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Exact semiclassical wave equation for stochastic quantum optics

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Abstract. Semiclassical (stochastic) wave equations are proposed for the coupled dynamics of atomic quantum states and semiclassical radiation field. All relevant predictions of standard unitary quantum dynamics are exactly reproducible in the framework of the stochastic wave equation model. We stress in such a way that the concept of stochastic wave equations is not to be restricted to the widely used Markovian approximation.

1. Introduction

For many years it has been understood that one cannot reproduce *all* the statistical predictions of quantum theory from purely classical statistics [1] but can do it for *certain* predictions. The reduced dynamics of quantum subsystems (i.e. effective dynamics of open quantum systems) can always be interpreted as hybrids of quantum and classical mechanisms. The corresponding *semiclassical* dynamics (which may also be called *semiquantized*) is described by *stochastic wave equations* (SWEs). For ten years they have attracted interest in the research of foundations [2] and, since the 1990s [3], in quantum optics, too.

Consider a system of atoms interacting with the radiation field. Basically, all attainable results are approximations: SWEs have been derived in the weak-coupling Markovian limit [4]. In the present work, however, we investigate the exact unitary dynamics of the atom + radiation system and we ask the following question. Can we describe the radiation field in terms of classical (stochastic) variables instead of quantum ones in such a manner that all relevant predictions remain *exactly* identical with those of the unitary quantum theory? The answer will be affirmative in almost all respects. The forthcoming results were anticipated previously [5] by detailed relativistic calculations. Here we intend to give a short account for exact SWEs. Readers interested in practical rather than conceptual aspects may, after reading section 2, understand SWEs directly from section 5.

2. The quantum model

For simplicity's sake, we consider single-mode (cavity) quantum electrodynamics. The Hamiltonian for the composite system of the atom plus radiation field has the following general form:

$$\hat{H} = \hat{H}^{\text{ato}} + \omega\hat{a}^\dagger\hat{a} + \hat{J}\hat{a}^\dagger + \hat{J}^\dagger\hat{a} \tag{1}$$

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where $\hat{H}^{\rm ato}$ is the atomic Hamiltonian, $\hat{a}$ is the absorption operator for the single radiation mode of frequency ω. In the interaction terms, $\hat{J}$ is the atomic operator proportional to charges and currents. As usual, we assume that at time $t = 0$ the quantum state of the system is a product of the atomic and cavity radiation states, respectively,

$$\Psi_0 = \psi_0^{\rm ato}\psi_0^{\rm rad}. \tag{2}$$

In an interaction picture, the quantum state Ψ evolves unitarily:

$$\frac{{\rm d}\Psi_t}{{\rm d}t} = -{\rm i}\hat{H}_I(t)\Psi_t \tag{3}$$

with interaction Hamiltonian

$$\hat{H}_I(t) = \hat{j}(t)\hat{a}^\dagger + {\rm HC} \tag{4}$$

where $\hat{j}(t) = {\rm e}^{{\rm i}\omega t}\hat{J}(t)$ is the 'rotated' version of the interaction picture current $\hat{J}(t)$. Though the present work concerns pure state equations it will nonetheless be convenient to also define a density operator $\hat{\rho} \equiv \Psi\Psi^\dagger$.

3. Stochastic field variables, semiclassical states and observables

The basic field variables $\hat{a}, \hat{a}^\dagger$ do not commute: $[\hat{a}, \hat{a}^\dagger] = 1$. We shall, nevertheless, establish a certain natural correspondence between them and their classical counterparts a, a^*. Let us introduce a special notation for symmetric products:

$$\hat{a}_c\hat{\mathcal{O}} \equiv \tfrac{1}{2}\left(\hat{a}\hat{\mathcal{O}} + \hat{\mathcal{O}}\hat{a}\right) = \{\hat{a}, \hat{\mathcal{O}}\} \tag{5}$$

where $\hat{\mathcal{O}}$ is an arbitrary operator and $\hat{a}_c$ is called a 'superoperator' (cf [5] and references therein). The superoperators $\hat{a}_c, \hat{a}_c^\dagger$ commute with each other [6]:

$$[\hat{a}_c, \hat{a}_c^\dagger]\hat{\mathcal{O}} \equiv \{\hat{a}, \{\hat{a}^\dagger, \hat{\mathcal{O}}\}\} - \{\hat{a}^\dagger, \{\hat{a}, \hat{\mathcal{O}}\}\} = 0 \tag{6}$$

hence we shall make the natural correspondence, mentioned above, between the classical complex variable a (or a^*) and the superoperator $\hat{a}_c$ (or $\hat{a}_c^\dagger$).

We describe the radiation field in terms of the classical stochastic variables a, a^* coupled to the quantized atomic ones. The state of the quantum system will then be represented by the *semiclassical* 'density':

$$\hat{\rho}(a, a^*) = {\rm tr}_{\rm rad}\left(\delta(a - \hat{a}_c)\delta(a^* - \hat{a}_c^\dagger)\hat{\rho}\right) \tag{7}$$

which is expected to be the density operator for the atom and phase space distribution for the field simultaneously. It should satisfy the positivity condition $\hat{\rho}(a, a^*) \geqslant 0$ for all complex values of a, a^*. Then ${\rm tr}_{\rm ato}\,\hat{\rho}(a, a^*)$ is the reduced phase space distribution $\rho^{\rm rad}(a, a^*)$ of the radiation field mode and, alternatively, $\int \hat{\rho}(a, a^*)\,{\rm d}a^*\,{\rm d}a$ is the reduced density operator $\hat{\rho}^{\rm ato}$ of the atom. Similarly to (7), we define the semiclassical counterpart of Hermitian observable $\hat{F}$ by

$$\hat{F}(a, a^*) = {\rm tr}_{\rm rad}(\delta(a - \hat{a}_c)\delta(a^* - \hat{a}_c^\dagger)\hat{F})\,. \tag{8}$$

We, however, do not consider all Hermitian observables but those where the correspondence is invertible:

$${\rm tr}\left(\hat{F}(\hat{a}_c, \hat{a}_c^\dagger)\hat{\mathcal{O}}\right) = {\rm tr}\left(\hat{F}\hat{\mathcal{O}}\right) \tag{9}$$

for all $\hat{\mathcal{O}}$. This includes a pretty large class of Hermitian operators.

The equivalence of the semiclassical picture with the full quantized one relies upon the following equation:

$$\mathrm{tr}\left(\hat{F}(\hat{a}_c, \hat{a}_c^\dagger)\hat{\rho}\right) = \mathrm{tr}_{\mathrm{ato}} \int \hat{F}(a, a^*)\hat{\rho}(a, a^*)\,\mathrm{d}a^*\,\mathrm{d}a \tag{10}$$

which follows from (7)–(9) and from the commutativity of $\hat{a}_c$ and $\hat{a}_c^\dagger$.

4. The positivity issue and its solution by coarse-graining

Let us write the phase space distribution of the radiation field, defined by tracing (7) over the atomic states as well, in the Fourier representation:

$$\rho^{\mathrm{rad}}(a, a^*) = \frac{1}{\pi^2} \int \exp(-\lambda a^* + \lambda^* a)\,\mathrm{tr}\left(\exp(-\lambda^* \hat{a}_c + \lambda \hat{a}_c^\dagger)\hat{\rho}\right)\mathrm{d}\lambda^*\,\mathrm{d}\lambda\,. \tag{11}$$

By substituting the identity

$$\exp(-\lambda^* \hat{a}_c + \lambda \hat{a}_c^\dagger)\hat{\rho} = \exp(-\lambda^* \hat{a}/2)\exp(\lambda \hat{a}^\dagger/2)\hat{\rho}\exp(\lambda \hat{a}^\dagger/2)\exp(-\lambda^* \hat{a}/2) \tag{12}$$

which follows from the rules (5), (6), one can apply the identity

$$\exp(\hat{A})\exp(\hat{B}) = \exp([\hat{A}, \hat{B}]/2)\exp(\hat{A} + \hat{B})$$

to obtain

$$\rho^{\mathrm{rad}}(a, a^*) = \frac{1}{\pi^2} \int \exp(-\lambda a^* + \lambda^* a)\,\mathrm{tr}\left(\exp(-\lambda^* \hat{a} + \lambda \hat{a}^\dagger)\hat{\rho}\right)\mathrm{d}\lambda^*\,\mathrm{d}\lambda\,. \tag{13}$$

One recognizes that $\rho^{\mathrm{rad}}(a, a^*)$ is identical to the well known Wigner function introduced long ago [7]. However, the Wigner function *cannot* be interpreted as phase space density since it may take negative values as well. From Husimi's work we know that a minimum coarse-graining will cure the problem [8]. Consequently, we apply a minimum coarse-graining to the 'sharp' distribution $\hat{\rho}(a, a^*)$ defined by (7). Let a_0, a_0^* be noisy complex field variables of vacuum distribution $(2/\pi)\exp(-2|a_0|^2)$. The coarse-grained semiclassical state thus reads

$$\bar{\hat{\rho}}(a, a^*) = \int \frac{\exp(-2|a_0|^2)}{\pi/2}\hat{\rho}(a + a_0, a^* + a_0^*)\,\mathrm{d}a_0^*\,\mathrm{d}a_0\,. \tag{14}$$

The corresponding coarse-grained phase space density $\bar{\rho}^{\mathrm{rad}}(a, a^*) = \mathrm{tr}\,\bar{\hat{\rho}}(a, a^*)$ is identical to the so-called Q-function of the radiation field (see, e.g., in [9]). As is well known, the Q-function is $1/\pi$ times the diagonal element of the density operator between coherent states. Accordingly, the corresponding relation holds true for $\bar{\hat{\rho}}(a, a^*)$ itself:

$$\bar{\hat{\rho}}(a, a^*) = \frac{1}{\pi}\langle a, a^*|\hat{\rho}|a, a^*\rangle \tag{15}$$

where $|a, a^*\rangle$ is the coherent state of the radiation field mode. (Two remarks on our notations are in order. First, we indicate the explicit dependence of coherent states on *both* a and a^*. Second, the quadratic form above has to be understood on the factor Hilbert-space of the cavity while the resulting expression is still an (a, a^*)-dependent density operator in the atom's Hilbert-space.) The form (15) guarantees the positivity of the coarse-grained semiclassical density.

One also introduces coarse-grained semiclassical observables:

$$\bar{\hat{F}}(a, a^*) = \int \frac{\exp(-2|a_0|^2)}{\pi/2}\hat{F}(a + a_0, a^* + a_0^*)\,\mathrm{d}a_0^*\,\mathrm{d}a_0\,. \tag{16}$$

Then a coarse-grained version of the 'sharp' equivalence equation (10) follows:

$$\mathrm{tr}\left(\bar{\hat{F}}(\hat{a}_c, \hat{a}_c^\dagger)\hat{\rho}\right) = \mathrm{tr}_{\mathrm{ato}} \int \hat{F}(a, a^*)\bar{\hat{\rho}}(a, a^*)\,\mathrm{d}a^*\,\mathrm{d}a \tag{17}$$

i.e. the statistics of coarse-grained quantum observables are still exactly reproducible from the coarse-grained semiclassical state $\bar{\hat{\rho}}(a, a^*)$.

One would worry because coarse-grained distributions are believed to lose information. In typical quantum optics applications things prove not so bad as long as one considers expectation values of polinoms of the absorption and emission operators. Then the additional noise is easy to subtract. Let us assume that we are interested in the expectation value of the photon number operator $\hat{a}^\dagger\hat{a}$ in the current quantum state $\hat{\rho}$ and we want to calculate it from $\bar{\hat{\rho}}(a, a^*)$. It is plausible to choose $\hat{F}(a, a^*) = |a|^2$. Then, via (16), let us calculate the corresponding coarse-grained observable $\bar{\hat{F}}(\hat{a}_c, \hat{a}_c^\dagger)$. We obtain $\overline{\hat{a}_c^\dagger\hat{a}_c} = \hat{a}_c^\dagger\hat{a}_c + \frac{1}{2}$. The equivalence condition (17) thus leads to

$$\mathrm{tr}\left((\hat{a}_c^\dagger\hat{a}_c + \tfrac{1}{2})\hat{\rho}\right) = \int |a|^2\bar{\rho}^{\mathrm{rad}}(a, a^*)\,\mathrm{d}a^*\,\mathrm{d}a\,. \tag{18}$$

Due to the identity $\mathrm{tr}((\hat{a}_c^\dagger\hat{a}_c + \frac{1}{2})\hat{\rho}) = \mathrm{tr}(\hat{a}^\dagger\hat{a}\hat{\rho}) + 1$, equation (18) yields

$$\mathrm{tr}(\hat{a}^\dagger\hat{a}\hat{\rho}) = \int |a|^2\bar{\rho}^{\mathrm{rad}}(a, a^*)\,\mathrm{d}a^*\,\mathrm{d}a - 1\,. \tag{19}$$

This is the simplest example to illustrate how exact quantum expectation values are reproduced from the coarse-grained semiclassical state $\bar{\hat{\rho}}(a, a^*)$.

5. Exact stochastic wave equation

We remind the reader that the composite system of the atom + radiation was originally assumed to be in a pure quantum state Ψ. Let us introduce a coherent state representation of Ψ:

$$\psi(a, a^*) = \frac{1}{\sqrt{\pi}}\langle a, a^*|\Psi\rangle\,. \tag{20}$$

The scalar product on the RHS is to be taken on the factor Hilbert-space of the cavity. (The author has failed to find a more suitable compact notation, see also the second remark after (15).) Strictly speaking, $\psi(a, a^*)$ is a wavefunction of the field-mode coordinates a, a^* while, on the other hand, it is state vector (of arbitrary representation) in the atomic Hilbert-space. It follows from (15) that the wavefunction (20) just yields the coarse-grained semiclassical density in the form

$$\bar{\hat{\rho}}(a, a^*) = \psi(a, a^*)\psi^\dagger(a, a^*)\,. \tag{21}$$

So, it is natural to call $\psi(a, a^*)$ a semiclassical wavefunction. Let us obtain its equation of motion.

In coherent state representation the following operator correspondences should be used (cf [10]):

$$\hat{a}^\dagger\Psi \leftrightarrow a^*\psi(a, a^*) \qquad \hat{a}\Psi \leftrightarrow \left(\frac{a}{2} + \frac{\partial}{\partial a^*}\right)\psi(a, a^*)\,. \tag{22}$$

Hence the Hamiltonian equation of motion (3) leads to the following equation of motion for the semiclassical wavefunction:

$$\frac{\mathrm{d}\psi_t(a, a^*)}{\mathrm{d}t} = -\mathrm{i}\left(a^*\hat{j}(t) + \frac{a}{2}\hat{j}^\dagger(t)\right)\psi_t(a, a^*) - \mathrm{i}\hat{j}^\dagger(t)\frac{\partial\psi_t(a, a^*)}{\partial a^*}\,. \tag{23}$$

This wave equation, combining unitary and stochastic dynamics, is our central result. By means of this equation, exact predictions of the unitary quantum theory can be obtained†.

Let us summarize the SWE method. Assume the atomic state at $t = 0$ is ψ_0^{ato} while the cavity's state is the vacuum state $|0, 0\rangle$. Then, according to (2), the semiclassical (stochastic) wavefunction (20) initially takes the form

$$\psi_0(a, a^*) = \psi_0^{\text{ato}} \frac{\exp(-|a|^2/2)}{\sqrt{\pi}} . \tag{24}$$

Let us switch on the interaction. Then the conditional atomic wavefunction $\psi_t(a, a^*)$ evolves as a function of the state (a, a^*) of the classical field, according to (23) while the (coarse-grained) probability distribution of the classical field variables a, a^* is given by

$$\rho_t(a, a^*) = \|\psi_t(a, a^*)\|^2 . \tag{25}$$

The expectation value of an arbitrary semiclassical observable $\hat{F}(a, a^*)$ will exactly reproduce the quantum expectation value of the corresponding coarse-grained Hermitian observable, i.e.

$$\text{tr}\big(\bar{\hat{F}}(\hat{a}_c, \hat{a}_c^\dagger)\hat{\rho}_t\big) = \int \psi_t^\dagger(a, a^*)\hat{F}(a, a^*)\psi_t(a, a^*)\, \mathrm{d}a^*\, \mathrm{d}a \tag{26}$$

where $\bar{\hat{F}}(a, a^*)$ is derived from $\hat{F}(a, a^*)$ by the minimum coarse-graining (16).

The existence of exact SWE was pointed out in [5] in the context of relativistic quantum-electrodynamics. That time, however, the stochastic field was not identified as a semiclassical radiation field. A generalization of our SWE (23) for infinite number of field modes being initially in thermal equilibrium states at non-zero temperature seems straightforward.

6. Outlook

The main result of the present work is a suggestion that semiclassical SWEs could *exactly* reproduce the quantum physics of both atomic *and* radiation degrees of freedom. In our opinion, the very existence of exact stochastic models is a novelty of fundamental interest. Conceptual elements of equivalence with unitary quantum theory are symmetrized products of non-commuting operators and a minimum coarse-graining of states and observables. Our SWE establishes the possibility of making efficient Monte Carlo simulations in the non-Markovian regime since using classical variables for the radiation field represents a fair simplification. Of course, the re-derivation of the extensively used Markovian SWEs is possible and desirable.

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† If we introduce the unnormalized wavefunction $\varphi(a^*)$ defined by $\psi(a, a^*) = \varphi(a^*)\exp(-|a|^2/2)/\sqrt{\pi}$ then the SWE (23) takes a much simpler form

$$\frac{\mathrm{d}\varphi_t(a^*)}{\mathrm{d}t} = -\mathrm{i}a^*\hat{j}(t)\varphi_t(a^*) - \mathrm{i}\hat{j}^\dagger(t)\frac{\partial\varphi_t(a^*)}{\partial a^*}$$

with the initial condition $\varphi_0(a^*) = \psi_0^{\text{ato}}$ instead of (24).

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