The Schrödinger Equation for Open Systems

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An universal exact description of kinetics of open quantum systems in terms of random wave functions and stochastic Schrödinger equation is suggested. It is shown that evolution of random quantum states of an open system is unitary on average, and this implies validity of the optical theorem for any inelastic scattering.

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1. As it is known, one not always can attribute to a quantum system some definite wave function. Instead a density matrix is necessary \[1\]. Anyway if the matter concerns an open system \(S\) which is a part of more complicated closed system \(S+W\) (where \(W\) is, for instance, “thermal bath” or “the rest of world”). In such a case even density matrix of \(S\) is not quite definite because it is impossible to write out an exact general equation for it. In practice one is supposed to manage with “kinetic equations” deduced either from the von Neumann equation for the whole system \(S+W\) or from speculative reasonings \[2, 3, 4, 5\]. Sometimes irreversible terms there are supplemented by noise terms to be averaged later. Somehow or other, usually one at first constructs approximate equations and then constructs a method of their approximate solving.

Meanwhile one may avoid such duplication of approximations if recruit “stochastic representation of quantum interactions” \[6\] (see also \[7, 8, 9\]). The latter produces a closed stochastic equation for \(S\) which is extremely simple, intuitively obvious and at the same time formally exact: if random sources in it reflect, by definite universal rules, internal dynamics of \(W\), then such sources act exactly as actual dynamic interaction of \(S\) with \(W\). Importantly, these random sources introduce at once noise and irreversibility as a statistical effect of the noise. Therefore approximation is required only once, under calculation of statistical averages. Related mathematical problems are similar to problems of theory of oscillations and waves in linear media with fluctuating parameters \[10\].

A purpose of the present article is to emphasize possibility to reformulate the approach suggested in \[6\] (see also \[9, 11, 12, 13\]) in terms of stochastic Schrödinger equation and thus generalize to open systems the concepts of pure quantum state and wave function. Correspondingly, one can apply to open systems, in an elementary statistical sense, the concept of unitarity of evolution which naturally coexists with irreversible evolution of averaged wave function and density matrix of \(S\). As the result, the problem of calculation of its averaged (that is true) density matrix can be substantially simplified. At that, an important roles is played by averaged wave function.

2. We will start with brief summary of the stochastic representation, following \[6\] (with not great difference of designations) and \[13\]. Let us divide the whole system Hamiltonian into three parts and write a part \(H_{int}\) responsible for the interaction as a bilinear form:

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

where operators \(S_j, W_j\) act in different Hilbert spaces of \(S\) and \(W\), respectively. Such decomposition of \(H_{int}\) frequently arises from very physical nature of the interaction and in any case is feasible in formal sense \[3\]. Then for any operator \(O\) introduce Liouville super-operator \(\mathcal{L}(O)\) and Jordan super-operator \(\Pi(O)\) as follows:

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

where \(A\) is arbitrary operator. Thus \(\mathcal{L}(H)\) is Liouville super-operator in the von Neumann equation \(\dot{\rho} = \mathcal{L}(H)\rho\) for density matrix \(\rho\) of the whole system \(S+W\). One can easy verify that correspondingly to \[11\] it expands to

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

Therefore, density matrix \(\rho_S(t) = Tr_W \rho(t)\) of \(S\) can be expressed by

\[
\rho_S(t) = Tr_W \exp \left[ \int_0^t \mathcal{L}_S(t') dt' \right] \rho(0),
\]

where \(\exp\) is chronologically ordered exponential,

\[
\mathcal{L}_S(t) \equiv \mathcal{L}(H_S) + \sum \left[ x_j(t) \mathcal{L}(S_j) + y_j(t) \Pi(S_j) \right],
\]

and \(x_j(t)\) and \(y_j(t)\) are time-varying super-operators,

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

whose action is completely localized in the \(W\)’s Hilbert space. The latter circumstance, if considered from the viewpoint of \(S\), allows us to treat \(x_j(t)\) and \(y_j(t)\) in \[3\] and \[4\] merely like arbitrary commutative (scalar) time-dependent variables. In other words, like “noises” or random processes. At that, the trace operation in \[3\] plays the role of statistical averaging in respect to the random processes \(x_j(t)\) and \(y_j(t)\).
In order to define effective statistical properties of
x_j(t) and y_j(t) in a simple unambiguous way, it is
covenient to assume that before some initial time moment
t_0, e.g. t_0 = 0, the subsystems $\mathcal{S}$ and $\mathcal{W}$ were non-
interacting and statistically independent one on another:
$\rho(t_0) = \rho_{S(t_0)}^{(in)} \rho_{W(t_0)}^{(in)}$. Then one can write
\[ \rho_S(t) = \langle R(t) \rangle , \quad \dot{R}(t) = \mathcal{L}_S(t)R(t) , \] (5)
where $R(t)$ is “random density matrix” of $\mathcal{S}$, which obeys “stochastic Liouville equation” with initial condition
$R(t_0) = \rho_{s(t_0)}^{(in)}$, and angle brackets symbolize the averaging:
\[ \langle \ldots \rangle = \text{Tr}_W \ldots \rho_{W}^{(in)} \]
On right-hand side here $x_j(t)$ and $y_j(t)$ are treated as the above super-operators while on left side as effective random processes. This is just the statistical definition of these processes. Evidently, it means that characteristic functional of random processes $x_j(t)$ and $y_j(t)$ can be presented by expressions
\[ \langle \exp \left[ \sum \left[ u_j(t) x_j(t) + f_j(t) y_j(t) \right] \right] \rangle = \text{Tr}_W \exp \left[ \int \mathcal{L}_W dt \right] \rho_{W}^{(in)} , \] (6)
where $u_j(t)$ and $f_j(t)$ are arbitrary probe functions,
\[ \mathcal{L}_W(t) \equiv \mathcal{L}(H_W) + \sum \left[ u_j(t) \Pi(W_j) + f_j(t) \mathcal{L}(W_j) \right] , \]
the integration begins at $t = t_0$ and by request one may move $t_0$ away to $-\infty$.

According to (4) (6), the processes $x(t)$ represent perturbation of $\mathcal{S}$ by $\mathcal{W}$ as directly prescribed by their Hamiltonian interaction. Analogously, $y(t)$ represent back action of $\mathcal{S}$ onto $\mathcal{W}$. In view of these observations, we can expect that $x(t)$ are quite usual random processes while, in opposite, $y(t)$ are rather unusual ones. Indeed, at $u(t) = 0$ the super-operator $\mathcal{L}_W(t)$ reduces to a Liouville super-operator, and then from (6) it follows that
\[ \langle y(t_1) \ldots y(t_n) \rangle = 0 . \] By the same reason, as we can see from (6), $\langle y(t) x(t_1) \ldots x(t_n) \rangle = 0$ if $t > \max_k(\tau_k)$. But generally $\langle x(t_1) \ldots x(t_m) y(t_1) \ldots y(t_n) \rangle \neq 0$ if $\max_k(\tau_k) > \max_k(t_k)$. Hence, $y(t)$ show their worth in conjunction with $x(t)$ only. At that, cross correlations of $y(t)$ with $x(t)$ represent response of $\mathcal{W}$ to its perturbation by $\mathcal{S}$ and eventually introduce to evolution of $\rho_S(t)$ dissipation and irreversibility. The condition $\max_k(\tau_k) > \max_k(t_k)$ comes from the chronological ordering in (6) and expresses the causality principle. Details and generalizations of such “stochastic representation of dynamic interactions” [6] can be found in [11] [12] [13] [14].

3. Now let us go to original theme of this paper.
If initially (before interaction between subsystem under interest $\mathcal{S}$ and “the world” $\mathcal{W}$ was switched on) $\mathcal{S}$ was in a pure state, $\rho_{S(t_0)}^{(in)} = |\Psi^{(in)}(t)\rangle \langle \Psi^{(in)}(t)|$, then solution to equation (5) is merely $R(t) = |\Psi(t)\rangle \langle \Psi(t)|$, where $\Psi(t)$ satisfies “stochastic Schrödinger equation”:
\[ \frac{d\Psi(t)}{dt} = -i \frac{\hbar}{\hbar} \left[ H_S + \sum w_j(t) S_j \right] \Psi(t) \] (7)
with initial condition $\Psi(t_0) = \Psi^{(in)}$ and
\[ w_j(t) \equiv x_j(t) + i\hbar y_j(t)/2 \]
being interpreted as complex random processes. In such sense, $\mathcal{S}$ at all times remains in a “random pure state”. Consequently, at arbitrary initial density matrix we can make its diagonalization, $\rho_S^{(in)} = \sum_\alpha |\Psi_\alpha^{(in)}\rangle \langle \Psi_\alpha^{(in)}|$, and then write
\[ R(t) = \sum_\alpha |\Psi_\alpha(t)\rangle P_\alpha \langle \Psi_\alpha(t)| , \]
where each of $\Psi_\alpha(t)$ satisfies (7) under initial condition $\Psi_\alpha(t_0) = \Psi_\alpha^{(in)}$, while the weights $P_\alpha$ stay constant.

Because of complexity of $w_j(t)$ an evolution described by equation (7) is not unitary:
\[ \frac{d}{dt} \langle \Psi_\alpha(t)|\Psi_\beta(t)\rangle = \sum y_j(t) \langle \Psi_\alpha(t)|S_j|\Psi_\beta(t)\rangle \neq 0 \]
Nevertheless, it is unitary on average:
\[ \frac{d}{dt} \langle \langle \Psi_\alpha(t)|\Psi_\beta(t)\rangle \rangle = \sum y_j(t) \langle \Psi_\alpha(t)|S_j|\Psi_\beta(t)\rangle \rangle = 0 \]
This statement directly follows from the above mentioned statistical properties of $\Psi(t)$ (that is factually from the causality principle). As the consequence,
\[ \langle \langle \Psi_\alpha(t)|\Psi_\beta(t)\rangle \rangle = \langle \Psi_\alpha^{(in)}|\Psi_\beta^{(in)}\rangle = \delta_{\alpha\beta} , \]
and one can say that the “random pure states” all the time are mutually orthogonal on average.

Let us suppose that the interaction by its nature is localized at time, that is has character of scattering process. In such a case, random time-varying state of $\mathcal{S}$ can be written as sum
\[ |\Psi(t)\rangle = |\Psi^0(t)\rangle + |\Psi^s(t)\rangle , \]
where $\Psi^0(t)$ represents free evolution of $\mathcal{S}$ while $\Psi^s(t)$ is contribution of the scattering, so that $\Psi^s(t_0) = 0$. Then, due to the unitarity on average, as well as unitarity of the free evolution, the equality
\[ \langle \langle \Psi(t)|\Psi(t)\rangle \rangle = \langle \Psi^0(t)|\Psi^0(t)\rangle \]
takes place. It implies that
\[ 2\text{Re} \langle \Psi^0(t)|\Psi^s(t)\rangle + \langle \langle \Psi^s|\Psi^s\rangle \rangle = 0 \] (10)
This is generalized “optical theorem” which is valid for arbitrary non-elastic scattering.
This result demonstrates that the average wave function $\langle \Psi(t) \rangle$ contains important information about an open system. It should be underlined that $\langle \Psi(t) \rangle$ is always unambiguously defined by equation (7) as soon as random processes $w(t)$ are defined by (10). Therefore, the average wave function is not less legitimate than the density matrix $\rho_S(t)$.

Notice also that if $w(t)$ in (7) are stationary random processes then average wave functions $\langle \Psi^s(t) \rangle$ in (10) and $\langle \Psi(t) \rangle = \Psi^0(t) + \langle \Psi^s(t) \rangle$ include those energies and frequencies only what already are present in $\Psi^0(t)$. Therefore non-elastic component of the scattering wholly comes from fluctuations $\Psi(t) - \langle \Psi(t) \rangle$, although the latter contribute to elastic component too. In view of this circumstance, relations (9) or (10) imply inequality

$$\mathcal{P}^{inel}(t) \leq 1 - \langle \langle \Psi(t) \rangle \rangle \langle \langle \Psi(t) \rangle \rangle \ ,$$

with $\mathcal{P}^{inel}(t)$ being total probability of non-elastic scattering. In case of a scattering center in one-dimensional conducting channel one can obtain additional inequality $\mathcal{P}^{inel} \leq 1/2$ [11, 13].

4. The stationarity condition realizes, for instance, when $\rho_W^{(in)} \propto \exp(-H_W/T)$, that is subsystem $W$ initially was thermodynamically equilibrium (all the more when $W$ is a thermostat). Then [6, 7, 9, 11, 13, 14]

$$\langle w_i^*(\tau), w_m(0) \rangle = K_{jm}(\tau) \ , $$
$$\langle w_i(\tau), w_m(0) \rangle = K_{jm}(\tau) \ , $$

$$K_{jm}(\tau) = \int_0^\infty \frac{e^{i\omega \tau} + \exp(h\omega/T)e^{-i\omega \tau}}{1 + \exp(h\omega/T)} \sigma_{jm}(\omega) \, d\omega \ ,$$

where $\sigma_{jm}(\omega)$ is a non-negatively defined real-valued spectrum matrix. This information about the random sources $w(t)$ is sufficient in the framework of the Born approximation or “one-loop” and “ladder” approximations and their analogues (such as “Bourret approximation”, “Kraichnan approximation”, etc. [10]). Moreover, if $w(t)$ possess Gaussian statistics ($W$ is “Gaussian thermostat”) then the spectrum $\sigma_{jm}(\omega)$ contains exhaustive information about them, and principally one can exactly find any average value. In all that cases, organization of the correlation matrix $K_{jm}(\tau)$ automatically ensures [6, 11, 14] balance of noise and dissipation (radiation and absorption of energy by $W$) in agreement with the fluctuation-dissipation theorem. If $w(t)$ are non-Gaussian then they obey also “generalized non-linear fluctuation-dissipation relations” [14].

5. Thus, the traditional approach to open systems based on model kinetic equations (or equivalent “Langevin equations”) has an alternative in the form of exact linear Liouville and Schrödinger stochastic equations supplemented by exact universal expression for characteristic functional of random sources (fluctuating parameters) in these equations. At this alternative approach it is possible to exploit concepts of wave functions and (pure) quantum states, their superposition and unitary evolution. Correspondingly, mathematical difficulties concentrate at statistical averaging of wave functions and density matrices over the sources. This allows to use many achievements of the theory of linear systems with randomly varying parameters [11]. In this respect it is useful to notice that non-Gaussian statistical models of fluctuating parameters sometimes are much better suitable for exact calculations than Gaussian ones [11]. Therefore development of simple Hamiltonian dynamical models of non-Gaussian thermostats is of great interest. From the other hand, as was shown by example applications of the new approach [2, 3, 11, 12], quite useful results can be obtained even without full statistical information about the sources.

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