted as a differential nuclear reaction experiment where an absorption is followed by a decay into an integral over outgoing states. The interior integral pair can be interpreted as a compound scattering density as a function of the decay position and momentum x_2, k_2. We can compare this to Goldberger and Watson's classic analysis of macroscopic wavepacket scattering ([65] chapter 3) to interpret the $\boldsymbol{V}_{x_1,k_1,\ell,a}$ operator. In particular, using a two particle wave packet defined as

$$\psi_2 = \int \mathrm{d}^3 k_1 \int \mathrm{d}^3 k_0 \alpha_1(\bar{k_1} - \bar{p_1}) \alpha_0(\bar{k_0} - \bar{p_0}) e^{i\bar{k_1}\cdot\bar{x_1}} e^{i\bar{k_0}\cdot\bar{x_0}} \chi_1 \chi_0 \tag{6.1.5.2}$$

where χ_1, χ_0 are internal states while the functions α_1, α_0 are the wave packet distributions.

This form has a standard justification for isolated systems that are translation invariant when you operate on both particles. Moreover, particles with an asymptotically small intrinsic scale relative to their wavepackets size can be reduced to a representation using relative coordinates. This is typical of the wavepackets that we are studying. In particular, since we are studying particles introduced into the free space by nuclear decays and nuclei have position uncertainties of atomic scales over a typical decay (or coupling) period, we

can use the atomic scale as an order of magnitude estimate to the macroscopic wavepacket width parameter, while the neutron and nucleus can both be modeled as individually less than a typical uranium nucleus effective radius in size. This guarantees that desired scale separation property. We will only use this observation to note that the usual central potentials of scattering theory are in fact available to us, even in a macroscopic wavepacket interaction scenario where the full system is not translation invariant.

Finally, we note that the wavepacket representation $\alpha_0(\bar{k_0} - \bar{p_0})e^{i\bar{k_0}\cdot\bar{x_0}}$ is identical in substance to our apparatus function definition. All that has changed is that the primary distribution is defined over momentum here rather than position. This is motivated by the fact that generally the S-matrix acquires its simplest physical definition as a function of momentum. This change can be effected easily by Fourier transform. Moreover, by unitary equivalence of inner products, this change leaves our transition rates invariant. This reveals that our choice of apparatus functions encodes both a fundamental spatial measurement theory and a deep connection to the theoretical foundations of scattering theory.

The formulation above can be understood as a relative of spectral representation in the sense that allows us to reduce a generic two-body quantum scattering problem to convolution in a subspace of L_2. Hence, given two approximate eigenstates of the intial and final configurations, χ_a and χ'_b respectively, we can write the transition probability in terms of the S matrix as

$$|\langle \chi'_b, S\psi_2\rangle|^2 = |\int \mathrm{d}^3k_1 \int \mathrm{d}^3k_0 \alpha_1(\bar{k_1} - \bar{p_1})\alpha_0(\bar{k_0} - \bar{p_0})e^{i\bar{k_1}\cdot\bar{x_1}}e^{i\bar{k_0}\cdot\bar{x_0}} \left(\delta_{a,b} - 2\pi i\delta(E_a - E_b)\langle b|\, T(\bar{k_1}, \bar{k_0})\,|a\rangle\right)|^2 \tag{6.1.5.3}$$

which can be simplified to

$$|\langle \chi'_b, S\psi_2\rangle|^2 = |\int \mathrm{d}^3k_1 \alpha_1(\bar{k_1} - \bar{p_1})e^{i\bar{k_1}\cdot\bar{x_1}}\tilde{T}_{a,b}(k_1, p_0, x_0)|^2 \tag{6.1.5.4}$$

where

$$\tilde{T}_{a,b}(k_1, p_0, x_0) = \int \mathrm{d}^3k_0 \alpha_0(\bar{k_0} - \bar{p_0})e^{i\bar{k_0}\cdot\bar{x_0}} \left(\delta_{a,b} - 2\pi i\delta(E_a - E_b)\langle b|\, T(\bar{k_1}, \bar{k_0})\,|a\rangle\right) \tag{6.1.5.5}$$

We note that the integrals of our phase space approximation instrument are over the analogues of the $(p_0, x_0), (p_1, x_1)$ variables, which function as macroscopic variables. On the other hand, the integral over k_0, k_1 is the representation of an inner product between states where the distribution of the non-neutron partner is subsumed into a reduced potential. Moreover, in our model, the nuclei are distributed about static locations so p_0, x_0 can be incorporated in the reaction index ℓ. Finally, by extending the x'_b state to an outgoing wave function with its own phase space distribution, we obtain a method for using scattering theory

to single-reaction PDP as a scattering event that provides the probability of a jump between a macroscopic wave function and a localized reaction channel.

From this point of view, we can understand $\boldsymbol{V}_{x_1,k_1,\ell,a}$ as a composite mapping between free macroscopic wavefunctions and a spectral subspace projected reaction state. A similar analysis of the decay process into a macroscopic wave function yields the following interpretation. The interior integrand

$$\frac{1}{(2\pi)^3}|\langle\alpha_{x_1,k_1}|\,\boldsymbol{V}_{x_1,k_1,\ell,a}\,|\boldsymbol{B}_{F,s_1}\psi\rangle|^2\;|\langle\alpha_{x_2,k_2}|\,\boldsymbol{V}_{x_2,k_2,\ell,d}\,|\boldsymbol{B}_{B,s_2-s_1}\boldsymbol{U}_{\ell,a}\alpha_{x_1,k_1}\rangle|^2 \tag{6.1.5.6}$$

can be understood as a probability density constructed in two stages. First, a transition occurs between a particle distributed according to the wavepacket ψ to a bound apparatus state with probability density $|\langle\alpha_{x_1,k_1}|\,\boldsymbol{V}_{x_1,k_1,\ell,a}\,|\boldsymbol{B}_{F,s_1}\psi\rangle|^2$. Then, a second event occurs after a time delay $s_2 - s_1$. Namely, the bound neutron decays back into the continuum in a given free apparatus state with probability density $|\langle\alpha_{x_2,k_2}|\,\boldsymbol{V}_{x_2,k_2,\ell,d}\,|\boldsymbol{B}_{B,s_2-s_1}\boldsymbol{U}_{\ell,a}\alpha_{x_1,k_1}\rangle|^2$. Although the joint distribution of absorption and decay events factors into a product of two sub-events, the absorptions and decays are not uncorrelated. In fact, the absorption-decay process can be strongly quantum correlated in this formulation by the fact that the absorption apparatus state of the first event uniquely determines the initial configuration of the quantum state that will eventually decay back into the continuum. By, discarding this correlation we obtain a Hauser-Fechbach memoryless compound reaction model. [59] As it is, this correlated version is easily compatible with a multi-channel generalized optical potential model. [59], [65] [50]

By choosing a differentially small exit volume at a microscopically large distance, we can recover the differential cross section and eliminate some of the macroscopic averaging effects to bring the two-reaction PDP formula into a form that is more closely aligned with the conventional functions of nuclear reaction theory. In order to do this properly, we would need to get into a lot of technical detail relating to the partial isometries of scattering theory and the spectral representation of Green's functions for unbounded operators. [125] This is necessary for future work in order to apply the technique to general scattering formulations but it is certainly possible. For now, it is sufficient to note that the reaction-transport PDP structure gives us a compound reaction model compatible with the statistical techniques used in finite-dimensional nuclear model spaces. [85] As such, this represents a viable mathematical foundation for solving the general data assimilation problem between differential and integral data sets.

6.2 PDP representation of Neutron Thermalization and the Approach to Equilibrium

We will conclude this section by introducing a particularly simple representation for a particle conserving reaction-transport process based on the theory outlined in chapter 5. The purpose here is to build on the interpretations of the previous section by defining a system with an explicitly defined set of reaction types and correlation tracking vector subspace. Where we have retained a degree of abstraction up to this point, this section introduces fairly severe limitations on the model and uses this simplified problem to identify a route to estimating quantum equilibrium distributions in general.

This model is predominantly intended as a simple model for conservative neutron thermalization in the presence of particle conserving resonance scattering events such as compound elastic scattering. In particular, this model is distinguished by having a continuous but static medium and a fixed finite number of particles that are completely independent. The result of this is a system of sequential absorptions and decays (that can be complemented in an obvious way by potential scattering from free states to free states) in order to handle all of the scattering processes that contribute to neutron thermalization. In the process of doing this, we will concretely define all of the operators that we have allowed to be defined abstractly up to this point. Moreover, in constructing and analyzing this model, we will construct a form for the Reaction-Transport Transition PMV measure for which there is a well developed theory of existence for equilibrium states. This will suggest a route forward for studying the formation of equilibrium states for more general models.

6.2.1 Example: Particle Conserving 3-Instrument Representation for Neutron Thermalization

Suppose we have a collection of neutrons scattering in a homogeneous medium composed of a single type of nucleus, where we have averaged the nuclear positions over a space of potential position in advance to produce a uniform field of density weighted reaction rates. We will treat this as an $\bar{x}$ dependent scale factor multiplying the individual absorption probability, such that

$$\boldsymbol{V}_{x_1,k_1,\ell,a} = (\rho_{\text{medium}}(x_1))^{1/2}\boldsymbol{V}_{k_1,\ell,a} \tag{6.2.1.1}$$

This allows us to forego the inclusion of any atom dependence in the set of ℓ, since the full medium dependence has already been included in the x dependence of the V operator functions. Moreover, the choice of the square root stems both from the fact that the scale factor is positive and from the probabilistic interpretation

of the single absorption formula 6.1.4.5. This density scaling factor should not appear in the decay potentials as they will depend only on the absorbed wave packet distribution relative to the medium's density.

Now we suppose there is a fixed number, $n \in \mathbb{N}$, of neutrons in the system. In an arbitrary initial state, these can be split in any definite way between the bound and the free subspaces. However, for simplicity, we will suppose that their initial configuration is entirely in the free space. Thus,

$$\boldsymbol{\rho} = \bigotimes_{i=1}^{n} \left|\psi_i^1\right\rangle \otimes c_B \otimes \bigotimes_{\ell=1}^{n_2} \left|v^\ell\right\rangle \bigotimes_{i=1}^{n} \left\langle\psi_i^1\right| \otimes c_B \otimes \bigotimes_{\ell=1}^{n_2} \left\langle v^\ell\right| \tag{6.2.1.2}$$

Next, we eliminate the Hilbert space for the medium and specify the set of reaction types. Since each neutron evolves independently and forms no quantum correlations with other particles through the medium, we can make the simplification of eliminating the separate Hilbert space for the medium and viewing the system as a pair of ideal gases with a quantum phase space distribution. These two gases trade particles back and forth at every point without limitation and therefore there is no need for excitation accounting. This reduction is satisfactory as long as the model is applied to systems at low enough densities that the medium is approximately unperturbed by interactions with the neutron gas.

Now, the set of reactions T can be divided up into a finite collection in the following way. For each pair of particle counts in the bound and free subspaces, say n_b and n_f, we can define single absorption or a single decay. We will also define a free to free jump that leaves the particle counts intact but transforms the momentum space distribution of one of the free particles by a partial isometry. The purpose of this additional event type is to account for the contribution of instantaneous potential scattering. Thus, for each

$$\boldsymbol{\rho} = \bigotimes_{i=1}^{n_f} \left|\psi_i^1\right\rangle \bigotimes_{i=1}^{n_b} \left|\phi_i^1\right\rangle \bigotimes_{i=1}^{n_f} \left\langle\psi_i^1\right| \bigotimes_{i=1}^{n_b} \left\langle\phi_i^1\right| \tag{6.2.1.3}$$

we can define a $\overline{\mathscr{J}}_a$ absorption operator restricted to the (n_f, n_b) subspace to be sum over the contribution from each element of the tensor product resulting in a state belonging to the $(n_f - 1, n_b + 1)$ subspace

$$\begin{aligned}\mathscr{J}_a^{n_f,n_b}(E_1, \boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1 \mathrm{d}^3k_1 \sum_{j=1}^{n_f} &|\langle\alpha_{x_1,k_1}| \boldsymbol{V}_{k_1,a} \left|\psi_j^1\right\rangle|^2 \rho_{\text{medium}}(x_1) \\ &\left|\bigotimes_{i=1}^{j-1} \psi_i^1 \bigotimes_{i=j+1}^{n_f} \psi_i^1 \otimes \bigotimes_{i=1}^{n_b} \phi_i^1 \otimes (\alpha_{x_1,k_1} \otimes e_2)\right\rangle \left\langle \bigotimes_{i=1}^{j-1} \psi_i^1 \bigotimes_{i=j+1}^{n_f} \psi_i^1 \otimes \bigotimes_{i=1}^{n_b} \phi_i^1 \otimes (\alpha_{x_1,k_1} \otimes e_2)\right|\end{aligned} \tag{6.2.1.4}$$

Note that we have defined $\boldsymbol{U}_a$ to be injection into a finite dimensional nuclear model space with no change to the phase space distribution. Furthermore, our reaction probability operator $\boldsymbol{V}_a$ has been made to take a particularly simple optical potential form, scaled by a density distribution. We can then define the full

absorption operator by summing over the finite set of allocations of n particles to the free and bound spaces such that at least one particle is free initially

$$\overline{\mathscr{J}}_a = \sum_{\ell=1}^{n} \Pi_{(\ell-1,n-\ell+1)} \mathscr{J}_a^{\ell,n-\ell} \Pi_{(\ell,n-\ell)} \tag{6.2.1.5}$$

The finite sum and subspace projectors can be pulled inside of the phase space integral to produce an operator of the form

$$\overline{\mathscr{J}}_a(E_1, \boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1 \mathrm{d}^3k_1 \overline{\mathscr{J}}_{x_1,k_1,a} \boldsymbol{\rho} \overline{\mathscr{J}}^*_{x_1,k_1,a} \tag{6.2.1.6}$$

on pure particle number states. This relies on the fact that a pure particle number state will have the same bound and free particle number allocation on both sides and so mixed terms would be killed by the resulting asymmetric projectors in the mixed terms acting on symmetric states.

In a similar way, we can define a $\overline{\mathscr{J}}_d$ decay operator restricted to the (n_f, n_b) subspace to be sum over the contribution from each element of the tensor product resulting in a state belonging to the (n_f+1, n_b-1) subspace. Specifically, suppose the internal states ϕ_i^1 are the product of a phase space distribution $\tilde{\phi}_i$ and a finite dimension complex vector v^i. Then we can introduce a matrix $\overline{\overline{M}}_d$ acting in the finite dimensional nuclear model space and contract it with a vector for an exit subspace for decaying back into the continuum via e_1. The resulting state is transformed by a positive scaling of a partial isometry represented by $\boldsymbol{S}_d$. This is a kind of finite dimensional analogue for coupled-channel based decay process.

$$\begin{aligned}\mathscr{J}_d^{n_f,n_b}(E_1, \boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1 \mathrm{d}^3k_1 \sum_{j=1}^{n_f} \left| \left\langle \alpha_{x_1,k_1}, \tilde{\phi}_j \left\langle e_1 \right| \overline{\overline{M}}_d \left| v^j \right\rangle \right\rangle \right|^2 \\ \left| \bigotimes_{i=1}^{n_f} \psi_i^1 \otimes \boldsymbol{S}_d \alpha_{x_1,k_1} \otimes \bigotimes_{i=1}^{j-1} \phi_i^1 \bigotimes_{i=j+1}^{n_b} \phi_i^1 \right\rangle \left\langle \bigotimes_{i=1}^{n_f} \psi_i^1 \otimes \boldsymbol{S}_d \alpha_{x_1,k_1} \otimes \bigotimes_{i=1}^{j-1} \phi_i^1 \bigotimes_{i=j+1}^{n_b} \phi_i^1 \right|\end{aligned} \tag{6.2.1.7}$$

We can then define the full decay operator by summing over the finite set of valid allocations of n particles to the free and bound spaces such that at least one particle is bound initially

$$\overline{\mathscr{J}}_d = \sum_{\ell=0}^{n-1} \Pi_{(\ell+1,n-\ell-1)} \mathscr{J}_d^{\ell,n-\ell} \Pi_{(\ell,n-\ell)} \tag{6.2.1.8}$$

The finite sum and subspace projectors can be pulled inside of the phase space integral to produce an operator of the form

$$\overline{\mathscr{J}}_d(E_1, \boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1 \mathrm{d}^3k_1 \overline{\mathscr{J}}_{x_1,k_1,d} \boldsymbol{\rho} \overline{\mathscr{J}}^*_{x_1,k_1,d} \tag{6.2.1.9}$$

on pure particle number states. This relies on the fact that a pure particle number state will have the same

bound and free particle number allocation on both sides and so mixed terms would be killed by the resulting asymmetric projectors in the mixed terms acting on symmetric states.

We can repeat this process for particle count subspace preserving scattering. We can define a $\overline{\mathscr{J}}_s$ decay operator restricted to the (n_f, n_b) subspace to be the sum over the contribution from each element of the tensor product resulting in a state belonging to the (n_f, n_b) subspace.

$$\mathscr{J}_s^{n_f,n_b}(E_1,\boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1\mathrm{d}^3k_1 \sum_{j=1}^{n_f} |\langle \alpha_{x_1,k_1}| \boldsymbol{V}_{k_1,s} \left|\psi_j^1\right\rangle|^2 \rho_{\text{medium}}(x_1) \left|\bigotimes_{i=1}^{j-1}\psi_i^1 \bigotimes_{i=j+1}^{n_f}\psi_i^1 \otimes \boldsymbol{S}\alpha_{x_1,k_1} \otimes \bigotimes_{i=1}^{n_b}\phi_i^1\right\rangle \left\langle \bigotimes_{i=1}^{j-1}\psi_i^1 \bigotimes_{i=j+1}^{n_f}\psi_i^1 \otimes \boldsymbol{S}\alpha_{x_1,k_1} \otimes \bigotimes_{i=1}^{n_b}\phi_i^1\right| \quad (6.2.1.10)$$

Note that we have defined $\boldsymbol{U}_s$ to be a positive scaling of a partial isometry represented by $\boldsymbol{S}$ and applied to the phase space distribution. Furthermore, our reaction probability operator $\boldsymbol{V}_s$ has been made to take a particularly simple potential scattering form, scaled by a density distribution. We can then define the full absorption operator by summing over the finite set of allocations of n particles to the free and bound spaces such that at ;east one particle is free initially

$$\overline{\mathscr{J}}_s = \sum_{\ell=1}^{n} \Pi_{(\ell,n-\ell)} \mathscr{J}_a^{\ell,n-\ell} \Pi_{(\ell,n-\ell)} \quad (6.2.1.11)$$

The finite sum and subspace projectors can be pulled inside of the phase space integral to produce an operator of the form

$$\overline{\mathscr{J}}_s(E_1,\boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1\mathrm{d}^3k_1 \overline{\mathscr{J}}_{x_1,k_1,s} \boldsymbol{\rho} \overline{\mathscr{J}}^*_{x_1,k_1,s} \quad (6.2.1.12)$$

on pure particle number states. This relies on the fact that a pure particle number state will have the same bound and free particle number allocation on both sides and so mixed terms would be killed by the resulting asymmetric projectors in the mixed terms acting on symmetric states.

Finally, our full reaction operator is given by

$$\mathscr{J}(E_1 \times \{a,d,s\}, \boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3x_1\mathrm{d}^3k_1 \sum_{\ell=1}^{n} \Pi_{(\ell,n-\ell)}\overline{\mathscr{J}}_{x_1,k_1,s}\Pi_{(\ell,n-\ell)}\boldsymbol{\rho}\Pi_{(\ell,n-\ell)}\overline{\mathscr{J}}^*_{x_1,k_1,s}\Pi^*_{(\ell,n-\ell)} \tag{6.2.1.13}$$

$$+ \int_{E_1} \mathrm{d}^3x_1\mathrm{d}^3k_1 \sum_{\ell=1}^{n} \Pi_{(\ell-1,n-\ell+1)}\overline{\mathscr{J}}_{x_1,k_1,a}\Pi_{(\ell,n-\ell)}\boldsymbol{\rho}\Pi_{(\ell,n-\ell)}\overline{\mathscr{J}}^*_{x_1,k_1,a}\Pi^*_{(\ell-1,n-\ell+1)} \tag{6.2.1.14}$$

$$+ \int_{E_1} \mathrm{d}^3x_1\mathrm{d}^3k_1 \sum_{\ell=0}^{n-1} \Pi_{(\ell+1,n-\ell-1)}\overline{\mathscr{J}}_{x_1,k_1,d}\Pi_{(\ell,n-\ell)}\boldsymbol{\rho}\Pi_{(\ell,n-\ell)}\overline{\mathscr{J}}^*_{x_1,k_1,d}\Pi^*_{(\ell+1,n-\ell-1)} \tag{6.2.1.15}$$

Note that this full reaction operator covers all reaction types and leaves the posterior density matrix as a finite sum of pure particle number density matrices so long as the prior density matrix is a finite sum of pure particle number density matrices. Note that if E_1 specifies a subset of reaction types, then $\mathscr{J}$ may only include one or two of the three potential contributing terms.

Now that we have specified the relationship between the Hilbert space models, the reaction types and their respective $\boldsymbol{U}_\ell$ and $\boldsymbol{V}_{x,k,\ell}$ operators, it remains to specify a set of free evolutions $\boldsymbol{B}_{F,t}$ and $\boldsymbol{B}_{B,t}$ that collectively satisfy the mesoscopic reaction rate consistency requirement. This is actually relatively easy to do using a trick from field theory for perturbed Hamiltonians. Suppose, we have a well defined reaction rate operator given by $\boldsymbol{R}$. Then a trivial direct computation gives us that for a free evolution $\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^*$, if $\boldsymbol{Y}$ is the generator of $\boldsymbol{B}_t$ then

$$\boldsymbol{Y} = -iH - \frac{1}{2}\boldsymbol{R} \tag{6.2.1.16}$$

satisfies the mesoscopic reaction rate constraint

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\left[\boldsymbol{S}_t\boldsymbol{\rho}\right] = -\mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{S}_t\boldsymbol{\rho}\right] \tag{6.2.1.17}$$

We can further simplify the form of the evolution by examining the projection onto free and bound fixed particle number subspaces. Specifically, we recall from the definition of the Collisionless Reaction Transport Propagator

$$\boldsymbol{S}_t\boldsymbol{\rho} = \boldsymbol{B}_t\boldsymbol{\rho}\boldsymbol{B}_t^* = \sum_{n+m=N}\sum_{n'+m'=N}(\Pi_F^n\boldsymbol{B}_t\Pi_F^n \otimes \Pi_B^m\boldsymbol{B}_t\Pi_B^m)\boldsymbol{\rho}(\Pi_F^{n'}\boldsymbol{B}_t\Pi_F^{n'} \otimes \Pi_B^{m'}\boldsymbol{B}_t\Pi_B^{m'})^*$$

Now, we can impose a more severely constrained but easily modeled form. Specifically, since bounded generator semigroups can be expanded as operator exponents and unbounded generator semigroups can

be expanded as exponents on each finite dimensional spectral subspace[91], it is more severe to apply the projection operator decomposition to the generator $\boldsymbol{Y}$. Indeed, if

$$\boldsymbol{Y} = \sum_{n+m=N} (\Pi_F^n \boldsymbol{Y} \Pi_F^n \otimes \Pi_B^m \boldsymbol{Y} \Pi_B^m) \tag{6.2.1.18}$$

then it follows from a limit of finite dimensional approximations that

$$\boldsymbol{B}_t = \sum_{n+m=N} (\Pi_F^n \boldsymbol{B}_t \Pi_F^n \otimes \Pi_B^m \boldsymbol{B}_t \Pi_B^m)$$

Therefore, we instead take 6.2.1.18 as our requirement. We will arrive at our model by constructing $\Pi_F^n \boldsymbol{Y} \Pi_F^n$ and $\Pi_B^m \boldsymbol{Y} \Pi_B^m$ independently. We will prove in the next section that the operator $\boldsymbol{R}$ for the $\mathscr{J}$ we specified above can be represented in this way without losing any information. It suffices to construct our Hamiltonian evolution on fixed bound and free particle number subspaces. In particular, since

$$\Pi_F^n \boldsymbol{Y} \Pi_F^n = -i \Pi_F^n H \Pi_F^n - \frac{1}{2} \Pi_F^n \boldsymbol{R} \Pi_F^n \tag{6.2.1.19}$$

$$\Pi_B^m \boldsymbol{Y} \Pi_B^m = -i \Pi_B^m H \Pi_B^m - \frac{1}{2} \Pi_B^m \boldsymbol{R} \Pi_B^m \tag{6.2.1.20}$$

it suffices to define $\Pi_F^n H \Pi_F^n$ for $\bigotimes_{i=1}^n \psi_i^1$ where $\psi_i^1 \in \mathscr{H}_F = L_2(\mathbb{R}^3)$ and $\Pi_B^m H \Pi_B^m$ for $\bigotimes_{i=1}^m \phi_i^1$ where $\phi_i^1 \in \mathscr{H}_B = L_2(\mathbb{R}^3) \otimes \mathbb{C}^k$. Moreover, we are modeling the particles as evolving independently, so

$$\Pi_F^n H \Pi_F^n = \bigotimes_{i=1}^n \Pi_F^1 H \Pi_F^1 \tag{6.2.1.21}$$

$$\Pi_B^m H \Pi_B^m = \bigotimes_{i=1}^m \Pi_B^1 H \Pi_B^1 \tag{6.2.1.22}$$

and it suffices to define the Hamiltonian on the single particle subspaces.

The bound subspace is meant to represent particles that are not propagating on macroscopic scales. As such, we will leave the phase space distribution unmodified and introduce a Hermitian matrix as the nuclear subspace Hamiltonian $\overline{\overline{H}}_{\text{nuc}} = \overline{\overline{H}}_{\text{nuc}}^*$. Then we have

$$\Pi_B^1 H \Pi_B^1 \phi_i^1 = \Pi_B^1 H \Pi_B^1 (\tilde{\phi}_i \otimes v) = \tilde{\phi}_i \otimes \overline{\overline{H}}_{\text{nuc}} v \tag{6.2.1.23}$$

The free subspace is meant to encode the typical semiclassical translation of the position distribution along the mean momentum vector. This can be achieved by using a Moyal bracket on the phase space representation to encode the simplest quantum generalization of the classical Poisson bracket for free propagation

along a linear path. [35][28] Using this structure, we can explicitly study the error induced by eliminating dispersion from the evolution when constructing computational approximations. However, for now it suffices to construct the evolution using a more standard free evolution operator: the minimal self-adjoint closure of the Laplacian

$$\Pi^1_F H \Pi^1_F \psi^1_i = -\Delta \psi^1_i = -\sum_{n=1}^{3} \frac{\mathrm{d}^2}{\mathrm{d}x_n^2} \psi^1_i \tag{6.2.1.24}$$

where the second equality holds on the dense subspace of continuously twice-differentiable functions in $\mathbb{R}^3$. Here we are again using natural units ($\hbar = c = 1$) for clarity.

This choice of operator is simple enough but it raises the question of how this is compatible with transport theory. Obviously, standard neutron transport theory is constructed from linear paths joined by scattering events. So why should this be a viable choice? Conversely, if this is the standard free model for quantum dynamics, why might a transport theory be a plausible approximation. The answer to this question relies on the context of the functions and time scales that we are studying. Indeed, since neutrons are not stable free particles, it only makes sense to require (as we did early in the construction of this measurement model) that neutrons be born in decays typical of the ones represented in the model. In that case, the single particle phase space distributions can be understood as small phase space volume integral representations using apparatus functions. Supposing for a moment that our apparatus function is a gaussian, we can examine the impact of a free evolution by a Laplacian. In fact, many people have done this. Given a near thermal velocity, the spreading of the wavepacket representing an atomically localized neutron will not be appreciable on distances much less than the distance between the earth and the moon. Apart from that spreading, the distribution does propagate linearly along the linear path determined by the mean momentum of the distribution. [112] [69] That is to say, in any real nuclear system, apparatus state spreading due to the Laplacian is negligible and the dynamics can be closely approximated by linear propagation as we desired. In order to study QSPs with other kinds of approximations to the free dynamics will require a closer examination of the Moyal bracket representation of the phase space evolution of an apparatus state.

Having completed the specification of $\mathscr{J}$ and $\boldsymbol{S}_t$ in a manner that is consistent with the existence of a mesoscopic reaction rate, we can obtain our model QSP directly from the PDP formula using the representation theorem 5.10.1. This completes the specification of a quantum field theoretic model for neutron thermalization and guarantees that it has all of the desired mathematical properties. Now we can perform some additional analysis of the reaction rate operator and so estimates to the system-wide reaction rate.

6.2.2 Reaction Observable for Particle Conserving 3-Instrument Representation

Now that we have carefully analyzed the measurement generators of the thermalization-like reaction transport process, we will need to explain how these operators can be expressed as familiar reaction rates that decompose over types. Since, $\overline{\mathscr{J}}_{x_1,k_1,a/s/d}$ transforms the bound and free subspaces separately and they are represented by the direct sum, it can always be decomposed as

$$\overline{\mathscr{J}}_{x_1,k_1,a/s/d} = \sum_{n+m=N} \sum_{n'+m'=N} \Pi_F^{n'} \overline{\mathscr{J}}_{x_1,k_1,a/s/d} \Pi_F^n \otimes \Pi_B^{m'} \overline{\mathscr{J}}_{x_1,k_1,a/s/d} \Pi_B^m \tag{6.2.2.1}$$

Thus using the linearity and permutation ordering of the trace inside the integral (as well as order reversing of operator compositions under adjoint), we have

$$\boldsymbol{R} = \sum_{\ell \in \{a,s,d\}} \sum_{n+m=N} \sum_{n'+m'=N} \int_{E_1} \mathrm{d}^3x_1 \mathrm{d}^3k_1 \left((\Pi_F^n \overline{\mathscr{J}}^*_{x_1,k_1,\ell} \Pi_F^{n'} \Pi_F^{n'} \overline{\mathscr{J}}_{x_1,k_1,\ell} \Pi_F^n \otimes \Pi_B^m \overline{\mathscr{J}}^*_{x_1,k_1,\ell} \Pi_B^{m'} \Pi_B^{m'} \overline{\mathscr{J}}_{x_1,k_1,\ell} \Pi_B^m) \right) \tag{6.2.2.2}$$

this proves our claim above that the reaction operator $\boldsymbol{R}$ can be decomposed as a sum over fixed bound and free particle number subspaces. We can go further and examine the interpretation of the trace against a state in terms of a sum over distinct reaction rates. Indeed, the simplest such observation comes from the outer most sum over reaction types. Namely, for N total neutrons,

$$\boldsymbol{R} = \boldsymbol{R}_s + \boldsymbol{R}_a + \boldsymbol{R}_d \tag{6.2.2.3}$$

$$\boldsymbol{R}_s = \sum_{n=1}^{N} \int \mathrm{d}^3x_1 \mathrm{d}^3k_1 \left(\Pi_F^n \overline{\mathscr{J}}^*_{x_1,k_1,s} \overline{\mathscr{J}}_{x_1,k_1,s} \Pi_F^n \otimes \mathbb{I} \right) \tag{6.2.2.4}$$

$$\boldsymbol{R}_a = \int \mathrm{d}^3x_1 \mathrm{d}^3k_1 \sum_{\ell=1}^{n} \Pi_{(\ell,n-\ell)} \mathscr{J}^{\ell,n-\ell *}_{x_1,k_1,a} \Pi_{(\ell-1,n-\ell+1)} \mathscr{J}^{\ell,n-\ell}_{x_1,k_1,a} \Pi_{(\ell,n-\ell)} \tag{6.2.2.5}$$

$$\boldsymbol{R}_d = \int \mathrm{d}^3x_1 \mathrm{d}^3k_1 \sum_{\ell=0}^{n-1} \Pi_{(\ell,n-\ell)} \mathscr{J}^{\ell,n-\ell *}_{x_1,k_1,d} \Pi_{(\ell+1,n-\ell-1)} \mathscr{J}^{\ell,n-\ell}_{x_1,k_1,d} \Pi_{(\ell,n-\ell)} \tag{6.2.2.6}$$

where we have introduced $\mathscr{J}^{\ell,n-\ell}_{x_1,k_1,a}$ as the integrand of $\mathscr{J}^{\ell,n-\ell}_a$ and $\mathscr{J}^{\ell,n-\ell}_{x_1,k_1,d}$ as the integrand of $\mathscr{J}^{\ell,n-\ell}_d$. The reaction intensity can be obtained directly from the reaction rate operator and a given state $\boldsymbol{\rho}$ as

$$I_{\mathrm{coll}}(t) = \mathrm{Tr}\left[\boldsymbol{R}\boldsymbol{\rho}(t)\right] \tag{6.2.2.7}$$

here we are using I_{coll} for the single event reaction rate as a reference to the collision intensity integral (integrated over all of phase space at a fixed time) from kinetic theory as these two should agree. As a result, we use our decomposition to find

$$I_{\text{coll}}(t) = I_{\text{scattering}}(t) + I_{\text{abs}}(t) + I_{\text{source}}(t) \tag{6.2.2.8}$$

$$I_{\text{scattering}}(t) = \text{Tr}\left[\boldsymbol{R}_s \boldsymbol{\rho}(t)\right] \tag{6.2.2.9}$$

$$I_{\text{abs}}(t) = \text{Tr}\left[\boldsymbol{R}_a \boldsymbol{\rho}(t)\right] \tag{6.2.2.10}$$

$$I_{\text{source}}(t) = \text{Tr}\left[\boldsymbol{R}_d \boldsymbol{\rho}(t)\right] \tag{6.2.2.11}$$

We can further extend this analysis by using it to study reaction rates in phase space subvolumes. The same trace manipulation argument can be used to directly construct the $\mathscr{J}(E)$ adjoint $\boldsymbol{R}_E$ for arbitrary phase space volumes E. This is a rate, it is not an absolute count of reactions in a time interval. In order to obtain a reaction count, we need to compute directly from the composite QSP generated by $\mathscr{J}$ and $\boldsymbol{S}_t$. In order to do this, we need to partition over different numbers of events and then split them into suballocations to the region of interest and to everywhere else. Then, for every count in the region of interest, we can determine the probability of the event by taking the trace. Multiplying this probability by the number of reactions detected and summing over counts will yield the expected reaction count in the volume in the time interval under consideration.

6.2.3 Non-Recurrence and Equilibrium Distributions of Particle Conserving 3-Instrument Representation

In the absence of absorption events with a cemetery state, we can use results from the theory of the generalized Wigner-Weisskopf atom [32] to prove that there is quantum equilibrium distribution arrived at in momentum space. We can do this by looking at operators of the form

$$\mathscr{J}(E_1, \boldsymbol{\rho}) = \int_{E_1} \mathrm{d}^3 x_1 \mathrm{d}^3 k_1 \boldsymbol{A}_{x_1,k_1} \boldsymbol{\rho} \boldsymbol{A}^*_{x_1,k_1} \tag{6.2.3.1}$$

We proved above that the reaction operators for the 3-instrument model of neutron thermalization can be represented as as finite sum over operators of this form where $\boldsymbol{A}_{x_1,k_1}$ satisfy

$$\int \mathrm{d}^3 x_1 \mathrm{d}^3 k_1 \text{Tr}\left[\boldsymbol{A}^*_{x_1,k_1} \boldsymbol{A}_{x_1,k_1}\right] < \infty \tag{6.2.3.2}$$

and are strongly continuous in phase space. It is sufficient to replace the spectral integrals with finite dimensional approximations and apply Davies' theory of transient and recurrent processes in quantum fields. This establishes that for every M-dimensional approximation $\mathscr{J}^M, \boldsymbol{S}_t^M, \boldsymbol{T}_t^M, \mathscr{H}_M$, there exists an equilibrium state $\boldsymbol{\rho}_{M,0}$ such that for all states $\boldsymbol{\rho}$,

$$\boldsymbol{T}_t^M \boldsymbol{\rho} \to \boldsymbol{\rho}_{M,0} \tag{6.2.3.3}$$

The nature of this convergence is somewhat more complex than for a classical neutron thermalization process, but the essential idea is in complete accord with the classical theory. For a point of comparison that uses radically different methods but is motivated by similar physical considerations, confer Parks. [117]

6.3 Mesoscopic Reaction Dynamics

Along the way to making a model that bridges the very large and very small scales of transport and scattering theory respectively, we have created a model for reaction-transport dynamics that applies at mesoscopic scales. While nonlinear macroscopic transport models can be viewed as law of large numbers type limits of this quantum stochastic theory, very small nuclear systems (say, <100 atoms across) will exhibit more subtle transport statistics such that an entirely new class of models proves necessary. In this case, we will need to directly approximate the distribution of reactions in the system using a discrete set of detectors. The goal would be to recover a discrete nonlinear, nonequilbrium Markov process on a network of detectors for modeling the mesoscopic dynamical system that would allow us to study phase transitions due to transmutations. [149], [72] As a precursor to such a coarse grained model, we propose a nonconservative quantum reactive-transport process with a finite number of nuclei.

6.3.1 Example: Non-Conserving Representations on Fock Space for Discrete Detectors

A second class of models derived from the theory outlined in 5 will now be introduced. These allow multiplicative processes and a dynamic medium but additionally require a finite fixed number of detectors (nuclei). This model is physically very similar to cell interaction theory of Osborn and Yip in its treatment of spatial cell structure medium. [115] As we did in the thermalization theory, it is relatively easy to introduce an additional kind of free to free space scattering that has the form of potential scattering.

Many of the essential ideas about subspace decompositions remain valid from the 3-instrument neutron thermalization model. The main modification that occurs in this model takes the form of the introduction of a finite number of detectors and a corresponding Hilbert space for the medium. This makes it impossible

to treat the neutrons as independent but enables us to study the formation of spatio-temporal correlations through interactions with the medium. We will proceed, as in the previous example, by first defining the Hilbert space and the enumeration of reaction types.

The main idea of this model is that the system consists of a finite set of detectors, each of which will have its reaction events counted separately. This is a fairly extreme version of the claim that reaction events are classically observable in a transport theory. However, without this assumption or something similar, explicit tracking of the medium as having a classical state cannot be incorporated into the theory.

So, where we previously had three reaction types, we now have $3N_m$ reaction types where N_m is the number of detectors. Thus,

$$T = \{a_1, s_1, d_1, a_2, s_2, d_2, \ldots, a_{N_m}, s_{N_m}, d_{N_m}\} \tag{6.3.1.1}$$

where a_i is an absorption event at detector i, s_i is a scattering event at detector i, and d_i is a decay event at detector i. Each $\boldsymbol{V}_{x_1,k_1,\ell}$ and $\boldsymbol{U}_\ell$ is then specific to the individual detection sites. In this way,

$$\frac{1}{(2\pi)^3}\int \mathrm{d}^3x_1\mathrm{d}^3k_1|\langle\alpha_{x_1,k_1}, \boldsymbol{V}_{x_1,k_1,a_i}\psi\rangle|^2 \tag{6.3.1.2}$$

can be thought of as the total probability of a single neutron ψ being absorbed by the detector i. Likewise $\boldsymbol{U}_{a_i}$ determines the internal state in the bound subspace of the ith detector that an absorbed particle is found in immediately after absorption. This dictates a number of requirements on the Hilbert space in order to coordinate the dynamics.

The free Hilbert subspace $\mathscr{H}_F$ can be modeled in the usual way as a particle number limited Fock space built up from products of single particle phase space wavefunctions.

$$\mathscr{H}_F = \bigoplus_{i=1}^{N_F}\bigotimes_{j=1}^{i} L_2(\mathbb{R}^3)\bigoplus c_F \tag{6.3.1.3}$$

The Hilbert subspace of the medium $\mathscr{H}_{\text{medium}}$ can be modeled as a product over finite dimensional subspaces

$$\mathscr{H}_{\text{medium}} = \bigotimes_{i=1}^{N_m}\mathbb{C}^{k_i} \tag{6.3.1.4}$$

Each of the spaces $\mathbb{C}^{k_i}$ represents the collection of possible internal population states of the ith detector. These transform in response to absorptions and decays in order track the residual set of particles in the system. If we wish to represent a system with an initial collection of $n_{F,0}$ free neutrons then the absolute

particle limit in the free space N_F but be chosen as greater than $n_{F,0} + \sum_{i=1}^{N_M} k_i$ so as to accommodate the maximum number of particles that can decay into the free space.

Finally, the bound subspace can be constructed in a number of ways. The main new requirement is that the detector that has absorbed the neutron must be able to be determined from the bound state. To this end, we extend the phase space dependence by a finite dimensional vector that encodes which bound subspace a given bound neutron lives in. In order to define a linear operator that can act equally well on all bound neutrons, we will construct each vector that includes all of the possible detector subspaces. This implies that a neutron can be in a superposition of detector subspaces in principle. However, we will generally attempt to define our transition operators so that a system that starts with all particles in pure free states or in detector pure bound states remains in a correspondingly pure state. This can be characterized efficiently in another number representation but we won't use that approach in the name of simplicity. At any rate, we can define $k_B = \sum_{i=1}^{N_m} k_{B_i}$ where $k_{B,i}$ is the dimensionality of the ith detector subspace. Then we have, for $\mathbb{C}^{k_B}$ organized into $k_{B,j}$ sized blocks by a well-ordereding of the detector indices,

$$\mathscr{H}_B = \bigoplus_{i=1}^{N_F} \bigotimes_{j=1}^{i} L_2(\mathbb{R}^3) \otimes \mathbb{C}^{k_B} \bigoplus c_B \tag{6.3.1.5}$$

Based on this construction, we can introduce our three operator families for the reaction-transport transition PMV measure using their restriction to well defined particle number subspaces. We suppose that we have an initial state given by

$$\boldsymbol{\rho} = \left| \bigotimes_{i=1}^{n_f} \psi_i^1 \otimes \bigotimes_{i=1}^{n_b} \phi_i^1 \bigotimes_{i=1}^{N_m} v^i \right\rangle \left\langle \bigotimes_{i=1}^{n_f} \psi_i^1 \otimes \bigotimes_{i=1}^{n_b} \phi_i^1 \bigotimes_{i=1}^{N_m} v^i \right| \tag{6.3.1.6}$$

Using $K_j = \sum_{i=1}^{j-1} k_{B,i}$ and $c_m \in C(\mathbb{R}^3, \mathbb{C})$ we can define a distribution in the internal space given by $\sum_{m=K_j+1}^{K_j+k_{B,j}} c_m(k_1) e_m \equiv u_j(k_1)$. We did not prove our primary sequence of theorems for a momentum dependence in the $\boldsymbol{U}_\ell$ operator. The extension is a primarily technical one but so useful for nuclear reaction modeling that it needs to be done. We can also introduce an operator D_j that scales and translates the absorbed apparatus state as a function of the detector site. This allows us to place the neutron in an interior phase space where it can undergo a collisionless bound evolution in its phase space distribution such that correlations formed as a result of the internal nuclear dynamics can be propagated back into the continuum. In the resulting operator, $\alpha_{x_1,k_1,j} \equiv (D_j \alpha_{x_1,k_1} \otimes u_j(k_1))$ We also make use of the shift operator on the medium vector as Sv_j, as described in the discussion of correlation encoding absorption operators. Finally, we note that the detection probability determining operator $\boldsymbol{V}_{x_1,k_1,a_j}$ is detection site dependent rather than

globally uniform. The absorption operator for the jth detector is given by,

$$\Psi^{n,m}_{a,j,m}(x_1,k_1) = \bigotimes_{i=1}^{m-1}\psi^1_i \bigotimes_{i=m+1}^{n_f}\psi^1_i \bigotimes_{i=1}^{n_b}\phi^1_i \otimes \alpha_{x_1,k_1,j}\bigotimes_{i=1}^{j-1}v^i \otimes Sv^j \bigotimes_{i=j+1}^{N_m} v^i \tag{6.3.1.7}$$

$$\mathscr{J}^{n_f,n_b}_{a_j}(E_1,\boldsymbol{\rho}) = \int_{E_1}\mathrm{d}^3x_1\mathrm{d}^3k_1\sum_{m=1}^{n_f}|\langle\alpha_{x_1,k_1}|\boldsymbol{V}_{x_1,k_1,a_j}\left|\psi^1_m\right\rangle|^2\left|\Psi^{n,m}_{a,j,m}(x_1,k_1)\right\rangle\left\langle\Psi^{n,m}_{a,j,m}(x_1,k_1)\right| \tag{6.3.1.8}$$

Most of the same notions apply to the definition of the decay operator as last time, except that we apply the inverse of the site dependent translation and scaling operator D_j^{-1} before computing the overlap with the apparatus state. The decay probability is computed from a site dependent interaction matrix on the finite dimensional nuclear space $\overline{\overline{M}}_{d,j}$. Finally, we also left shift the medium vector as S^*v^j. The decay operator for the jth detector is given by,

$$\Psi^{n,m}_{d,j}(x_1,k_1) = \bigotimes_{i=1}^{n_f}\psi^1_i \otimes \boldsymbol{S}_{d,j}\alpha_{x_1,k_1}\bigotimes_{i=1}^{j-1}\phi^1_i \bigotimes_{i=j+1}^{n_b}\phi^1_i \bigotimes_{i=1}^{j-1}v^i \otimes S^*v^j \bigotimes_{i=j+1}^{N_m} v^i \tag{6.3.1.9}$$

$$\mathscr{J}^{n_f,n_b}_{d_j}(E_1,\boldsymbol{\rho}) = \int_{E_1}\mathrm{d}^3x_1\mathrm{d}^3k_1\left|\left\langle\alpha_{x_1,k_1},D_j^{-1}\tilde{\phi}_j\left\langle e_1\right|\overline{\overline{M}}_{d,j}\left|u^j\right\rangle\right\rangle\right|^2\left|\Psi^{n,m}_{d,j}(x_1,k_1)\right\rangle\left\langle\Psi^{n,m}_{d,j}(x_1,k_1)\right| \tag{6.3.1.10}$$

The potential scattering operator for the jth detector is left almost unchanged,

$$\Psi^{n,m}_{s,j,m}(x_1,k_1) = \bigotimes_{i=1}^{m-1}\psi^1_i \bigotimes_{i=m+1}^{n_f}\psi^1_i \otimes \boldsymbol{S}\alpha_{x_1,k_1}\bigotimes_{i=1}^{n_b}\phi^1_i \bigotimes_{i=1}^{N_m} v^i \tag{6.3.1.11}$$

$$\mathscr{J}^{n_f,n_b}_{s_j}(E_1,\boldsymbol{\rho}) = \int_{E_1}\mathrm{d}^3x_1\mathrm{d}^3k_1\sum_{m=1}^{n_f}|\langle\alpha_{x_1,k_1}|\boldsymbol{V}_{x_1,k_1,s_j}\left|\psi^1_m\right\rangle|^2\left|\Psi^{n,m}_{s,j,m}(x_1,k_1)\right\rangle\left\langle\Psi^{n,m}_{s,j,m}(x_1,k_1)\right| \tag{6.3.1.12}$$

In the above forms, we used a single absorption and single decay structure. It is easy to extend this to multiple neutrons created in the bound state for a single absorption. This is achieved by duplicating the detected apparatus state in the bound state with a momentum dependent multiplication weight $\gamma_i(k_1)$. There is a corresponding shift in the medium state by $S^{*(1-r)}$ where r is the number of secondary neutrons excited into an active bound state from the finite quiescent medium. The process of multiple particles decaying into the medium then proceeds by individual, temporally isolated decays.

These can be extended to the full space using the subspace composition methods of section 6.2.1. The free evolutions can be defined as in the last section but with a block diagonal form on the detector internal evolutions by a finite Hermitian matrix and an identity operator on any vector in the medium. The resulting model can be very complex in general but is finally rich enough to track the evolution of a system where individual transmutations materially effect the medium in a way that cannot be ignored. This enables a new class of mixed quantum and classical correlation structures to be studied in nuclear systems. These

systems will exhibit strong nonlinearities when restricted to either subspace and approximated classically. As the size of the system grows and densities shrink, the nonlinearity weakens to the point that it can be safely ignored over a large range of states and we can recover the classical linear neutron transport theory.

Chapter 7

Future Work

The purpose of this work is to form a bridge between two other interesting classes of problems. In particular, using this framework, problems in nuclear science would reduce to three modeling stages. First, one would develop a quantum statistical model of a single neutron collision with a nucleus having macroscopic motion that was atomically coupled to the medium. This would include the design and validation of nuclear reaction models, condensed matter flow and kinetic energy distribution models, and decay displacement modeling. Second, one would incorporate these models explicitly into reaction transport PDP with appropriate spatial inhomogeneity constraints. Finally, one would derive a nonlinear Markov branching process associated to the reaction transport QSP using interacting particle system methods. This would then provide a classical predictive model that preserves a subset of important reaction rate measurements while modeling other reaction rates with bounded error.

The first stage would be amenable to uncertainty quantification and model selection for non-parametric statistics. The third stage would support the incorporation of simplifying symmetries to obtain benchmark solutions and it would support the development of novel computational approximations. Both of these classes of problems are exciting and interesting. However, in the absence of a well developed set of tools for the second step in this analysis process, they would not function as a cohesive whole. In this sense, the current text functions as a guidebook for the second modeling step. This work effectively constrains the space of valid models for the first step. This work also provides some basic assumptions and approximation tools that are guaranteed to be valid when setting out on the third step. Thus, the progress made in this work has opened new possibilities for solving more familiar problems in both the phenomenological nuclear reaction modeling and in the direct simulation spaces. We will outline some of those goals and the relevant references and tools in this chapter.

7.1 Nuclear Model Selection and Uncertainty Quantification

We discussed the nuclear data assimilation problem in some detail in section 6.1. We have provided a tool for explicitly modeling nuclear processes and transport processes in a single framework and identified the elements of the reaction-transport PDP in terms of scattering operators. In order to actually begin to address the underlying statistical problem, this would need to be incorporated into an uncertainty quantification calculation for practical nuclear models and real detector measurements from a nuclear reactor. This would require both fundamental metrological work on the validity of measurements and uncertainty modeling. [140],[104] This also implies a need to further extend model selection technologies to functional data.[49],[138] This need particularly stems from the fact that for many systems we can faithfully characterize and fit the pure continuum scattering channel of the reaction. However, characterization of non-isolated resonances in this system requires merging a continuous scattering measurement and fitted potential data with discrete channel absorption measurements. This is well-suited to analysis by semi-parametric estimation methods like approximation by empirical measures. [84][144] Moreover, the empirical measure approximation approach can be neatly connected with the stochastic simulation picture of neutron transport. [110] This set of relationships suggests an opportunity to leverage the analysis that we have done in this work to develop a new statistical tool for fitting resonance structures.

It may also be possible to approach the data assimilation problem directly by starting from data measured in multiple systems (differential and integral) and represent them all as measurements of quantum stochastic processes. We can then fit the evaluated measurement functions $|\langle \alpha_{x_1,k_1}, \boldsymbol{V}_{x_1,k_1,a_i}\psi\rangle|^2$ using functional maximum likelihood methods. [45],[46] This can then be cast as a set of noisy measurements for a scattering system and we can perform a statistical inverse scattering analysis.[75],[22] The result would be a jointly fitted set of quantum potentials that should have a broad range of efficacy and include both the pure scattering dynamics and a kind of renormalization by the medium to make them appropriate to application in transport problems.

This problem would also require direct modeling of reaction detection in the macroscopic system. In a practical sense, this would almost certainly require the use of classical thermodynamic limit approximations to the event density. The tools of quantum stochastic process simulation would likely not be able to cope with the number of particles that would need to be modeled. This implies a need for more efficient simulation tools that still can handle the propagation of reaction rate information directly from the nuclear models. This brings us to our second modeling problem.

7.2 Classical Transport Methods as an Approximation to Reaction-Transport PDPs

One of the motivating ideas that inspired the reaction-transport PDP quantization that we are using was the nonlinear quantum simulation method for studying quantum stochastic detection processes [6] and its natural analogy to the classical PDP type behavior of particle simulation Monte Carlo. [89], [110] Dautray and Lions gave seemingly restrictive conditions for modeling macroscopic cross sections based purely on PDE considerations. It is the contention of this work that the real limitations on the use of transport models can be understood in terms of the convergence of scaled sums of sampled neutron path trees on the full path space. We can take a few tentative steps down this path and at the same time shed some light on the interpretation of the PDP formula as a operator-valued precursor to particle simulation via empirical processes.

Reaction-transport PDPs have a nearly classical behavior between collision events and the collision probabilities (or reaction intensities in the Pál-Bell theory) can be approximated by $\mathrm{Tr}\,[\boldsymbol{R}_E\boldsymbol{\rho}]$. So, we can think of the approach to classical transport as a pathwise application of the generalized Ehrenfest theorem. The approach of quantum trajectories to classical trajectories has been studied extensively as part of the semiclassical theory of Gurtzweiller and Bohmian dynamics. [14],[97] The relation to stochastic simulation on a pathwise basis and its relationship to decoherence models has been studied extensively in the quantum information literature since Belavkin's original work. [16] The idea that reaction-transport PDPs can yield nonlinear transport equations for scattering in a correlated medium can be investigated from a few different perspectives. We will discuss three of these perspectives in what follows as well as two modeling technique for obtaining classical approximations to the structural operators of the reaction-transport QSP from other theories.

7.2.1 Classical Field Optimizing Distance

It is possible to construct a direct comparison of bounded reaction rate quantum stochastic processes with classical transport processes. That is, there is a method for investigating the quality of a classical approximation entirely in the space of quantum stochastic processes. In the context of coherent state methods in quantum field theory, Davies presents a technique for mapping random walks μ_t on the underlying LCH index space (for us the typed geographic phase space) into a full dynamical semigroup $\boldsymbol{T}_{\mu,t}$.

Thus, by comparing the semigroup induced by individual random walks for the evolution of a single

neutron to the full dynamical semigroup of our quantum PDP model $\boldsymbol{T}_t$ we can construct a measure of nearness on the single particle subspace. Specifically, the quantity $|\mathrm{Tr}\,[\boldsymbol{T}_{\mu,t}\boldsymbol{\rho} - \boldsymbol{T}_t\boldsymbol{\rho}]|$ maximized over the single particle states $\boldsymbol{\rho}$ gives the distance from any single particle random walk μ_t on G to our reaction-transport QSP. By minimizing this distance we may be able to identify an optimal random walk for modeling neutron dynamics.

Moreover, if we can generalize Davies' result (say, using more modern coherent states methods [1]) then we can extend the technique to the study of multi-particle states and possibly even study the convergence in a scaling limit. By suitably constraining the class of random walks that we study, we may be able to establish the optimality of a given choice of transition rates for a given Pál-Bell equation. Another interesting direct of extension would be to generalize the theorem from Davies to map random walks on a number-geographic space to an event conditioned QSP. This would make it possible to optimize our choice of transition rates to optimize the accuracy of our predictions for particular types of detection events.

7.2.2 ISPs, Classical PDPs, and Transport Monte Carlo Simulation

A radically different approach to classical model optimization is to make use of the idea that Monte Carlo simulation gives rise to valid (although potentially nonlinear) kinetic equations. There are two different approaches to this: "particle simulation" or generalized law of large numbers. We will discuss both options separately but they are actually related through interacting particle systems theory and concentration inequalities.

The first approach involves modeling the quantum stochastic process using simulation methods. Indeed, quantum stochastic systems that can be understood as continuous measurements can generally be recast as nonlinear pathwise simulations using vectors rather than density matrices. [16],[67] Given that mutiparicle states are not symmetrized by virtue of particle localization [111], and the evolutions are integrals over purity preserving operations, this is a particularly simple transition to make. Moreover, once we are simulating vectors along quantum trajectories, we can make use of the previously mentioned semiclassical approximation to obtain classical evolutions along the free trajectories. [14],[97] Then it is simply a matter of replacing the reaction rate operators with their expected values and we can have a pathwise simulation for an interacting particle system. The approximation can be studied directly on individual paths and it is obvious that any information related to the phase will immediately be lost once we compress down to the classical trajectory. However, this will yield a result that can be formulated as an interacting particle system that converges weakly under repeated simulation as an empirical measure.[144],[109],[110] Depending on how carefully this evolution is tracked, the result will be a measure-valued branching process or simply an expected number

density. If we simply sum and scale paths without retaining particle number information we will obtain an expected number density much like in a scaling limit from traditional IPS theory. [96],[89] If we retain particle number information, we can recover a measure-valued branching process which is much closer to the objective of this theory. [94],[43],[47],[34] Moreover, if we split the bound and free populations and take scaling limits separately, we can obtain a two species model akin to those used in viral propagation studies. [105] Then, we can treat the free neutron kinetic equation and bound neutron kinetics using dramatically different tools as is typical in nuclear engineering.

In order to implement the second approach, we need to construct two distinct approximation steps since we won't be using convergence as an average over paths. First, we need to replace the quantum stochastic process by a nonlinear but commutative Markov process. Second, we need to apply a generalized law of large numbers to directly obtain a kinetic equation for the full system. The first step can be done somewhat circuitously. Our QSP is conservative when you look at it in the right light. We don't allow for unbounded growth stemming from interactions with an infinite fermi sea. Depletion of the medium is possible by repeatedly increasing the free population. Thus, the evolution operators involved can actually be thought of as being bounded. As such, we can always construct a suitable dilated theory such that our quantum stochastic process can be recovered by compression on to a subspace.[135] Then, the resulting Hamiltonian theory can be mapped to a path integral relative to a classical stochastic process by using stochastic spectral methods. [36],[98] This can be reduced to a strictly classical process on some constrained set of measurements. There is a complex problem to address here involving quantum measurement theory and how to identify the measurements that could be left intact as we reduce the path integration to a process on the base space rather than a Hilbert space. Supposing we can do that, then it is possible to invoke the existing theory for a generalized law of large numbers for nonlinear Markov processes. [83] This is actually an application of concentration inequalities to the reduction of a stochastic process to a density satisfying a generator equation. It may be possible, as Kolokoltsov notes, to generalize this to a direct reduction of a QSP.

7.2.3 Moyal Bracket Dynamics for Classical Field Approximation

A third technique for studying the reduction of our reaction-transport QSP to a classical process is to employ the techniques developed for non-equilibrium field theory that we discussed in the review of literature. The cluster expansion followed by correlation function decay rate bounding methodology that we outlined can be applied to quantum systems as well as classical systems.[4] The main challenge amounts to choosing a representation of the quantum system that is amenable to this. However, there is already an extensive body

of work on phase space quantization and the Wigner transform to draw on in this effort.[55],[1],[25],[35],[28] We can use the techniques that have been developed for studying phase space quantized systems to simplify the dynamics the reaction-transport PDP into a framework reminiscent of the Liouvillan dynamics on phase space but with a Moyal bracket used in place of the Poisson bracket. The reaction transition operators have also been chosen to take a particularly simple form under the action of the Wigner transform. This approach has been used in other contexts for the study of nonequilibrium dynamics of many-body systems and has been shown to be successful. The most concerning challenge would be the representation and approximation of the bound state dynamics in terms of Moyal brackets.

It is worth noting that in our construction of the free propagator in chapter 6, we used a Laplacian applied to each particle for the free dynamics. By using the Moyal bracket, we can study the approximation of this by streaming terms in a more wholistic sense than we could have using the path simulation method. This is useful for understanding in a deeper way what is lost from the free propagation in the transition to a classical kinetic equation.

7.2.4 Beam Averaging for Detector Efficiencies in terms of Scattering Theory

We have discussed three (arguably four) different approaches to the construction of classical neutron transport theories from a fitted reaction-transport PDP. It is worth considering how we would actually obtain a fitted PDP from other experimental data. The underlying systems can be very complicated and it is worth identifying how we can model the data without using the full power of the individual quantum field theories for nuclear scattering and condensed matter dynamics.

One useful simplification is in the analysis of the reaction events with probabilities encoded by the terms $|\langle \alpha_{x_1,k_1}, \boldsymbol{V}_{x_1,k_1,a_i}\psi\rangle|^2$. Per our discussion in the review of literature, it is generally not enough to use the bare cross section. The interaction needs to be renormalized into an effective interaction to account for coupling to other parts of the medium. In analyzing this process, we have an operator family $\boldsymbol{V}_{x_1,k_1,\ell}$ and an apparatus function α to fit. The function α may be used in other analyses (such as a scaling argument) so over reliance on a particular form of α should be avoided. This still gives us an enormous amount of leeway for modeling. In order to avoid trying to account for every possible scattering feature, it is useful to recall the underlying purpose of this analysis. We are attempting to recover a more reliable classical stochastic model. All of the techniques that we have proposed for doing so ultimately rely on integrals over path distributions. One approach to simplifying this work is to replace the full potential $\boldsymbol{V}_{x_1,k_1,\ell}$ with an averaged potential $\langle \boldsymbol{V}_{x_1,k_1,\ell}\rangle$. In particular, because any scaling limit will involve a distribution that is integrated over angles of approach, we can average the potential over possible incident beams. Techniques based this idea have

been in use in nuclear engineering for both slow neutron scattering and resonance integral approximation for many years.[117],[137] The proposal here is simply that this same approximation scheme applies to the full quantum potential when it is used directly in the computation of transition probabilities in a quantum field theory.

7.2.5 Condensed Matter Fluctuation Averaging and Apparatus Function Sensitivity

Another useful simplification that can be introduced is a recognition that the condensed matter physics can be replaced by a static equivalent. Although neutron fluctuations propagate at high speeds, our information about the particular vibrational state of atoms in the lattice at any given time is very limited. Indeed, phonons and other condensed matter phenomena will impact the interaction of neutrons and nuclei, through Doppler broadening and amplified scattering rates. However, the electronic dynamics is extremely complex and not necessarily useful to model from the standpoint of a macroscopic measurement. The point of view we take here is that the fully dynamic medium can be replaced by an equilibrium mean field that exhibits phase space widths that represent the mean deviation over a sufficiently long cycle. The validity of a static medium approximation becomes something of an ergodic problem in this light, but the essential approximation is easy to implement. We don't need to make the potentials $\boldsymbol{V}_{x_1,k_1,\ell}$ an explicit function of time so long as we average them over a typical dynamical period so that the potential has a width that is representative of the range of motion of a nucleus in an oscillating atom and energies are smoothed to account for the Maxwellian distribution of velocities in advance.

7.3 Extension of Absorption and Decay Operators to More General Creation and Annihilation Processes

We have introduced a fairly simple model of the reaction dynamics of a system. There are several improvements that we can make that would expand the range of possible applications. In particular, examining unbounded absorption and decay processes provides a route to studying the quantum neutron dynamics without using a discrete medium. This will produce a result that is more closely related to the Pál-Bell equation. This will require additional technicalities from more modern quantum stochastic process theories.[119]

There is also work to be done in expanding the range of condensed matter models that this technique can apply to. Right now, we only allow static atomic systems that transmute dynamically. This can fairly easily be extended to flowing systems that evolve independently of the collision dynamics. However, this

will require some additional methods from measure transport theory. [2]

Finally, we currently only allow nonlinear coupling of neutrons through interactions with the medium where transmutations have occurred. This ignores correlations induced by condensed matter disruptions. For example, a neutron that induces fission will create local fluctuations in the condensed matter distribution (including for nuclei that the neutron itself never specifically interacted with). This will then alter the collision probabilities for other neutrons passing through the "damaged" region. These second order effects can be dramatic and have never been quantified from the perspective of neutron transport. This would require the introduction of another Hilbert subspace associated to the condensed matter medium from an atomic perspective and the modeling of disruptions due to collisions would need to be handled by some generalization of the methods of radiation energy deposition from health physics.[142]

7.4 Direct Comparison to Other Non-Equilibrium Quantum Theories

So far, we have developed a new theory with novel capabilities. However, given that fact that this includes features that make it effectively bounded, it is likely that this theory supports a representation in other existing non-equilibrium quantum field theories. A direct comparison of the results for neutron thermalization to the cell function method of Osborn and Yip is an obvious first step. However, there has also been an enormous amount of recent work by quantum field theorists for nuclear matter, quantum liquids, and nanotechnology that is superficially very different from the quantum optical approach that we adopt here. [126],[18],[76],[29] Most of these authors (except for Dalton who draws more on the Wigner function tradition) extend the work of Kadanoff and Baym in one sense or another. [8] For this reason, it appears that the initial construction of this theory in one of the other frameworks would have proven difficult and would not have connected as nicely to particle simulation methods. However, the evolution of non-equilibrium field theory has been significant and rapid enough in recent years that it is likely that a comparison of the methods would yield significant new approximation tools and greater insight into how to optimally fit the free parameters of our theory.

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