# Mixed classical-quantal representation for open quantum systems

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LETTER TO THE EDITOR

# Mixed classical-quantal representation for open quantum systems

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**Abstract.** For all but the simplest open quantum systems, quantum trajectory Monte Carlo methods, including quantum jump and quantum state diffusion (QSD) methods, have besides their intuitive insight into the measurement process a numerical advantage over direct solutions for the density matrix, especially where many degrees of freedom are involved. For QSD the trajectories are continuous, and often localize to small near-minimum uncertainty wave packets which follow approximately classical paths in phase space. The mixed representation discussed here takes advantage of this localization to reduce computing space and time by a further significant factor, using a quantum oscillator representation that follows a classical path. The classical part of this representation describes the time evolution of the expectation values of position and momentum in classical phase space, while the quantal part determines the degree of localization of the quantum mechanical state around this phase space point. The method can be applied whether or not the localization is produced by a measuring apparatus.

In this letter a numerical method for solving master equations of open quantum systems is introduced. It combines two general elements which offer numerical advantages, namely

(i) a Monte Carlo method for solving the master equation for the density operator of a quantum statistical ensemble by stochastic simulation, and
(ii) an appropriately chosen time dependent basis for solving the relevant stochastic Schrödinger equation for the quantum state.

In the method introduced here the recently developed quantum state diffusion method (QSD) [1–7] is combined with a representation of the corresponding nonlinear, stochastic Schrödinger equation in a basis of eigenstates of a shifted harmonic oscillator. This oscillator is centred around the instantaneous position and momentum of the quantum system. This way the general phenomenon of localization of QSD state vectors in configuration and momentum space [5–7] is taken into account. This approach promises considerable advantages in solving QSD equations of realistic open quantum systems with a few degrees of freedom.

The quantum state diffusion (QSD) method describes the time evolution of individual quantum systems under the influence of physical processes which destroy quantum coherence [1–7]. In QSD theory the evolution is represented through a unique correspondence between the master equation for the ensemble density operator $\rho(t)$ and an Itô–Langevin

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diffusion equation for the normalized state vector $|\psi(t)\rangle$ of an individual system of the ensemble. If $H$ is the Hamiltonian describing the dynamics of a quantum system and $L_m$ are the Lindblad operators which describe statistically independent decohering processes, then the most general master equation is given by [8,9]

$$\dot{\rho}(t) = -\frac{\mathrm{i}}{\hbar}[H, \rho(t)] + \frac{1}{2}\sum_m ([L_m, \rho(t)L_m^\dagger] + [L_m\rho(t), L_m^\dagger]). \tag{1}$$

The associated QSD equation for an individual quantum system of the ensemble is given by the stochastic Itô equation [1–7]

$$|\mathrm{d}\psi(t)\rangle = -\frac{\mathrm{i}}{\hbar}H\,|\psi(t)\rangle\,\mathrm{d}t + \sum_m (L_m - \langle L_m\rangle_{\psi(t)})\,|\psi(t)\rangle\,\mathrm{d}\xi_m$$

$$+ \sum_m (\langle L_m^\dagger\rangle_{\psi(t)}L_m - \frac{1}{2}L_m^\dagger L_m - \frac{1}{2}\langle L_m^\dagger\rangle_{\psi(t)}\langle L_m\rangle_{\psi(t)})\,|\psi(t)\rangle\mathrm{d}t \tag{2}$$

with $\langle L_m\rangle_{\psi(t)} = \langle\psi(t)|L_m|\psi(t)\rangle$. The complex Wiener processes $\xi_m(t)$ [10] satisfy the relations

$$M\mathrm{d}\xi_m = 0$$

$$\mathrm{d}\xi_m\mathrm{d}\xi_{m'} = 0$$

$$\mathrm{d}\xi_m^*\mathrm{d}\xi_{m'} = \delta_{mm'}\mathrm{d}t. \tag{3}$$

The density operator of the ensemble $\rho(t)$ and the quantum state of the individual system $|\psi(t)\rangle$ are related by

$$\rho(t) = M\,|\psi(t)\rangle\langle\psi(t)| \tag{4}$$

with $M$ denoting a mean over the ensemble. According to equation (2) the time evolution of an individual quantum system under the influence of a decohering process is continous but not (almost nowhere) differentiable [10]. A crucial feature of the unique correspondence between equations (2) and (1) is the invariance of both equations with respect to arbitrary unitary transformations in the Hilbert space spanned by the Lindblad operators, i.e.

$$L_m \to \overline{L_m} = \sum_j u_{mj}L_j \tag{5}$$

with $\sum_m u_{mj}u_{mj'}^* = \delta_{jj'}$. It is this invariance property which makes the correspondence between any master equation of the general Lindblad form of (1) and the corresponding stochastic Itô equation (2) unique. Furthermore, this uniqueness is essential for a satisfactory physical interpretation of the solutions of (2) as the evolution of an individual member of the ensemble under the influence of the decohering process irrespective of any measurement [3].

The numerical method for solving the QSD equation (2) presented in this letter is based on a mixed representation of the quantum state vector which is partly classical and partly quantal. Advantage is thereby taken of the localization of QSD state vectors in configuration and momentum space [5–7, 11]. This type of localization takes place under quite general conditions as long as the Lindblad operators $L_m$ are nearly linear in the position and canonical momentum operators over domains in phase space with areas of the order of $\hbar$ [7, 11]. Typically, in this case the state vector $|\psi(t)\rangle$ localizes towards an approximate Gaussian wave packet with small or even minimum Heisenberg indeterminacy product of position and momentum. Furthermore, the centre of this wave packet evolves in time approximately according to the laws of classical mechanics.

In order to put the problem into perspective let us consider the simplest non-trivial quantum system with one degree of freedom and a Hamiltonian $H(Q, P)$ which is a nonlinear perturbation of a linear oscillator $H_0(Q, P)$, namely

$$H(Q, P) = H_0(Q, P) + H_1(Q, P). \tag{6}$$

The Lindblad operators $L_m$ are assumed to be linear in $Q$ and $P$. The main idea of the mixed representation consists in solving the QSD equation (2) with Hamiltonians of the type given in (6) in an appropriately chosen moving basis which is defined by the instantaneous expectation values

$$\begin{aligned} \langle Q\rangle_t &= \langle\psi(t)|Q|\psi(t)\rangle \\ \langle P\rangle_t &= \langle\psi(t)|P|\psi(t)\rangle \end{aligned} \tag{7}$$

of position and canonical momentum. Therefore at each time $t$ the state of the system $|\psi(t)\rangle$ is specified by a 'classical part', i.e. the point $(\langle Q\rangle_t, \langle P\rangle_t)$ in classical phase space, and a 'quantal part' which is determined by the expansion coefficients with respect to the instantaneous basis. A convenient choice for these basis states $|n(t)\rangle$ are the eigenstates of the shifted harmonic oscillator

$$H_{\mathrm{sh}}(Q, P, t) = H_0(Q + \langle Q\rangle_t, P + \langle P\rangle_t) \tag{8}$$

which is centred around the classical phase space point $(\langle Q\rangle_t, \langle P\rangle_t)$. In terms of the energy eigenstates $|n\rangle$ of the unshifted harmonic oscillator $H_0(Q, P)$ they are given by

$$|n(t)\rangle = \exp\left(-\mathrm{i}\langle Q\rangle_t P/\hbar + \mathrm{i}\langle P\rangle_t Q/\hbar\right)|n\rangle. \tag{9}$$

The ground state of the shifted harmonic oscillator, i.e. $|n(t) = 0\rangle$, is a coherent state of the original harmonic oscillator $H_0(Q, P)$ whereas the basis states with values $n(t) > 0$ are 'excited coherent states'. In a numerical integration procedure which is based on this mixed representation the propagation of the state $|\psi(t)\rangle$ from time $t_0$ to time $t_0 + \Delta t$ is broken up into two steps. In the first step $|\psi(t_0)\rangle$ is propagated from $t_0$ to $t_0 + \Delta t$ in the basis $|n(t_0)\rangle$. In the second part of the step the basis is also changed to $|n(t_0 + \Delta t)\rangle$ thus obtaining

$$|\psi(t_0 + \Delta t)\rangle = \sum_{n=0}^{\infty} c_n(t_0 + \Delta t)\,|n(t_0 + \Delta t)\rangle. \tag{10}$$

Thus in the mixed representation the state $|\psi(t)\rangle$ is defined by the set of quantities

$$\{(\langle Q\rangle_t, \langle P\rangle_t); c_n(t)\}. \tag{11}$$

When there is little phase space localization, the mixed représentation has little or no advantage over a representation of $|\psi(t)\rangle$ in the basis of eigenstates of $H_0(Q, P)$, for example. But in the case of significant phase space localization, the mixed representation offers considerable advantages. In particular, if the phase space localization is complete, the only non-zero quantum amplitude in the mixed representation is the vacuum amplitude $c_0(t)$ which has modulus one. In that case the quantum part of the mixed representation can be ignored and it reduces to a pure classical representation. For strong but incomplete localization only a few 'excited coherent states' are significant and the mixed representation constitutes an efficient practical tool for solving the QSD equation (2). It should be mentioned that numerical methods for solving the ordinary time dependent Schrödinger equation, which are based on wave packet approaches, have a long history particularly in the chemical physics literature. Originally in these approaches Gaussian wave packets with variable widths are propagated along prescribed classical trajectories (see, for example, [12]). However, as the ordinary Schrödinger equation does not exhibit the phenomenon of localization in phase space, the applicability of these type of wave packet approaches is

very restricted. In particular, it breaks down as soon as an initially localized wave packet is spread out over a large fraction of configuration space.

As an example demonstrating the practical significance of the mixed classical-quantal representation consider the one-dimensional dynamics of a driven, weakly anharmonic oscillator with Hamiltonian

$$H(Q, P) = \hbar\Delta\omega a^\dagger a + \hbar f a + \hbar f^* a^\dagger + \hbar\mu(a^\dagger a)^2. \tag{12}$$

The destruction and creation operators of the harmonic oscillator are denoted $a$ and $a^\dagger$. The parameters $\mu$ and $f$ measure the strength of an anharmonic perturbation and an oscillating driving force, respectively, and $\Delta\omega$ is the detuning of the frequency of the driving force from the oscillator frequency. In a one-dimensional, adiabatic approximation model Hamiltonians of this form have been used to describe various physical phenomena such as optical bistability [13] or the weakly relativistic motion of a resonantly driven charged particle in a harmonic ion trap [14]. The damping of this driven, weakly anharmonic oscillator with rate $\gamma$, for example by radiative decay, can be described by the Lindblad operator $L = (\gamma)^{1/2}a$ [15]. Thus, in this case the time evolution implied by (2) is expected to lead to localization towards an eigenstate of the destruction operator $a$, i.e. a coherent state with $|c_0(t)|^2 = 1$.

In figure 1 the time evolution of the real and imaginary parts of the expectation value $\alpha(t) = \langle a \rangle(t)$ is shown as evaluated from (2) with the mixed representation method for two realizations of the decohering Wiener process $\xi(t)$. As a weakly delocalized initial state $|\psi(t = 0)\rangle = |n(t = 0) = 12\rangle$ has been chosen with $\alpha(t = 0) = 10$. The two realizations shown in figure 1 converge to two different stationary states, because the initial state and the parameters of the Hamiltonian (12) lead to bistable dynamics. The bars centred around the expectation values $\alpha(t)$ indicate the uncertainties $\Delta\,\mathrm{Re}[\alpha(t)]$ and $\Delta\,\mathrm{Im}[\alpha(t)]$ which are a measure for the degree of localization of the quantum state $|\psi(t)\rangle$ in phase space. In the case of complete localization $|\psi(t)\rangle$ becomes a coherent state and both uncertainties assume the value $\frac{1}{2}$. The dashed curve in figure 1 clearly shows complete localization in phase space towards a coherent state in the stationary limit. Thus with increasing time the mixed representation becomes purely classical with $|c_0(t)|^2 = 1$. The time evolution of the dotted curve in figure 1 is more complicated but nevertheless it also localizes in phase space. In particular, this realization of the QSD equation (2) performs strong oscillations and converges very slowly towards the second stationary state. This different stability behaviour of the two stable stationary states is characteristic of bistable behaviour. Furthermore, in the course of its time evolution the dotted curve also passes the neighbourhood of a nearby unstable stationary state whose position is known from previous semiclassical treatments [13, 14] and is indicated by an arrow in figure 1.

The actual saving in computation time and space implied by the mixed classical–quantal representation discussed here depends mainly on two factors, namely the initial condition $|\psi(t = 0)\rangle$ and the magnitude of typical values of $\alpha(t)$ of the problem considered. The more closely the initial condition resembles a coherent state and the larger are typical values of $\alpha(t)$, the larger the saving. Compared with an expansion in terms of energy eigenstates of $H_0(Q, P)$, for example, in the ideal case of complete localization in one space dimension the maximum saving in space and computation time per time step $\Delta t$ is expected to be a factor of the order of $\sqrt{|\alpha(t)|^2}$, for large values of $|\alpha(t)|^2$. This is due to the fact that in the unshifted harmonic oscillator basis of $H_0(Q, P)$ at least of the order of $\sqrt{|\alpha(t)|^2}$ basis states are needed to represent this coherent state properly. As an example for a non-ideal situation, consider the time evolution of $|\psi(t)\rangle$ shown by the dotted curve in figure 1. Despite the complicated bistable dynamics and the moderate values of

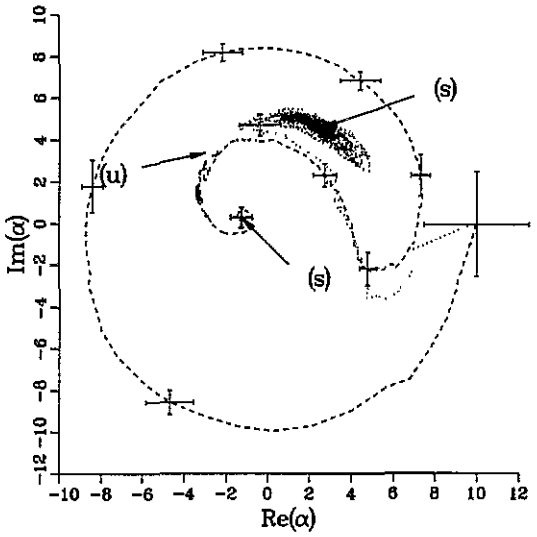


**Figure 1.** Time evolution of real and imaginary parts of the expectation value $\alpha(t) = \langle a \rangle(t)$ as evaluated from equation (2) for two realizations of $\xi(t)$ (dashed and dotted curves) with identical initial conditions $\alpha(t = 0) = 10$ and $\Delta\,\mathrm{Re}[\alpha(t = 0)] = \Delta\,\mathrm{Im}[\alpha(t = 0)] = 2.5$. The bars indicate the uncertainties $\Delta\,\mathrm{Re}[\alpha(t)]$ and $\Delta\,\mathrm{Im}[\alpha(t)]$. Stable (s) and unstable (u) stationary states are positioned at the tips of the corresponding arrows. The values of the parameters are $\mu = 0.1\gamma$, $f = -6\gamma$ and $\Delta\omega = -5\gamma$.

$\alpha(t)$, even in this case comparisons with calculations performed with a simple expansion of $|\psi(t)\rangle$ in energy eigenstates of $H_0(Q, P)$ indicate a saving in computation time of at least a factor of 2. This modest value is mainly due to the delocalized nature of the initial state. Thus it might be considered as a lower bound. In realistic applications to the dynamics of charged particles in ion traps, for example, typical initial conditions are well represented by minimum uncertainty wave packets. Therefore in such cases the time gain increases significantly. Nevertheless, a rough estimate based on this lower bound indicates at least a saving of a factor of the order of $2^D$ for similar systems with $D$ degrees of freedom. Thus the mixed classical–quantal representation discussed here promises considerable advantages in solving QSD equations of realistic open quantum systems with a few degrees of freedom.

In summary, a mixed classical–quantal method for solving QSD equations numerically has been introduced. Advantage is thereby taken of the localization of solutions to small near-minimum uncertainty wave packets which follow approximately classical paths in phase space. In particular, in open quantum systems with a few degrees of freedom this proposed numerical method is expected to reduce computing time and space by a significant amount. In comparison with the simulation methods [16–18] this conclusion is also supported by a recent comparison [16] which has shown that, even if no advantage is taken of this localization of solutions, simulations of the dynamics of open quantum systems by QSD equations are as efficient numerically as the recently proposed quantum jump methods [17, 18]. Therefore the method proposed here is well suited for realistic numerical studies on the time evolution of individual dissipative quantum systems. Applications of this method to the two dimensional motion of charged particles in a Penning trap are in progress and will be presented elsewhere.

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