Simulation of open quantum systems

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received 5 December 2008; accepted in final form 15 May 2009
published online 24 June 2009

PACS 02.70.Ss – Quantum Monte Carlo methods
PACS 03.65.Sq – Semiclassical theories and applications
PACS 03.65.Yz – Decoherence; open systems; quantum statistical methods

Abstract – We present an approach for the semiclassical treatment of open quantum systems. An expansion into localized states allows restriction of a simulation to a fraction of the environment that is located within a predefined vicinity of the system. Adding and dropping environmental particles during the simulation yields an effective reduction of the size of the system that is being treated.

Dynamics of open quantum systems is attracting a growing interest since advances in experimental techniques allow to create and probe coherent superpositions of different states of growing size and complexity [1,2]. The larger such systems and the more “different” the respective states in such a superposition are, the more important is the influence of an environment on the coherence of such states. Whereas superpositions of different atomic hyperfine states may survive the interaction with the electromagnetic field as their environment for several seconds [3], coherent superpositions of states that are separated by an optical transition typically dephase on the time scale of at best microseconds, and coherence times for classical objects like the famous textbook example of a cat are so short that there is no prospect of ever observing coherent superpositions of such classical objects. On the other hand, coherent superpositions of mesoscopic objects have been observed experimentally [4–6], what has resulted in conjectures that signatures of quantum coherence can also be observed, \textit{e.g.}, in biological systems [7–10]. Whereas, ideas of coherence-based biological effects are rather recent, the question about the stability of coherent superpositions of different many-body states in engineered quantum systems is not so new, since, for example, the speed up of a quantum computer as compared to its classical version is based on the existence of coherent superpositions of many substantially different states of an at least mesoscopic quantum register.

Any theoretical treatment of open system dynamics, however, is impeded by the \textit{de facto} impossibility of simulating the dynamics of a system comprised of the system of interest and the typically macro-, or at least mesoscopic environment. Numerous prior approaches end up with \textit{effective} equations of motion for the system itself, where the dynamics of the environment is eliminated, such as a Lindblad equation [11,12] that describes the influence of an environment onto a system. Such an effective theory, however, is always subject to approximations, \textit{e.g.}, a Markov approximation, and/or taking the system-bath interaction to be linear, and/or the environment itself to be harmonic.

In this paper we would like to take a different approach. Since large quantum systems naturally imply semiclassical behavior, we describe here an approach to open system dynamics in the semiclassical regime. Our approach is based on the propagation of Gaussian states. That is, an initial state is expanded in terms of Gaussian states, and each of these components is then propagated individually. Under the evolution of a general Hamiltonian an initial Gaussian state will not remain Gaussian. However, for well localized wave packets the Hamiltonian can be approximated to be locally harmonic, so that the Gaussian character is preserved [13–15]. Such techniques have proven to accurately describe dynamical properties of various closed systems, thermodynamic properties [16,17], and also open quantum systems [18,19].

In the following we consider a manybody quantum systems with continuous degrees of freedom and smooth (twice differentiable) interaction potentials that vanish for arbitrarily large separation of the respective particles. We make use of the expansion into \textit{localized} states which permits effectively reducing the size of the environment to
Alternatively, one may also describe the dynamics of the environment outside $V$ in terms of “frozen” wave packets. This reduces the environment dynamics outside the interaction area to a classical problem that can be treated for comparatively many particles, and an environment particle can be incorporated in the full wave packet simulation if its classical trajectory enters $V$.

The quantum state of both the system and the environment particles will be described in the following in terms of Gaussian states. Such a state is completely characterized in terms of the expectation values of all coordinates and momenta $x = [r_1, p_1, r_2, p_2, \ldots, r_n, p_n] = \text{Tr} \hat{H} \rho$, and the corresponding covariances

$$\Sigma_{ij} = \text{Tr} \left( \frac{-\hat{H}}{\hbar} \right) \rho - x_i x_j.$$  \hspace{1cm} (1)

Here, the $r_i$ are the coordinates of the respective particles, and the $p_i$ are the corresponding momenta. Knowledge of these quantities allows to recover the underlying Gaussian quantum state $\rho$, however the explicit parametrization of $\rho$ in terms of those parameters is a rather lengthy expression, so that the quantum state itself is not the most convenient quantity for our purposes. The Weyl symbol of the density matrix, i.e. the Wigner function

$$W(\vec{r}, \vec{p}) = \int d^n q \left( \hat{r} - \frac{\hat{q}}{2} \right) \left( \hat{r} + \frac{\hat{q}}{2} \right) e^{i \hat{p} \hat{q}}$$  \hspace{1cm} (2)

is significantly more suitable, because it has the simple parametrization

$$W(x) = \frac{1}{\sqrt{\pi^n |\det \Sigma|}} e^{-\frac{1}{2} (x - \vec{x})^T \Sigma^{-1} (x - \vec{x})},$$  \hspace{1cm} (3)

The evolution of a Gaussian quantum state due to a quadratic Hamiltonian gives rise to Newton’s equations of motion $\dot{x} = S \nabla H$ with the symplectic matrix $S$, and

$$\frac{\partial \Sigma}{\partial t} = 2 (\Sigma H S - S H \Sigma),$$  \hspace{1cm} (4)

where $H$ contains the second derivatives of the Hamiltonian $H$ with respect to the coordinates and momenta, i.e. $H_{ij} = \frac{1}{2} \frac{\partial^2 H}{\partial x_i \partial x_j}$. A general Hamiltonian can be approximated as quadratic if the width of the wave packet is so narrow that it covers a domain in phase space only, in which the anharmonicity can be neglected. In this case, the $H_{ij}$ are evaluated at the location in phase space at which the quantum state is centered at any instance of time. That is, the many-body wave packet sits in a co-moving harmonic Hamiltonian, where the shape of the harmonic potentials vary in time in accordance with the shape of the exact potentials around the wave packet.

Equation (4) describes the unitary evolution of the system and its surrounding environment. Any dissipative nature of the the dynamics is due to tracing over environmental degrees of freedom, or a (thermal) average over different environment states. The efficiency with which partial traces can be performed therefore influences the efficiency of an open system simulation significantly. The present description of a quantum state in terms of phase space variables and covariances allows a very straightforward method for this, which is based on the fact that the expectation value of any observable $A$ on particles that are not being traced over are unaffected by the partial tracing

$$\text{Tr} A \rho = \text{Tr}_V A (\text{Tr}_V \rho).$$  \hspace{1cm} (5)
Here, “Tr” denotes the trace over the entire system, “Tr_V” denotes the trace over all particles inside V and “Tr_{V'}” denotes the trace over all particles outside V. This holds true in particular also for the values of x and Σ; and since the parametrization of the Wigner function in eq. (3) is valid for systems with an arbitrary number of particles, tracing over some degrees of freedom is equivalent to simply dropping all components of x and Σ corresponding to the degrees of freedom being traced over. In turn, adding a particle corresponds to extending x and Σ by the respective quantities, with vanishing correlations between the added particle, and the residual system.

So far, we have been assuming the initial state be a narrow Gaussian wave packet, where the term “narrow” implies that the wave packet is localized in a domain in phase space in which the Hamiltonian can be approximated quadratically. This condition, however, is often not satisfied, and for wider wave packets the harmonic approximation breaks down. Nevertheless, any quantum state |ψ⟩ (pure or mixed) can be decomposed into an incoherent mixture of coherent, i.e. Gaussian states |ψ⟩ = \int dμ(α)P_α(β)⟨α|ψ⟩ |α⟩, with the P-function P_α(β). Since, this holds also for pure states, P_α cannot always be a probability distribution, i.e. it can adopt negative values. The central merit of this representation is that different initial states |α⟩ can be propagated individually, and the overall final state is then the incoherent sum over the individually propagated states. In the present framework of an open system, this implies that partial traces can be taken at any instant. The big disadvantage of such a representation is the often wild behavior of P_α. In particular for nonclassical states P_α is rapidly oscillating, and close to singular, which severely limits its usefulness for practical purposes.

Often it is significantly easier to expand the state |Ψ⟩ into a coherent sum of Gaussian states |Ψ⟩ ≃ \sum α |ψ⟩(α). Due to the linearity of the Schrödinger equation, one can of course propagate each initial term |ψ⟩(α) individually, and, then reconstruct the final state

\[ U_t |Ψ⟩ = \sum α U_α |ψ⟩(α) \approx \sum α U_α^0 |ψ⟩(α), \]

where \[ U_α^0 = T \exp(-i/\hbar \int dt H_α(t)) \] is the approximate propagator, and H_α is the locally quadratic approximation of H expanded around x_α(t).

In order to take partial traces, however, one needs to consider the corresponding density matrix:

\[ \rho_t = \sum_{αβ} U_{αβ}^* U_α |β⟩⟨β|U_β |α⟩ = \sum_{αβ} U_{αβ}^0 |β⟩⟨β|U_β^0 |α⟩. \]

Here, \[ U_{αβ}^0 \] is the unitary transformation generated by the Hamiltonian H expanded around the classical positions of the states |α(t)⟩ and |β(t)⟩, respectively. Thus, in the following, we will consider the evolution of the individual operators \[ ρ_{αβ} \] resulting from |α⟩⟨β|. Since those operators are not necessarily normalized, all expectation values will be defined including normalization \[ \langle A \rangle_ρ = \text{Tr}_ρ Aρ/\text{Tr}_ρ ρ \].

Doing so, one obtains the equations of motion

\[ \frac{∂Σ}{∂t} = 2(ΣH_+S - S H_+Σ) - \frac{i}{\hbar}S H_-S - \frac{2i}{\hbar} Σ H_- Σ, \]

with \[ H_+ = 1/2(H_α + H_β) \], and \[ H_- = H_α - H_β; \] and with \[ H_α, H_β \] being the second-order expansion coefficients of H taken along the phase space positions \[ x_α = ⟨α|x⟩, x_β = ⟨β|x⟩ \] as depicted in fig. 2. The equations of motion for the positions and momenta x are a bit more lengthy, and they are most conveniently characterized by the relation

\[ x = \frac{1}{2}(x_α + x_β) - i/\hbar ΣS(x_α - x_β) + δx. \]

The Weyl symbol corresponding to those complex phase space coordinates and uncertainties is given by eq. (3) up to the additional factor \[ \exp(η) \] with

\[ η = \frac{1}{2\hbar^2} (x_α - x_β) ΣΣS(x_α - x_β) - i\hbar (\vec{p}_α - \vec{p}_β)(\vec{r}_α - \vec{r}_β) + δη. \]

and a phase \[ ϕ \] whose evolution is given by \[ ϕ = L_α - L_β - \frac{i}{2\hbar} \text{Tr}_ρ ΣΣH_--. \] Here, \[ L_i, (i = 1, 2) \] is the Lagrange function with variables \[ \vec{r}_i \], and \[ \vec{p}_i \]. Similarly to eq. (9), we have introduced a term \[ δη \] in eq. (10) that vanishes for pure state, that, however, will adopt finite values upon the execution of partial traces. As argued above, the dynamical variables x, and Σ remain unchanged.
partial tracing. However, $x_\alpha$, and $x_\beta$ are propagated rather than $x$, and for a general state any entry of $x$ depends on all the entries of $x_\alpha$, and $x_\beta$ as shown in eq. (9). Therefore, one may not simply drop the entries of $x_\alpha$, and $x_\beta$ that belong to a particle that is traced over, but one needs to consider their contributions to $x$ first: let us decompose $x$ into a vector $x_V$ that contains the elements that are kept and a vector $x_p$ that contains the elements that are dropped because of a partial trace, so that $x = x_V \oplus x_p$. Similarly, also $\Sigma$ can be divided into a part $\Sigma_V$ that is associated only with $x_V$, $\Sigma_p$ that is associated only with $x_p$ and a term $\Sigma_{V,V}$ that is associated with the correlations between $x_V$ and $x_p$, such that $\Sigma$ reads

$$
\Sigma = \left[ \begin{array}{cc} \Sigma_V & \Sigma_{V,V} \\
\Sigma_{V,V}^T & \Sigma_p \end{array} \right].
$$

The $V$-components of $x$ do not only depend on the $V$-components of $x_\alpha$, and $x_\beta$, but there is the term

$$
\delta x_V = -\frac{i}{\hbar} \left[ \begin{array}{c} 0 \\
\Sigma_{V,V} \end{array} \right] \mathcal{S} (x_\alpha - x_\beta),
$$

(11)

that depends on the $V$-components of the phase space variables and covariances. Thus, for $\alpha \neq \beta$ a partial trace can not be performed by simply dropping all the $V$-components as can be done for the case $\alpha = \beta$. Instead, the term $\delta x_V$ has to be kept track of. This is the reason for the term $\delta x$ in eq. (9). At each partial trace, there is the increment $\delta x_V$ to the term $\delta x$. The same reasoning also applies to $\eta$, where there is the increment

$$
\delta \eta_V = \frac{1}{2\hbar^2} (x_\alpha - x_\beta) S \left[ \begin{array}{c} 0 \\
\Sigma_{V,V} \end{array} \right] \mathcal{S} (x_\alpha - x_\beta)
$$

$$
- \frac{i}{\hbar} \left( \bar{p}_V^x \bar{p}_V^\beta + \bar{p}_V^\beta \bar{p}_V^x \right) (\bar{r}_V^\alpha - \bar{r}_V^\beta).
$$

(12)

to $\delta \eta$ at any partial trace.

These increments directly result in a decrease of the norm of the terms $\varrho_{\alpha,\beta}$ for $\alpha \neq \beta$. For a sufficiently large phase distance $x_\alpha - x_\beta$ these terms can be interpreted as off-diagonal matrix elements of the quantum state $\varrho$. Both increments $\delta x_V$ and $\delta \eta_V$ depend on the phase space distances $|x_V^\alpha - x_V^\beta|$ of the wave packets associated with the environment particles in $V$.

For the interpretation of these increments let us consider the case of an initially distant environmental particle that approaches the system, interacts with it, gets separated from the system and is therefore traced over. Typically, the state $|\Psi\rangle$ of this composite system cannot be described by a single Gaussian wave packet, but has to be described by a superposition of several narrow wave packets, $|\Psi\rangle \simeq \sum_{\alpha} \Psi_\alpha |\alpha\rangle = \sum_{\alpha,\alpha_\xi} \Psi_{\alpha,\alpha_\xi} |\alpha\rangle \otimes |\alpha_\xi\rangle$. Here, the index “$s$” refers to “system”, the index “$e$” refers to “environment” and $\alpha$ is a multi-index for the pair $\alpha_\xi$ and $\alpha_e$. That is, the density matrix for this composite system reads

$$
\varrho = \sum_{\alpha_\xi,\alpha_e} \Psi_{\alpha_\xi,\alpha_e}^* \Psi_{\alpha_e,\alpha_\xi} |\alpha_\xi\rangle \langle \alpha_\xi | \otimes |\alpha_e\rangle \langle \alpha_e |.
$$

(13)

Let us consider first a term of the system density matrix that results from a trace over the environment degrees of freedom of a wave packet with $\alpha_\xi = \beta_\xi$ and $\alpha_e = \beta_e$. This describes a regular wave packet, i.e. a diagonal element of the density matrix, that has interacted with a wave packet of the environment particle. Such a wave packet does not acquire any increments; it may just have exchanged energy with wave packets of environment particles and have changed its widths. This is different for a term that describes a coherence of the system particle, that is, a term where initially $\alpha_\xi \neq \beta_\xi$ and $\alpha_e = \beta_e$. For such an initial state amplitude, the final state amplitudes $|\alpha_e\rangle$ and $|\beta_e\rangle$ will typically not coincide anymore, due to the interaction between the environment and the system particle. Therefore, the corresponding system operator $\varrho_{\alpha_\xi,\beta_e}$ has acquired the increments of eqs. (11) and (12). Via the phase space distances $|x_V^\alpha - x_V^\beta|$ the magnitude of these increments depends on how strongly the trajectories of environment particles’ wave packets are dependent on the individual state-amplitudes $\alpha_\xi$ and $\beta_\xi$ of the system particle. In other words, the norm of $\varrho_{\alpha_\xi,\beta_e}$ decreases significantly if the environment particle contains a lot of information about the system particle, or, if it has performed a good which way measurement. Finally, there are also initial state components with $\alpha_\xi \neq \beta_e$ which typically will be responsible for differences between a classical and a quantum environment. In general the effect on coherence properties of the system state is qualitatively similar as for the case $\alpha_e = \beta_e$: the larger the phase space separation between the initial states $|\alpha_\xi\rangle$ and $|\beta_\xi\rangle$ of the system particle is, the larger will also be the final phase space separation of the final environment particle states $|\alpha_e\rangle$ and $|\beta_e\rangle$, and —in turn— the larger will be the increments of eqs. (11) and (12). However, due to the exponentially small overlap of different coherent states with a sizeable phase space separation, contributions of initial amplitudes with $\alpha_e \neq \beta_e$ will only have a non-negligible contribution to the quantum state of the system particle if $\alpha_e \simeq \beta_e$.

In order to illustrate the present method, we will apply it to the investigation of decoherence rates of superpositions of harmonic-oscillator coherent states $|\alpha\rangle + |\beta\rangle$. The decoherence rate is predicted [20,21] and experimentally verified [22,23] to grow quadratically with increasing phase space separation $\delta x$ between $|\alpha\rangle$ and $|\beta\rangle$. However, this quadratic dependence holds only for small phase space separations, and once the separation is much larger than the range of the interaction potential a saturation is expected [24,25]. We consider the full 3-dimensional problem with a thermal environment of mutually noninteracting particles that, however, interact with the oscillator via a short-range Gaussian interaction. The environment is dilute so that only two-body interactions are taken into account. Since the initial state of the oscillator is pure, we take the initial state of the many-body system to be a direct product of the oscillator state and states of the environment particles. A thermal environment is
Decay constant of about $10 \times 10^7$ during the entire integration would yield $8 \times 10^7$ simulations of the entire system with all particles present. However, the integration of 182 coupled differential equations, where the relative phase space separation $\delta x$ between $|\alpha\rangle$ and $|\beta\rangle$ is chosen to be 10, 20, 30, and 40 oscillator length. The coherence decays exponentially, and the decays are faster for larger initial phase space separations.

realized via an average over 2000 realizations of an environment consisting of 1500 particles. Due to the possibility of adding and removing particles this requires the integration of 182 coupled differential equations, whereas the simulation of the entire system with all particles present during the entire integration would yield $8 \times 10^7$ differential equations.

Figure 3 shows the decay of the Hilbert Schmidt norm $\text{Tr} \mathcal{g}_{\alpha\beta} \mathcal{G}_{\alpha\beta}$, i.e. the magnitude of coherence as a function of time for different initial phase space separations 10, 20, 30 and 40 oscillator lengths. The individual curves show an exponential decay $\exp(-\gamma t)$ (with time given in multiples of the oscillator period) with some remaining noise due to the average over a finite sample of environment realizations, and allow the extraction of a decay constant $\gamma$. Figure 4 displays this decay constant as a function of the initial phase space separation. Even for $\delta x = |\delta x|$ vanishing, there is some decoherence with a decay constant of about $10^{-5}$, since a coherent state is not an eigenstate to the interaction potential, but the decay time for this case is significantly longer than that for a coherent superposition of two coherent states. For small values of $\delta x$, we recover the predicted quadratic increase of the decay constant, and once the phase space separation exceeds the range of the interaction potential (25 oscillator lengths in this case), the increase with $\delta x$ gets slower and, as expected, saturation sets in. This behaviour can easily be interpreted in terms of the increments in eqs. (11) and (12). For separations $\delta x$ that are significantly smaller than the system-environment interaction range, any environment particles can perform only a poor which-way measurement, i.e. trajectories of environment particles depend only weakly on whether the system is in state $|\alpha\rangle$ or $|\beta\rangle$. The larger the phase space separation of the system states $|\alpha\rangle$ or $|\beta\rangle$ is, the larger are the final separations $|x_0^- - x_0^+|$ of environment particles after the interaction with the system, and the faster does the off-diagonal term $\mathcal{g}_{\alpha\beta}$ get damped out. However, if the separation between the system states $|\alpha\rangle$ or $|\beta\rangle$ exceeds the system-bath interaction range, a further increase of this separation can not improve a which-way measurement of an environment particle, so that there is the saturation of decoherence times in fig. 4.

The present techniques allow treatment of general situations of quantum systems embedded in an environment, but the effort that is necessary for a simulation depends on the specific situation: the more delocalized a given state is, the more wave packets are required in an expansion; however, the number of required wave packets grows quadratically with the phase space volume that is occupied by the state to be simulated. Such a quadratic increase is moderate and does not pose too severe constraint, in particular, since the propagation of different wave packets can be parallelized “trivially”. Another factor that influences the efficiency of the present method is the size of the domain in which environment particles are taken into account. The radius of this domain has to be larger than the interaction range between system and environment particles to guarantee that environment particles are traced over when their influence on the system is negligible and that they are taken into account in the equations as soon as they have an impact on the system. For systems of strongly interacting environment particles that radius may be chosen even larger than the system-environment interaction to make sure that environment particles that are added to the system have enough time to thermalize with the rest of the bath before they interact with the actual system.
The crucial condition that has to be satisfied for the validity of the present approach is that the second derivative of the system-potentials, i.e. system-environment interaction, inter-environment interaction or external potentials, vary slowly over the typical width of the wave packets that are used. Therefore, long-range and short-range interactions have two mutually exclusive advantages and disadvantages in the present framework: short-range interactions allow restriction the actual simulation to a comparatively small neighborhood, however, require rather narrow wave packets, since the range over which the anharmonicities of the potentials occur are limited by the interaction range; long-range interactions, on the other hand, require the simulation of a comparatively large neighborhood, but typically allow the use of rather broad wave packets, so that the computational effort that increases with the size of this neighborhood is balanced by the reduced number of wave packets that are needed. For coulomb interactions it might be questionable to simply drop leaving environmental particles since the interaction energy is fully compensated by the increasing number of environment particles that are found at a given distance from the system. However, in such cases, one can replace the environment outside the simulation-environment by an effective external potential that describes the influence of the distant environment on the system.

Since wave packets spread spatially over time in many systems the present approximations may become questionable after some period of time. Nevertheless, since decoherence typically takes place on time scales that are significantly shorter than other damping phenomena, it is rather the short-term than the long-term behavior that is of importance for open quantum systems. It is also important to note in this context that an environment interaction can result in a narrowing of the system wave packet, so that with an environment there is an effect counteracting the spreading.

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We would like to thank T. Paul, T. Pohl, and E. Polack for stimulating discussions. Financial support by the Alexander von Humboldt foundation is gratefully acknowledged.

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