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Feynman, Wigner, and Hamiltonian Structures Describing the Dynamics of Open Quantum Systems

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Abstract

This paper discusses several methods for describing the dynamics of open quantum systems, where the environment of the open system is infinite-dimensional. These are purifications, phase space forms, master equation and liouville equation forms. The main contribution is in using Feynman-Kac formalisms to describe the infinite-demsional components.

This paper discusses several approaches for describing the dynamics of open quantum systems. Open quantum systems play an important role in modelling physical systems coupled to their environment and, in particular, for the emerging field of quantum feedback control theory (see [12]). Thus, in studying coherent quantum feedback, models consisting of a quantum system related to quantum control system, so that each of these systems turns out to be open, are considered.

Generally the master equation is presented in the theoretical physics literature as the central description of an open quantum system. In practice, however, it is these solutions that are important for potential applications, rather than the master equations themselves. Our goal is to solve the exact master equations, which describe the reduced dynamics of subsystems of certain large systems generated by the dynamics of these large systems: these master equation arise from a number of different approaches which we will consider.

In fact, we examine four approaches for describing subsystems dynamics, and in each case we exploit Feynman type formulas (see [1, 2]). Moreover, we assume that the quantum systems under consideration are obtained by the Schrödinger quantization [3] of classical Hamiltonian systems.

1. Our first approach is based on a representation of mixed states as random pure ones, where the dynamics of a subsystem of the isolated quantum

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system is described by a random process taking values in the Hilbert space of the subsystem. The random process is then defined by using the Feynman formula for the solution of the Schrödinger equation for the united system.

2. The second approach uses the Wigner function [4] and also its infinite dimensional analogue, the Wigner measure, which was introduced in [5]. If the phase space of the classical Hamiltonian system generating the quantum system under consideration is finite dimensional, then the density of the Wigner measure with respect to the standard Lebesgue measure coincides with the Wigner function. As shown in [5], the evolution of the Wigner measure of a closed quantum system is described by a Liouville-Moyal type equation; in order to obtain a solution of the master equation for the dynamics of the Wigner measure (or function) of a subsystem of the initial system from a solution of this equation represented by using a Feynman type formula, it suffices to integrate this representation over the coordinates of the phase space of the corresponding classical subsystem. Another approach for describing the evolution of the Wigner function of a subsystem is discussed in [6].

3. The third approach again uses the Feynman formulas for the Schrödinger equation for a quantum system and its environment, but this time these formulas are used to describe the evolution of the density operator of each part; it is given by the corresponding partial trace of the evolving density operator of the united system.

4. The final approach considered here is based on the representation of any state of the quantum system by a probability measure on its Hilbert space. In the case of a closed system, the evolution of this measure is described by the Liouville equation generated by the Hamiltonian structure, and here the Hamiltonian equation coincides with the Schrödinger equation (see [7-9]). At the same time, the correlation operator of this measure coincides with the density operator [10], so knowing the evolution of the density operator of the subsystem allows us to obtain the evolution of the probability measure on its Hilbert space and hence solve the master equation generated by the associated Liouville equation. It should perhaps be emphasized that the technique for treating Wigner measures by employing a suitable projection of the (pseudo)measure defined on the space of the combined classical system, is not applicable in this situation because the Hilbert space of the united system is the tensor product, rather than the Cartesian product.

This paper focuses on the algebraic structures related to the problems under consideration, and we do not explicitly state the analytical details.

1 STATES OF OPEN QUANTUM SYSTEMS

Let $\mathfrak{H}_1$ and $\mathfrak{H}_2$ be the Hilbert spaces of states of two quantum systems. In what follows, we refer to the first system (as well as to its classical counterpart) as the *open system* and to the second as *the environment*, respectively. These two systems form a composite system, whose Hilbert space is the Hilbert tensor product [3] $\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2$.

Let $\mathcal{Q}_1$ and $\mathcal{Q}_2$ be the configuration spaces of the corresponding classical open system and the environment, respectively. We assume that $\mathcal{Q}_1$ and $\mathcal{Q}_2$ are real separable Hilbert spaces. In both cases we shall assume that we have measures ν_j $(j = 1, 2)$ defined on the σ-algebra of Borel subsets of the corresponding spaces. We then set

$$\mathfrak{H}_1 = L^2(\mathcal{Q}_1, \nu_1), \quad \mathfrak{H}_2 = L^2(\mathcal{Q}_2, \nu_2)$$

and in particular the composite Hilbert space is then

$$\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2 \cong L^2(\mathcal{Q}_1 \times \mathcal{Q}_2, \nu_L \otimes \nu_2).$$

The open system we wish to describe will be quantum mechanical, so we have $\dim \mathcal{Q}_1 < \infty$, and fix ν_1 to be standard Lebesgue measure on $\mathcal{Q}_1$ for definiteness.

The dimension of $\mathcal{Q}_2$ will typically be infinite, in this case, according to the well-known result of Weil, there does not exist a non-zero σ-finite countably additive locally finite Borel measure on $\mathcal{Q}_2$. Instead, we fix a Gaussian measure ν_2 on $\mathcal{Q}_2$ (this is a matter of convenience, however, and non-Gaussian measures may be used as well).

If $\varphi \in L^2(\mathcal{Q}_1 \times \mathcal{Q}_2, \nu_1 \otimes \nu_2)$ is normalized, that is,

$$\int_{\mathcal{Q}_1 \times \mathcal{Q}_2} |\varphi(q_1, q_2)|^2 \, \nu_1(dq_1)\nu_2(dq_2) = 1,$$

then the *marginal distributions* ρ_k are defined by

$$\rho_1(q_1) \triangleq \int_{\mathcal{Q}_2} |\varphi(q_1, q_2)|^2 \, \nu_2(dq_2)$$

$$\rho_2(q_2) \triangleq \int_{\mathcal{Q}_1} |\varphi(q_1, q_2)|^2 \, \nu_1(dq_1)$$

A probability measure $\mathbb{P}_2$ on $\mathcal{Q}_2$ is then defined by

$$\mathbb{P}_2(dq_2) = \rho_2(q_2) \, \nu_2(dq_2),$$

so $\mathbb{P}_2$ is absolutely continuous with respect ν_2 with Radon-Nikodym density ρ_2, and describes the results of measurements of the environment coordinates. The pair $(\mathcal{Q}_2, \mathbb{P}_2)$ is a Kolmogorov probability space.

Taking the fixed pure state φ, we may define a $\mathfrak{H}_1 (= L^2(\mathcal{Q}_1, \nu_1))$-valued random variable on $(\mathcal{Q}_2, \mathbb{P}_2)$ by

$$\Psi_1 : q_2 \mapsto \varphi(\cdot, q_2). \tag{1}$$

If we fix an operator $\hat{A}_1$ on $\mathfrak{H}_1$, then

$$
\begin{aligned}
\mathbb{E}_2\left[\frac{\langle\Psi_1|\hat{A}_1|\Psi_1\rangle_{\mathfrak{H}_1}}{\langle\Psi_1|\Psi_1\rangle_{\mathfrak{H}_1}}\right] &= \int_{\mathscr{Q}_2}\frac{\langle\Psi_1|\hat{A}_1|\Psi_1\rangle_{\mathfrak{H}_1}(q_2)}{\langle\Psi_1|\Psi_1\rangle_{\mathfrak{H}_1}(q_2)}\mathbb{P}_2(dq_2) \\
&= \int_{\mathscr{Q}_2}\frac{\int_{\mathscr{Q}_1}\varphi(q_1,q_2)^*(\hat{A}_1\otimes I_2\,\varphi)(q_1,q_2)\nu_1(dq_1)}{\int_{\mathscr{Q}_1}|\varphi(q_1',q_2)|^2\nu_1(dq_1')}\mathbb{P}_2(dq_2) \\
&= \int_{\mathscr{Q}_1}\int_{\mathscr{Q}_2}\varphi(q_1,q_2)^*(\hat{A}_1\otimes I_2\,\varphi)(q_1,q_2)\nu_1(dq_1)\nu_2(dq_2) \\
&\equiv \langle\varphi|\hat{A}_1\otimes I_2|\varphi\rangle_{\mathfrak{H}_1\otimes\mathfrak{H}_2} \\
&\equiv \operatorname{tr}_{\mathfrak{H}_1}[\hat{\varrho}_1\hat{A}_1].
\end{aligned}
$$

where $\hat{\varrho}_1$ is the von Neumann density operator corresponding the the marginal state of the open system.

Proposition 1. *The correlation operator of the probability measure on $L^2(\mathscr{Q}_1,\nu_1)$, which is the distribution of results of measurements of the random pure state Ψ_1 given in (1), coincides with the von Neumann density operator.*

In Dirac notation, we may write $langle q_1|\Psi\rangle$ for the complex-valued random variable $\langle q_1|\Psi : q_2\mapsto\varphi(q_1,q_2)$, then

$$
\mathbb{E}_2\left[\frac{\langle q_1|\Psi_1\rangle\langle\Psi_1|q_1'\rangle}{\langle\Psi_1|\Psi_1\rangle_{\mathfrak{H}_1}}\right]=\varrho(q_1,q_1'),
$$

where $\varrho(q_1,q_1')$ is the kernel operator of $\hat{\varrho}_1$.

Remark 1. It is useful to compare the following two approaches for calculating the probability distribution of the results of measurements of the coordinate q_1 of the first system, one of which directly uses the function $\varphi\in L^2(\mathscr{Q}_1\times\mathscr{Q}_2,\nu_1\otimes\nu_2)$, which represents the pure state of the composite system, and the other one uses the $L^2(\mathscr{Q}_1,\nu_1)$-valued random variable Ψ_1. In the former case, the marginal probability density ρ_1 giving the results of measurements of the coordinate q_1. In the second approach, the density ρ_1 can be obtained by using the Chapman-Kolmogorov formula, the random variable F, and the probability $\mathbb{P}_2$ as

$$
\begin{aligned}
\rho_1(q_1) &= \int_{\mathscr{Q}_2}\rho_1(q_1|q_2)\mathbb{P}_2(dq_2) \\
&= \int_{\mathscr{Q}_2}\frac{|\varphi(q_1,q_2)|^2}{\int_{\mathscr{Q}_1}|\varphi(q_1',q_2)|^2\nu_1(dq_1')}\int_{\mathscr{Q}_1}|\varphi(q_1'',q_2)|^2\,\nu_1(dq_1'')\nu_2(dq_2) \\
&\equiv \int_{\mathscr{Q}_2}|\varphi(q_1,q_2)|^2\,\nu_2(dq_2),
\end{aligned}
$$

where the conditional probability density $\rho_1(q_1|q_2)$ is defined by $\rho_1(q_1|q_2)=|\varphi(q_1,q_2)|^2/\int_{\mathscr{Q}_1}|\varphi(q_1',q_2)|^2\nu_1(dq_1')$.

Remark 2. Of course, the Hilbert-valued random variable representing a mixed state of the open system is not uniquely determined; e.g., instead of the *coordinate representation* $L^2(\mathcal{Q}_1, \nu_1)$ of the Hilbert space $\mathfrak{H}_1$, we can use a *momentum representation* of this Hilbert space.

Remark 3. It also follows from the above considerations that the evolution of the open system can be described by a random process taking value in the same Hilbert space. However, this process is not uniquely determined either; thus, the corresponding master equation (which is an equation with a time dependent random coefficient) is not uniquely determined.

2 RANDOM PROCESSES DESCRIBING THE EVOLUTION OF OPEN SYSTEMS

We recall that the Feynman formulas are representations of Schrödinger groups or semigroups as limits of integrals over finite Cartesian products of some space $\mathscr{X}$, (see, e.g., [1, 2]). If $\mathscr{X}$ coincides with the domain Ω of functions from the space on which these groups or semigroups act and $\Omega \subset \mathscr{Q} = \mathscr{Q}_1 \times \mathscr{Q}_2$ then the corresponding Feynman formula is said to be *Lagrangian*; if $\mathscr{X} = \Omega \times \mathscr{P}$, where $\mathscr{P} = \mathscr{P}_1 \times \mathscr{P}_2$ is the momentum space of the classical version of the quantum system under consideration, then the Feynman formula is said to be Hamiltonian (not all Feynman formulas belong to one of these two classes)[1].

We identify (see [4, 10]) $\mathscr{P}_j$ with $\mathscr{Q}_j^*$ and $\mathscr{Q}_j$ with $\mathscr{P}_j^*$ $(j = 1, 2)$. These identifications generate isomorphisms (cf. [4])

$$J : \mathscr{Q}_j \times \mathscr{P}_j \ni (q, p) \mapsto (p, q) \in (\mathscr{Q}_j \times \mathscr{P}_j)^* \qquad (2)$$

and a similar isomorphism between the spaces

$$\mathscr{Q} \times \mathscr{P} \triangleq (\mathscr{Q}_1 \times \mathscr{Q}_2) \times (\mathscr{P}_1 \times \mathscr{P}_2) \qquad (3)$$

and $(\mathscr{Q} \times \mathscr{P})^*$.

Let $\psi_1 \in \mathfrak{H}_1 \left(= L^2(\mathscr{Q}_1, \nu_1)\right)$ be the initial state of the open system, and let ψ_2 be the initial state of the environment, which is called the *reference state*. We have $(\psi_1 \otimes \psi_2)(q_1, q_2) = \psi_1(q_1)\psi_2(q_2)$. Suppose that a classical Hamiltonian function $H : \mathscr{Q} \times \mathscr{P} \mapsto \mathbb{R}$ is defined by

$$H(q_1, p_1, q_2, p_2) \triangleq H_1(q_1, p_1) + H_2(q_2, p_2) + H_{12}(q_1, p_1, q_2, p_2) \qquad (4)$$

---

[1] The Feynman-Kac formulas are representations of the same groups and semigroups as integrals over the space consisting of functions of a real variable taking values in the same space $\mathscr{X}$. The multiple integrals in the Feynman formulas approximate the (infinite dimensional) integrals in the Feynman-Kac formulas. In the case of the Schrödinger semigroups generated by Hamiltonians quadratic in momenta, the infinite dimensional integrals in the Feynman-Kac formulas turn out to be integrals with respect to probability measures; however, in the case of Schrödinger groups, there appear integrals with respect to the so-called Feynman pseudo-measures or their analogues in the Feynman-Kac formulas (in many realistic situations, integrals with respect to pseudo-measures are defined as the limits of appropriate sequences of finitely many integrals).

The Hamiltonian observable $\hat{H}$ governing the evolution of the composite system may be written as

$$\hat{H} = \hat{H}_1 \otimes I_2 + I_1 \otimes \hat{H}_2 + \hat{H}_{12}, \tag{5}$$

where $\hat{H}_j$ is the pseudo-differential operator on $\mathfrak{H}_j$ with Weyl symbol H_j for $j = 1, 2$ and $\hat{H}_{12}$ is the pseudo-differential operator on with Weyl symbol H_{12} (for the definition of pseudo-differential operators on spaces of functions square integrable with respect to a measure different from the Lebesgue measure, see [2, 10]). It is useful to assume that $\hat{H}_1$ governs the internal dynamics of the open system, $\hat{H}_2$ governs the internal dynamics of the environment, and $\hat{H}_{12}$ describes the interaction.

Theorem 1. *Suppose that, for each $t = 0$, $\varphi(t) \in H_1 \otimes H_2$ denotes the state of the composite system at the moment t. Then, for all $(q_1, q_2) \in \mathscr{Q}_1 \times \mathscr{Q}_2$,*

$$\begin{aligned}
\varphi(t)(q_1, q_2) &= \left(e^{it\hat{H}} \psi_1 \otimes \psi_2 \right)(q_1, q_2) = \lim_{n \to \infty} \left(\widehat{e^{i\frac{t}{n}H}} \right)^n \psi_1 \otimes \psi_2 (q_1, q_2) \\
&= \lim_{n \to \infty} \left(\widehat{e^{i\frac{t}{n}H_1 \otimes I_2}} \circ \widehat{e^{i\frac{t}{n}I_1 \otimes H}} \circ \widehat{e^{i\frac{t}{n}H_{12}}} \right)^n \psi_1 \otimes \psi_2 (q_1, q_2).
\end{aligned}$$

The proof is based on Chernoff's theorem [11].

Remark 4. The substitution of the explicit expressions for the pseudo-differential operators on the right-hand side of the last relation turns this relation into a Feynman type formula.

We now define two random processes describing the dynamics of the open quantum system. Suppose that, for each $t \geq 0$, $\mathbb{P}_t$ is a probability measure on a copy $\mathscr{Q}_2^t$ of the space $\mathscr{Q}_2$ whose density $\rho_t(\cdot)$ with respect to ν_2 is defined as

$$\rho_t(q_2) \triangleq \int_{\mathscr{Q}_1} \left| \lim_{n \to \infty} \left(\widehat{e^{i\frac{t}{n}H}} \right)^n \psi_1 \otimes \psi_2 (q_1, q_2) \right|^2 \nu_1(dq_1), \tag{6}$$

$\mathbb{P}$ is the probability measure on the product space $\mathscr{X}$ of the family of spaces $\{\mathscr{Q}_2^t : t \geq 0\}$ defined as the product of the measures $\mathbb{P}_t$, and $\psi^{\mathbb{P}} : [0, \infty) \times (\mathscr{X}, \mathbb{P}) \mapsto L^2(\mathscr{Q}_1)$ is the $L^2(\mathscr{Q}_1)$-valued random process defined by

$$\psi^{\mathbb{P}}(t, q) = \psi_t^{\mathbb{P}}(q) \triangleq \varphi(t)(\cdot, q(t)) \tag{7}$$

where $q(= q(\cdot)) \in \mathscr{X}$ and φ is the pure state function appearing in Theorem 1. Suppose also that, for the same t, $\gamma(t)$ is a bijection between $\mathscr{Q}_2$ and $\mathscr{Q}_2^t$, which determines an isomorphism between the measure space $(\mathscr{Q}_2, \nu_2)$ and the measure space $(\mathscr{Q}_2^t, \mathbb{P}_t)$, and $\psi_v : [0, \infty) \times (\mathscr{Q}_2, \nu_2) \mapsto L^2(\mathscr{Q}_1, \nu_1)$ is the random process defined by

$$\psi_\nu(t, q) \triangleq \varphi(t)(\cdot, \gamma(t)(q)). \tag{8}$$

Theorem 2. *Under the above assumptions, the state of the open quantum system at a moment of time t is described by the $L_2(\mathscr{Q}_1, \nu_1)$-valued random variables $\psi^{\mathbb{P}}(t, \cdot)$ (on $(\mathscr{X}, \mathbb{P})$) and $\psi_{\nu_2}(t, q)$ (on $(\mathscr{Q}_2, \nu_2)$).*

3   THE WIGNER EVOLUTION FUNCTIONS OF THE OPEN QUANTUM SYSTEM

Given a density operator T on $\mathfrak{H}$, the Weyl function generated by T is the function $W_T : \mathscr{Q} \times \mathscr{P} \mapsto \mathbb{R}$ defined by

$$W_T(H) \triangleq \mathrm{tr}\left\{ T e^{-i\hat{H}} \right\}, \tag{9}$$

where $\hat{H}$ is the pseudo-differential operator on $\mathfrak{H} = L^2(\mathscr{Q}, \nu_1 \otimes \nu_2)$ with symbol $JH \in \mathscr{Q}^* \times \mathscr{P}^*$ [5]. The *Wigner measure* on $\mathscr{Q} \times \mathscr{P}$ generated by the density operator T is defined by

$$\int_{\mathscr{Q} \times \mathscr{P}} e^{i(\mathfrak{p}_1 \mathfrak{q}_2 - \mathfrak{q}_1 \mathfrak{p}_2)} W_T^M\,(d\mathfrak{q}_1, d\mathfrak{p}_1) = W_T\,(\mathfrak{q}_1, \mathfrak{p}_2)\,, \tag{10}$$

with $(\mathfrak{q}, \mathfrak{p}) \in \mathscr{Q} \times \mathscr{P}$, cf. [5].

The Wigner measure $W_{T_1}^M$ on $\mathscr{Q}_1 \times \mathscr{P}_1$ generated by a density operator T_1 on $\mathfrak{H}_1$ is defined in a similar way. The density of the measure $W_{T_1}^M$ with respect to ν_1 coincides with the classical Wigner function (see [5]).

Theorem 3. *If T is a density operator on H and T_1 is the corresponding reduced density operator on H_1, then*

$$W_{T_1}^M\,(\cdot) = \int_{\mathscr{Q}_2 \times \mathscr{P}_2} W_T^M\,(\cdot, dq_2, dp_2)\,.$$

Using this theorem and the Feynman formula for the solution of the Moyal type equation which describes the evolution of the Wigner measure on $\mathscr{Q} \times \mathscr{P}$, we can obtain a formula describing the evolution of the Wigner measure (and, thereby, the Wigner function) on $\mathscr{Q}_1 \times \mathscr{P}_1$.

4   HAMILTONIAN STRUCTURES

This section considers the third and the fourth approach for describing the dynamics of open quantum systems, which are closely related to each other. We assume that ψ_1, ψ_2, and $\mathfrak{H}$ are the same as above and $T(\cdot)$ is a function describing the dynamics of the open system, whose values are density operators on $\mathfrak{H}_1$.

Theorem 4. *If, for each $t > 0$, $k_T(t)$ is the integral kernel of a trace-class operator $T(t)$ on H_1, then*

$$
\begin{aligned}
k_T\,(t, q_1, q_2) \;=\; & \int_{\mathscr{Q}_2} \left[\lim_{n \to \infty} \left(\widehat{e^{i \frac{t}{n} H}} \right)^n \psi_1 \otimes \psi_2\,(q_1, q) \right] \\
& \times \left[\lim_{n \to \infty} \left(\widehat{e^{i \frac{t}{n} H}} \right)^n \psi_1 \otimes \psi_2\,(q_2, q) \right] \nu_2(dq).
\end{aligned}
$$

Theorem 5. *Let $\nu_2(\cdot)$ be a function of a real variable such that, for each t, $\nu_{2,t}$ is a Gaussian measure on $\mathfrak{H}_1$ with correlation operator $T(t)$. Then the function $\nu_{2,t}$ satisfies the master (Liouville) equation.*

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