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Deriving the Jarzynski Relation From Doi-Peliti Field Theory

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DERIVING THE JARZYNSKI RELATION FROM DOI-PELITI FIELD THEORY

by

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Abstract

Recently, a number of strict equalities have been developed for far from equilibrium statistical mechanical systems that relate work done on a system and its change in free energy. We develop a field-theoretic description of non-equilibrium work relations using Doi-Peliti field theory. Specifically, we create the Doi-Peliti field theory for thermal systems and use it to derive the well-known Jarzynski equality. Our resulting framework can be extended to other non-equilibrium relations. We consider classical particles on a lattice that experience pair-wise interactions and a local potential. These particles hop with rates determined by coupling to a thermal bath. Work protocols are imposed by varying the local potential, which drives the system out of equilibrium. In this framework, work relations appear simply as the result of a gauge-like transformation combined with a time-reversal. We present the derivation with a one-dimensional system on a lattice and conclude with the generalization to multiple dimensions and the continuum limit.

Chapter 1

Introduction

To motivate the derivation of the Jarzynski relation, we begin with a practical example. A common problem in polymer physics and biochemistry is determining how a system changes due to a non-equilibrium process. For instance, let us assume that we have an RNA strand with both ends connected to beads as shown in Fig. 1.1. We fix the bead at one end to a micropipette and place the other bead in a laser trap. The laser trap allows us to apply force to the bead and cause the RNA strand to extend. From the bead's displacement in the laser trap, we determine the force on the bead. Thus, we are able to quantify the amount of work done on the RNA strand during its extension. For our non-equilibrium process, let us extend the bead from an initial separation of λ_1 to a final separation λ_2, done at a specified rate. This process is known as a work protocol.

We record the work required to complete this protocol for multiple trials. By plotting the data in a histogram, we are able to produce a work distribution similar to the one shown in Fig. 1.2. Assume that for our system, we have an initial state A and associated equilibrium Helmholtz free energy F_A. Then if the system undergoes a process leading to a final state B with equilibrium Helmholtz free energy F_B, the change in Helmholtz free energy, $\Delta F = F_B - F_A$, may be negative or positive. If our system were large, the work distribution produced by this process would be a sharply peaked function (Dirac delta function) centered at the average work value $\langle W \rangle$. Classically, the change in free energy of the system, ΔF, due to the work protocol would be bounded by the second law of thermodynamics: $\langle W \rangle \geq \Delta F$.

However, our example system is not in the thermodynamic limit and hence our

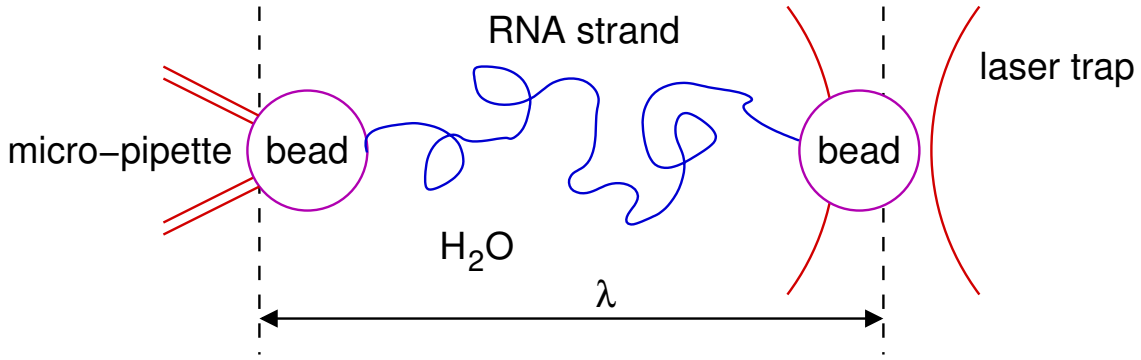

Figure 1.1: An example system of an RNA molecule attached to two beads that are being forced to make the system undergo a non-equilibrium process. The first bead is fixed to a micropipette, and the second bead is in a laser trap applies force to the RNA molecule and increases the extension λ.

work distribution is not a Dirac delta function. As shown in Fig. 1.2, for our small system non-equilibrium process we have a wide distribution of work values produced from the work protocol. To understand how the work distribution is produced, let us imagine multiple trials that all follow the specified work protocol. Since we have such a small system, fluctuations in the water bath surrounding the RNA molecule cause differing amounts of work required to extend the RNA molecule. For instance, during one trial more water molecules may strike the particle to the right than to the left requiring more work than usual to extend the RNA molecule. Alternatively, more water molecules may strike the RNA molecule to the right, requiring less work. Note, there are values of work less than the change of free energy of the system, and hence the second law of thermodynamics is not particularly insightful. However, the Jarzynski relation provides an equality that is always able to determine the change in free energy from the work distribution. This is experimentally shown in [12, 13, 14, 15].

The Jarzynski equality is a non-equilibrium statistical mechanics relation and is explicitly

$$\langle e^{-W/k_BT} \rangle = e^{-\Delta F/k_BT}, \tag{1.1}$$

where W is the work done on the system, T is the temperature, k_B is Boltzmann's constant, and ΔF is the change in free energy. The angle brackets around the term containing the work indicate an average over an infinite number of realizations of the system undergoing the same work protocol. Generally, a work protocol is a specified sequence of values for the control parameter of the system that occurs regardless of the energetic cost.

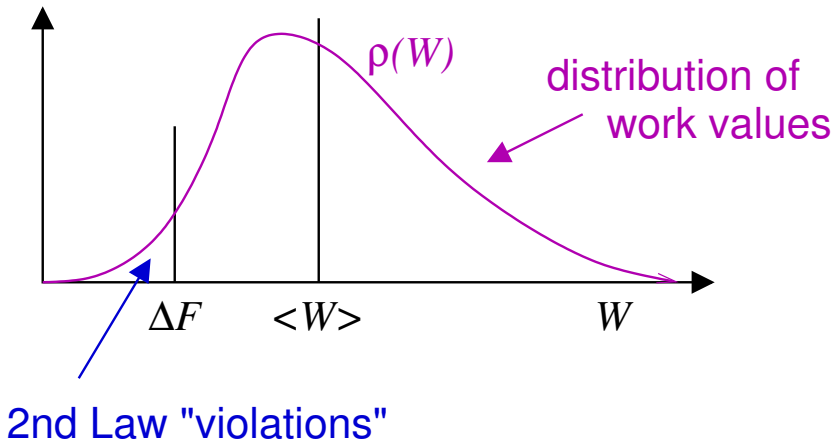

Figure 1.2: The work distribution produced from multiple trials of extending an RNA strand according to a given work protocol. Both the average work the RNA molecule requires to extend, $\langle W \rangle$ and the systems corresponding change in free energy due to this process, ΔF are labelled. The work values that violate the second law of thermodynamics are less than ΔF and shown above.

The second law of thermodynamics like most statistical mechanical and thermodynamic relations, is based on using the overwhelming likelihood of more probable states for very large systems, typically Avogadro's number of particles. While the second law is powerful in its generality, it only applies for large thermodynamic systems, and describes system variables in terms of inequalities for all non-quasistatic processes. The fundamental statistical mechanics and thermodynamic relations used in this paper can be found in Ref. [1]. Currently, a series of relations such as the Crook's relation [2, 3], the fluctuation theorem [4, 5], and the Jarzynski equality [6] have succeeded in removing the near equilibrium requirement. They describe the system in terms of equalities instead of inequalities [7, 8, 9, 10, 11]. Interestingly, the Jarzynski equality holds true for systems of any size as well as systems very far from equilibrium. Thanks to this universality, the relation has been the focus of many recent studies.

Other pedagogical examples of the Jarzynski relation such as a harmonic oscillator with a varying spring stiffness can be found in Ref. [16]. Additionally, a quantum mechanical derivation for the harmonic oscillator was demonstrated by Ref. [17]. However, there is one important caveat for the Jarzynski relation: the initial state must be an equilibrium state with the same temperature T.

Another aspect of the relation is that it holds for a wide variety of systems.

Both quantum and classical systems obey the relation, whether they are stochastic or deterministic, either on a lattice or taken to the continuum limit [6, 18, 19, 20, 21]. Previous studies have shown that the Jarzynski relation results from a time-reversal symmetry. We will produce the Jarzynski relation in the mathematical framework of the Doi-Peliti field theory [25]. By casting the relation in this field theory, we have not only derived it in this context, but we have also created the foundation for producing similar relations such as the Crook's relation in this framework. Previous field-theoretic formulations of the Jarzynski relation were found by Mallick, Moshe, and Orland [22] as well as Täuber [23]. Their derivations were phenomenological due to assumptions about the particle dynamics that are generally only valid for large systems near an equilibrium critical point. Contrary to their derivations, Doi Peliti field theory is based on first principles and is generally valid, with no restrictions on system size or location in a phase diagram.

Before we dive into the model, we now give a quick description of Doi-Peliti field theory. Field theories are mathematical frameworks (see Ref. [24] for more detail) and in this instance, Doi-Peliti field theory is used to describe classical particles and their dynamics. Most field theories involve phenomenology where they include terms that have been specifically created to satisfy an appropriate symmetry. Doi-Peliti field theory has the advantage that it properly maps classical particle behavior to a field theory without having to make ad hoc assumptions about the dynamics. Previous uses of Doi-Peliti field theory were for athermal systems such as irreversible chemical reactions [25]. For our derivation, we seek to create a new formulation of the field theory that applies to thermal systems.

Chapter 2

Model and Statistical Mechanics

The model that we will be working with is a finite-sized lattice with a finite and conserved number of particles undergoing a stochastic hopping process as shown in Fig. 2.1. All particles obey classical rules, and each lattice site may contain multiple particles at a given time. We will explain the theory on a one dimensional lattice for simplicity, but we may extend it to a hypercubic lattice of arbitrary dimension. For a given particle, there is an inhomogeneous energy landscape on this lattice as shown in Fig. 2.2 due to pair interactions between the particles and a local site-by-site lattice potential that can vary with time. Statistical mechanical rules bias a particle to have a higher probability of existing at a lattice site with a lower energy. Likewise, the hopping rates are biased by the energy transition between the initial and final states of the hopping process. We use the term *state* to mean a specific configuration of all of the particles in a system. Throughout the paper, we will indicate the number of particles at a given site i known as the occupation number of the site by n_i, and a specific state configuration of the system with the term $\{n\} = (n_1, n_2, n_3, \ldots n_L)$, where L is the number of lattice sites. The local potential $\tilde{U}_i(t)$ of each lattice site may change with time. The coefficient V_{ij} determines the strength of the pair interactions between two particles at site i and j and is constant with respect to time. The variation of the $U_i(t)$ will be the mechanism through which the work protocol will be enacted in order to produce the Jarzynski relation.

We characterize the system with the probabilities of the states $P(\{n\}, t)$ for all states $\{n\}$. The system dynamics such as the hopping rates affect the time derivative of $P(\{n\}, t)$. In other words, the dynamics of the system and how the system evolves are encapsulated in the probabilities of the states. For instance, the probabilities

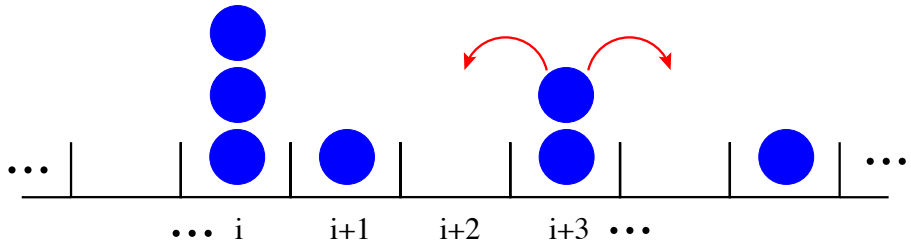

Figure 2.1: Particles are allowed to hop between lattice sites with their hopping rates determined by the difference in energy between the state of the system before the hop and the state after. While shown in one dimension here, we allow for multiple dimensions in our model.

of the system will be initially stationary because the system is in equilibrium. As the local lattice potential varies with time, the probabilities of the system existing in given states will change due to the shift in the lattice energetics.

2.1 Energy

In equation form, we may represent the total energy for a given state as

$$E(\{n\},t) = \frac{1}{2}\sum_{i=1}^{L}\sum_{j=1}^{L} n_i V_{ij} n_j - \frac{1}{2}\sum_{i=1}^{L} V_{i,i} n_i + \sum_{i=1}^{L} n_i \tilde{U}_i(t), \tag{2.1}$$

where the first two terms represent the pair potential contributions, the coefficient $V_{i,j}$ indicates the strength of these pair interactions, the third term indicates the contributions from the lattice site potentials, and i, j are lattice site indices. The second pair potential term $\frac{1}{2}\sum_i V_{i,i} n_i$ compensates for the over-counting of the same-site pair potentials in the first pair potential term. Since this term is also linear in terms of the occupation number n_i, we group it with the local potential $\tilde{U}_i$ to form

$$U_i = \tilde{U}_i + \frac{1}{2} V_{i,i}. \tag{2.2}$$

Using this definition in Eq. (2.1), we have

$$E(\{n\},t) = \frac{1}{2}\sum_{i=1}^{L}\sum_{j=1}^{L} n_i V_{ij} n_j + \sum_{i=1}^{L} n_i U_i(t). \tag{2.3}$$

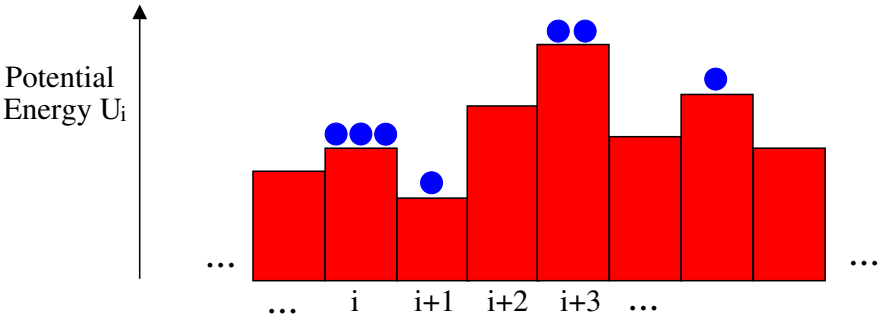

Figure 2.2: A representative model of the potential at each lattice site. While sites with a lower potential are more likely to have more particles, it is not necessitated as they are subject to thermal fluctuation. On average, they will follow Boltzmann statistics.

Boltzmann statistics provides the equilibrium probability for the system to exist in a given state. In particular, the probability of a given state is proportional to the exponent of the negative state's energy. Expressed as an equation, we have

$$P(\{n\},t) = \frac{1}{Z} e^{-E(\{n\},t)/k_B T}, \tag{2.4}$$

where Z is a normalization factor known as the partition function and $E(\{n\},t)$ is the energy of the state $\{n\}$ at time t. Since the initial state for the Jarzynski relation is an equilibrium state, the state is governed by these statistics and is referred to as the Boltzmann state.

2.2 Master Equation

To evolve the system forward in time, we turn to the master equation:

$$\partial_t P(\{n\},t) = \sum_{\{m\}\neq\{n\}} \Big[\underbrace{w_{\{m\}\to\{n\}} P(\{m\},t)}_{\text{Gain Term}} - \underbrace{w_{\{n\}\to\{m\}} P(\{n\},t)}_{\text{Loss Term}} \Big], \tag{2.5}$$

which relates a given state's probability's rate of change $\partial_t P(\{n\},t)$ to the current state of the system. The rate constants $w_{\{m\}\to\{n\}}$ represent the rate at which any dynamical process causes a transition from state $\{m\}$to state $\{n\}$. With no information about the rate constants $w_{\{m\}\to\{n\}}$, this master equation is extraordinarily

general as the only assumption about the system dynamics is that they are Markovian. Markovian dynamics only depend on the instantaneous probabilities $P(\{n\},t)$ and not on the state of the system at earlier times. In essence, the equation is a basic flow in versus flow out differential equation for the probabilities that determines the current likelihood of a certain state. The gain term is the probability gained from all states $\{m\}$ that can become state $\{n\}$ at rate $w_{\{m\}\to\{n\}}$. Similarly, the loss term is probability lost to all states $\{m\}$ at rate $w_{\{m\}\to\{n\}}$.

For the Jarzynski equality to hold, the system must initially be in a equilibrium state governed by Boltzmann statistics. However, this does not indicate that particles are not moving; it implies that the probabilities are stationary. A natural assumption that satisfies this condition is known as detailed balance.

Detailed balance is the assumption that the flow term into a given state $w_{\{m\}\to\{n\}}P(\{m\},t)$ must precisely equal the flow out of the state $w_{\{n\}\to\{m\}}P(\{n\},t)$ in order to maintain equilibrium. When the system is in equilibrium, the particles obey Boltzmann statistics for their given distributions. Note that for all following calculations we will use $\beta = 1/k_BT$ where k_B is the Boltzmann constant, and T is the temperature of the state. Thus, the $P(\{n\},t)$ is $e^{-\beta E(\{n\},t)}$, where $E(\{n\},t)$ indicates the energy of the $\{n\}$ state. When formulating the probabilities for the states, we must also consider how many states are able to make the transition as each state contributes to the probability of the transition. We count the number of possible configurations of the particles could form a state $\{n\}$ with the multinomial coefficient

$$M(\{n\}) = \frac{N!}{n_1!n_2!n_3!\cdots} = \frac{N!}{\prod_i n_i!}, \tag{2.6}$$

where index i indicates lattice site, and N is the sum of all n_i. Hence, the probability of being in a given state $\{n\}$ is

$$P(\{n\},t) = \frac{1}{Z}\frac{N!}{\prod_i n_i!}e^{-\beta E(\{n\},t)}. \tag{2.7}$$

By reformulating the original equality of detailed balance, we connect the rates in and out of a state via:

$$\frac{w_{\{n\}\to\{m\}}}{w_{\{m\}\to\{n\}}} = \frac{P(\{m\},t)}{P(\{n\},t)} = \left(\prod_i \frac{n_i!}{m_i!}\right)e^{-\beta(E(\{m\},t)-E(\{n\},t))}. \tag{2.8}$$

By changing the lattice site potentials U_i, we force the system out of equilibrium. Since the model is coupled to a thermal reservoir, we are able to give and receive

energy from the bath. Due to heat flow, this would eventually lead to the system achieving equilibrium if not for the change in the lattice site potentials U_i. To simulate this, we make an assumption about the relation of the two states known as Glauber dynamics. Glauber dynamics states that the hopping rates are

$$w_{\{n\}\to\{m\}} = \Gamma \frac{\alpha(\{n\})e^{\beta E(\{n\},t)}}{e^{\beta E(\{n\},t)} + e^{\beta E(\{m\},t)}}, \tag{2.9}$$

where Γ is an overall rate constant related to how quickly particles transition between states, and α is determined by the number of particles in the state $\{n\}$ that are capable of making the specific transition to $\{m\}$. We will elaborate on α in Sec. (2.3). The rate constant Γ is the discrete space equivalent of the continuous space diffusion constant D. The energy terms are the same as Eq. (2.3). With a substitution into Eq. (2.8), one can show that this satisfies detailed balance.

We will now define the state transition rules for our system. If we observe the system during a small enough time frame, at most one particle moves at a given time. Likewise, particles are only allowed to hop to adjacent lattice sites. For instance, if a particle has moved two lattice sites away from its original location, the particle must have transitioned through the lattice site between the initial and final sites. Additionally, each particle hops independently from all other particles. These rules markedly restrict the possible state transitions of our system. If the system is in state $\{n\}$, the states $\{m\}$ available for transition to state $\{n\}$ must be exactly one particle out of alignment with state $\{n\}$, and that particle must be exactly one nearest neighbor hop away from creating the state $\{n\}$.

2.3 Two Lattice Site Example

To provide a simplified example of possible transitions, let us assume that we have two sites on our lattice. We will focus on transitions for the state $\{n\} = (n_1, n_2)$. As defined before, we only allow one nearest neighbor hop in an arbitrarily small window of time. Hence, states $\{m\}$ that are able to transition to or from (n_1, n_2) are $(n_1 + 1, n_2 - 1)$ and $(n_1 - 1, n_2 + 1)$. Let us now set up the master equation for our miniature system.

We start with transitions to and from the state (n_1+1, n_2-1). Since (n_1+1, n_2-1) has one more particle on site 1 and one less on site 2, we may simply express the energy

of the (n_1+1, n_2-1) as a shift of the (n_1, n_2) state's energy:

$$E(n_1+1, n_2-1, t) = E(n_1, n_2, t) + U_1 + \sum_{j=1}^{2} V_{1j} n_j - U_2 - \sum_{j=1}^{2} V_{2j} n_j. \tag{2.10}$$

To begin, we determine the detailed balance ratio for this transition:

$$\begin{aligned}
\frac{w_{(n_1+1,n_2-1)\to(n_1,n_2)}}{w_{(n_1,n_2)\to(n_1+1,n_2-1)}} &= \frac{(n_1+1)!(n_2-1)!}{n_1! n_2!} \frac{e^{\beta E(n_1+1,n_2-1,t)}}{e^{\beta E(n_1,n_2,t)}} \\
&= \frac{(n_1+1)}{n_2} \frac{e^{\beta(E(n_1,n_2,t)+U_1+\sum_{j=1}^{2} V_{1j} n_j - U_2 - \sum_{j=1}^{2} V_{2j} n_j)}}{e^{\beta E(n_1,n_2,t)}} \\
&= \frac{(n_1+1)}{n_2} \frac{e^{\beta(U_1+\sum_{j=1}^{2} V_{1j} n_j)}}{e^{\beta(U_2+\sum_{j=1}^{2} V_{2j} n_j)}}.
\end{aligned} \tag{2.11}$$

Since this notation is cumbersome, we define

$$\epsilon_i \equiv U_i + \sum_{j=1}^{L} V_{ij} n_j. \tag{2.12}$$

Using Eq. (2.12), we create the Glauber dynamics for the transition $(n_1+1, n_2-1) \to (n_1, n_2)$:

$$w_{(n_1+1,n_2-1)\to(n_1,n_2)} = \Gamma \frac{(n_1+1) e^{\beta \epsilon_1 n_1}}{e^{\beta \epsilon_1} + e^{\beta \epsilon_2}}. \tag{2.13}$$

For the reverse transition $(n_1, n_2) \to (n_1+1, n_2-1)$, we have

$$w_{(n_1,n_2)\to(n_1+1,n_2-1)} = \Gamma \frac{n_2 e^{\beta \epsilon_2}}{e^{\beta \epsilon_1} + e^{\beta \epsilon_2}}. \tag{2.14}$$

Using the same logic as the previous transition, we create the rates for $(n_1-1, n_2+1) \to (n_1, n_2)$:

$$w_{(n_1-1,n_2+1)\to(n_1,n_2)} = \Gamma \frac{(n_2+1) e^{\beta \epsilon_2}}{e^{\beta \epsilon_1} + e^{\beta \epsilon_2}}. \tag{2.15}$$

For the reverse transition $(n_1, n_2) \to (n_1-1, n_2+1)$, we have

$$w_{(n_1,n_2)\to(n_1-1,n_2+1)} = \Gamma \frac{n_1 e^{\beta \epsilon_1}}{e^{\beta \epsilon_1} + e^{\beta \epsilon_2}}. \tag{2.16}$$

Our two-lattice-site master equation is:

$$\begin{aligned}\partial_t P(n_1,n_2,t) = w_{(n_1-1,n_2+1)\to(n_1,n_2)}P(n_1-1,n_2+1,t) - w_{(n_1,n_2)\to(n_1-1,n_2+1)}P(n_1,n_2,t)\\ + w_{(n_1+1,n_2-1)\to(n_1,n_2)}P(n_1+1,n_2-1,t) - w_{(n_1,n_2)\to(n_1+1,n_2-1)}P(n_1,n_2,t).\end{aligned} \tag{2.17}$$

Inputting the rates, we have

$$\begin{aligned}\partial_t P(n_1,n_2,t) =&\Gamma\frac{1}{e^{\beta\epsilon_1}+e^{\beta\epsilon_2}}\Big[(n_2+1)e^{\beta\epsilon_2}P(n_1-1,n_2+1,t) - n_1e^{\beta\epsilon_1}P(n_1,n_2,t)\\ &+ (n_1+1)e^{\beta\epsilon_1}P(n_1+1,n_2-1,t) - n_2e^{\beta\epsilon_2}P(n_1,n_2,t)\Big]\end{aligned} \tag{2.18}$$

With a slight regrouping of terms, our master equation may be expressed as:

$$\begin{aligned}\partial_t P(n_1,n_2,t) =&\frac{\Gamma}{e^{\beta\epsilon_1}+e^{\beta\epsilon_2}}\Big\{e^{\beta\epsilon_1}\Big[(n_1+1)P(n_1+1,n_2-1,t) - n_1P(n_1,n_2,t)\Big]\\ &+ e^{\beta\epsilon_2}\Big[(n_2+1)P(n_1-1,n_2+1,t) - n_2P(n_1,n_2,t)\Big]\Big\}\end{aligned} \tag{2.19}$$

To extend this to all lattice sites, let us focus specifically on particle transitions involving the ith site of the lattice. The state of the system is $\{n\}$, specifying n_i particles at site i. All states that can transition to or from state $\{n\}$, restricted to transitions including site i, are only one particle out of alignment with state $\{n\}$. To generalize the two site example, imagine that the full lattice is a series of two site transitions. We may extend the two site example to general lattice sites by taking sites 1 and 2 and identifying them as sites i and $i+1$ for general i, and then summing over all sites i. Hence for our model, we use the following master equation:

$$\begin{aligned}\partial_t P(\{n\},t) = \Gamma\sum_{i=1}^{L}\Bigg[&\frac{e^{\beta\epsilon_i}}{e^{\beta\epsilon_i}+e^{\beta\epsilon_{i+1}}}\Big((n_i+1)P(\ldots,n_i+1,n_{i+1}-1,\ldots,t) - n_iP(\{n\},t)\Big)\\ &+\frac{e^{\beta\epsilon_{i+1}}}{e^{\beta\epsilon_i}+e^{\beta\epsilon_{i+1}}}\Big((n_{i+1}+1)P(\ldots,n_i-1,n_{i+1}+1,\ldots,t) - n_{i+1}P(\{n\},t)\Big)\Bigg].\end{aligned} \tag{2.20}$$

Since the system has left-right symmetry, every part of the left-moving term (top line) has a counterpart in the right-moving term (bottom line) with its direction reversed.

2.4 First Law

Let us differentiate the average total energy of the system with respect to time to produce an expression akin to the first law of thermodynamics:

$$\frac{d}{dt}\langle E\rangle = \frac{d}{dt}\sum_{\{n\}} P(\{n\},t)E(\{n\},t) = \sum_{\{n\}}\frac{dP}{dt}E + \sum_{\{n\}} P\frac{dU}{dt}, \tag{2.21}$$

where the $P(\{n\},t)$ is the probability of a given state configuration $\{n\}$, and $E(\{n\},t)$ is the energy of the state. Via differentiating and the product rule, we produce two terms, one where the probability of the states change and the other where the lattice potential changes.

First, let us imagine that the lattice potentials U_i are fixed. Thus, the $\frac{dU}{dt}$ term vanishes, and we are left with the first term on the right of Eq. (2.21). Particles will change their state configuration $P(\{n\},t)$ to attempt to reach equilibrium with a coupled thermal reservoir. As the particles move, they exchange energy with the reservoir. Since only the probabilities of the particle configurations are changing with time, the total energy changes solely via exchange with the coupled reservoir. Hence, the first term of Eq. (2.21) naturally represents the system's heat flow dQ/dt.

Inversely, by locking the particles in place but allowing the lattice site potentials U_i to change, we remove our heat flow term. However, the total energy now varies due to lattice site potential U_i in the form of the second term of Eq. (2.21). By raising or lowering a site's lattice potential, the particles at that site are forced up or down in energy in a manner analogous to doing work on them. More succinctly, the second term represents our definition of the derivative of work dW/dt for the system. Note that since the pair potential coefficient does not change with time, it does not contribute to the work term. Therefore, the change in the lattice potential U_i is the only term that produces work.

Chapter 3

The Doi Representation

The time derivative $\partial_t P(\{n\}, t)$ in the master equation for our system Eq. (2.20), depends on the occupation numbers n_i. While explicitly describing the state's evolution, the occupation number is difficult to deal with directly in the master equation. The master equation is a set of linear equations where there is mixing of different states, which would represent off-diagonal terms in a matrix representation. To ease the manipulation of these equations, we exploit that each particle hops identically and independently. We use the Doi representation of the master equation to remove the explicit dependence on the occupation number. Derivation of the Doi representation is presented by Doi in Ref. [26].

Doi mechanics utilizes annihilation and creation operators $\hat{a}, \hat{a}^\dagger$, respectively, defined similarly to their quantum mechanics definitions. Doi mechanics have constant coefficients with respect to the occupation number in the master equation. Just as each site had an occupation number, sites $i, j, \ldots$ will have associated creation operators $\hat{a}_i^\dagger, \hat{a}_j^\dagger, \ldots$ and annihilation operators $\hat{a}_i, \hat{a}_j, \ldots$ to increase and decrease the number of particles at a site by 1, respectively. For all integers greater than or equal to zero, our model lacks restrictions for the occupation numbers. Hence the creation and annihilation operators are analogous to bosonic operators (Ref. [27]), which means that the operators follow these relations:

$$\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij}, \qquad \left[\hat{a}_i, \hat{a}_j\right] = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0, \tag{3.1}$$

where $[A, B] = AB - BA$ indicates a commutation relation. Since a site may have zero particles, we define our ground state $|0\rangle$ via

$$\hat{a}_i |0\rangle = 0, \tag{3.2}$$

as the state that is destroyed by any annihilation operator. Similarly, we shall define the nth state $|n\rangle$ through repeated application of the creation operator on the ground state:

$$|n_i\rangle = (\hat{a}_i^\dagger)^{n_i} |0\rangle . \tag{3.3}$$

As its name implies, the creation operator $\hat{a}_i^\dagger$ increases the occupation number on site i by one. This follows directly from its definition:

$$\hat{a}_i^\dagger |n_i\rangle = \hat{a}_i^\dagger (\hat{a}_i^\dagger)^{n_i} |0\rangle = (\hat{a}_i^\dagger)^{n_i+1} |0\rangle = |n_i + 1\rangle . \tag{3.4}$$

This definition differs from the usual quantum mechanics definition of $\hat{a}^\dagger$ by a normalization constant. Similarly, the annihilation operator $\hat{a}_i$ decreases the occupation number for site i by one and also produces a constant due to the operator relation:

$$\hat{a}_i |n_i\rangle = n_i |n_i - 1\rangle , \tag{3.5}$$

which also differs by a normalization constant from the usual quantum mechanics definition. This proof may be found in Appendix (A). In combination, these two definitions allow us to define the number operator $\hat{a}_i^\dagger \hat{a}_i$ such that it leaves the state unchanged but produces a constant coefficient of n_i:

$$\hat{a}_i^\dagger \hat{a}_i |n_i\rangle = \hat{a}_i^\dagger n_i |n_i - 1\rangle = n_i \hat{a}_i^\dagger |n_i - 1\rangle = n_i |n_i\rangle . \tag{3.6}$$

The number operator allows us to extract information about occupation numbers for a given state.

Through these operators and states, we create an algebraic construction known as a Fock space. The purpose of the Fock space is to encode all information of the system at a given time into a single state $|\Psi(t)\rangle$, defined by

$$|\Psi(t)\rangle = \sum_{\{n\}} P(\{n\}, t) |\{n\}\rangle , \tag{3.7}$$

where $|\Psi(t)\rangle$ contains all the probabilities of any site containing any number of particles at a given time. There is an important difference between this representation and a quantum mechanical state; the Doi state is linear in $P(\{n\}, t)$ while the quantum mechanical state is not. Information about state number and probability is extracted via use of operators, most commonly the number operator.

By utilizing the Fock space states, we remove from the master equation the dependence on the occupation number. We express the master equation as an imaginary-time Schrödinger equation using a Hamiltonian to determine the rate at which the system evolves,

$$\partial_t |\Psi(t)\rangle = -\hat{H} |\Psi(t)\rangle , \tag{3.8}$$

where the Hamiltonian $\hat{H}$ depends on the dynamics of the given system.

If we had a constant Hamiltonian $\hat{H}$, the solution to Eq. (3.8) would be

$$|\Psi(t)\rangle = e^{-\hat{H}(t-t_1)} |\Psi(t_1)\rangle , \tag{3.9}$$

where $|\Psi(t_1)\rangle$ is the state of the system at the initial time t_1.

3.1 Two Site Example (Continued)

To move our full lattice master equation to the Fock space, we first return to the simplified two site lattice for which we developed the master equation, Eq. (2.19), in the previous chapter. We will create the Doi representation of this master equation by creating a Hamiltonian $\hat{H}$, which contains all of the dynamics of the system. This allows us to re-express the master equation as an imaginary-time Schrödinger equation like Eq. (3.8).

Let us input this into our state equation form of the master equation:

$$\partial_t |\Psi(t)\rangle = \sum_{n=0}^{\infty} \partial_t P(n,t) |n\rangle \tag{3.10}$$

$$= \sum_{n_1,n_2=0}^{\infty} \frac{\Gamma}{e^{\beta\epsilon_1} + e^{\beta\epsilon_2}} \Big\{ e^{\beta\epsilon_1} \Big[(n_1+1)P(n_1+1, n_2-1, t) - n_1 P(n_1, n_2, t) \Big] + e^{\beta\epsilon_2} \Big[(n_2+1)P(n_1-1, n_2+1, t) - n_2 P(n_1, n_2, t) \Big] \Big\} |n\rangle . \tag{3.11}$$

To simplify the derivation of a Hamiltonian $\hat{H}$, let us first work with random unbiased diffusion, i.e. the case where $\epsilon_i = 0$ for all i. Hence we have

$$\partial_t |\Psi(t)\rangle = \sum_{n_1,n_2=0}^{\infty} \Gamma \Big[(n_1+1)P(n_1+1, n_2-1, t) - n_1 P(n_1, n_2, t) + (n_2+1)P(n_1-1, n_2+1, t) - n_2 P(n_1, n_2, t) \Big] |n_1, n_2\rangle . \tag{3.12}$$

The loss terms are produced through an application of the number operator $\hat{a}_i^\dagger \hat{a}_j$ for $i = 1, 2$. Conversely, the gain terms appear like number operators, but instead of

having the same site for both operators, we swap them. However, we must also shift over the sum. Let us act apply the operator, $\hat{a}_1^\dagger \hat{a}_2$ to the general state $|n_1, n_2\rangle$:

$$\sum_{n_1,n_2=0}^{\infty} \hat{a}_1^\dagger \hat{a}_2 |n_1, n_2\rangle = \sum_{n_1,n_2=0}^{\infty} n_2 |n_1 + 1, n_2 - 1\rangle . \tag{3.13}$$

Since the sum indices are arbitrary, we may shift them by $n_1 \to n_1 - 1$ and $n_2 \to n_2 + 1$. The gain term then becomes

$$\sum_{n_1,n_2=0}^{\infty} (n_2 + 1) |n_1, n_2\rangle \to \sum_{n_1=1,n_2=-1}^{\infty} (n_2 + 1) |n_1, n_2\rangle . \tag{3.14}$$

Since the $n_2 = -1$ state does not exist, we may shift the lower limit of the sum to $n_2 = 0$. Likewise, the $n_1 = 0$ state contributes 0 to the sum. Hence, we may add it to the sum without affecting it. This results in

$$\sum_{n_1,n_2=0}^{\infty} \hat{a}_1^\dagger \hat{a}_2 |n_1, n_2\rangle = \sum_{n_1,n_2=0}^{\infty} (n_2 + 1) |n_1, n_2\rangle . \tag{3.15}$$

Through a similar procedure, $\hat{a}_2^\dagger \hat{a}_1$ produces:

$$\sum_{n_1,n_2=0}^{\infty} \hat{a}_2^\dagger \hat{a}_1 |n_1, n_2\rangle = \sum_{n_1,n_2=0}^{\infty} (n_1 + 1) |n_1, n_2\rangle . \tag{3.16}$$

Combining these terms and applying negative signs where appropriate, we create the Hamiltonian for diffusion:

$$\begin{aligned} \hat{H} &= \Gamma(\hat{a}_2^\dagger \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_1) \\ &= \Gamma(\hat{a}_2^\dagger - \hat{a}_1^\dagger)(\hat{a}_2 - \hat{a}_1). \end{aligned} \tag{3.17}$$

Now let us add back in the energy potentials such that $\epsilon_i \neq 0$. The local lattice potential component of ϵ_i is a simple scalar U_i. Unfortunately, the pair interaction term is more complicated as it has the occupation number in the exponent. To create this, we expand the exponent via its Taylor series resulting in

$$e^{\sum_i V_{ij} n_j} = \sum_m \frac{\left(\sum_i V_{ij} n_j\right)^m}{m!} \tag{3.18}$$

Hence if we create the appropriate operators for $\left(\sum_i V_{ij} n_j\right)^m$ where m is an integer index, we may then input this term into the series to produce the exponent. Conveniently, the occupation number raised to a power is produced through repeated applications of the number operator $\hat{a}_j^\dagger \hat{a}$ to the state. Thus,

$$e^{\sum_i V_{ij} \hat{a}_j^\dagger \hat{a}_j} \left|\{n\}\right\rangle = e^{\sum_i V_{ij} n_j} \left|\{n\}\right\rangle . \tag{3.19}$$

Since this exponential needs to act on the $|\{n\}\rangle$ state and leaves the states unaltered, this operator acts on the state before any other operator acts on the state. Otherwise, the result of this operator would be changed by an operator which did not leave the state unchanged.

Therefore, the dynamics of our system are described by the $\hat{H}$:

$$\hat{H} = \Gamma \frac{(\hat{a}_2^\dagger - \hat{a}_1^\dagger)\left(\hat{a}_2 e^{U_2 + \sum_j V_{2j} \hat{a}_j^\dagger \hat{a}_j} - \hat{a}_1 e^{U_1 + \sum_j V_{1j} \hat{a}_j^\dagger \hat{a}_j}\right)}{e^{U_2 + \sum_j V_{2j} \hat{a}_j^\dagger \hat{a}_j} + e^{U_1 + \sum_j V_{1j} \hat{a}_j^\dagger \hat{a}_j}}. \tag{3.20}$$

Again, we may extend the two state model to the full system via a sum over all lattice sites. First let us define the operator $\hat{\epsilon}_i = U_i + \sum_j V_{ij} \hat{a}_j^\dagger \hat{a}_j$. Hence for the system model that we are using to produce the Jarzynski relation, we have the Hamiltonian

$$\hat{H} = \Gamma \sum_i \frac{(\hat{a}_{i+1}^\dagger - \hat{a}_i^\dagger)\left(\hat{a}_{i+1} e^{\hat{\epsilon}_{i+1}} - \hat{a}_i e^{\hat{\epsilon}_i}\right)}{e^{\hat{\epsilon}_{i+1}} + e^{\hat{\epsilon}_i}}. \tag{3.21}$$

The energy potentials associated with the terms are the same as the Glauber dynamics found in the original master equation, Eq. (2.20). While this Hamiltonian appears unwieldy, we will see that the equation simplifies significantly in the continuum limit.

Chapter 4

Computing Averages

To produce the Jarzynski equality, we need to be able to produce an average while using the Fock space representation. By definition, the average of some function $F(\{n\}, t)$ at time t in this system is

$$\langle F(\{n\}, t)\rangle = \sum_{\{n\}} F(\{n\})P(\{n\}, t). \tag{4.1}$$

This average is linear in terms of the probability $P(\{n\}, t)$. As we noted before, the Doi state $|\Psi(t)\rangle$ is also linear in terms of the probability. Hence, we are unable to use the usual quantum mechanical expectation value $\langle\Psi(t)|\,\hat{F}\,|\Psi(t)\rangle$, which would be quadratic in the probability. Instead, the solution is to use $\langle P|\,\hat{F}\,|\Psi(t)\rangle$ where $\langle P|$ is the projection state, and $\hat{F}$ is the operator representation of the function $F(\{n\}, t)$.

Typically, the Doi representation of the projection state is

$$\langle P| = \langle 0|\prod_{i=1}^{L} e^{\hat{a}_i} = \langle 0|\, e^{\sum_i \hat{a}_i}. \tag{4.2}$$

Note that P here does not indicate probability, but instead is the symbol for the projection state. Expanding with the Taylor series of the $e^{\hat{a}_i}$, this state enables us to act any power of $\hat{a}_i^\dagger$ to the left and receive the same state back, as shown in Appendix A. In other words, it is a left eigenstate of the $\hat{a}_i^\dagger$ operators, with eigenvalue 1. Because we have a fixed number of particles, the exponential form of the projection state is superfluous. In terms of the Taylor expansion for the state, we require the terms up to n_i (the total number of particles at a given site) as we have an equivalent

number of $\hat{a}_i^\dagger$. Simplifying the state further, we may limit the sum of all occupation numbers n_i and hence $\hat{a}_i^\dagger$ to be N. We Taylor expand Eq. (4.2) producing

$$\langle P| = \langle 0| \sum_{N=0}^{\infty} \frac{\left(\sum_{i=1}^{L} \hat{a}_i\right)^N}{N!} = \sum_{N=0}^{\infty} \langle P_N| \tag{4.3}$$

where we have introduced the N particle projection state $\langle P_N|$ defined by

$$\langle P_N| = \langle 0| \frac{1}{N!}\left(\sum_{i}^{L} \hat{a}_i\right)^N, \tag{4.4}$$

This state forms every combination of number operators for exactly N particles.

Our system begins in equilibrium. Accordingly, the distribution of particles in the initial state is governed by Boltzmann statistics. Note that we will work in units of $k_B T = 1$ for the rest of the derivation. First, let us assume that there are no energy differences between lattice sites. Therefore in equilibrium, we have fully unbiased random hops between lattice sites known as diffusion. The probability distribution for the initial state for diffusion is

$$P_{\text{diff}}(\{n\}) = \frac{M(\{n\})}{Z}, \tag{4.5}$$

where $M(\{n\})$ is the multinomial coefficient defined in Eq. (2.6). The initial state for diffusion $|\Psi_{\text{diff}}\rangle$, is then:

$$|\Psi_{\text{diff}}\rangle = \sum P(\{n\})\,|\{n\}\rangle = \sum_{\{n\}} \frac{M(\{n\})}{Z} \prod_i (\hat{a}_i^\dagger)^{n_i}\,|0\rangle = \frac{1}{ZN!}\left(\sum_i^L \hat{a}_i^\dagger\right)^N |0\rangle\,, \tag{4.6}$$

where the sums denoted by $\{n\}$ are limited such that the upper bound of each sum n_i sum to $\sum_i n_i = N$ and N is the total number of particles. If not for the additional partition function Z coefficient, this would be the Hermitian adjoint of the projection state for a fixed number of particles Eq. (4.4). We now reintroduce the lattice site potentials U_i but leave the pair interactions for later. This modifies our probabilities of the initial state, a Boltzmann state, to be

$$P_B(\{n\}) = \frac{M(\{n\}) e^{-\sum_i n_i U_i}}{Z}. \tag{4.7}$$

This produces an initial Boltzmann state very similar to the diffusion state but with the local energy potentials included

$$|\Psi_B\rangle = \sum P(\{n\})\,|\{n\}\rangle = \frac{1}{N!Z}\left(\sum_i^L \hat{a}_i^\dagger e^{U_i}\right)^N |0\rangle\,. \tag{4.8}$$

Next, we re-implement the pair interactions in the system. Following the same procedure as before, we have created a Boltzmann $|\Psi_B\rangle$ such that

$$\begin{aligned} |\Psi_B\rangle =& \sum P(\{n\})\,|\{n\}\rangle \\ =& \frac{1}{N!Z} e^{-\frac{1}{2}\sum_{ij}\hat{a}_i^\dagger \hat{a}_i V_{ij} \hat{a}_j^\dagger \hat{a}_j} \left(\sum_{i=1}^{L} \hat{a}_i^\dagger e^{-U_i}\right)^N |0\rangle\,. \end{aligned} \tag{4.9}$$

All three forms are highly analogous to the projection state. We will return to this symmetry when producing the Jarzynski relation.

Chapter 5

Peliti Field Theory

In this chapter, we will exploit the lack of dependence on the occupation numbers in the Doi Hamiltonian to integrate the dynamics of the system and map the system to the field theory. The presentation here closely follows Ref. [25] and the original field theory derivations may be found in Refs. [28, 29]. To introduce this concept, let us move back from attempting to average the work and instead average a generic function $F(\{n\},t)$ at some time t. If we had a constant Hamiltonian, we would have

$$\langle F(\{n\},t)\rangle = \langle P_N|\,\hat{F}\,|\Psi(t)\rangle = \langle P_N|\,\hat{F}e^{-\hat{H}(t-t_1)}\,|\Psi_B\rangle\,, \tag{5.1}$$

where $\hat{F}$ is the operator representation of $F(\{n\},t)$. Commonly, the solution $|\Psi(t)\rangle$ to the imaginary-time Schrödinger equation is expanded using the Trotter formula to make manipulation easier:

$$e^{\hat{H}t} = \lim_{\Delta t\to 0}(1-\hat{H}\Delta t)^{t/\Delta t}. \tag{5.2}$$

Inputting this equation into our average of $F(\{n\},t)$, we have

$$\langle F(\{n\},t)\rangle = \langle P_N|\,\hat{F}(1-\hat{H}\Delta t)(1-\hat{H}\Delta t)\cdots(1-\hat{H}\Delta t)\,|\Psi_B\rangle\,. \tag{5.3}$$

However, our system does not have a constant Hamiltonian. Hence, we must use a solution to Eq. (3.8) that does not require the Hamiltonian to be fixed. We integrate the dynamics by time stepping:

$$\frac{|\Psi(t+\Delta t)\rangle - |\Psi(t)\rangle}{\Delta t} = -\hat{H}\,|\Psi(t)\rangle\,. \tag{5.4}$$

Since we have a Hamiltonian $\hat{H}$ that varies with time, we use the time stepping formula repeatedly to span the time between the initial time t_1 and the final time t_2. Letting each time t have its own Hamiltonian $\hat{H}_t$, we have

$$|\Psi(t)\rangle = (1 - \hat{H}_{t_2}\Delta t)(1 - \hat{H}_{t_2-\Delta t}\Delta t)\cdots(1 - \hat{H}_{t_1}\Delta t)\,|\Psi_B\rangle\,. \tag{5.5}$$

We use this to produce an average similar to Eq. (5.3) but with a Hamiltonian that changes with time. In order to evaluate this non-constant Hamiltonian average, we must again borrow from quantum mechanics and introduce coherent states, which are left and right eigenstates of the $\hat{a}^\dagger$ and $\hat{a}$ operators, respectively. Explicitly,

$$\langle\phi|\,\hat{a}^\dagger = \langle\phi|\,\bar{\phi} \;\text{ and }\; \hat{a}\,|\phi\rangle = \phi\,|\phi\rangle\,, \tag{5.6}$$

where $\langle\phi|$ and $|\phi\rangle$ are coherent states. They are defined by

$$\langle\phi| = \langle 0|\,e^{\bar{\phi}\hat{a}}e^{-|\phi|^2/2} \;\text{ and }\; |\phi\rangle = e^{\phi\hat{a}^\dagger}e^{-|\phi|^2/2}\,|0\rangle\,, \tag{5.7}$$

where ϕ is a complex number and $\bar{\phi}$ is its complex conjugate. Due to the $e^{-|\phi|^2/2}$ terms, the states are normalized: $\langle\phi|\phi\rangle = 1$. In particular we are going to utilize the relation,

$$\mathbf{1} = \int \frac{d^2\phi}{\pi}\,|\phi\rangle\,\langle\phi|\,, \tag{5.8}$$

where $d^2\phi = d(\mathrm{Re}\phi)d(\mathrm{Im}\phi)$. A useful equation that is related to the normalization of the states is the overlap relation. The overlap relation is the inner product of two different coherent states $|\phi_1\rangle$ and $\langle\phi_2|$. This results in

$$\langle\phi_1|\phi_2\rangle = \exp\Big(\bar{\phi}_1\phi_2\Big)\exp\Big(-\tfrac{1}{2}|\phi_1|^2 - \tfrac{1}{2}|\phi_2|^2\Big). \tag{5.9}$$

Proofs for each of these relations may be found in Appendix (B).

We now map to the field theory. Every time slice has a different Hamiltonian $\hat{H}_t$, and hence we must have a different set of coherent states $|\phi_t\rangle$ associated with that time. Note that to indicate the different lattice sites we use $\{\phi\} = (\phi_1, \phi_2, \phi_3, \ldots, \phi_L)$, where

$$|\{\phi\}\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes |\phi_3\rangle \ldots, \tag{5.10}$$

is the vector product of the states. Since the coherent states at different lattice sites are orthogonal, the complete set of states for coherent states may extend to all lattice sites via

$$\mathbf{1} = \int\left(\prod_i \frac{d^2\phi_i}{\pi}\right)|\{\phi\}\rangle\,\langle\{\phi\}| = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi\,|\{\phi\}\rangle\,\langle\{\phi\}|\,, \tag{5.11}$$

where $\mathcal{D}\bar{\phi}_\tau \mathcal{D}\phi_\tau = \prod_{i,\tau} d^2\phi_{i,\tau}/\pi$ and τ is the time index. Moving back to our average of $F(\{n\}t)$, we now insert a set of coherent states at each time slice into the average resulting in

$$\langle F(\{n\},t)\rangle = \mathcal{N}^{-1} \int \prod_{t_i=t_1}^{t_2} \mathcal{D}\bar{\phi}_{t_i}\mathcal{D}\phi_{t_i} \langle P_N| \hat{F} |\{\phi_{t_2}\}\rangle \langle\{\phi_{t_2}\}| (1-\hat{H}_{t_2}\Delta t) |\{\phi_{t_2-\Delta t}\}\rangle \langle\{\phi_{t_2-\Delta t}\}| \cdots \\ \cdots (1-\hat{H}_{t_2-\Delta t}\Delta t) \langle\{\phi_{t_1+\Delta t}\}| (1-\hat{H}_{t_1}\Delta t) |\{\phi_{t_1}\}\rangle \langle\{\phi_{t_1}\}|\Psi_B\rangle , \tag{5.12}$$

where $\mathcal{N}$ is a normalization constant determined by ensuring the average $\langle 1\rangle = 1$, and $\phi_{i,t}$ indicates the field variable for lattice site i at time t. We make this into a closed form equation by writing the multiple Hamiltonian components as a product. Let each time slice in Eq. (5.12) be labeled with a time index τ that increments in steps of Δt from the initial time t_1 to the final time t_2. Rewriting Eq. (5.12) with this notation, we have

$$\langle F(\{n\},t)\rangle = \mathcal{N}^{-1} \lim_{\Delta t\to 0} \int \prod_{\tau=\Delta t+t_1}^{t_2} \left[\left(\mathcal{D}\bar{\phi}_\tau \mathcal{D}\phi_\tau\right) \langle\{\phi\}_\tau| 1-\hat{H}_\tau \Delta t |\{\phi\}_{\tau-\Delta t}\rangle \right] \\ \times \left(\mathcal{D}\bar{\phi}_{t_1}\mathcal{D}\phi_{t_1}\right) \langle P_N| \hat{F} |\{\phi\}_{t_2}\rangle \langle\{\phi\}_{t_1}|\Psi_B\rangle . \tag{5.13}$$

We must evaluate the three main components of this expression: the projection state contribution, the Boltzmann state contribution, and the bulk action. Encoding the dynamics of the system, the bulk action term contains all of the contributions from the Hamiltonian. To evaluate this component, we need to know how to act the Hamiltonian on the coherent states. For a general operator $\hat{A}$, we are able to express it as a function of the coherent state variables $A(\{\phi\}_1, \{\phi\}_2)$ via

$$A(\{\bar{\phi}\}_2, \{\phi\}_1) \equiv \frac{\langle\{\bar{\phi}\}_2| \hat{A} |\{\phi\}_1\rangle}{\langle\{\bar{\phi}\}_2|\{\phi\}_1\rangle}. \tag{5.14}$$

Next let us deal with the projection state contribution $\langle P_N| \hat{F} |\{\phi\}_{t_2}\rangle$:

$$\langle P_N| \hat{F} |\{\phi\}_{t_2}\rangle = F(\{\phi\}_{t_2}) \langle 0| \frac{\left(\sum_i \hat{a}_i\right)^N}{N!} |\{\phi\}_{t_2}\rangle = F(\{\phi\}_{t_2}) \frac{\left(\sum_i \phi_i(t_2)\right)^N}{N!} e^{-\sum_i |\phi_{i,t_2}|^2/2}. \tag{5.15}$$

Note that $F(\{\phi\}_{t_2})$ is strictly a function of $\{\phi_{t_2}\}$ as all $\hat{a}_i^\dagger$ in the expression act on the projection state producing the eigenvalue of 1.

Finally, we deal with the Boltzmann contribution. We will first explain the case where the particles do not interact and the local lattice potential is the only energy term and then describe the interacting case in a later section. For now, we will call the vector product $\Psi_B(\{\phi\}_{t_1})$, but exclude the normalization factor $e^{-\sum_i |\phi_{i,t_1}|^2/2}$ of the coherent state from the term. Explicitly, we have

$$\langle\{\phi\}_{t_1}|\Psi_B\rangle = \Psi_B(\{\bar{\phi}\}_{t_1})e^{-\sum_i |\phi_{i,t_1}|^2/2}. \tag{5.16}$$

Armed with this definition, we may re-express Eq. (5.13) as

$$\begin{aligned}\langle F(\{n\},t)\rangle = \mathcal{N}^{-1}\lim_{\Delta t\to 0}\int\prod_{\tau=\Delta t+t_1}^{t_2}\left[\left(\mathcal{D}\bar{\phi}_\tau\mathcal{D}\phi_\tau\right)\langle\{\phi\}_\tau|\{\phi\}_{\tau-\Delta t}\rangle\left(1-H(\{\phi\}_\tau,\{\phi\}_{\tau-\Delta t})\Delta t\right)\right]\\ \times\left(\mathcal{D}\bar{\phi}_{t_1}\mathcal{D}\phi_{t_1}\right)F(\{\phi_{t_2}\})\left(\sum_i\phi_{i,t_2}\right)^N\Psi_B(\{\bar{\phi}\}_{t_1})e^{\sum_i(-\frac{1}{2}|\phi_{i,t_2}|^2-\frac{1}{2}|\phi_{i,t_1}|^2)}.\end{aligned} \tag{5.17}$$

The angle bracket factor after the differentials is evaluated using the overlap relation Eq. (5.9) and results in

$$\begin{aligned}\langle\{\phi\}_\tau|\{\phi\}_{\tau-\Delta t}\rangle &= \prod_i\exp(-\tfrac{1}{2}|\phi_{i,\tau}|^2-\tfrac{1}{2}|\phi_{i,\tau-\Delta t}|^2+\bar{\phi}_{i,\tau}\phi_{i,\tau-\Delta t})\\ &= \prod_i\exp(-\bar{\phi}_{i,\tau}[\phi_{i,\tau}-\phi_{i,\tau-\Delta t}])\exp(\tfrac{1}{2}|\phi_{i,\tau}|^2-\tfrac{1}{2}|\phi_{i,\tau-\Delta t}|^2).\end{aligned} \tag{5.18}$$

Since the time steps are infinitesimally small, we use a Taylor expansion to reduce the difference found in the first term of Eq. (5.18) to a derivative:

$$\exp(-\bar{\phi}_{i,\tau}[\phi_{i,\tau}-\phi_{i,\tau-\Delta t}]) = \exp(-\bar{\phi}_{i,\tau}[(d\phi_{i,\tau}/dt)\Delta t+\mathcal{O}(\Delta t^2)]), \tag{5.19}$$

where the higher order powers of Δt vanish in the limit $\Delta t\to 0$. Inputting Eq. (5.18) into the average Eq. (5.17), the second term of Eq. (5.18) combines repeatedly due to the product over the index τ resulting in

$$\prod_\tau\exp(\tfrac{1}{2}|\phi_{i,t}|^2-\tfrac{1}{2}|\phi_{i,t-\Delta t}|^2) = \exp(\tfrac{1}{2}|\phi_{i,t_2}|^2-\tfrac{1}{2}|\phi_{i,t_1}|^2). \tag{5.20}$$

The first term cancels with the $\exp(-\sum_i \frac{1}{2}|\phi_{i,t_2}|^2)$ in the projection state contribution, Eq. (5.15). Conversely, the second term combines with the an identical term from the initial Boltzmann state, Eq. (5.16), to form $\exp(-\sum_i \frac{1}{2}|\phi_{i,t_1}|^2)$. In the limit as $\Delta t \to 0$, the product of the overlap relation in combination with normalization factors from the projection state and Boltzmann state form

$$\begin{aligned}
&\lim_{\Delta t\to 0} e^{-\sum_i \frac{1}{2}|\phi_{i,t_2}|^2 - \sum_i \frac{1}{2}|\phi_{i,t_1}|^2} \prod_\tau \langle \{\phi\}_\tau | \{\phi\}_{\tau-\Delta t}\rangle \\
&= \lim_{\Delta t\to 0} \exp\Bigg(\sum_i \Big[-|\phi_{i,t_1}|^2 - \sum_\tau \Delta t \bar{\phi}_{i,\tau}(\partial_t \phi_{i,\tau} + \mathcal{O}(\Delta t^2)\Big]\Bigg) \\
&= \exp\Bigg(\sum_i \Big[-|\phi_i(t_1)|^2 - \int_{t_1}^{t_2} dt\, \bar{\phi}_i(t)\partial_t \phi_i(t)\Big]\Bigg),
\end{aligned} \tag{5.21}$$

where $\phi_i(t)$ is a continuous function of time for the field variable at site i.

Before moving on to the Jarzynski average, the last component of the field that we will calculate is the contribution of $1 - H(\{\bar{\phi}\}_\tau, \{\phi\}_{\tau-\Delta t})$. In the limit $\Delta t \to 0$, the $\mathcal{O}(\Delta t)$ difference in the arguments of $H(\{\bar{\phi}\}_\tau, \{\phi\}_{\tau-\Delta t})$ is assumed negligible. In this limit, we have

$$\lim_{\Delta t\to\infty} \prod_{\tau=\Delta t+t_1}^{t_2} \Big(1 - H(\{\bar{\phi}\}_\tau, \{\phi\}_{\tau-\Delta t}\Big) = \exp\Bigg(-\int_{t_1}^{t_2} dt\, H(\{\bar{\phi}(t)\}, \{\phi(t)\})\Bigg). \tag{5.22}$$

In combination with Eq. (5.21), we rewrite Eq. (5.17) as

$$\langle F(\{n\}, t)\rangle = \mathcal{N}^{-1} \int \Bigg[\Big(\mathcal{D}\bar{\phi}\mathcal{D}\phi\Big) F(\{\phi(t_2)\})\Bigg(\sum_i \phi_i(t_2)\Bigg)^N \Psi_B(\{\bar{\phi}(t_1)\}) e^{-S[\{\bar{\phi}\},\{\phi\}]}, \tag{5.23}$$

where $\mathcal{D}\bar{\phi}\mathcal{D}\phi$ now indicates the product of all $\mathcal{D}\bar{\phi}_\tau \mathcal{D}\phi_\tau$ between time t_1 and t_2:

$$\mathcal{D}\bar{\phi}\mathcal{D}\phi = \lim_{\Delta t\to 0} \prod_{\tau=t_1}^{t_2} \mathcal{D}\bar{\phi}_\tau \mathcal{D}\phi_\tau. \tag{5.24}$$

The exponentiated term is known as the statistical action of field theory and is

$$S[\{\bar{\phi}\}, \{\phi\}] = \sum_i |\phi_i(t_1)|^2 + \int_{t_1}^{t_2} dt\, \Big(\sum_i \bar{\phi}_i(t)\partial_t \phi_i(t) + H(\{\bar{\phi}(t)\}, \{\phi(t)\})\Big). \tag{5.25}$$

Chapter 6

Jarzynski Average

We will now produce the Jarzynski average using the Doi-Peliti field theory and a gauge-like transformation. The crux of the problem is averaging the exponent of the work: $\langle e^{-W} \rangle$. To average this work, we must slightly modify the Doi-Peliti averaging procedure from the previous chapter. Since the work is a continuous process for our system, we cannot calculate the value of a work function at a final time as the work depends on how the system evolves and at the final time, that information is lost. Hence, we must average the work while we evolve the system forward in time.

In a manner similar to updating the system with Eq. (5.4), we also increment the work dW for every time step Δt. Hence for every time step, we now have a factor of $1 - \frac{d\hat{W}_\tau}{dt}\Delta t$ as the expansion of the exponentiated work protocol at some time τ. Note that $dW = \frac{d\hat{W}_\tau}{dt}\Delta t$ in the limit of $\Delta t \to 0$. As shown in Sec. (2.4), the change in the lattice site potential U_i is solely responsible for producing the work. Thus, we replace $1 - \frac{d\hat{W}}{dt}$ with

$$\prod_{i=1}^{L}\left(1 - \frac{dU_{i,\tau}}{dt}\hat{a}_i^\dagger \hat{a}_i \Delta t\right), \tag{6.1}$$

where as before τ indicates the time step. This modifies Eq. (5.13) to be

$$\langle e^{-W} \rangle = \mathcal{N}^{-1} \lim_{\Delta t \to 0} \int \prod_{\tau=\Delta t+t_1}^{t_2} \Big[\left(\mathcal{D}\bar{\phi}_\tau \mathcal{D}\phi_\tau\right) \langle \{\phi\}_\tau | \prod_{i=1}^{L}\left(1 - \frac{dU_{i,\tau}}{dt}\hat{a}_i^\dagger \hat{a}_i \Delta t\right) \left(1 - \hat{H}_\tau \Delta t\right) |\{\phi\}_{\tau-\Delta t}\rangle \Big] \times \left(\mathcal{D}\bar{\phi}_{t_1} \mathcal{D}\phi_{t_1}\right) \langle P_N | \{\phi\}_{t_2} \rangle \langle \{\phi\}_{t_1} | \Psi_B \rangle \,.$$

Note that there is no function between the projection state and the final coherent state. In the limit of $\Delta t \to 0$, all Δt^2 and higher terms are negligible. We will simplify this expression by implicitly removing the Δt^2 term at each time step resulting in

$$\prod_{i=1}^{L}\Big(1 - \frac{dU_{i,\tau}}{dt}\hat{a}_i^\dagger \hat{a}_i \Delta t\Big)\Big(1 - \hat{H}_\tau \Delta t\Big) = (1 - \sum_i \frac{dU_{i,\tau}}{dt}\hat{a}_i^\dagger \hat{a}_i \Delta t - \hat{H}_\tau \Delta t\Big) \tag{6.2}$$

We will now act the operators on the coherent states as before. Every term existed in the previous expression except for the contribution of the work. This is easily acted on the coherent states to form:

$$\langle\{\phi\}_\tau| \frac{dU_{i,\tau}}{dt}\hat{a}_i^\dagger \hat{a}_i \Delta t\, |\{\phi\}_{\tau-\Delta t}\rangle = \frac{dU_{i,\tau}}{dt}\bar{\phi}_i \phi_i \Delta t\, \langle\{\phi\}_\tau|\{\phi\}_{\tau-\Delta t}\rangle\,. \tag{6.3}$$

We may group this term with the Hamiltonian term and move it to the statistical action. Hence, we have the same integral for the average as before except there is an additional work term in the statistical action:

$$\langle e^{-W}\rangle = \mathcal{N}^{-1}\int\Big(\mathcal{D}\bar{\phi}\mathcal{D}\phi\Big)\Big(\sum_i \phi_i(t_2)\Big)^N \Psi_B(\{\bar{\phi}(t_1)\})e^{-S[\{\bar{\phi}\},\{\phi\}]}. \tag{6.4}$$

where the statistical action is

$$S[\{\bar{\phi}\},\{\phi\}] = \sum_i\Big[|\phi_i(t_1)|^2 + \int_{t_1}^{t_2} dt\,\Big(\sum_i\Big[\bar{\phi}_i(t)\partial_t\phi_i(t) + \bar{\phi}_i(t)\phi_i(t)\partial_t U_i(t)\Big] + H(\bar{\phi}_i(t),\phi_i(t))\Big)\Big] \tag{6.5}$$

6.1 Non-Interacting Case

For clarity of the derivation, we will begin with the case where there are no particle interactions, i.e. $V_{ij} = 0$. Our Boltzmann state for this situation is defined by

Eq. (4.8). Now we will define $\Psi_B(\{\bar{\phi}\}_{t_1})$ for this instance. We have

$$\Psi_B(\{\bar{\phi}\}_{t_1}) = \langle\{\phi\}_{t_1}|\Psi_B\rangle\, e^{\sum_i \frac{1}{2}|\phi_{i,t_1}|^2} \tag{6.6}$$

$$= \langle\{\phi\}_{t_1}|\, \frac{1}{N!Z}\left(\sum_i^L \hat{a}^\dagger e^{U_i(t_1)}\right)^N |0\rangle$$

$$= \frac{1}{N!Z}\left(\sum_i^L \bar{\phi}_i(t_1) e^{U_i(t_1)}\right)^N. \tag{6.7}$$

Inserting this into the modified version of Eq. (5.23) for the Jarzynski relation, we have

$$\langle e^{-W}\rangle = \mathcal{N}^{-1}\int \mathcal{D}\bar{\phi}\mathcal{D}\phi\left(\sum_i \phi_i(t_2)\right)^N \frac{1}{N!Z}\left(\sum_i^L \bar{\phi}_i(t_1)e^{U_i(t_1)}\right)^N e^{-S[\{\bar{\phi}\},\{\phi\}]}, \tag{6.8}$$

where $S[\{\bar{\phi}\},\{\phi\}]$ is defined by Eq. (6.5). However, we must define the component $H(\{\bar{\phi}\},\{\phi\})$ of $S[\{\bar{\phi}\},\{\phi\}]$ for the non-interacting case. The Hamiltonian that we will use to create this term does not have the pair potentials included,i.e. $V_{ij} = 0$. Hence the energy term $\epsilon_{i,j}$ is reduced to the local potential term U_i and the Hamiltonian in Eq. 3.21 reduces to

$$\hat{H} = \Gamma\frac{1}{e^{U_{i+1}} + e^{U_i}}\sum_i (\hat{a}_{i+1}^\dagger - \hat{a}_i^\dagger)\Big(\hat{a}_{i+1}e^{U_{i+1}} - \hat{a}_i e^{U_i}\Big). \tag{6.9}$$

Since we are already in the continuum limit with respect to time, we will act the Hamiltonian on the same $\{\phi\}$ states to the left and right for simplicity. We have

$$H(\{\bar{\phi}\},\{\phi\}) = \frac{\langle\{\phi\}|\,\hat{H}\,|\{\phi\}\rangle}{\langle\{\phi\}|\{\phi\}\rangle}$$

$$= \frac{\langle\{\phi\}|\,\Gamma\Big(\sum_i \frac{1}{e^{U_{i+1}}+e^{U_i}}(\hat{a}_{i+1}^\dagger - \hat{a}_i^\dagger)(e^{U_{i+1}}\hat{a}_{i+1} - e^{U_i}\hat{a}_i)\Big)\,|\{\phi\}\rangle}{\langle\{\bar{\phi}\}|\{\phi\}\rangle}$$

$$= \Gamma\sum_i \frac{(\bar{\phi}_{i+1} - \bar{\phi}_i)(e^{U_{i+1}}\phi_{i+1} - e^{U_i}\phi_i)}{e^{U_{i+1}} + e^{U_i}}. \tag{6.10}$$

Using this definition of $H(\{\bar{\phi}\},\{\phi\})$ of $S[\{\bar{\phi}\},\{\phi\}]$ in our statistical action, we rewrite the non-interacting statistical action as

$$S[\{\bar{\phi}\},\{\phi\}] = \sum_i\Big[|\phi_i(t_1)|^2 + \int_{t_1}^{t_2} dt\,\Big(\bar{\phi}_i(t)\partial_t\phi_i(t)$$

$$+ \Gamma\frac{(\bar{\phi}_{i+1} - \bar{\phi}_i)(e^{U_{i+1}}\phi_{i+1} - e^{U_i}\phi_i)}{e^{U_{i+1}} + e^{U_i}} + \bar{\phi}_i(t)\phi_i(t)\partial_t U_i(t)\Big)\Big]. \tag{6.11}$$

6.1.1 Gauge-like Transformation

We produce the relation by performing a gauge-like transform on the field variables. The gauge-like transform rescales the field variables by an associated energy term. Specifically the rescaling is

$$\phi_i(t) \to \bar{\psi}_i(t)e^{-U_i(t)}, \quad \text{and} \quad \bar{\phi}_i(t) \to \psi_i(t)e^{U_i(t)}, \tag{6.12}$$

where $\psi_i(t)$ is also a complex field variable associated with the same site i at time t. This transformation is convenient for several reasons. First, the Jacobian of the transformation is equal to one. Hence, the differentials in Eq. (6.8) transform as

$$\mathcal{D}\bar{\phi}\mathcal{D}\phi \to \mathcal{D}\bar{\psi}\mathcal{D}\psi. \tag{6.13}$$

Additionally, all bilinear (linear in ϕ and $\bar{\phi}$) terms are invariant under the transformation:

$$\bar{\phi}_i(t)\phi_i(t) \to \psi_i(t)e^{U_i(t)}e^{-U_i(t)}\bar{\psi}_i(t) = \bar{\psi}_i(t)\psi_i(t). \tag{6.14}$$

Second, the spatial contributions of the Hamiltonian are invariant under the transformation. For the transformation $H(\{\bar{\phi}\},\{\phi\}) \to H(\{\bar{\psi}\},\{\psi\})$ we have

$$\Gamma\sum_i \frac{(\bar{\phi}_{i+1}-\bar{\phi}_i)(e^{U_{i+1}}\phi_{i+1}-e^{U_i}\phi_i)}{e^{U_{i+1}}+e^{U_i}} \to \Gamma\sum_i \frac{(e^{U_{i+1}}\psi_{i+1}-e^{U_i}\psi_i)(\bar{\psi}_{i+1}-\bar{\psi}_i)}{e^{U_{i+1}}+e^{U_i}}. \tag{6.15}$$

Since the field variables commute with their complex conjugates, these two forms are equivalent. We will refer to the ith component of this term as $H(\bar{\psi}_i(t),\psi_i(t))$.

The transformation of the time derivative term and the work term are the most vital parts of this transformation. Simultaneously performing the transformation on their sum, we have

$$\bar{\phi}_i(t)\partial_t\phi_i(t) + |\phi_i(t)|^2\partial_t U_i(t) \to \psi_i(t)e^{U_i(t)}\partial_t(\bar{\psi}_i(t)e^{-U_i(t)}) + |\psi_i(t)|^2\partial_t U_i(t), \tag{6.16}$$

which may be simplified to

$$\psi_i(t)\partial_t\bar{\psi}_i(t) - |\psi_i(t)|^2\partial_t U_i(t) + |\psi_i(t)|^2\partial_t U_i(t) = \psi_i(t)\partial_t\bar{\psi}_i(t). \tag{6.17}$$

Thus, the transformation cancels the term associated with the work in the statistical action. However, the time derivative is currently acting on $\bar{\psi}$ instead of ψ. To recreate

our original expression in terms of ψ, we use the method of integration by parts on the integral to produce

$$\int_{t_1}^{t_2} dt\, \psi_i(t)\partial_t\bar{\psi}_i(t) = |\psi_i(t_2)|^2 - |\psi_i(t_1)|^2 + \int_{t_2}^{t_1} dt\, \bar{\psi}_i(t)\partial_t\psi_i(t). \tag{6.18}$$

Combining this with the term $|\psi_i(t_1)|^2$, this becomes

$$|\psi_i(t_1)|^2 + \int_{t_1}^{t_2} dt\, \psi_i(t)\partial_t\bar{\psi}_i(t) = |\psi_i(t_2)|^2 + \int_{t_2}^{t_1} dt\, \bar{\psi}_i(t)\partial_t\psi_i(t). \tag{6.19}$$

The total rescaling for the statistical action is therefore

$$S[\{\bar{\psi}\},\{\psi\}] = \sum_i \Big[|\psi_i(t_2)|^2 + \int_{t_2}^{t_1} dt\, \Big(\bar{\psi}_i(t)\partial_t\psi_i(t) - H(\bar{\psi}_i(t),\psi_i(t))\Big)\Big]. \tag{6.20}$$

where the Hamiltonian term receives a negative sign because the integral bounds have been reversed. Now the average integrates from the final time t_2 to the initial time t_1, reversing time.

The final piece to the puzzle is the contribution of the initial Boltzmann state and the final projection state. We will show that the two contributions swap roles under the rescaling, moving the Boltzmann state from time t_1 to t_2. For the non-interacting Boltzmann state, the gauge-like transformation is

$$\Psi_B(\{\bar{\phi}\}) = \frac{1}{Z_{t_1}N!}\Big(\sum_i^L \bar{\phi}_i(t_1)e^{-U_i(t_1)}\Big)^N \to \frac{1}{Z_{t_1}N!}\Big(\sum_i^L \psi_i(t_1)\Big)^N, \tag{6.21}$$

where Z_{t_1} is the partition function at time t_1. This transformed Boltzmann state is precisely the contribution of the projection state at time t_1 for ψ except it has an additional reciprocal of the partition function Z_{t_1}. In a similar fashion, the contribution of the projection state rescales to be

$$\frac{1}{N!}\Big(\sum_i^L \psi_i(t_1)\Big)^N \to Z_{t_2}\frac{1}{Z_{t_2}N!}\Big(\sum_i^L \bar{\psi}_i(t_2)e^{-U_i(t_2)}\Big)^N, \tag{6.22}$$

where Z_{t_2} is the partition function at time t_2. The rescaling has made the projection state into the Boltzmann state except now it has an extra factor of the partition function at the final time.

The total transformation creates

$$\langle e^{-W} \rangle = \mathcal{N}^{-1} \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \frac{1}{N! Z_{t_1}} \left(\sum_i \psi_i(t_1) \right)^N Z_{t_2} \frac{1}{Z_{t_2} N!} \left(\sum_i^L \bar{\psi}_i(t_2) e^{-U_i(t_2)} \right)^N e^{-S[\{\bar{\psi}\},\{\psi\}]}. \tag{6.23}$$

Unlike before the transformation, the action does not contain a work term. Hence, the action is the same as if we were averaging one, except we are now working backwards in time. Fortunately, the initial and final states outside of the action have swapped, excluding the extra partition functions. Thus, we are able to integrate over time, simply in reverse. According to statistical mechanics, the ratio of the partition functions is the exponent of negative change of the Helmholtz free energy (with a factor of β). Explicitly writing β and factoring out the extra partition functions from the average, we have

$$\langle e^{-\beta W} \rangle = \frac{Z_{t_2}}{Z_{t_1}} \langle 1 \rangle = e^{-\beta \Delta F}. \tag{6.24}$$

Thus, for the case of non-interacting particles on a lattice, the Jarzynski relation is produced.

6.2 Continuum Limit

We can generalize our results from the previous section by moving from the lattice model to continuous space for our particles behaviors. Explicitly, the continuum limit occurs when we take the limit of the lattice spacing h approaching zero. This occurs after we act the Doi operators on the coherent states because lattice site operators acting on a specific site loses meaning in the limit.

When moving to the continuum limit, $\phi_i(t)$ becomes a function of the spatial variable x such that $\phi(x,t)$. Most parts of the average may directly swap from the discretized lattice form to the continuous functional representation. A slight complexity is introduced with the Hamiltonian. Since the Hamiltonian has a difference between the field variables ϕ at neighboring sites ($\bar{\phi}$ does as well), we must change the differences into derivatives. By definition, we have

$$\partial_x \phi(x) = \lim_{h \to 0} \frac{\phi_{i+1} - \phi_i}{h}, \tag{6.25}$$

where h is the space between the lattice sites, and i is some arbitrary lattice site that corresponds to the spatial position x. Additionally, sums over all lattice sites become integrals over all space. We do not explicitly show the time argument for the $\phi(t)$ function for brevity in this section. As in the previous section, we assume that their are no particle interactions and hence have the same Hamiltonian Eq. (6.9).

After acting the Hamiltonian on the coherent states as shown in Eq. (6.10), we multiply it by $1 = e^{-(\Delta U)/2}/e^{-(\Delta U)/2}$ resulting in

$$\begin{aligned} H(\{\bar{\phi}\},\{\phi\}) &= \Gamma \sum_i \frac{(\bar{\phi}_{i+1} - \bar{\phi}_i)(e^{\Delta U/2}\phi_{i+1} - e^{-\Delta U/2}\phi_i)}{e^{\Delta U/2} + e^{-\Delta U/2}} \\ &= \Gamma \sum_i \frac{(\bar{\phi}_{i+1} - \bar{\phi}_i)(e^{\Delta U/2}\phi_{i+1} - e^{-\Delta U/2}\phi_i)}{2\cosh \Delta U/2}, \end{aligned} \tag{6.26}$$

where $\Delta U = (U_{i+1} - U_i)$. Moving to the continuum limit, we have

$$H(\{\bar{\phi}\},\{\phi\}) = \lim_{h\to 0} \Gamma h^2 \sum_i \frac{(\bar{\phi}_{i+1} - \bar{\phi}_i)}{h} \frac{(e^{\Delta U/2}\phi_{i+1} - e^{-\Delta U/2}\phi_i)}{h} \frac{1}{2\cosh \Delta U/2}. \tag{6.27}$$

To take this limit, we must expand the exponentials containing $\Delta\epsilon$ like terms. For the term associated with ϕ, we have

$$\frac{e^{\Delta U/2}\phi_{i+1} - e^{-\Delta U/2}\phi_i}{h} = \frac{(1 + \Delta U/2 + \mathcal{O}(\Delta U^2))\phi_{i+1} - (1 - \Delta U/2 + \mathcal{O}(\Delta U^2))\phi_i}{h}. \tag{6.28}$$

Since ΔU^2 terms in the continuum limit are negligible, we have

$$\frac{e^{\Delta U/2}\phi_{i+1} - e^{-\Delta U/2}\phi_i}{h} = \frac{\phi_{i+1} - \phi_i + (\phi_{i+1} + \phi_i)(\Delta U/2)}{h}. \tag{6.29}$$

Taking the limit for this term, we have

$$\begin{aligned} \lim_{h\to 0} \frac{\phi_{i+1} - \phi_i + (\phi_{i+1} + \phi_i)(\Delta U/2)}{h} &= \partial_x \phi(x) + (2\phi(x))\partial_x U(x)/2 \\ &= \partial_x \phi(x) + (\phi(x))\partial_x U(x). \end{aligned} \tag{6.30}$$

Note that $\lim_{h\to 0} \phi_{i+1} + \phi_i = 2\phi(x)$ as the difference between ϕ_{i+1} and ϕ_i is negligible in the limit.

In a similar manner, we may take the limit for the $\cosh \Delta U/2$ and produce

$$\begin{aligned} \lim_{h\to 0} \cosh \Delta U/2 &= \lim_{h\to 0} 1 + \mathcal{O}(\Delta U^2) \\ &= 1. \end{aligned} \tag{6.31}$$

Explicitly writing the time argument and taking the Hamiltonian's limit, we have

$$H(\{\bar{\phi}(t)\},\{\phi(t)\}) = D\int dx\,\partial_x\bar{\phi}(x,t)\Big(\partial_x\phi(x,t)+\phi(x,t)\partial_x U(x,t)\Big). \tag{6.32}$$

where $D=\Gamma h^2/2$ and is a diffusion constant. Hence, the full average becomes

$$\langle e^{-W}\rangle = \mathcal{N}^{-1}\int\Big(\mathcal{D}\bar{\phi}\mathcal{D}\phi\Big)\left(\int dx\,\phi(x,t_2)\right)^N \Psi_B(\{\bar{\phi}(t_1)\})e^{-S[\{\bar{\phi}\},\{\phi\}]}. \tag{6.33}$$

where the statistical action is

$$\begin{aligned} S[\{\bar{\phi}\},\{\phi\}] = \int dx\,\Bigg[&|\phi(x,t_1)|^2 \\ &+\int_{t_1}^{t_2} dt\,\Big(\bar{\phi}(x,t)\partial_t\phi(x,t)+\bar{\phi}(x,t)\phi(x,t)\partial_t U(x,t) \\ &+D\partial_x\bar{\phi}(x,t)(\partial_x\phi(x,t)+\phi(x,t)\partial_x U(x,t))\Big)\Bigg] \end{aligned} \tag{6.34}$$

We are able to perform the gauge transformation in an analogous form to the original lattice transformation found in Sec. (6.1). The only difference between the two derivations is that the $\bar{\phi}$,ϕ, and U are all functions of the spatial variable x instead of associated with a single lattice site. This is also true for the gauge transformation variables $\bar{\psi}$ and ψ.

6.3 Interacting Case

With the pair-interactions included in the energetics, we return the V_{ij} term to the energy ϵ_i resulting in the full Hamiltonian shown in Eq. (3.21). To begin, we will move this Hamiltonian to the continuum limit as before under the ϵ_i notation. Exactly analogous to the previous derivation for U_i, we produce the continuum limit for the ϵ_i such that the Hamiltonian is

$$H(\{\bar{\phi}(t)\},\{\phi(t)\}) = D\int dx\,\partial_x\bar{\phi}(x,t)\Big(\partial_x\phi(x,t)+\phi(x,t)\partial_x\epsilon(x,t)\Big) \tag{6.35}$$

where $\partial_x\epsilon(x,t)$ is explicitly

$$\partial_x\epsilon(x,t) = \partial_x U(x,t)+\int dy\,\bar{\phi}(y,t)\phi(y,t)V(x-y) \tag{6.36}$$

where y is a spatial variable independent of x but over the same dimension. The term dependent on the pair interactions in Eq. 6.36 is produced through the same Taylor expansion that produces the local potential U_i term.

We now will produce the Jarzynski relation through a similar gauge-transformation process as seen in Sec. 6.1.1, but with a pair interaction term. For the transformations for $\bar{\phi}$ and ϕ, we use

$$\phi(x,t) \rightarrow \bar{\psi}(x,t) e^{-U(x,t) - \int dy\, \bar{\phi}(y,t)\phi(y,t)V(x-y)} \tag{6.37}$$

and

$$\bar{\phi}(x,t) \rightarrow \psi(x,t) e^{U(x,t) + \int dy\, \bar{\phi}(y,t)\phi(y,t)V(x-y)}. \tag{6.38}$$

As before, the differentials $\mathcal{D}\bar{\phi}\mathcal{D}\phi$ and all bilinear terms are invariant under this transformation,

$$\begin{aligned}\bar{\phi}(x,t)\phi(x,t) \rightarrow & \bar{\psi}(x,t) e^{-U(x,t) - \int dy\, \bar{\phi}(y,t)\phi(y,t)V(x-y)} e^{U(x,t) + \int dy\, \bar{\phi}(y,t)\phi(y,t)V(x-y)} \psi(x,t) \\ = & \psi(x,t)\bar{\psi}(x,t).\end{aligned} \tag{6.39}$$

The spatial terms in the Hamiltonian,

$$D \int dx\, \partial_x \bar{\phi}(x,t) \Big(\partial_x \phi(x,t) + \phi(x,t) \partial_x \epsilon(x,t) \Big), \tag{6.40}$$

are invariant under the transformation.

Again, we use the transformation of the time derivative term to cancel the work term. For only the time derivative (excluding the work term temporarily), we have

$$\begin{aligned}\bar{\phi}(x,t)\partial_t \phi(x,t) \rightarrow & \ \psi(x,t) e^{U(x,t) + \int dy\, \bar{\phi}(y,t)\phi(y,t)V(x-y)} \partial_t \bar{\psi}(x,t) e^{-U(x,t) - \int dy\, \bar{\phi}(y,t)\phi(y,t)V(x-y)} \\ = & \ \psi(x,t) \bigg(\partial_t \bar{\psi}(x,t) - \bar{\psi}(x,t) \partial_t \Big(U(x,t) + \int dy\, |\phi(y,t)|^2 V(x-y) \Big) \bigg).\end{aligned} \tag{6.41}$$

The second term of Eq. 6.41 cancels the work term. A new term from the non-interacting case has appeared as the final term of this equation. To understand its function, we integrate by parts to produce

$$\begin{aligned}\int dx |\psi(x,t)|^2 \partial_t \int dy\, |\psi(y,t)|^2 V(x-y) = & |\psi(x,t)|^2 \int dy\, |\psi(y,t)|^2 V(x-y) \Big|_{t=t_1}^{t_2} \\ & - \int dx \big[\partial_t |\psi(x,t)|^2 \int dy\, |\psi(y,t)|^2 V(x-y) \big].\end{aligned} \tag{6.42}$$

We should note that $V(x-y)$ is symmetric with respect to x and y. Since x and y are arbitrary variables that we integrate over, the final term on the right in Eq. (6.42) is identical (excluding the negative sign) to the term we were originally attempting to integrate on the left. Hence, if we add this term to both sides of the equation and divide by 2, Eq. (6.42) becomes

$$\int dx|\psi(x,t)|^2\partial_t \int dy\,|\psi(y,t)|^2 V(x-y) = \frac{1}{2}\int dx|\psi(x,t)|^2 \int dy\,|\psi(y,t)|^2 V(x-y)\Big|_{t=t_1}^{t_2} \tag{6.43}$$

This pair potential term depends on the initial and final conditions of the system. As such, we will return to it when we are reversing the contributions of the initial and final states.

The contribution from the projection state is identical to the non-interacting case. Hence we have

$$\frac{1}{N!}\left(\int dx\,\psi(x,t_1)\right)^N \to Z_{t_2}\frac{1}{Z_{t_2}N!}\left(\int dx\,\bar{\psi}(x,t_2)e^{-U(x,t_2)-\int dy\,|\phi(y,t_2)|^2 V(x-y)}\right)^N, \tag{6.44}$$

Due to the pair interactions, the manipulation of the initial Boltzmann state, Eq. (4.9), is slightly modified compared to the non-interacting case. Since we are back at the operator level, we are no longer in the continuum limit and instead have individual lattice sites i. We begin by acting the coherent state $\langle\{\phi\}_{t_1}|$. First we insert an additional complete set of coherent states labeled by $\{\phi\}_0$, a set of field variables at time t_1 but different $\{\phi\}_{t_1}$, between the pair potential term and the contribution from the non-interacting Boltzmann state:

$$\frac{1}{N!Z_{t_1}}\int \mathcal{D}\bar{\phi}_0\mathcal{D}\phi_0\,\langle\{\phi\}_{t_1}|\,e^{-\frac{1}{2}\sum_{ij}\hat{a}_i^\dagger\hat{a}_i V_{ij}\hat{a}_j^\dagger\hat{a}_j}\,|\{\phi\}_0\rangle\,\langle\{\phi\}_0|\left(\sum_{i=1}^{L}\hat{a}_i^\dagger e^{-U_i}\right)^N|0\rangle\,. \tag{6.45}$$

Starting by acting the non-interacting term to the left (the term between the right most bra and ket in Eq.(6.45)), we have

$$\left(\sum_{i=1}^{L}\bar{\phi}_i(t_1)e^{-U_i(t_1)}\right)^N e^{-\frac{1}{2}\sum_i|\phi_{i,0}|^2}. \tag{6.46}$$

We first act the pair potential term in the limit where V_{ij} is weak. Hence we may expand our pair potential term according to its Taylor series and act it on the coherent

states:

$$\begin{aligned}\langle\{\phi\}_{t_1}|\, e^{-\frac{1}{2}\sum_{ij}\hat{a}_i^\dagger\hat{a}_i V_{ij}\hat{a}_j^\dagger\hat{a}_j}\,|\{\phi\}_0\rangle &= \langle\{\phi\}_{t_1}|\left(1-\frac{1}{2}\sum_{ij}\hat{a}_i^\dagger\hat{a}_i V_{ij}\hat{a}_j^\dagger\hat{a}_j\right)|\{\phi\}_0\rangle \\ &= \Big(1-\frac{1}{2}\sum_{ij}\bar{\phi}_{i,t_1}\phi_{i,0}V_{ij}\bar{\phi}_{j,t_1}\phi_{j,0}\Big) \\ &\quad \exp\Big(\sum_i -\frac{1}{2}|\phi|^2_{i,t_1}-\frac{1}{2}|\phi|^2_{i,0}+\bar{\phi}_{i,t_1}\phi_{i,0}\Big) \qquad (6.47)\end{aligned}$$

Combining the overlap from Eq. (6.47) and the normalization factor from Eq. (6.46) results in:

$$\exp\Big(\sum_i \phi_{i,0}(\bar{\phi}_{i,t_1}-\bar{\phi}_{i,0})\Big)\exp\Big(-\sum_i\frac{1}{2}|\phi|^2_{i,t_1}\Big). \qquad (6.48)$$

The integral $\int \mathcal{D}\bar{\phi}_0\mathcal{D}\phi_0$ extends over the entire complex plane. Rotating the plane has no effect on the outcome of the integral because the entirety of the plane is always integrated. This process is known as a Wick rotation and allows us to produce a delta function from Eq. (6.48) by integrating over the imaginary axis of ϕ_0. Then, we integrate over the real axis and collapse the delta function. This integration forces all $\phi_{i,0}$ to become ϕ_{i,t_1}. Hence the Boltzmann state contribution is

$$\frac{1}{N!Z_{t_1}}\Big(1-\frac{1}{2}\sum_{ij}\bar{\phi}_i(t_1)\phi_i(t_1)V_{ij}\bar{\phi}_j(t_1)\phi_j(t_1)\Big)\Big(\sum_{i=1}^{L}\bar{\phi}_i(t_1)e^{-U_i(t_1)}\Big)^N e^{-\frac{1}{2}\sum_i|\phi_{i,0}|^2}. \qquad (6.49)$$

Since we are in the weak V_{ij} limit, we may replace the expanded term with the original exponential resulting in

$$\frac{1}{N!Z_{t_1}}e^{-\frac{1}{2}\sum_{ij}\bar{\phi}_i(t_1)\phi_i(t_1)V_{ij}\bar{\phi}_j(t_1)\phi_j(t_1)}\Big(\sum_{i=1}^{L}\bar{\phi}_i(t_1)e^{-U_i(t_1)}\Big)^N e^{-\frac{1}{2}\sum_i|\phi_i(t_1)|^2}. \qquad (6.50)$$

Last, we must move to the continuum limit in the same fashion as before

$$\frac{1}{N!Z_{t_1}}e^{-\frac{1}{2}\int dxdy\,\bar{\phi}(x,t_1)\phi(x,t_1)V(x-y)\bar{\phi}(x,t_1)\phi(x,t_1)}\Big(\int dx\,\bar{\phi}(x,t_1)e^{-U(x,t_1)}\Big)^N e^{-\frac{1}{2}\int dx|\phi(x,t_1)|^2}. \qquad (6.51)$$

We now perform the gauge transformation on the Boltzmann state contribution. All bilinear terms in the pair interaction term are invariant under the transformation.

The non-interacting component becomes

$$\left(\int dx\, \bar{\psi}(x,t_1) e^{\int dy\, \bar{\psi}(y,t)\psi(y,t)V(x-y)}\right)^N e^{-\frac{1}{2}\int dx\, |\psi(x,t_1)|^2}. \tag{6.52}$$

The pair interaction term inside here may be drawn out at the cost of an additional integral over x in the exponent. Hence, the positive V_{ij} exponent (with field variable and integral implicit) from the Boltzmann state combines with the initial $-\frac{1}{2}V_{ij}$ exponent and the $-\frac{1}{2}V_{ij}$ from the time derivative, Eq. (6.43), and cancels. Conversely, there is a positive $\frac{1}{2}V_{ij}$ exponent from the time derivative that combines with the pair interaction component of the projection state that produces a negative $-\frac{1}{2}V_{ij}$ exponent at time t_2. Lumping the normalization from the Boltzmann state into the statistical action $S[\{\bar{\phi}\},\{\phi\}]$ as usual, the average becomes

$$\langle e^{-W}\rangle = \mathcal{N}^{-1}\int \mathcal{D}\bar{\phi}\mathcal{D}\phi \frac{Z_{t_2}}{(N!)^2 Z_{t_1}}\left(\sum_i \psi_i(t_1)\right)^N \tag{6.53}$$

$$\frac{1}{Z_{t_2}}\left(\sum_i^L \bar{\psi}_i(t_2) e^{-U_i(t_2)}\right)^N e^{-\frac{1}{2}\sum_{ij}\bar{\phi}_i(t_2)\phi_i(t_2)V_{ij}\bar{\phi}_j(t_2)\phi_j(t_2)} e^{-S[\{\bar{\psi}\},\{\psi\}]}. \tag{6.54}$$

where all terms in the action are now appropriately transformed. As before, this produces the Jarzynski relation since the average is now an average of one with partition functions found at the appropriate times. Future work involves further clarification of the initial condition rescaling for the pair interactions.

6.4 Multiple Dimensions

Our next step is to generalize the average to an arbitrary number of dimension d. At the Fock space level, the previously defined operator relations hold as indices i, j simply indicate different lattice sites; the lattice sites are not confined to a single dimension. The differentials $\mathcal{D}\bar{\phi}\mathcal{D}\phi$ extend to all d dimensions. Time derivatives and all non-spatial terms remain unaffected by the shift to multiple dimensions.

As the Hamiltonian contains the spatial dependence, we are interested in how the Hamiltonian transforms when moved to multiple dimensions. If we imagine having two dimensions instead of one, we now have two additional lattice sites which a given lattice site could use to make transitions to and from a given state. These terms would

be identical to the terms already found in the Hamiltonian as shown in Eq. (3.21). Extrapolating on this behavior, we produce additional and synonymous terms as those found in Eq. (3.21) for each dimension. We shall express the field variables as functions of all dimensions specified by $\phi(\mathbf{x}, t)$ such that $\mathbf{x} = (x_1, x_2, x_3 \ldots)$ where x_i is a single spatial dimension specified by index i. In the continuum limit and adhering to Einstein summation notation, the Hamiltonian becomes:

$$H(\{\bar{\phi}\}, \{\phi\}) = D \int d\mathbf{x} \Big(\partial_i \bar{\phi}(\mathbf{x}, t) \partial_i \phi(\mathbf{x}, t) + \partial_i \bar{\phi}(\mathbf{x}, t) \phi(\mathbf{x}, t) \partial_i U(\mathbf{x}, t) + \partial_i \bar{\phi}(\mathbf{x}, t) \phi(\mathbf{x}, t) \int d\mathbf{y} |\phi(\mathbf{y}, t)|^2 \partial_i V(\mathbf{x} - \mathbf{y}) \Big). \tag{6.55}$$

Einstein summation notation indicates an implied sum over a repeated index. For example, $\sum_i x_i y_i = x_i y_i$ in this notation. The index i subscript denotes a derivative with respect to the x_i spatial variable. In combination with the other terms that comprise the action, we create the statistical action for the interacting particle case:

$$S[\{\bar{\phi}\}, \{\phi\}] = \int d\mathbf{x} \Bigg[|\phi(\mathbf{x}, t_1)|^2 + \int_{t_1}^{t_2} dt \Big(\bar{\phi}(\mathbf{x}, t) \partial_t \phi(\mathbf{x}, t) + D \int d\mathbf{x} \Big(\partial_i \bar{\phi}(\mathbf{x}, t) \partial_i \phi(\mathbf{x}, t) + \partial_i \bar{\phi}(\mathbf{x}, t) \phi(\mathbf{x}, t) \partial_i U(\mathbf{x}, t) + \partial_i \bar{\phi}(\mathbf{x}, t) \phi(\mathbf{x}, t) \int d\mathbf{y} |\phi(\mathbf{y}, t)|^2 \partial_i V(\mathbf{x} - \mathbf{y}) \Big) \Bigg]. \tag{6.56}$$

The derivation of the Jarzynski relation for multiple dimensions follows the same transform as the previous section except now the field variables are functions of multiple dimensions.

Chapter 7

Conclusions

In chapter (6), we demonstrated that the Jarzynski relation can be produced from a gauge-like transformation of the fields in addition to a time reversal of the dynamics. Now that we have developed the field theory for thermal systems, our goal is to understand the underlying mechanism so that we can see how the relation holds, if it can be extended, and if it will be broken under any circumstances. We have previously noted that there is a series of non-equilibrium work relations, all tightly connected, that can be produced by modifying the Jarzynski relation. We hope to use the field-theoretic framework to define other thermodynamic quantities for non-equilibrium systems in terms of strict equalities. Specifically, we hope to extend the Doi-Peliti field theory framework to address other thermodynamic properties such as entropy production [11].

One of the most remarkable features of our formalism is that it requires no assumptions about the form of the particle interactions. Our pair-wise potentials V_{ij} were defined such that they could encompass any interaction between two particles. Hence, our derivation holds for types of particle interactions including but not limited to dilute gases, liquid-gas phase transitions, and crystallization phase dynamics. In the future, we plan to extend the derivation to multiple species of particles and chemical reactions.

Being able to generalize the Jarzynski relation would be useful for a variety of fields. For instance in fields such as biology and polymer chemistry, the change of free energy between a stretched and unstretched polymer chain such as DNA is an important question. Waiting for the chain to uncoil due to thermal fluctuations

in equilibrium takes a prohibitively long time, making the measurement impossible. With the development of the Jarzynski relation, we now may force the polymer to extend and use the relation to determine the change in free energy [12, 13, 14, 15]. Similarly, computer models of thermal systems are able to utilize the relation enabling them to also forgo the equilibrium requirement. Previous to the Jarzynski relation, processes such as these were very difficult to quantify. Our goal is to use the field-theoretic framework developed here to produce more relations like the Jarzynski relation that would quantify these small-scale processes.

Appendix A

Doi Relations

A.1 Hermitian Conjugation

If we have matrix A, its Hermitian adjoint $A^\dagger$ is equivalent to taking the transpose of the A and then complex conjugating each entry in that matrix. Operators and states may be represented by matrices, and hence have Hermitian adjoint. For $\hat{a}$, $\hat{a}^\dagger$ is by definition its Hermitian adjoint. Analogous to quantum mechanical states, left and right Doi states are Hermitian conjugates of each other. For instance, the state $\langle n|$ is the Hermitian adjoint of $|n\rangle$. For further detail, refer to Ref. [27].

A.2 Annihilation Operator Acting on the nth State

We will prove $\hat{a}_i |n_i\rangle = n_i |n_i - 1\rangle$ Eq. (3.5) using induction. Let $P(n_i)$ be the preceding statement for $n_i \in \mathbb{N}$.
1) For the base step, we have $n_i = 0$. Hence, $\hat{a}_i |0\rangle = 0$ by the definition found in section 2 and $P(0)$ holds.
2) For the induction step, we will assume that $P(n_i)$ is true. Thus, we have

$$\hat{a}_i |n_i\rangle = n_i |n_i - 1\rangle . \tag{A.1}$$

We will show that $P(n_i + 1)$ holds. First let us take the commutator relation

$$\left[\hat{a}_i, \hat{a}_i^\dagger\right] = \hat{a}_i \hat{a}_i^\dagger - \hat{a}_i^\dagger \hat{a}_i = 1, \tag{A.2}$$

and rewrite it as

$$\hat{a}_i\hat{a}_i^\dagger = \hat{a}_i^\dagger\hat{a}_i + 1. \tag{A.3}$$

Utilizing this relation, we have

$$\hat{a}_i \left|n_i + 1\right\rangle = \hat{a}_i(\hat{a}_i^\dagger)^{n_i+1}\left|0\right\rangle = \hat{a}_i\hat{a}_i^\dagger(\hat{a}_i^\dagger)^{n_i}\left|0\right\rangle = (\hat{a}_i^\dagger\hat{a}_i + 1)\left|n_i\right\rangle. \tag{A.4}$$

By the induction hypothesis Eq. (A.1), we have

$$(\hat{a}_i^\dagger\hat{a}_i + 1)\left|n_i\right\rangle = \left|n_i\right\rangle + \hat{a}_i^\dagger n_i\left|n_i - 1\right\rangle = \left|n_i\right\rangle + n_i\left|n_i\right\rangle = (n_i + 1)\left|n_i\right\rangle. \tag{A.5}$$

Thus, $P(n)$ holds for all $n \in \mathbb{N}$ by the principle of mathematical induction.

A.3 Projection State

We will prove that the projection state $\left|P\right\rangle$ is a right eigenstate of the creation operator $\hat{a}$ with eigenvalue of 1. To begin, we Taylor expand the projection state's exponent resulting in

$$\begin{aligned}
\hat{a}\left|P\right\rangle &= \hat{a}e^{\hat{a}^\dagger}\left|0\right\rangle \\
&= \hat{a}\left(1 + \hat{a}^\dagger + \frac{(\hat{a}^\dagger)^2}{2!} + \frac{(\hat{a}^\dagger)^3}{3!} + \cdots\right)\left|0\right\rangle \\
&= \left(\hat{a} + \hat{a}\hat{a}_i^\dagger + \frac{\hat{a}(\hat{a}^\dagger)^2}{2!} + \frac{(\hat{a}\hat{a}_i^\dagger)^3}{3!} + \cdots\right)\left|0\right\rangle \\
&= \hat{a}\left|0\right\rangle + \hat{a}\left|1\right\rangle + \frac{\hat{a}\left|2\right\rangle}{2!} + \frac{\hat{a}\left|3\right\rangle}{3!} + \cdots.
\end{aligned} \tag{A.6}$$

Using Eq. (3.5), we have

$$\begin{aligned}
&= 0 + 1\left|0\right\rangle + \hat{a}\left|1\right\rangle + \frac{\hat{a}\left|2\right\rangle}{2!} + \cdots \\
&= \left(1 + \hat{a}^\dagger + \frac{(\hat{a}^\dagger)^2}{2!} + \frac{(\hat{a}^\dagger)^3}{3!} + \cdots\right)\left|0\right\rangle \\
&= e^{\hat{a}^\dagger}\left|0\right\rangle = \left|P\right\rangle.
\end{aligned} \tag{A.7}$$

By Hermitian conjugation, we also know that $\left\langle P\right|$ is the left eigenstate of $\hat{a}_i^\dagger$.

Appendix B

Coherent State Relations

We will prove the validity of Eq. (5.6), (5.8), (5.9) and normalization for coherent states.

B.1 Coherent States as Eigenstates

We will now prove that $\langle\phi|\,\hat{a}^\dagger = \langle\phi|\,\bar{\phi}$ and $\hat{a}\,|\phi\rangle = \phi\,|\phi\rangle$. Starting with the right eigenstate and the definition of the coherent state, we have

$$\hat{a}\,|\phi\rangle = \hat{a}e^{-|\phi|^2/2}e^{\hat{a}^\dagger\phi}\,|0\rangle\,. \tag{B.1}$$

Now we expand the exponential according to its Taylor series and produce

$$\begin{aligned}\hat{a}\,|\phi\rangle &= \hat{a}e^{-|\phi|^2/2}\Big(1+\phi\hat{a}^\dagger+\frac{(\phi\hat{a}^\dagger)^2}{2!}+\cdots\Big)\,|0\rangle \\ &= e^{-|\phi|^2/2}\Big(\hat{a}+\phi\hat{a}\hat{a}^\dagger+\frac{\phi^2\hat{a}(\hat{a}^\dagger)^2}{2!}+\cdots\Big)\,|0\rangle\,.\end{aligned} \tag{B.2}$$

Realizing that this is a superposition of all n states and using Eq. (3.5), we have

$$\begin{aligned}\hat{a}\,|\phi\rangle &= e^{-|\phi|^2/2}\Big(\hat{a}\,|0\rangle + \phi\hat{a}\,|1\rangle + \frac{\phi^2\hat{a})}{2!}\,|2\rangle + \cdots\Big)\\ &= e^{-|\phi|^2/2}\Big(0 + \phi\,|0\rangle + \phi^2\,|1\rangle + \cdots\Big)\\ &= e^{-|\phi|^2/2}\Big(\phi + \phi^2\hat{a}^\dagger + \cdots\Big)\,|0\rangle\\ &= \phi e^{-|\phi|^2/2}e^{\hat{a}^\dagger\phi}\,|0\rangle = \phi\,|\phi\rangle\,, \end{aligned} \tag{B.3}$$

yielding our result. Since $\langle\phi|$ is the Hermitian conjugation of $|\phi\rangle$, we may take the Hermitian of $\hat{a}\,|\phi\rangle = \phi\,|\phi\rangle$ to produce the left eigenstate equivalent. Hence, $\langle\phi|\,\hat{a}^\dagger = \langle\phi|\,\bar{\phi}$ follows.

B.2 Complete Set of States

We will prove that

$$\mathbf{1} = \int \frac{d^2\phi}{\pi}\,|\phi\rangle\,\langle\phi|\,,$$

Eq. (5.8) where $d^2\phi = d(\mathrm{R}\phi)d(\mathrm{Im}\phi)$ and the integral is over the entire complex plane. Beginning with the right hand side of the equation and expanding the exponentials in the coherent states, we have

$$\int \frac{d^2\phi}{\pi}\,|\phi\rangle\,\langle\phi| = \int \frac{d^2\phi}{e^{|\phi|^2}\pi}e^{\hat{a}^\dagger\phi}\,|0\rangle\,\langle 0|\,e^{\hat{a}\bar{\phi}} = \int \frac{d^2\phi}{e^{|\phi|^2}\pi}\sum_{m,n}\frac{\phi^m(\bar{\phi})^n}{n!m!}\,|m\rangle\,\langle n|\,, \tag{B.4}$$

where n and m are indices of sums that range from zero to infinite. All complex numbers maybe represented using polar coordinates for their value on the complex plane. We define $\phi = re^{i\theta}$ and thus $\bar{\phi} = (re^{-i\theta})$ where r is the magnitude of ϕ and θ contains the phase information. The differentials $d^2\phi$ becomes $rdrd\theta$, and we integrate over all space. Inputting the polar representation, we have

$$\begin{aligned}\int \frac{d^2\phi}{\pi}\,|\phi\rangle\,\langle\phi| &= \int \frac{d^2r dr d\theta}{e^{r^2}\pi}\sum_{m,n}\frac{(re^{i\theta})^m((re^{-i\theta}))^n}{n!m!}\,|m\rangle\,\langle n|\\ &= \int_0^\infty dr\int_0^{2\pi} d\theta\frac{1}{e^{r^2}\pi}\sum_{m,n}\frac{r^{m+n+1}e^{i(m-n)\theta}}{n!m!}\,|m\rangle\,\langle n|\,. \end{aligned} \tag{B.5}$$

Since $e^{iN\theta}$ is oscillatory in terms of θ where N is a non-zero integer constant, when integrated between 0 and 2π this integral will evaluate to zero. However when $N = 0$, $e^{i0} = 1$. Hence, the θ integral will be zero except when $m = n$ where the integral would become equal to 2π creating a Kronecker delta function. Evaluating the integral and then using the Kronecker delta function to collapse a sum, we have

$$\begin{aligned}\int \frac{d^2\phi}{\pi} |\phi\rangle \langle\phi| &= \int_0^\infty dr \frac{1}{e^{r^2}\pi} \sum_{m,n} \frac{r^{m+n+1}(2\pi\delta_{m,n})}{n!m!} |m\rangle \langle n| \\ &= \int_0^\infty dr \frac{2}{e^{r^2}} \sum_n \frac{r^{2n+1}}{(n!)^2} |n\rangle \langle n| . \end{aligned} \tag{B.6}$$

We now evaluate the r integral via a variable substitution and integration by parts. Let $u = r^2$ and $du = 2rdr$. With this substitution,

$$\begin{aligned}\int \frac{d^2\phi}{\pi} |\phi\rangle \langle\phi| &= \int_0^\infty du \sum_n \frac{e^{-u}u^n}{(n!)^2} |n\rangle \langle n| \\ &= \sum_n \frac{1}{n!} |n\rangle \langle n| \qquad \text{by repeated integration by parts.} \end{aligned} \tag{B.7}$$

This is the definition of a complete set of states for a quantum harmonic oscillators where

$$\sum_n \frac{1}{n!} |n\rangle \langle n| = \mathbf{1}. \tag{B.8}$$

Hence, we have proved that Eq. (5.8) is true.

B.3 Overlap Relation and Normalization

We will first show that the overlap relation Eq. (5.9)

$$\langle\phi_1|\phi_2\rangle = \frac{e^{\bar{\phi}_1}e^{\phi_2}}{e^{(|\phi_1|^2+|\phi_2|^2)/2}},$$

where ϕ_1 and ϕ_2 are different complex variables. Beginning with the left-hand side, we have

$$\begin{aligned}\langle\phi_1|\phi_2\rangle &= \langle 0| e^{\bar{\phi}_1\hat{a}} e^{-|\phi_1|^2/2} |\phi_2\rangle \\ &= e^{-(|\phi_1|^2)/2} \langle 0| (1 + \bar{\phi}_1\hat{a} + \frac{(\bar{\phi}_1\hat{a})^2}{2!} + \cdots) |\phi_2\rangle . \end{aligned} \tag{B.9}$$

Referring to Eq. (5.6), we can evaluate the $\hat{a}$ to the right producing

$$\langle\phi_1|\phi_2\rangle = e^{-|\phi_1|^2/2}\langle 0|\,(1+\bar{\phi}_1\phi_2+\frac{(\bar{\phi}_1\phi_2)^2}{2!}+\cdots)\,|\phi_2\rangle = e^{-|\phi_1|^2/2}\langle 0|\,e^{\bar{\phi}_1\phi_2}\,|\phi_2\rangle\,. \quad \text{(B.10)}$$

Now we take the inner product $\langle 0|\,|\phi_2\rangle$ and have

$$\langle 0\phi_2\rangle = \langle 0|\,e^{\hat{a}^\dagger\phi_2}e^{-|\phi_2|^2/2}\,|0\rangle = e^{-|\phi_2|^2/2}, \quad \text{(B.11)}$$

by acting all of the $\hat{a}^\dagger$ in the Taylor expansion of the exponent on the vacuum state to the left. This yields the final result of

$$\langle\phi_1|\phi_2\rangle = e^{-|\phi_2|^2/2}e^{-|\phi_1|^2/2}e^{\bar{\phi}_1\phi_2}, \quad \text{(B.12)}$$

which is the overlap relation.

Next, we will use the overlap relation to prove normalization for a single ϕ eigenstate: $\langle\phi|\phi\rangle = \mathbf{1}$. Using the overlap relation for the same state, we have

$$\langle\phi|\phi\rangle = e^{-|\phi|^2}e^{\bar{\phi}\phi} = 1. \quad \text{(B.13)}$$

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