Classical non-equilibrium statistical mechanics and an “open system dynamics” perspective on quantum-classical analogy *

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Abstract

It is well known that the statistics of closed classical systems evolves according to the Liouville theorem. Here we study the dynamics of the marginal statistics of classical systems coupled to external degrees of freedom, by developing a time-local equation of motion using Green’s functions and a series expansion method. We also compare this equation of motion with its supposed quantum counterpart, namely the quantum master equation, which we hope could shed some light on quantum-classical analogy (QCA) from the perspective of “open system dynamics”. We notice an apparent exception to QCA in this case, as the first-order classical equation of motion derived herein contains a term that does not appear to have a quantum analogue. We also propose possible ways of getting around this tension, which may help re-establish QCA (in first perturbative order). We do not draw a definitive conclusion about QCA in the context of open system dynamics but hope to provide a starting point for investigations along this line.

1 Motivations

Classical non-equilibrium statistical mechanics

The probability density of a closed classical system evolves according to an exact, time-local equation of motion, namely the Liouville theorem. This

*This is a first draft of the manuscript. On a side note, the author is not familiar with the research fields of classical statistical mechanics or open classical systems, and this work is a spin-off from the author’s research on quantum dynamics, in part motivated by curiosity about quantum-classical analogy.
readily gives a clear understanding of the dynamics of a closed classical system’s probability density. However, if a classical system is coupled to other, “external” degrees of freedom, the evolution of its (marginal) probability density does not generally follow the Liouville theorem, and there is generally no simplistic description of its dynamics. We call such a system an “open classical system”. (See also [16, 17, 18, 19, 20] for previous works on open classical systems through different approaches.)

It would be of theoretical interest to have an equation of motion for the marginal probability density of general open classical systems. In doing so, one should be able to see the “properties” of the dynamics of an open classical system’s marginal density, exact to every perturbative order. One may gain insights into the general nature of such dynamics by examining the equation of motion without necessarily solving it. On the other hand, most real-world physical systems are coupled to external degrees of freedom. Thus such an equation of motion might also have pragmatic value as it may be applied to real-world open classical systems to study the evolution of their (marginal) statistics.

Notably, the author has noticed that the early proposal of the “time-convolutionless projection operator” method [22, 23, 24] may be applicable to open classical systems as well. If this is the case, then it should ultimately yield results equivalent to the results we obtain in this work, as any formally exact theory should be mathematically equivalent to any other formally exact theory on the same subject. However, their derivation is different from ours, wherein they use more constructs such as the projection operator technique and antichronological time-ordering. In any case, our formalism is developed independently from [22, 23, 24]; it is mainly inspired by our work on quantum master equation for open systems [3] and in part motivated by curiosity about quantum-classical analogy [8]. All the steps in our derivation are naturally motivated and all the intermediate terms are intuitively defined. Lastly but importantly, our derivation is direct and “by construction”, as it does not use any “inverse” as ansatz, whereas the “inverse” was invariably invoked in the derivations in [22, 23, 24].

Quantum-classical analogy from an open system dynamics perspective

First, it should be cautioned that what we mean by quantum-classical analogy here is not necessarily the same thing as the quantum-classical “correspondence principle”. [11, 8] Rather, we mean, broadly speaking, some kind of resemblance and/or parallelism between quantum theory and classical theory of physics. [8] Moreover, in the author’s opinion, the criteria for what qualifies as an adequate analogy might involve some extent of subjectivity.

Quantum-classical analogy has been studied from various perspectives. [8]

1It also appears that our derivation leads to an additional term as compared to the results from their derivation, as will be seen later.
For example, it has been examined from a “state” perspective, by looking at the states of quantum systems in the phase space representation and their classical counterparts. It has also been studied from a “dynamics” perspective, with an emphasis on chaos. Our work is also on dynamics. By developing an equation of motion for the marginal probability density of a general open classical system, we open up the possibility of formally comparing it with the master equation for the reduced density matrix of open quantum systems. (See [3, 4, 5] for examples of master equations for open quantum systems.) In doing so, one might look at quantum-classical analogy from a formal, “reduced dynamical” perspective, that is, by looking at the evolution of a general open system’s marginal statistics in both quantum and classical settings.

We will outline some background thoughts here. First, we choose to consider the quantum density operator and what may be considered its classical counterpart - the probability density distribution of classical system’s states, which we shall loosely refer to as “classical density” herein. Second, we note that, under the aforementioned consideration, there is an (obvious) analogy between the equation of motion for the quantum density (i.e. the von Neumann equation) and the equation of motion for the classical density (i.e. the Liouville theorem) in the closed system scenario. Thus, in this case, we may already reasonably identify a quantum-classical analogy at the level of closed system dynamics. Third, we may not have a priori reason to assume that the quantum-classical analogy found at the level of closed system dynamics would automatically (or necessarily) imply an adequate quantum-classical analogy at the level of open system dynamics. Therefore, deriving an equation of motion for a general open classical system’s probability density may facilitate a better examination of quantum-classical analogy in the open system scenario. This could be of importance/relevance considering that most systems in the real world, in both quantum and classical settings, are open systems.

2 Derivations

2.1 Basic concepts

Phase space and probability density

Suppose we are dealing with a system of \( N \) particles in one dimension. Let’s denote the position and momentum of the \( n \)-th particle as \( q_n \) and \( p_n \) respectively. Let’s denote the collection of all classical degrees of freedom as \( x \equiv \{ q_1, p_1, q_2, p_2, \ldots q_N, p_N \} \in \mathbb{R}^{2N} \), where \( \mathbb{R}^{2N} \) is the 2N-dimensional phase space.

In classical statistical mechanics, an important quantity is the probability density (referred to as the density function in [1]) - it is a scalar field on the phase space. At any time \( t \), an instance of the probability density function \( \rho_t(x) \) is a state of the scalar field. Herein we will use the “vector” \( \vec{\rho} \) to denote a state
of the field and \{\rho(x)\} to denote the components of the vector. Each vector component \(\rho(x)\) is just (the numerical value of) the probability density at a “phase point” \(x\).

**Liouville’s theorem**

The equation of motion (EOM) for the evolution of probability density in classical statistical mechanics is given by the Liouville theorem:

\[
\frac{\partial}{\partial t} \rho_t(x) = \{H_t(x), \rho_t(x)\}_x,
\]

where \(H_t(x)\) is the Hamiltonian and the Poisson bracket on arbitrary functions \(f_t(x)\) and \(g_t(x)\) with respect to variables \(x \equiv \{q_1, p_1, q_2, p_2, \ldots q_N, p_N\}\) is defined as:

\[
\{f_t(x), g_t(x)\}_x = \sum_{k=1}^{N} \left( \frac{\partial f_t(x)}{\partial q_k} \frac{\partial g_t(x)}{\partial p_k} - \frac{\partial f_t(x)}{\partial p_k} \frac{\partial g_t(x)}{\partial q_k} \right).
\]

Note that this EOM is of first order in time, which means the values of \(\{\rho_t(x)\}\) for \(\forall x \in \mathbb{P}^{2N}\) (equivalently the vector \(\vec{\rho}_t\)) is properly a “state” of the field. That is, \(\{\rho_t(x)\}\) contains all (statistical) information about the physical system under consideration and all subsequent evolution of the classical statistics of the system is completely determined by \(\{\rho_t(x)\}\). We shall call this the “statistical state” of the system to avoid possible confusion with the “physical state” of the system, the latter of which means the system is in some definitive state characterized by variables \(x\) as in classical mechanics.

**Green’s function**

Because of linearity, we introduce the Green’s function \([13, 14]\) \(G_t(x, y)\) formally, such that the following equality holds for arbitrary \(\rho_0(y)\):

\[
\rho_t(x) = \int \text{d}y \, G_t(x, y) \rho_0(y).
\]

Physically, this equality may be interpreted in the following way: The probability (density) \(\rho_t(x)\) at \(x\) at time \(t\) comes from the probability sources \(\rho_0(y)\) all across phase space \(\forall y \in \mathbb{P}^{2N}\) at time \(t = 0\) with respective weights \(G_t(x, y)\). To be more precise, the initial probability \(\rho_0(y_1)\) of the system being at physical

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2The state of the scalar field may be thought of as an (infinite-dimensional) vector. The term “vector” here does not necessarily mean a proper vector that transforms in certain ways under coordinate transformation in the rigorous mathematical sense. Rather we simply mean a set of numbers like a column vector.
state $y_1$ contributes to the final probability $\rho_t(x)$ with a weight $G_t(x, y_1)$, the initial probability $\rho_0(y_2)$ at $y_2$ contributes to the final probability $\rho_t(x)$ by adding up contributions from all the initial probabilities $\{\rho_0(y)\}$ for $\forall y \in \mathbb{P}^{2N}$, each contribution weighed by $G_t(x, y)$. In other words, the larger the Green’s function $G_t(x, y)$ is for some $y$, the bigger “bang for the buck” the initial probability $\rho_0(y)$ at that particular $y$ has on the final probability $\rho_t(x)$.

Let’s now work out the Green’s functions. First, plugging Eq. (3) into the Liouville’s equation Eq.(1) yields

$$\int dy \rho_0(y) \frac{\partial}{\partial t} G_t(x, y) = \int dy \rho_0(y) \{H_t(x), G_t(x, y)\}_x.$$ (4)

Now we know that Eq.(4) must hold for arbitrary $\rho_0(y)$, we may choose to set $\rho_0(y) = \delta(y, Y)$ for some parameter $Y \in \mathbb{P}^{2N}$, where $\delta(a, b)$ is the multi-variate delta function. Then we have

$$\int dy \delta(y, Y) \frac{\partial}{\partial t} G_t(x, y) = \int dy \delta(y, Y) \{H_t(x), G_t(x, y)\}_x,$$ (5)

$$\Rightarrow \frac{\partial}{\partial t} G_t(x, Y) = \{H_t(x), G_t(x, Y)\}_x.$$ (6)

Moreover, the parameter $Y$ is arbitrary, therefore Eq.(6) must hold for $\forall Y \in \mathbb{P}^{2N}$. Thus we conclude that the Green’s function $G_t(x, y)$ formally introduced in Eq.(3) obeys the following EOM

$$\frac{\partial}{\partial t} G_t(x, y) = \{H_t(x), G_t(x, y)\}_x,$$ (7)

for $\forall x, y \in \mathbb{P}^{2N}$ and for all $t$.

### 2.2 Perturbative method

#### Power series expansion

Let’s parametrize the Hamiltonian by a prefactor $\lambda$, which can be thought of as controlling the strength of the Hamiltonian $\lambda H_t(x)$. Then the EOM for the Green’s function Eq.(7) becomes

$$\frac{\partial}{\partial t} G_t(x, y) = \lambda \{H_t(x), G_t(x, y)\}_x.$$ (8)

By analogy with the perturbation technique widely used in quantum mechanics [11, 3, 6, 7], let’s suppose the solution to this EOM can be written as a
power series in the parameter $\lambda$:

$$G_t(x, y) = \sum_{n=0}^{\infty} \lambda^n G_{t,n}(x, y). \quad (9)$$

Plugging Eq. (9) into Eq. (8), we have

$$\sum_{n=0}^{\infty} \lambda^n \frac{\partial}{\partial t} G_{t,n}(x, y) = \sum_{n=0}^{\infty} \lambda^{n+1} \{H_t(x), G_{t,n}(x, y)\}_x. \quad (10)$$

Because $\lambda$ is arbitrary, in order for Eq. (10) to hold identically, the equality must hold for each of the $n$th power term of $\lambda$. That is,

$$\frac{\partial}{\partial t} G_{t,0}(x, y) = 0, \quad (n = 0) \quad (11)$$

$$\frac{\partial}{\partial t} G_{t,n}(x, y) = \{H_t(x), G_{t,n-1}(x, y)\}_x. \quad (n = 1, 2, \ldots) \quad (12)$$

Eq. (11) implies that $G_{t,0}(x, y)$ does not have explicit dependence on time. To find its precise form (as function of $x$ and $y$), let’s set $\lambda = 0$, which implies

$$G_t(x, y) = \sum_{n=0}^{\infty} \lambda^n G_{t,n}(x, y) = G_{t,0}(x, y), \quad (13)$$

because all terms in the series Eq. (9) vanish except the zeroth order term. In this case, Eq. (3) implies

$$\rho_t(x) = \int dy G_t(x, y) \rho_0(y)$$

$$= \int dy G_{t,0}(x, y) \rho_0(y). \quad (14)$$

On the one hand, $\lambda = 0$ also implies

$$\frac{\partial}{\partial t} \rho_t(x) = 0, \quad (15)$$

$$\Rightarrow \rho_t(x) = \rho_0(x), \quad (16)$$

because of the vanishing Hamiltonian. Comparing Eq. (10) with Eq. (14), we have

$$\rho_0(x) = \int dy G_{t,0}(x, y) \rho_0(y). \quad (17)$$

In order for Eq. (17) to hold for arbitrary $x \in \mathbb{P}^2$, we must have

$$G_{t,0}(x, y) = \delta(x, y). \quad (18)$$
Setting \( n = 1 \) in Eq. (12) yields

\[
\frac{\partial}{\partial t} G_{t,1}(x,y) = \{ H_t(x), G_{t,0}(x,y) \}_x
\]

\[
= \{ H_t(x), \delta(x,y) \}_x,
\]

which implies

\[
G_{t,1}(x,y) = \int_0^t dt' \{ H_{t'}(x), \delta(x,y) \}_x.
\]

Similarly, higher-order terms \( G_{t,n}(x,y) \) for \( n = 2,3,\ldots \) in Eq. (9) can be worked out iteratively using Eq. (12) and will hereafter be treated as known functions.

### Dynamical map

Now we are ready to write down the probability density \( \rho_t(x) \) at arbitrary \( x \in \mathbb{P}^{2N} \) at arbitrary time \( t \) as a functional of the initial state \( \overrightarrow{\rho}_0 \) of the probability density field on phase space.

With Eqs. (3, 9), we have

\[
\rho_t(x) = \int dy \ G_t(x,y) \rho_0(y)
\]

\[
= \sum_{n=0}^{\infty} \lambda^n \int dy \ G_{t,n}(x,y) \rho_0(y)
\]

\[
= \sum_{n=0}^{\infty} \lambda^n L_{t,n}[\overrightarrow{\rho}_0](x),
\]

where \( L_{t,n}[\overrightarrow{\rho}](x) \) is a functional of any “vector” \( \overrightarrow{\rho} \) (i.e. depending on all values \( \{\rho(y)\} \) for \( \forall y \in \mathbb{P}^{2N} \)) defined as

\[
L_{t,n}[\overrightarrow{\rho}](x) \equiv \int dy \ G_{t,n}(x,y) \rho(y).
\]

### 2.3 System’s statistics

#### System-environment bifurcation

Suppose we are interested in the statistics of a subset of variables only, maybe because we are able to observe/measure those variables only. Let \( x \equiv \{q_1, p_1, q_2, p_2, \ldots, q_{NS}, p_{NS}\} \) denote the degrees of freedom we are interested in and call it the “system”; let \( x' \equiv \{q'_1, p'_1, q'_2, p'_2, \ldots, q'_{NE}, p'_{NE}\} \) denote the other degrees of freedom and call it the “environment”. This idea is similar to the bifurcation of system and environment in quantum mechanics. [5]
The full dynamics of system and environment \((x, x') \in \mathbb{P}^{2N}\) obeys the Liouville equation, with \(N = N_S + N_E\), and the same derivation above still applies. It can be shown that the probability density at time \(t\) is

\[
\rho_t(x, x') = \int dy \int dy' G_t(x, x'; y, y') \rho_0(y, y')
\]

\[
= \sum_{n=0}^{\infty} \lambda^n \int dy \int dy' G_{t,n}(x, x'; y, y') \rho_0(y, y')
\]

\[
\equiv \sum_{n=0}^{\infty} \lambda^n L_{t,n} [\rho_0] (x, x'),
\]

where \(L_{t,n} [\rho_0] (x, x')\) is a functional of any “vector” \(\rho_0\) (i.e. depending on all values \(\{\rho(y, y')\}\) for \(\forall (y, y') \in \mathbb{P}^{2N}\)) defined as

\[
L_{t,n} [\rho_0] (x, x') \equiv \int dy \int dy' G_{t,n}(x, x'; y, y') \rho(y, y'),
\]

and

\[
G_{t,0} (x, x'; y, y') = \delta(x, x'; y, y') \equiv \delta(x, y)\delta(x', y'), \ (n = 0)
\]

\[
G_{t,1} (x, x'; y, y') = \int_0^t dt' \{ H_{t'} (x, x'), \delta(x, y)\delta(x', y') \}_{(x,x')}, \ (n = 1)
\]

\[
G_{t,n} (x, x'; y, y') = \int_0^t dt' \{ H_{t'} (x, x'), G_{t,n-1}(x, x'; y, y') \}_{(x,x')} , \ (n \geq 2)
\]

**Initial statistical independence**

For the purpose of our discussion, let’s suppose at time \(t = 0\) the joint probability density is a product of the initial probability density of the system and that of the environment.

This condition can also be motivated/justified on physical grounds. Suppose the system’s degrees of freedom, say the position and momentum of a billiard ball, does not interact with the environment’s degrees of freedom, say the position and momentum of a second billiard ball, before \(t = 0\); that is, ball 1 and ball 2 have never collided by \(t = 0\). In this case, though we are not certain about the either billiard ball’s precise physical state and thus can only describe both in probabilistic terms \(\rho_{0,0}^S (x)\) and \(\rho_{0,0}^E (x')\) respectively, we are certain about the fact that the statistics of ball 1 is independent of the statistics of ball 2, because now that they have never interacted they could not have influenced one another. In other words, the joint probability density is just a product of the
two probability densities, \[ \rho_0(x, x') = \rho_0^S(x)\rho_0^E(x'). \] (28)

**Marginal probability**

We may integrate the joint probability density over some degrees of freedom to obtain the marginal probability density on other degrees of freedom. In particular, if we want to know the statistics of the system without regards to that of the environment, we may integrate the joint probability density over the environment’s degrees of freedom \( x' \equiv \{ q_{1}', p_{1}', q_{2}', p_{2}', \ldots q_{N_E}', p_{N_E}' \} \) to find the marginal probability density on the system’s degrees of freedom \( x \equiv \{ q_1, p_1, q_2, p_2, \ldots q_{N_S}, p_{N_S} \} \). Thus, given the joint probability density \( \rho_t(x, x') \) at any time \( t \), the marginal probability density of the system is

\[ \rho_t^S(x) = \int dx' \rho_t(x, x') \]

\[ = \sum_{n=0}^{\infty} \lambda^n \int dx' \int dy' G_{t,n}(x, x'; y, y') \rho_0(y, y') \]

\[ = \sum_{n=0}^{\infty} \lambda^n \int dx' \int dy' G_{t,n}(x, x'; y, y') \rho_0^S(y)\rho_0^E(y') \]

\[ = \sum_{n=0}^{\infty} \lambda^n \mathcal{E}_{t,n} \left[ \rho_0^S \right] (x), \] (29)

where we have made use of Eqs. (23, 28) and introduced the following definition

\[ \mathcal{E}_{t,n} \left[ \rho_0^S \right] (x) = \int dy \left( \int dx' \int dy' G_{t,n}(x, x'; y, y') \rho_0^E(y') \right) \rho_0^S(y), \] (30)

which precisely speaking is a functional of any “vector” \( \rho_0^S \) (i.e. depending on all values \( \{ \rho_0^S(y) \} \) for \( \forall y \in \mathbb{P}^{2N_S} \)).

The zeroth-order term of series can be worked out explicitly using Eq. (28),

\[ \mathcal{E}_{t,0} \left[ \rho_0^S \right] (x) = \int dy \left( \int dx' \int dy' G_{t,0}(x, x'; y, y') \rho_0^E(y') \right) \rho_0^S(y) \]

\[ = \int dy \left( \int dx' \delta(x, y)\delta(x', y') \rho_0^E(y') \right) \rho_0^S(y) \]

\[ = \left( \int dy \delta(x, y)\rho_0^S(y) \right) \left( \int dx' \int dy' \rho_0^E(y') \right) \]
\[ \rho^S(x) \int dx' \rho_0^E(x') = \rho^S(x); \] (31)

its time derivative is
\[ \dot{\mathcal{E}}_{t,0} \left[ \tilde{\rho}^S \right](x) = \frac{\partial}{\partial t} \left[ \tilde{\rho}^S \right](x) = 0. \] (32)

The first-order term can be worked out explicitly using Eq. (26),
\[ \mathcal{E}_{t,1} \left[ \tilde{\rho}^S \right](x) = \int dy \left( \int dx' \int dy' G_{t,1}(x, x'; y, y') \rho_0^E(y') \right) \rho^S(y) \]
\[ = \int dy \left( \int dx' \int dy' \int_0^t dt' \{ H_V(x, x'), \delta(x, y)\delta(x', y') \}_{x, x'} \rho_0^E(y') \right) \rho^S(y) \]
\[ = \int_0^t dt' \int dx' \left\{ H_V(x, x'), \int dy \rho^S(y) \delta(x, y) \right\}_x \int dy' \rho_0^E(y') \delta(x', y') \]
\[ + \int_0^t dt' \int dy \rho^S(y) \delta(x, y) \int dx' \left\{ H_V(x, x'), \int dy' \rho_0^E(y') \delta(x', y') \right\}_x \]
\[ = \int_0^t dt' \int dx' \left\{ H_V(x, x'), \rho^S(x) \right\}_x \rho_0^E(x') \]
\[ + \int_0^t dt' \rho^S(x) \int dx' \left\{ H_V(x, x'), \rho_0^E(x') \right\}_x \]
\[ = \int_0^t dt' \left\{ \left( \int dx' \rho_0^E(x') H_V(x, x') \right), \rho^S(x) \right\}_x \]
\[ + \int_0^t dt' \left( \int dx' \left\{ H_V(x, x'), \rho_0^E(x') \right\}_x \right) \rho^S(x); \] (33)

its time derivative is
\[ \dot{\mathcal{E}}_{t,1} \left[ \tilde{\rho}^S \right](x) = \left\{ \left( \int dx' \rho_0^E(x') H_V(x, x') \right), \rho^S(x) \right\}_x \]
\[ + \left( \int dx' \left\{ H_V(x, x'), \rho_0^E(x') \right\}_x \right) \rho^S(x). \] (34)

Higher-order terms \( \mathcal{E}_{t,n} \left[ \tilde{\rho}^S \right](x) \) for \( n \geq 2 \) can as well be worked out using the higher-order Green's functions \( G_{t,n}(x, x'; y, y') \) in Eq. (27).
In summary, from Eq.\((29)\) we have
\[
\rho^S_t(x) = \mathcal{E}_{t,0} \left[ \rho^S_0 \right](x) + \sum_{n=1}^{\infty} \lambda^n \mathcal{E}_{t,n} \left[ \rho^S_0 \right](x)
\]
\[
= \rho^S_0(x) + \mathcal{E}_t \left[ \rho^S_0 \right](x),
\]
where
\[
\mathcal{E}_t \left[ \rho^S \right] \equiv \sum_{n=1}^{\infty} \lambda^n \mathcal{E}_{t,n} \left[ \rho^S \right](x),
\]
with \(\mathcal{E}_{t,n} \left[ \rho^S \right](x)\) defined as in Eq.(30).

2.4 Equation of motion

The \(Y_{N,t}\) map

Following the approach in \cite{3}, let’s define a linear map that will be central to our derivation/construction:
\[
Y_{N,t} \left[ \rho^S_0 \right](x) \equiv \sum_{n=0}^{N} (-1)^n \mathcal{E}_{t}^{(n)} \left[ \rho^S \right](x),
\]
where \(\mathcal{E}_{t}^{(n)} \left[ \rho^S \right](x) \equiv \mathcal{E}_t \left( \mathcal{E}_t \left( ... \mathcal{E}_t \left[ \rho^S \right] \right) \right)(x)\) is a composition of \(n\) \(\mathcal{E}_t\) maps.

Note that Eq.(36) implies \(\mathcal{E}_t \left[ \rho^S \right](x) \sim O(\lambda)\) and thus \(\mathcal{E}_{t}^{(n)} \left[ \rho^S \right](x) \sim O(\lambda^n)\).

First-order equation of motion

Following the same reasoning as in \cite{3}, if we want to obtain an \(M\)th-order approximate equation of motion, we can choose \(N = M - 1\) in Eq.(37), so that the neglected terms are of the order \(O(\lambda^{N+2}) \sim O(\lambda^{M+1})\). Thus, to obtain a first-order equation of motion, let’s apply the Y map Eq.(37) to \(\rho^S_t\) with \(N = M - 1 = 0\), which yields
\[
Y_{0,t} \left[ \rho^S_0 \right](x) = (-1)^0 \mathcal{E}_t \left( \rho^S_0 \right)(x)
\]
\[
= \rho^S_0(x)
\]
\[
= \rho^S_0(x) + \mathcal{E}_t \left[ \rho^S_0 \right](x),
\]
(38)
where in the last equality we have made use of Eq.\((35)\). Rearranging terms in Eq.\((38)\), we can express \(\rho^S_0(x)\) in terms of \(\rho^S_t(x)\) up to zeroth order \(\rho^S_0(x) = \rho^S_t(x) - E_t \left[ - \rightarrow \rho^S_0 \right](x) = \rho^S_t(x) + \mathcal{O}(\lambda) \), \(39\)
or, in an alternative “vector” notation, \(\rightarrow \rho^S_0 = \rightarrow \rho^S_t + \mathcal{O}(\lambda) \). \(40\)

Now, to derive an equation of motion up to first order, we partial differentiate both sides of Eq.\((35)\) with respect to time, which yields
\[
\frac{\partial}{\partial t} \rho^S_t(x) = \frac{\partial}{\partial t} \rho^S_0(x) + \frac{\partial}{\partial t} \mathcal{E}_t \left[ - \rightarrow \rho^S_0 \right](x) = 0 + \mathcal{E}_t \left[ - \rightarrow \rho^S_0 \right](x) = \mathcal{E}_t \left[ - \rightarrow \rho^S_t \right](x) + \mathcal{O}(\lambda^2) = \lambda \mathcal{S}_{t,1} \left[ - \rightarrow \rho^S_t \right](x) + \mathcal{O}(\lambda^2), \tag{41}\]
where in the third equality we have made use of Eq.\((40)\) and in the last equality we have made use of Eq.\((36)\). Neglecting \(\mathcal{O}(\lambda^2)\) terms in Eq.\((41)\), using Eq.\((34)\) for the first term, and setting \(\lambda = 1\) formally, we arrive at a first-order equation of motion:
\[
\frac{\partial}{\partial t} \rho^S_t(x) = \mathcal{E}_t \left[ - \rightarrow \rho^S_t \right](x) = \left\{ \left( \int dx' \rho^E_0(x') H_t(x, x') \right), \rho^S_t(x) \right\}_x + \left( \int dx' \left\{ H_t(x, x'), \rho^E_0(x') \right\}_x \right) \rho^S_t(x). \tag{42}\]

Note that in order to obtain an equation of motion up to first order only, we have not followed the full treatment as we did in \([3]\), but have instead used a somewhat short-cut approach here. But it is in the same spirit as the full treatment in \([3]\).

2.5 Main results

So we have a time-local equation of motion for the probability density \(\rho^S_t(x)\) on the system’s phase space \(x \equiv \{q_1, p_1, q_2, p_2, \ldots q_{NS}, p_{NS} \} \in \mathbb{P}^{2NS}\) to first
perturbative order

$$\frac{\partial}{\partial t} \rho_t^S(x) = \left\{ H_t^{eff}(x), \rho_t^S(x) \right\}_x + B_t(x) \rho_t^S(x), \quad (43)$$

where the effective Hamiltonian $H_t^{eff}(x)$ and the prefactor $B_t(x)$ are

$$H_t^{eff}(x) \equiv \int dx' \rho_0^E(x') H_t(x,x'), \quad (44)$$

$$B_t(x) \equiv \int dx' \left\{ H_t(x,x'), \rho_0^E(x') \right\}_{x'}. \quad (45)$$

Provided that the formalism in [22, 23, 24] is in fact applicable to the case of open classical systems, the first-order results therein, albeit in an abstract form, should have served the purpose of finding first-order corrections to the classical Liouville dynamics like we have done here. We notice, however, that even to first perturbative order, our derivation leads to a term $B_t(x) \rho_t^S(x)$ that doesn’t appear to have a counterpart in their result. For example, the first-order term Eq.(31a) of Ref.[24] is (roughly speaking) some "average of the perturbing Liouvillian", which is a prima facie counterpart of the first term in Eq.(43) only. This issue may be worth further investigation.  

3 Discussions

Apparent tension with quantum master equation

Quantum master equations are used to describe the evolution of open quantum systems. The quantum master equation can be considered counterpart to the equation of motion for marginal classical probability density as we develop in this paper, just like the von-Neumann equation for closed quantum systems can be considered counterpart to the Liouville equation for full classical probability density. Thus it makes sense to compare the main result here with a quantum master equation.

Formally exact master equations can be found in [3, 4, 5]. We will compare the main result herein with the master equation in [3]. Our equation of motion to first order is Eqs.(43-45) above, which is to be compared with the first-order

\footnote{The author speculates that, in regard to open classical systems, it is possible that their derivation might have implicitly assumed some condition(s) which might be "reasonable" for practical purposes but might not be strictly (necessarily) true, and as a result might have left out something which could have been included, whereas our treatment might be (arguably) more careful in the sense that it makes as few assumptions as possible. However, it must be stressed that such speculation is mere guesswork, based only on "gut feeling" but not grounded on any sound knowledge or rigorous reasoning, and is meant to guess some possibility for mere exploratory purpose.}
master equation in [3]:

\[
\frac{d}{dt} \rho^S_t = -\frac{i}{\hbar} \left[ H_{\text{eff}}(t), \rho^S_t \right],
\]

(46)

where

\[
H_{\text{eff}}(t) = \sum_n \text{Tr} (\rho_{E0} E_n(t)) S_n(t)
= \sum_n \text{Tr} \left( S_n(t) \otimes \rho_{E0} E_n(t) \right)
= \text{Tr} \left( (\mathbb{I}_S \otimes \rho_{E0}) \sum_n S_n(t) \otimes E_n(t) \right)
= \text{Tr} \left( (\mathbb{I}_S \otimes \rho_{E0}) H_{\text{SE}}(t) \right).
\]

(47)

Now, if we were to identify the marginal probability density \( \rho^S_t(x) \) in the classical case with the reduced density operator \( \rho^S_t \) in the quantum case, the classical Poisson bracket \( \{ A(x), B(x) \}_x \) with the quantum commutator \( -\frac{i}{\hbar} [A, B] \), the classical effective Hamiltonian density \( H^{\text{eff}}_{\text{t}}(x) = \int dx' \rho^E_0(x') H_t(x, x') \) with the quantum effective Hamiltonian \( H_{\text{eff}}(t) = \text{Tr} \left( (\mathbb{I}_S \otimes \rho_{E0}) H_{\text{SE}}(t) \right) \), where in turn the integral over classical environmental degrees of freedom \( \int dx' \ldots \) were compared with the partial trace over quantum environmental degrees of freedom \( \text{Tr} E(\ldots) \), then we can see that the first-order equation of motion developed herein Eq.(43) agrees with its quantum counterpart Eq.(46) except having an extra term \( B_t(x) \rho^S_t(x) \), where \( B_t(x) = \int dx' \{ H_t(x, x'), \rho^E_0(x') \}_x \). Therefore, at face value, we do not appear to have established QCA at the subsystem (i.e. open system) level even to the lowest (first) perturbative order.

Note that this is unlike in the case of the whole system (i.e. closed system) level, where one can easily identify the QCA between the quantum von Neumann equation \( \frac{d}{dt} \rho_t = -\frac{i}{\hbar} [H(t), \rho_t] \) and the classical Liouville equation \( \frac{d}{dt} \rho_t(x) = \{ H_t(x), \rho_t(x) \}_x \).

The apparent tension between the classical and quantum scenarios in the case of open system lies in the second term of Eq.(43), namely \( B_t(x) \rho^S_t(x) \), which does not appear to have a counterpart in the first-order quantum master equation in [3]. In the followings, we will present two ways of possibly getting around this apparent tension.

Possible solution 1

A closer look at the prefactor \( B_t(x) = \int dx' \{ H_t(x, x'), \rho^E_0(x') \}_x \) might offer some hint. For an integral over the environmental variables \( x' \equiv \{ q'_1, p'_1, q'_2, p'_2, \ldots q'_N_E, p'_N_E \} \), we have

\[
B_t(x) = \int dx' \{ H_t(x, x'), \rho^E_0(x') \}_x.
\]
where in the last line we have defined the factor $B_{t,k}(x,x')$ accordingly. Let’s examine the factor $B_{t,k}(x,x')$ for an arbitrary $k$ in Eq. (48) in greater detail:

$$B_{t,k}(x,x') = \int_{-\infty}^{+\infty} dq'_k \int_{-\infty}^{+\infty} dp'_k \left( \frac{\partial H_t(x,x')}{\partial q'_k} \frac{\partial \rho_0^E(x')}{\partial p'_k} - \frac{\partial H_t(x,x')}{\partial p'_k} \frac{\partial \rho_0^E(x')}{\partial q'_k} \right)$$

$$= \int_{-\infty}^{+\infty} dq'_k \left( \int_{-\infty}^{+\infty} dp'_k \frac{\partial H_t(x,x')}{\partial q'_k} \frac{\partial \rho_0^E(x')}{\partial p'_k} \right)$$

$$- \int_{-\infty}^{+\infty} dp'_k \left( \int_{-\infty}^{+\infty} dq'_k \frac{\partial H_t(x,x')}{\partial p'_k} \frac{\partial \rho_0^E(x')}{\partial q'_k} \right)$$

$$= \int_{-\infty}^{+\infty} dq'_k \left( \frac{\partial H_t(x,x')}{\partial q'_k} \rho_0^E(x') \bigg|_{p'_k=\pm\infty} - \int_{-\infty}^{+\infty} dp'_k \frac{\partial^2 H_t(x,x')}{\partial q'_k \partial p'_k} \rho_0^E(x') \right)$$

$$- \int_{-\infty}^{+\infty} dp'_k \left( \frac{\partial H_t(x,x')}{\partial p'_k} \bigg|_{q'_k=\pm\infty} - \int_{-\infty}^{+\infty} dq'_k \frac{\partial^2 H_t(x,x')}{\partial q'_k \partial p'_k} \rho_0^E(x') \right)$$

$$= - \int_{-\infty}^{+\infty} dq'_k \int_{-\infty}^{+\infty} dp'_k \frac{\partial^2 H_t(x,x')}{\partial p'_k \partial q'_k} \rho_0^E(x')$$

$$+ \int_{-\infty}^{+\infty} dp'_k \int_{-\infty}^{+\infty} dq'_k \frac{\partial^2 H_t(x,x')}{\partial q'_k \partial p'_k} \rho_0^E(x')$$

$$= 0,$$

where in the third equality we have used integration by parts, in the fourth equality we have assumed the following quantities vanish at infinity (for an arbitrary $k$),

$$\frac{\partial H_t(x,x')}{\partial q'_k} \rho_0^E(x') \big|_{p'_k=\pm\infty} = \frac{\partial H_t(x,x')}{\partial p'_k} \rho_0^E(x') \big|_{q'_k=\pm\infty} = 0,$$
and in the last equality we have assumed the symmetry of second derivatives
(for an arbitrary \( k \)), that is,
\[
\frac{\partial^2 H_t(x, x')}{\partial q'_k \partial p'_k} = \frac{\partial^2 H_t(x, x')}{\partial p'_k \partial q'_k},
\]
and throughout we have assumed the orders of integrals are interchangeable.
With these assumptions (under these conditions), we may say \( B_{t,k}(x, x') = 0 \)
for an arbitrary \( k \); plugging this into Eq.\((48)\), we may say \( B_t(x) = 0 \).

Thus we have shown that the extra term \( B_t(x) \rho_s^S(x) \) in Eq.\((43)\) vanishes
with the aforementioned assumptions. One might argue that these assumptions/conditions
are apparently satisfiable in “normal” (i.e. sufficiently “well-behaved”) situations. For example, looking at Eq.\((50)\), we note that the probability density \( \rho_E^0(x') \) should vanish at infinity because of normalization requirement for a probability distribution
\[
\int dx' \rho_E^0(x') = 1,
\]
thus provided that \( \frac{\partial H_t(x, x')}{\partial q'_k} |_{q'_k = \pm \infty} \) and \( \frac{\partial H_t(x, x')}{\partial p'_k} |_{p'_k = \pm \infty} \) do not blow up, the condition Eq.\((50)\)
would be satisfied. With the vanishing of \( B_t(x) \rho_s^S(x) \), the first-order equation
of motion Eq.\((43)\) would then become
\[
\frac{\partial}{\partial t} \rho_s^S(x) = \left\{ H_t^{\text{eff}}(x), \rho_s^S(x) \right\}_x,
\]
which we might now say has an apparent QCA with the first-order quantum master equation \( \frac{\hbar}{i} \rho_t^S = - \frac{i}{\hbar} \left[ H_t^{\text{eff}}(t), \rho_t^S \right] \). It should be stressed that we do not claim rigour in these arguments.

One might still ask whether we have satisfactorily established quantum-classical analogy with this approach, because the vanishing of \( B_t(x) \rho_s^S(x) \) is apparently not a priori. If in the case of first-order quantum master equation there were a priori nothing beyond the commutator \( - \frac{i}{\hbar} \left[ H_t^{\text{eff}}(t), \rho_t^S \right] \), whereas in the case of classical equation of motion there were something beyond the Poisson bracket \( \left\{ H_t^{\text{eff}}(x), \rho_t^S(x) \right\}_x \), which turned out to vanish given some conditions (albeit possibly “reasonable” ones), does this adequately qualify as QCA? Or is it too weak a sense to talk about QCA?

Possible solution 2

In response to the questions above, let’s have a closer look at the first-order quantum master equation in Eq.\((3)\). For \( H_{SE}(t) = \sum_n S_n(t) \otimes E_n(t) \), the original expression for the first-order term is
\[
\mathcal{L}_{1,t} (\rho_t^S) = - \frac{i}{\hbar} \left( \sum_n Tr_E \left( S_n(t) \rho_t^S \otimes E_n(t) \rho_E^0 \right) - \sum_n Tr_E \left( \rho_t^S S_n(t) \otimes \rho_{E0} E_n(t) \right) \right),
\]
(53)
and thus the first-order master equation may be worked out more carefully as follows:

\[
\frac{d}{dt} \rho_i^S = -\frac{i}{\hbar} \left( \sum_n T_{RE} \left( S_n(t) \rho_i^S \otimes E_n(t) \rho_{E0} \right) - \sum_n T_{RE} \left( \rho_i^S S_n(t) \otimes \rho_{E0} E_n(t) \right) \right)
\]

\[
= -\frac{i}{\hbar} \sum_n \left( S_n(t) \rho_i^S T_{RE} \left( E_n(t) \rho_{E0} \right) - \rho_i^S S_n(t) T_{RE} \left( \rho_{E0} E_n(t) \right) \right)
\]

\[
= -\frac{i}{\hbar} \sum_n \left( S_n(t) \rho_i^S T_{RE} \left( \rho_{E0} E_n(t) \right) - \rho_i^S S_n(t) T_{RE} \left( \rho_{E0} E_n(t) \right) \right)
\]

\[
= -\frac{i}{\hbar} \sum_n \left( T_{RE} \left( S_n(t) \otimes E_n(t) \left( I_S \otimes \rho_{E0} \right) \right) \rho_i^S - T_{RE} \left( \left( I_S \otimes \rho_{E0} \right) S_n(t) \otimes E_n(t) \right) \rho_i^S \right)
\]

\[
= -\frac{i}{\hbar} \left[ \sum_n T_{RE} \left( S_n(t) \otimes \rho_{E0} E_n(t) \right) , \rho_i^S \right]
\]

\[
- \frac{i}{\hbar} \left( T_{RE} \left( \sum_n S_n(t) \otimes E_n(t) \left( I_S \otimes \rho_{E0} \right) \right) \rho_i^S \right)
\]

\[
- \frac{i}{\hbar} \left( -T_{RE} \left( \left( I_S \otimes \rho_{E0} \right) \sum_n S_n(t) \otimes E_n(t) \right) \rho_i^S \right)
\]

\[
= -\frac{i}{\hbar} \left[ T_{RE} \left( \left( I_S \otimes \rho_{E0} \right) \sum_n S_n(t) \otimes E_n(t) \right) , \rho_i^S \right]
\]

\[
- \frac{i}{\hbar} \left( T_{RE} \left( H_{SE}(t) \left( I_S \otimes \rho_{E0} \right) \right) \rho_i^S - T_{RE} \left( \left( I_S \otimes \rho_{E0} \right) H_{SE}(t) \right) \rho_i^S \right)
\]

\[
= -\frac{i}{\hbar} \left[ T_{RE} \left( \left( I_S \otimes \rho_{E0} \right) H_{SE}(t) \right) , \rho_i^S \right]
\]

\[
+ T_{RE} \left( -\frac{i}{\hbar} \left[ H_{SE}(t) , \left( I_S \otimes \rho_{E0} \right) \right] \right) \rho_i^S
\]

\[
= -\frac{i}{\hbar} \left[ H_{eff}(t) , \rho_i^S \right] + B(t) \rho_i^S ,
\]

(54)

where

\[
H_{eff}(t) \equiv T_{RE} \left( \left( I_S \otimes \rho_{E0} \right) H_{SE}(t) \right) ,
\]

(55)

\[
B(t) \equiv T_{RE} \left( -\frac{i}{\hbar} \left[ H_{SE}(t) , \left( I_S \otimes \rho_{E0} \right) \right] \right) .
\]

(56)
Now we see an extra term $B(t)\rho^S_t$ beyond the commutator $-\frac{i}{\hbar} [H_{eff}(t), \rho^S_t]$ in the first-order quantum master equation. Note that the difference between this derivation and the original derivation in [3], the latter of which does not give rise to the term $B(t)\rho^S_t$, lies in the third equality of Eq.(54). In the original derivation in [3] we simply assume $\text{Tr}_E (\rho_{E0} E_n(t)) = \text{Tr}_E (E_n(t) \rho_{E0})$, whereas here in Eq.(54) we do not assume the same, but formally work out the difference between $\text{Tr}_E (\rho_{E0} E_n(t))$ and $\text{Tr}_E (E_n(t) \rho_{E0})$. The result of this new treatment is the second term of Eq.(54), namely $B(t)\rho^S_t$.

Comparing the first-order quantum master equation Eq.(54) with its classical counterpart Eq.(43), we may now see a better analogy between them. In particular, the second term of Eq.(43)

$$B_t(x)\rho^S_t(x) = \int dx' \{H_t(x, x'), \rho^E_0(x')\} x', \rho^S_t(x) \quad (57)$$

now has an analogous term in Eq.(54)

$$B(t)\rho^S_t = \text{Tr}_E \left( -\frac{i}{\hbar} [H_{SE}(t), (I_S \otimes \rho_{E0})] \right) \rho^S_t, \quad (58)$$

if we were again to identify $\{A(x), B(x)\}_{x'}$ and $\int dx' \ldots$ in the former with $-\frac{i}{\hbar} [A, B]$ and $\text{Tr}_E \ldots$ in the latter. In view of this, one may argue that QCA is plausibly re-established.

One might still ask further questions, for example, whether the vanishing of $B_t(x)\rho^S_t$ in the quantum case is subject to analogous (or "corresponding") conditions as the vanishing of $B_t(x)\rho^S_t(x)$ in the classical case is, so that whenever one vanishes the other would also vanish accordingly/correspondingly.

Regardless of the possibility of further questions, the formal analogy between $B_t(x)\rho^S_t(x)$ in the classical case and $B_t(x)\rho^S_t$ in the quantum case apparently holds anyway. One might even argue that, in some sense, this might be the right kind of quantum-classical analogy one would be looking for.

Summary

In the above, we might have possibly/arguably established quantum-classical analogy at the level of open system dynamics, up to the leading (first) perturbative order. It should be noted that we do not have a definitive conclusion regarding whether QCA is sufficiently established here, nor do we claim rigour in our discussions. We only mean to provide some heuristics for the issue and possibly some starting point for further discussions.

Besides the issue of QCA per se, this work also helps us notice the formal existence of the term $B(t)\rho^S_t$ in the first-order quantum master equation, an issue that was neglected in [3]. Thus one contribution our formalism could have is that the classical equation of motion derived herein might shed light on its quantum counterpart and possibly help us notice issues that might have been
overlooked in the works of open quantum systems.

4 Conclusions

In this work we develop a formalism to study the evolution of the marginal probability density of open classical systems, using Green’s functions and a series expansion method.

We have worked out the equation of motion for a general open classical system’s marginal probability density up to first order, namely Eq. (43). With this framework, higher-order terms can be worked out systematically, by using the $Y_{N,t}$ map as in Eq. (37). (Also, see [3] for a treatment using the $Y_{N,t}$ map in the context of open quantum systems.) By working out higher-order terms, one will be able to see how system-environment coupling further modifies the (idealistically Liouville) dynamics of classical systems. For example, it may be interesting to examine the second-order term. In the case of open quantum systems, quantum decoherence generally arises as a second-order effect. It might be interesting if we could see some counterpart of “decoherence” in the context of open classical system’s statistics using our formalism.

Besides such general study of a formal nature, our formalism may be applied to real-world classical systems to study the evolution of their (marginal) statistics when coupled to external degrees of freedom. This practicality can be a direction for future efforts.

This work may also contribute to the study of quantum-classical analogy from an open system dynamics perspective, by comparing the first-order equation of motion Eq. (43) (or any higher-order equation of motion that can be worked out with our framework) with what could be considered its quantum counterpart (e.g. the quantum master equation in [3]). We notice an apparent tension between quantum and classical open system dynamics in first order; we also present possible ways of getting around the tension. However, we claim no definitive conclusion about a sufficient quantum-classical analogy, but only hope to provide some starting point for further investigations along this line.

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