Exact stochastic Liouville and Schrödinger equations for open systems

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Abstract

An universal form of kinetic equation for open systems is considered which naturally unifies classical and quantum cases and allows to extend concept of wave function to open quantum systems. Corresponding stochastic Schrödinger equation is derived and illustrated by the example of inelastic scattering in quantum conduction channel.

Key words: statistical mechanics, kinetic theory, open systems, quantum transport, inelastic scattering, stochastic Liouville equation, stochastic Schrödinger equation

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1. Introduction

It is seldom when one can say about a quantum system that it is in a pure state described by certain wave function, \( \Psi(t) \). Even closed system generally is in a mixed state and should be described by density matrix \[ |P(H)\rangle \equiv \sum_{\alpha} P_{\alpha} |\Psi_{\alpha}(t)\rangle |\Psi_{\alpha}(t)\rangle \]

where \( \Psi_{\alpha}(t) \) is a full set of mutually orthogonal solutions to system’s Schrödinger equation ( \( \langle \Psi_{\alpha}(t)|\Psi_{\beta}(t)\rangle = 0 \) at \( \alpha \neq \beta \) ), time-independent \( P_{\alpha} \) are their statistical weights, and whole \( R(t) \) is solution to the von Neumann equation.

All the more if a system \( S \) interacts with some other system \( W \), e.g. “the rest of the World”. In such case representation (1) loses meaning and density matrix of \( S \) becomes “thing in itself” to be found from von Neumann equation of total closed system \( S+W \).

There are many different approaches to this vast problem [1-3]. However, any of them results in either approximate kinetic and stochastic equations for \( S \) or formally exact but too complicated ones. In present paper, in part following [4-7], one more approach is described which leads to such kinetic equation which is at once simple and exact. Its other advantages are intuitive obviousness, explicit separation of contributions from \( S \) and \( W \) and possibility to reformulate it in terms of wave function of \( S \) itself, thus rehabilitating representation (1) as applied to open systems.

2. Stochastic treatment of dynamic interactions

As usually, let us divide Hamiltonian \( H \) of the whole system \( S+W \) into three parts and assume that the interaction part, \( H_{int} \), has bilinear form:

\[ H = H_S + H_W + H_{int}, \quad H_{int} = \sum_j S_j W_j, \quad (2) \]

where operators \( S_j \) and \( W_j \) act at different Hilbert spaces of \( S \) and \( W \), respectively. Such a decomposition of the interaction Hamiltonian is always possible (and, as a rule, it directly follows from physics of interaction). For any operator \( O \) define Liouville and Jordan super-operators:

\[ \mathcal{L}(O)A = \frac{i}{\hbar} (OA - AO), \quad \Pi(O)A = \frac{1}{2} (OA + AO), \]

where \( A \) is arbitrary operator. Thus \( \mathcal{L}(H) \) is the Liouville evolution operator of \( S+W \). One can see that correspondingly to (2) it decomposes to

\[ \mathcal{L}(H) = \mathcal{L}(H_S + H_W + \sum_j S_j W_j) = \mathcal{L}(H_S) + \mathcal{L}(H_W) + \sum_j [\mathcal{L}(S_j) \Pi(W_j) + \Pi(S_j) \mathcal{L}(W_j)] \]

From the viewpoint of \( S \) it is formally equivalent to

\[ \mathcal{L}_S(t) = \mathcal{L}(H_S) + \sum_j [x_j(t) \mathcal{L}(S_j) + y_j(t) \Pi(S_j)] \quad (4) \]

where \( x_j(t) \) and \( y_j(t) \) play as arbitrary scalar time functions although in respect to \( W \) they are super-operators

\[ x_j(t) = e^{\mathcal{L}(H_W)t} \Pi(W_j) e^{\mathcal{L}(H_W)t}, \]

\[ y_j(t) = e^{\mathcal{L}(H_W)t} \mathcal{L}(W_j) e^{\mathcal{L}(H_W)t}. \]
$y_j(t) = e^{-L(H_W) t} L(W_j) e^{L(H_W) t}$

In detail, if $\rho(t)$ denotes joint density matrix of $S+W$, which undergoes the von Neumann equation $\dot{\rho} = L(H) \rho$, and $\rho_S(t) = \text{Tr}_W \rho(t)$ density matrix of $S$, then

$$\rho_S(t) = \text{Tr}_W \tilde{\exp} \left[ \int_0^t L_S(t') \, dt' \right] \rho(0),$$

where $\tilde{\exp}$ means chronologically ordered exponential.

These facts prompt us to consider $x_j(t)$ and $y_j(t)$ as random processes while operation $\text{Tr}_W$ in (5) as statistical moment integrations begin at $t = -\infty$, moved away to $t = \infty$.

More details about them and various generalizations of the “stochastic representation” can be found in [5,7,8,10].

3. Stochastic Schrödinger equation

If initially (before the interaction) $S$ was in a pure state, $\rho_S^{(in)} = |\Psi^{(in)}(t)\rangle \langle \Psi^{(in)}(t)|$, then equation (7) has a solution which all the time keeps such form: $R(t) = |\Psi(t)\rangle \langle \Psi(t)|$, where $\Psi(t)$ satisfies stochastic Schrödinger equation

$$\frac{d\Psi(t)}{dt} = -\frac{i}{\hbar} \left[ H_S + \sum_j w_j(t) S_j \right] \Psi(t)$$

with initial condition $\Psi(t_0) = \Psi^{(in)}$, and

$$w_j(t) \equiv x_j(t) + \hbar y_j(t)/2$$

are mentioned as complex-valued random processes. Hence, solution to (7) under arbitrary initial condition $R(t_0)$, let $\rho_S^{(in)} = \sum_{\alpha} |\Psi_{\alpha}^{(in)}\rangle P_{\alpha} |\Psi_{\alpha}^{(in)}\rangle$ in the diagonal form, can be written in the form (1) where each of $\Psi_{\alpha}(t)$ evolves according to (9) but all $P_{\alpha}$ stay constant.

Because of complexity of $w_j(t)$, the evolution governed by (9) is not unitary:

$$\frac{d}{dt} \langle \Psi_{\alpha}(t) | \Psi_{\beta}(t) \rangle = \sum_{\gamma} y_{j}(t) \langle \Psi_{\alpha}(t) | S_{j} | \Psi_{\beta}(t) \rangle \neq 0 \quad (10)$$

Nevertheless it is unitary on average:

$$\frac{d}{dt} \langle \Psi_{\alpha}(t) | \Psi_{\beta}(t) \rangle \equiv \left\langle \sum_{\gamma} y_{j}(t) \langle \Psi_{\alpha}(t) | S_{j} | \Psi_{\beta}(t) \rangle \right\rangle = 0 ,$$

$$\langle \Psi_{\alpha}(t_0) | \Psi_{\beta}(t_0) \rangle \propto \delta_{\alpha \beta} \quad (11)$$

This statement directly follows from the above mentioned specific statistical properties of $y_j(t)$.

Let the interaction by its nature is time-localized, that is has a character of scattering. In such situation for any particular “stochastic pure state” one can write

$$|\Psi(t)\rangle = |\Psi^0(t)\rangle + |\Psi^s(t)\rangle$$
with $|\Psi^0(t)\rangle$ describing free evolution of $\mathcal{S}$ and $|\Psi^s(t)\rangle$ at $t \rightarrow \infty$ representing result of the scattering. Then due to
$$\langle \langle \Psi^s(t) | \Psi^s(t) \rangle \rangle = |\Psi^0| \langle \Psi^0 \rangle$$
and consequently
$$2 \text{Re} \langle \Psi^0 | \langle \Psi^s \rangle \rangle + \langle \langle \Psi^s | \Psi^s \rangle \rangle = 0 \quad (12)$$
This is nothing but “the optical theorem on average” which equally holds for both elastic and inelastic scattering. It demonstrates also that average wave function $\langle \Psi(t) \rangle$ can bring useful information about an open quantum system.

### 4. Interaction with thermal bath

Of special interest are cases when $\mathcal{W}$ is very large system in thermodynamical equilibrium, $\rho_{\mathcal{W}}^{(in)} \propto \exp(-H_{\mathcal{W}}/T)$, so that all $x_j(t)$, $y_j(t)$ and $w_j(t)$ are stationary random processes. If one assumes (without loss of generality) that $\text{Tr}_W W_j \rho_{\mathcal{W}}^{(in)} = 0$, then all the processes have zero mean values and all their pair correlations reduce to function
$$K_{jm}(\tau) \equiv \text{Tr}_W W_j \exp(-i\tau H_{\mathcal{W}}/\hbar) W_m \rho_{\mathcal{W}}^{(in)}$$
One can routinely verify that
$$K_{jm}(\tau) = K_{mj}^*(\tau),$$
$$\langle w_j^s(\tau) w_m(0) \rangle = K_{jm}(\tau),$$
$$\langle w_j(\tau) w_m(0) \rangle = \langle w_j^s(\tau) w_m^s(0) \rangle^* = K_{jm}(\tau) \theta(\tau) + K_{jm}^*(\tau) \theta(-\tau),$$
$$K_{jm}^{xy}(\tau) \equiv \langle x_j(\tau) x_m(0) \rangle = \text{Re} K_{jm}(\tau),$$
$$K_{jm}^{xy}(\tau) = \langle x_j(\tau) y_m(0) \rangle = (2/\hbar) \theta(\tau) \text{Im} K_{jm}(\tau),$$
$$K_{jm}(\tau - i\hbar/2T) = K_{jm}(\tau - i\hbar/2T),$$
where $\theta(t)$ is the Heaviside step function. The last equality expresses equivalence of $\mathcal{W}$ and in its turn implies definite relation between $K_{jm}^{xy}(\tau)$ and $K_{jm}^{xy}(\tau)$:
$$K_{jm}^{xy}(\tau) = \int_0^\infty \cos(\omega \tau) \sigma_{jm}(\omega) d\omega,$$
$$K_{jm}^{yx}(\tau) = -\frac{2\theta(\tau)}{\hbar} \int_0^\infty \sin(\omega \tau) \tan \left( \frac{\hbar \omega}{2T} \right) \sigma_{jm}(\omega) d\omega,$$
where $\sigma_{jm}(w)$ is non-negatively defined spectrum matrix. In essence, this is usual fluctuation-dissipation theorem.

Of course, the $\mathcal{W}$’s equilibrium results also in definite relations between higher-order correlators of $x(t)$ and $y(t)$. They were discussed in [11]. In the classical limit all they can be summarized by symbolic equality
$$\varepsilon_j y_j(-t) \simeq y_j(t) + \frac{1}{T} \frac{dx_j(t)}{dt},$$
where $\simeq$ means statistical equivalence under time inversion, $t \rightarrow -t$, and $\varepsilon_j \equiv 1$ indicates time parity of variable $x_j(t)$ from viewpoint of Hamiltonian mechanics, so that $x_j(-t) \simeq \varepsilon_j x_j(t)$. Correspondingly, the second-order relation expressed by (14) in the classical limit simplifies to
$$K_{jm}^{xy}(\tau) = \frac{\theta(\tau)}{T} \frac{d}{d\tau} K_{jm}^{yx}(\tau)$$

### 5. Inelastic scattering center in conducting channel

Let $\mathcal{S}$ be one-dimensional conduction channel formed by discrete sites ($n = \ldots -1, 0, 1, \ldots$), $\mathcal{W}$ be thermostat, and their interaction realizes through randomly varying potential localized at only one site, for certainty, $n = 0$. Then $\langle H_S \rangle_{n_n} = \epsilon [\delta_{n_{n-1}} - \delta_{n_{n+1}}]/2$, where $\epsilon$ is channel’s bandwidth, and $\sum w_j(t) S_j = w(t) S$, where $S_{n_n} = \delta_{n_0} \delta_{n_0}$. We want to consider evolution of wave function $\Psi(t, n)$ which initially, at $t = t_0 < 0$, represents a wide wave packet placed on the left from $n = 0$ and moving to the right with momentum $\hbar k_0 > 0$. Thus let us divide it into free and scattered parts: $\Psi(t, n) = \Psi^0(t, n) + \Psi^s(t, n)$, where $\Psi^0 = -iH_S \Psi^0 / \hbar$, so that (9) transforms to
$$\frac{d\Psi^0(t, n)}{dt} = -i \frac{\hbar}{\hbar} \langle H_S \Psi^0(t, n) + w(t) \delta_{n_0} \Psi(t, 0) \rangle,$$
with initial condition $\Psi^0(t_0, n) = 0$.

Strictly speaking, such division presumes that particle scattered by fluctuating potential can not be captured by it. If it is really so, that is $\Psi^0(t, n) \rightarrow 0$ at $t \rightarrow \infty$ for any given finite $n$ (first of all, $n = 0$), then at large enough $t > 0$ after scattering we can determine probabilities of reflection, $\mathcal{R}$, and transmission, $\mathcal{T}$, as
$$\mathcal{T} = \sum_{n \geq 0} |\Psi^s|^2,$$
$$\mathcal{R} = \sum_{n < 0} |\Psi^s|^2$$
(16)
Here we took into account mirror symmetry of scattered wave, $\Psi^0(t, -n) = \Psi^s(t, n)$, which obviously follows from (15). After averaging (16) over the thermostat and combining with general “optical theorem” (17) we have
$$\langle \mathcal{R} \rangle = 1 - \langle \mathcal{T} \rangle = -\text{Re} \sum_n \Psi^0(t, n) \langle \Psi^s(t, n) \rangle,$$
(17)
Alternatively, we can describe the scattering in terms of outgoing wide wave packets with discrete wave numbers $k$ (separated by a width of ingoing packet in reciprocal space) and amplitudes $\Psi_k = \Psi^0_k + \Psi^s_k$. Then $\Psi^0_k = \delta_{k k_0}$, and optical theorem (17) takes form
$$\langle \mathcal{R} \rangle = -\text{Re} \langle \Psi^0_{k_0} \rangle = -\text{Re} \langle \Psi^s_{k_0} \rangle,$$
(18)
The second equality here is again consequence of the mirror symmetry of scattering which implies $\Psi^s_{-k} = \Psi^s_k$.
Next, let us divide $\mathcal{R}$ and $\mathcal{T}$ into elastic and inelastic parts marked by “el” and “in”, respectively, so that
$$\mathcal{R}^e = |\Psi_{-k_0}|^2, \quad \mathcal{T}^e = |\Psi_{k_0}|^2,$$
(19)
and use obvious general inequalities
\[
|\langle \Psi_k \rangle|^2 \geq |\langle \Psi_k \rangle|^2 \geq \langle \Re \langle \Psi_k \rangle \rangle^2
\]
By applying them to (19) and combining with (18) it is easy to obtain
\[
\langle R^{in} \rangle = \langle R \rangle - \langle R \rangle^2 \leq \langle R \rangle - \langle R \rangle^2,
\]
\[
\langle T^{in} \rangle = \langle T \rangle - \langle T \rangle^2 \leq \langle T \rangle - \langle T \rangle^2
\]
(20)
In fact these are identical inequalities since \( R^{in} = T^{in} \) already due to the mirror symmetry. Their sum gives us restriction on total probability of inelastic scattering, \( P^{in} \):
\[
P^{in} = \langle R^{in} \rangle + \langle T^{in} \rangle \leq 2 \langle R \rangle (1 - \langle R \rangle) \leq 1/2
\]
(21)
This seems important and interesting consequence from the “unitarity on average”.

More careful consideration bases on stochastic integral equation for \( \psi(t) \equiv \Psi(t, 0) \) which follows from (12):
\[
\psi(t) = \Psi^0(t, 0) - \frac{i}{\hbar} \int_0^t G_0(t - t', 0) w(t') \psi(t') dt',
\]
\[
G_0(\tau, n) \equiv \int_0^\pi \exp \left[ i nk - i E(k) \tau / \hbar \right] \frac{dk}{2\pi},
\]
with \( E(k) = \epsilon \{ 1 - \cos k \} / 2 \) being dispersion of the channel. Let us confine ourselves by weak scattering, in the sense that \( \langle w(t) \rangle = 0 \) and \( \sigma(\omega) \ll \hbar \epsilon \), where spectrum \( \sigma(\omega) \) of the fluctuating potential is mentioned like in (14) as spectrum of its real part \( x(t) = \Re w(t) \): \( \langle x(\tau), x(0) \rangle = \int_0^\infty \cos(\omega \tau) \sigma(\omega) d\omega \). Thus, according to (13–14),
\[
\langle w(\tau) w(0) \rangle = K(\{ |\tau| \}), \quad \langle w^* (\tau) w(0) \rangle = K(\tau),
\]
\[
K(\tau) = \int_0^\infty \frac{e^{i\omega \tau} + \exp(\hbar \omega / T) e^{-i\omega \tau}}{1 + \exp(\hbar \omega / T)} \sigma(\omega) d\omega
\]
(23)
Then simple analysis of equation (22) in the corresponding standard “one-loop” approximation (or, in other words, “the Bourett approximation” [12]) yields
\[
\langle R \rangle = \frac{C}{1 + C}, \quad C \approx \frac{1}{\sqrt{E_0(\epsilon - E_0)}} \times
\]
\[
\times \int_{-E_0 / \hbar}^{(\epsilon - E_0) / \hbar} \frac{\sigma(\omega)}{1 + \exp(\hbar \omega / T)} \sqrt{(E_0 + \hbar \omega)(\epsilon - E_0 - \hbar \omega)} d\omega,
\]
where \( E_0 \equiv E(k_0) \). In fact, due to our assumption, \( C \ll 1 \) and at that, naturally, almost all the scattering is inelastic, except may be case of very small particle’s energy \( E_0 \) (for more details see [9]). Contributions to the integral from \( \omega > 0 \) and \( \omega < 0 \) correspond to scattering with energy radiation or absorption by the thermostat, respectively.

6. Conclusion

We just had a chance to make sure that there exists universal form of stochastic Liouville and Schrödinger equations which is exactly valid for arbitrary open quantum system \( S \) representable as a part of some closed system \( S + W \). Simultaneously there exist universal exact recipes for determination of statistical characteristics of random sources, or noises, \( w(t) \), what enter these equations.

Peculiarity of thus stated “stochastic representation of dynamic interactions” (between \( S \) and \( W \)) is that stochastic images, \( w(t) \), of Hermitian operator variables \( W(t) \) of \( W \) behave like a \( c \)-number (purely commutative) complex-valued random processes. Their imaginary parts, \( y(t) = \Im w(t) \), introduce dissipation into \( S \)’s evolution by means of virtual violation of its unitarity. Nevertheless, due to specific statistical properties of \( y(t) \), statistical averaging restores the unitarity although keeps the dissipation.

It is useful to underline that our approach to open systems makes it possible to obtain final results under interest without conventionally thought “kinetic equations”, i.e. omit stages of approximate derivation of a kinetic equation and then its approximate solving. Illustrations were done in [5,7,8,9] and just above. From the other hand, our approach gives all tools for correct construction of kinetic equations as well as “Langevin equations” for \( S \)’s variables [10].

Importantly, Hamiltonian character of joint dynamics of \( S + W \) implies general statistical connections between real and imaginary components of \( w(t) \) (especially when \( W \) is a thermostat [11]), which help to convert simple abstract models of stochastic processes into our approach. At that, one can exploit all the theory of linear dynamic systems with randomly varying parameters (including theory of waves in random media [12]).

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