PHYSICAL REVIEW
LETTERS

VOLUME 83 | 13 DECEMBER 1999 | NUMBER 24

Quantum Trajectories for Brownian Motion

Walter T. Strunz,[1] Lajos Diósi,[2] Nicolas Gisin,[3] and Ting Yu[3]
[1]*Fachbereich Physik, Universität GH Essen, 45117 Essen, Germany*
[2]*Research Institute for Particle and Nuclear Physics, POB 49, 1525 Budapest 114, Hungary*
[3]*Group of Applied Physics, University of Geneva, 1211 Geneva 4, Switzerland*
(Received 30 July 1999)

We present the stochastic Schrödinger equation for the dynamics of a quantum particle coupled to a high temperature environment and apply it to the dynamics of a driven, damped, nonlinear quantum oscillator. Apart from an initial slip on the environmental memory time scale, in the mean, our result recovers the solution of the known non-Lindblad quantum Brownian motion master equation. A remarkable feature of our powerful stochastic approach is its localization property: individual quantum trajectories remain localized wave packets for all times, even for the classically chaotic system considered here, the localization being stronger as $\hbar \to 0$.

PACS numbers: 05.40.Jc, 03.65.Sq, 05.45.Mt, 42.50.Lc

The understanding of the dynamics of open or dissipative quantum systems is of fundamental importance both from a practical and a conceptual point of view. The archetype of such a system is the standard quantum Brownian motion (QBM) model [1] which describes a particle with Hamiltonian $H(q, p)$, coupled to an environment of harmonic oscillators (q_λ, p_λ) via its position q, such that the total Hamiltonian of system and environment reads

$$H_{\rm tot}(q, p, q_\lambda, p_\lambda) = H(q, p) + \sum_\lambda \left\{ \frac{p_\lambda^2}{2m_\lambda} + \frac{1}{2} m_\lambda \omega_\lambda^2 \left(q_\lambda - \frac{g_\lambda}{m_\lambda \omega_\lambda^2} q \right)^2 \right\}. \tag{1}$$

Up to now, in order to determine the time dependent dynamics of the open "system," the standard procedure was the derivation of a master equation for the reduced density operator, which, for the high temperature case considered below, is widely accepted to read

$$\hbar \dot{\rho}_t = -i[H, \rho_t] - i \frac{\gamma}{2} [q, \{p, \rho_t\}] - \frac{m\gamma kT}{\hbar} [q, [q, \rho_t]], \tag{2}$$

where γ is the damping rate. This master equation is a Markov master equation *not*, however, of Lindblad form [2], and indeed it turns out that it may violate the positivity of ρ_t on very short time scales, which has led to an ongoing debate about its range of applicability [3]. We will briefly address this issue later on in this Letter.

Our new approach to quantum Brownian motion is very different and circumvents the derivation of a master equation for ρ_t altogether. Instead, we use a stochastic Schrödinger equation, derived straight from the microscopic model (1), for pure states $\psi_t(z)$ *(quantum trajectories)*. Our construction recovers the reduced density operator as the ensemble mean $M[\cdots]$ over many of these quantum trajectories, in principle without any approximation:

$$\rho_t = M[|\psi_t(z)\rangle\langle\psi_t(z)|]. \tag{3}$$

The mean $M[\cdots]$ is taken over the process z_t which drives the stochastic Schrödinger equation. We are thus able to determine ρ_t in a Monte Carlo sense without an explicit master equation for its time evolution.

Quantum trajectory methods have been used extensively in recent years, mainly in the quantum optics community, due to their numerical efficiency, their intimate connection to (continuous) measurement, and their illustrative power

0031-9007/99/83(24)/4909(5)$15.00

helping to gain physical insight. The master equations encountered in quantum optics are of standard Lindblad type, for which Markov quantum trajectory methods are known for some time now: there are jump processes [4] and diffusive processes [5] recovering the reduced density operator. Despite being possibly the best known of all master equations, the quantum Brownian motion master equation (2), being *not* of Lindblad form, has so far been excluded from a treatment with these powerful methods.

Only recently the authors managed to extend the quantum trajectory concept to *non-Markovian* situations [6]; more precisely, we were able to determine a stochastic Schrödinger equation for the dynamics of a quantum system coupled to a bath of harmonic oscillators as in (1), without using the concept of a master equation for ρ_t. An alternative approach to non-Markovian quantum trajectories, emphasizing more the continuous measurement point of view, has now also been established [7].

In its linear version [8], our *non-Markovian quantum state diffusion* (QSD) stochastic Schrödinger equation for the quantum Brownian motion model (1) takes the form

$$\hbar\dot{\psi}_t(z) = -iH'\psi_t(z) + qz_t\psi_t(z) - q\int_0^t ds\,\alpha(t,s)\,\frac{\delta\psi_t(z)}{\delta z_s}, \quad (4)$$

where we assumed a factorized total initial density operator $\rho_{\rm tot} = |\psi_0\rangle\langle\psi_0| \otimes \rho_T$ with a pure system state $|\psi_0\rangle$ and an environmental thermal density operator ρ_T. The influence of the environment on the system is encoded in the bath correlation function $\alpha(t,s) = \langle F(t)F(s)\rangle_{\rho_T}$ where $F(t) = \sum_\lambda g_\lambda q_\lambda(t)$ is the quantum force in (1) and z_t is thus a complex Gaussian stochastic c number force with correlation $M[z_t^* z_s] = \alpha(t,s)$. In the usual high temperature limit $kT \gg \hbar\Lambda \gg \hbar\omega, \hbar\gamma$, where Λ is an environmental cutoff frequency and ω, γ are the typical system frequency and damping rate, respectively, one finds [1]

$$\alpha(t,s) = 2m\gamma kT\Delta(t-s) + i\hbar m\gamma\dot{\Delta}(t-s), \quad (5)$$

where $\Delta(t)$ is a deltalike function decaying on the environmental "memory" time scale Λ^{-1} [here we use $\Delta(t) = \frac{\Lambda}{2}e^{-\Lambda|t|}$]. In (4), the Hamiltonian $H' = H(q,p) + \frac{1}{2}m\gamma\Lambda q^2$ contains an additional potential term that turns out to be counterbalanced by a similar term arising from the memory integral.

Equation (4) is exact; it provides a quantum trajectory method for Brownian motion for any temperature and any distribution of environmental oscillators in the model (1), i.e., for any $\alpha(t,s)$. In order to compute numbers, however, we have to express the functional derivative under the memory integral in (4) in terms of elementary operators. In the high temperature limit considered here, we simply need to expand in terms of the time delay $(t-s)$,

$$\frac{\delta\psi_t(z)}{\delta z_s} = \frac{1}{\hbar}\left(q - \frac{p}{m}(t-s) + \ldots\right)\psi_t(z), \quad (6)$$

where the dots denote terms of the order $(t-s)^2$ and higher, leading to corrections of the order ω/Λ, γ/Λ and can therefore be neglected (see [9] for a general theory of such "post-Markov" open systems). With (6), the memory integral in (4) takes the form

$$\int_0^t ds\,\alpha(t,s)\,\frac{\delta\psi_t(z)}{\delta z_s} = [g_0(t)q - g_1(t)p]\psi_t(z), \quad (7)$$

where we introduce time dependent coefficients $g_0(t) = \frac{1}{\hbar}\int_0^t ds\,\alpha(t,s)$ and $g_1(t) = \frac{1}{m\hbar}\int_0^t ds(t-s)\alpha(t,s)$. The imaginary part of $g_0(t)$ will be compensated by the additional potential term in H'. The imaginary part of $g_1(t)$ gives rise to damping. The real part of $g_0(t)$ describes diffusion, and as the real part of $g_1(t)$ also gives rise to diffusion, yet smaller by a factor ω/Λ, the latter can be neglected compared to the former in the regime we are interested in.

In order to get an efficient Monte Carlo method (importance sampling [10]), we go over to the nonlinear version of (4), which keeps the trajectories $\psi_t(z)$ normalized at all times while retaining the correct ensemble mean (3); see [6]. Using (7), the relevant stochastic Schrödinger equation for Brownian motion reads

$$\hbar\dot{\psi}_t(z) = -iH\psi_t(z) - i\left(\frac{1}{2}m\gamma\Lambda + \mathrm{Im}\{g_0(t)\}\right)q^2\psi_t(z) + (q - \langle q\rangle)z_t\psi_t(z) - \mathrm{Re}\{g_0(t)\}[(q-\langle q\rangle)^2 - \langle\!\langle (q-\langle q\rangle)^2\rangle\!\rangle]\psi_t(z) + i\,\mathrm{Im}\{g_1(t)\}(qp - \langle qp\rangle + m\langle\dot{q}\rangle q - \langle q\rangle p)\psi_t(z). \quad (8)$$

Normalized quantum trajectories $\psi_t(z)$ whose ensemble mean gives the desired reduced density operator according to (3) can now be propagated using (8), where $\langle\dot{q}\rangle = \frac{d}{dt}\langle q\rangle$, a quantity which has to be determined numerically along with $\psi_t(z)$. In (8), after a short *initial slip* $t \gg \Lambda^{-1}$, the time dependent coefficients approach their asymptotic values $g_0(t) \to \frac{m\gamma kT}{\hbar} - \frac{i}{2}m\gamma\Lambda$ and $\mathrm{Im}\{g_1(t)\} \to -\frac{\gamma}{2}$.

We now highlight the power of our stochastic Schrödinger equation for Brownian motion (8) by investigating the dynamics of a driven, damped, nonlinear, noisy system, the Duffing oscillator, where $H = \frac{1}{2}p^2 + \frac{1}{4}q^4 - \frac{1}{2}q^2 + gq\cos(t)$, here coupled to a heat bath at temperature T. This system has been studied before using the master equation (2) (see [11] and references therein), including a straight numerical solution which requires the propagation of a huge matrix. In our new approach, one propagates pure states $\psi_t(z)$ according to (8), a great reduction in resources, with the need, however, to solve (8) many times in order to evaluate the mean values. For Lindblad master equations, the power of quantum

trajectory methods for investigating classically chaotic dissipative systems was shown in [12] (see also [13]).

We use parameters $g = 0.3$ with a damping rate $\gamma = 0.25$; thus the classical problem is chaotic [14]. The environment is furthermore characterized by $kT = 0.3$, and a cutoff frequency $\Lambda = 5$. With $\hbar$ of the order 10^{-2} and smaller (see various choices of $\hbar$ below), the parameters are in the required regime. As the initial condition we chose a standard coherent state located at $\langle q\rangle = 0.1, \langle p\rangle = 0.1$.

In Fig. 1 we show the ensemble mean $M[W_z(q, p, t = 4)]$ over 1000, 5000, and 10 000 Wigner functions of pure state trajectories $\psi_t(z)$ obtained solving (8) numerically up to a time $t = 4$. According to our construction, this quantity converges to the Wigner function of the reduced density operator for many realizations. Here we have chosen $\hbar = 0.01$, a phase space area corresponding approximately to the extension of the wave packets shown in Fig. 2.

In Fig. 2 we show contour plots of Wigner functions $W_z(q, p, t = 4)$ of four realizations of (8), many of which add up to the Wigner function of the desired reduced density matrix shown in Fig. 1. One can see clearly that these individual Wigner functions are well localized in phase space compared to the phase space spread of the ensemble, even for this classically chaotic system.

This remarkable feature of the QBM stochastic Schrödinger equation (8) is highlighted again in Fig. 3, where we show the mean position spread, $M[\Delta q] = M[\sqrt{\langle(q - \langle q\rangle)^2\rangle}]$ and the mean uncertainty product $M[\Delta q \Delta p/\hbar]$ in units of $\hbar$ of individual trajectories as a function of time for three different choices of $\hbar$.

The quantities shown in Fig. 3 can only be given sense in the framework of quantum trajectories; they have no meaning from a density operator point of view as they are the ensemble mean over an expression nonquadratic in $\psi_t(z)$. It is apparent from Fig. 3 that individual trajectories are well localized in phase space for all times, the localization being stronger the smaller $\hbar$. As can be seen, our quantum trajectories remain almost "classical" states, yet recover the fully quantum master equation (2). Thus, the representation (3) expresses the reduced density operator of quantum Brownian motion explicitly as a mixture of almost classical states.

The observed localization property of QSD is well known in the Markov case and has been studied, for instance, in [13]. Here we see that similar properties hold for the generalized non-Markovian QSD equation (8) which has now been applied to quantum dynamics beyond the class of Lindblad master equations.

Finally, let us briefly address the connection between our approach and the widely used QBM master equation (2). Since a quantum trajectory approach strictly preserves positivity of the reduced density operator, our QBM stochastic Schrödinger equation (8) cannot be identical to (2) in the mean, as the latter is known to violate positivity on short time scales. Taking the ensemble mean $M[\cdots]$ in (3) with (4) analytically, we were able to show

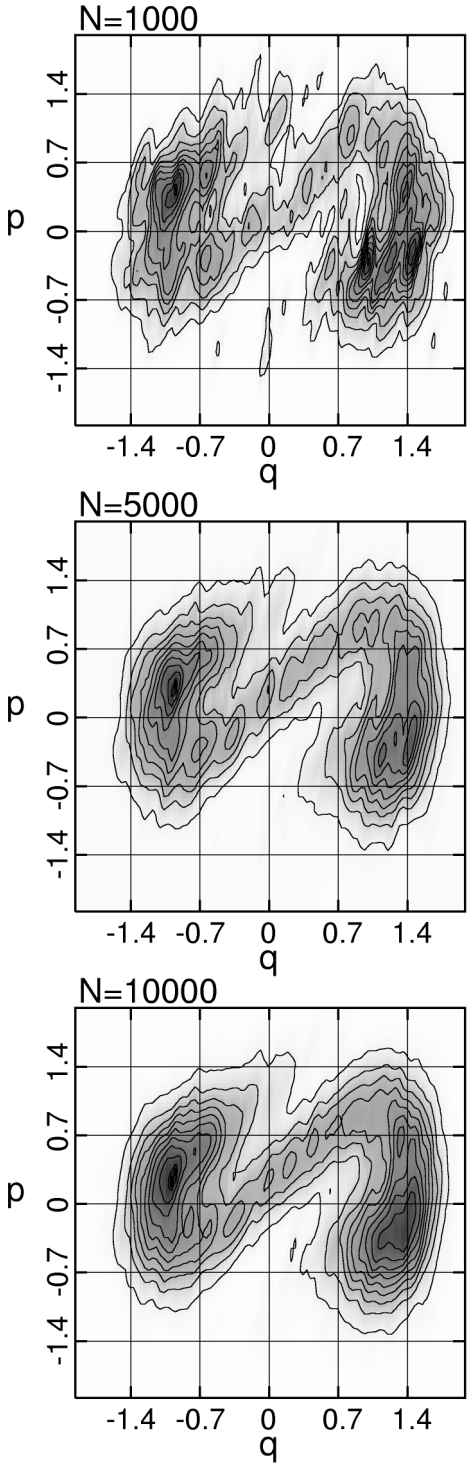

FIG. 1. Contour plots of the Wigner function $W(q, p, t = 4)$ of the reduced density operator of the thermal Duffing oscillator with $\hbar = 0.01$ (for the phase space area corresponding to this $\hbar$, see Fig. 2). The contour plots show the ensemble mean over 1000, 5000, and 10 000 Wigner functions $W_z(q, p, t = 4)$ of individual quantum trajectories obtained solving the quantum Brownian motion stochastic Schrödinger equation (8).

in [9] that in the regime considered in this Letter the evolution of the ensemble mean (3) is well described by the master equation

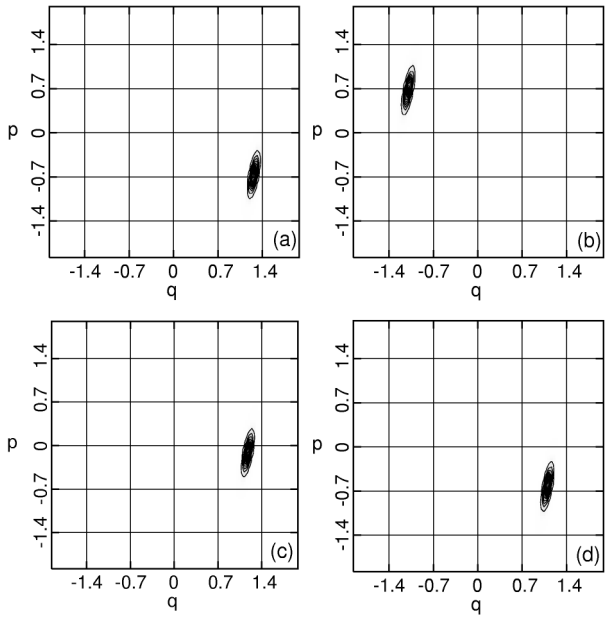

FIG. 2. Contour plots of Wigner functions $W_z(q, p, t = 4)$ of four individual quantum trajectories obtained solving the quantum Brownian motion stochastic Schrödinger equation (8) for the thermal Duffing oscillator. Individual trajectories remain well localized in phase space with respect to the overall spread of the ensemble mean, even for this classically chaotic system. The chosen value of $\hbar = 0.01$ is slightly smaller than the phase space area covered by these states.

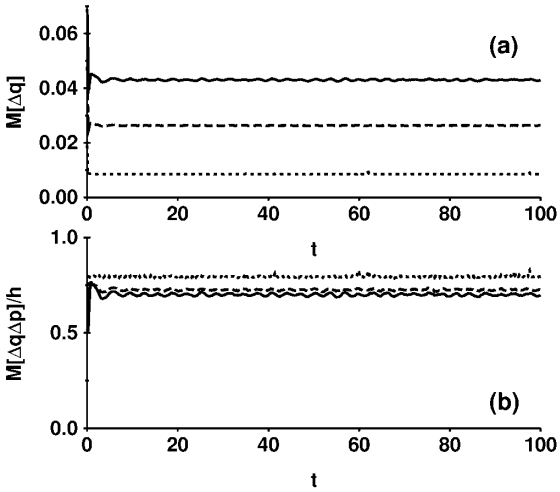

FIG. 3. Localization property of the QBM stochastic Schrödinger equation. Individual runs are well localized in phase space, the localization being stronger the smaller $\hbar$: (a) the average position spread $M[\Delta q] = M[\sqrt{\langle (q - \langle q \rangle)^2 \rangle}]$ of solutions of the QBM stochastic Schrödinger equation for the choices $\hbar = 0.01$ (solid line), $\hbar = 0.005$ (dashed line), and $\hbar = 0.001$ (dotted line). (b) Shows the mean uncertainty product $M[\Delta q \Delta p]/\hbar$, which remains of the order 1 almost independently of $\hbar$. Thus the quantum trajectories remain almost minimum uncertainty wave packets for all times.

$$\hbar\dot{\rho} = -i[H, \rho] - i\left(\frac{1}{2} m\gamma\Lambda + \mathrm{Im}\{g_0(t)\}\right)[q^2, \rho] + i\,\mathrm{Im}\{g_1(t)\}[q, \{p, \rho\}] - \mathrm{Re}\{g_0(t)\}[q, [q, \rho]], \tag{9}$$

which reduces to (2) for times larger than the environmental memory time, $t \gg \Lambda^{-1}$, due to the asymptotics of the coefficients $g_0(t), g_1(t)$. Thus, apart from an initial slip on the environmental memory time scale Λ^{-1}, our approach recovers (2) in the mean. It is known in the case of the exact master equation for a damped harmonic oscillator [15] that such time dependent coefficients may ensure the positivity of the reduced density operator for non-Lindblad master equations, a result that is here supported for general system Hamiltonian $H(q, p)$.

To conclude, we have presented the stochastic Schrödinger equation for Brownian motion. It is compatible with the standard QBM master equation yet allows one to compute states rather than a matrix, a huge reduction in resources, which becomes even more relevant for QBM in more than one space dimension. Individual trajectories are well localized in phase space, the localization being stronger the smaller $\hbar$. Thus, in (3), the reduced density operator for Brownian motion is explicitly represented as an ensemble of almost classical states.

We thank F. Haake and I. C. Percival for helpful comments. W. T. S. thanks the Deutsche Forschungsgemeinschaft for support through the SFB 237 "Unordnung und große Fluktuationen." N. G. and T. Y. thank the Swiss National Science Foundation.

[1] R. P. Feynman and A. R. Vernon, Ann. Phys. (N.Y.) **24**, 118 (1963); A. O. Caldeira and A. J. Leggett, Physica (Amsterdam) **121A**, 587 (1983); H. Grabert, P. Schramm, and G.-L. Ingold, Phys. Rep. **168**, 115 (1988); C. W. Gardiner, *Quantum Noise* (Springer, Berlin, 1991); U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 1993).

[2] G. Lindblad, Commun. Math. Phys. **48**, 119 (1973).

[3] Ph. Pechukas, in *Large Scale Molecular Systems*, edited by W. Gans *et al.* (Plenum Press, New York, 1991); L. Diósi, Physica (Amsterdam) **199A**, 517 (1993); S. Gnutzmann and F. Haake, Z. Phys. B **101**, 263 (1996); A. Rocco and P. Grigolini, Phys. Lett. A **252**, 115 (1999); K. Jacobs, I. Tittonen, H. M. Wiseman, and S. Schiller, Phys. Rev. A **60**, 538 (1999).

[4] J. Dalibard, Y. Castin, and K. Mölmer, Phys. Rev. Lett. **68**, 580 (1992); H. Carmichael, *An Open System Approach to Quantum Optics* (Springer, Berlin, 1994); M. B. Plenio and P. L. Knight, Rev. Mod. Phys. **70**, 101 (1998).

[5] N. Gisin and I. C. Percival, J. Phys. A **25**, 5677 (1992); **26**, 2233 (1993); **26**, 2245 (1993).

[6] W. T. Strunz, L. Diósi, and N. Gisin, Phys. Rev. Lett. **82**, 1801 (1999); L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **58**, 1699 (1998).

[7] M. W. Jack, M. J. Collett, and D. F. Walls, Phys. Rev. A **59**, 2306 (1999).

[8] L. Diósi and W. T. Strunz, Phys. Lett. A **235**, 569 (1997);

L. Diósi, Quantum Semiclass. Opt. **8**, 309 (1996); W. T. Strunz, Phys. Lett. A **224**, 25 (1996).

[9] T. Yu, L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **60**, 91 (1999); T. Yu, L. Diósi, N. Gisin, and W. T. Strunz, quant-ph/9905006 (to be published).

[10] N. Metropolis *et al.*, J. Chem. Phys. **21**, 1087 (1953); K. Binder, in *Monte-Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979).

[11] S. Habib, K. Shizume, and W. H. Zurek, Phys. Rev. Lett. **80**, 4361 (1998).

[12] T. P. Spiller *et al.*, J. Low Temp. Phys. **101**, 1037 (1995).

[13] N. Gisin and I. C. Percival, J. Phys. A **26**, 2233 (1993); T. Steimle, G. Alber, and I. C. Percival, J. Phys A **28**, L491 (1995); R. Schack, T. Brun, and I. C. Percival, J. Phys. A **28**, 5401 (1995); T. Brun *et al.*, J. Phys. A **29**, 2077 (1995); W. T. Strunz and I. C. Percival, J. Phys. A **31**, 1801 (1998).

[14] J. Guckenheimer and P. Holmes, *Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vector Fields* (Springer, New York, 1997).

[15] F. Haake and R. Reibold, Phys. Rev. A **32**, 2462 (1985); B. L. Hu, J. P. Paz, and Y. Zhang, Phys. Rev. D **45**, 2843 (1992); **47**, 1576 (1993).