
Relaxation of Quantum Hydrodynamic Modes

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ABSTRACT: In this article, we develop a series of hierarchical mode-coupling equations for the momentum cumulants and moments of the density matrix for a mixed quantum system. Working in the Lagrange representation, we show how these can be used to compute quantum trajectories for dissipative and nondissipative systems. This approach is complementary to the de Broglie–Bohm approach in that the moments evolve along hydrodynamic/Lagrangian paths. In the limit of no dissipation, the paths are the Bohmian paths. However, the “quantum force” in our case is represented in terms of momentum fluctuations and an osmotic pressure. Representative calculations for the relaxation of a harmonic system are presented to illustrate the rapid convergence of the cumulant expansion in the presence of a dissipative environment. © 2002 Wiley Periodicals, Inc. *Int J Quantum Chem* 89: 313–321, 2002

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Introduction

Over the past few years, there has been an tremendous surge of interest in developing new methods for quantum dynamics based upon hydrodynamic representations. Many of these [1–9] are based upon the de Broglie–Bohm (dBB) [11–17] description of quantum mechanics, semiclassical Liouville space representations [18], or semiclassical initial value representations [19, 20]. One potential

advantage to be gained is the development of adaptive grids [21] and systematic partitioning between quantum and classic variables.

In this article, we develop a hydrodynamic moment expansion for the quantum density matrix. In what follows, we show that each term in the series expansion of the density matrix about the diagonal can be related term by term to a corresponding moment of the momentum space distribution of the Wigner function. Moreover, the time–evolution of each of these moments follows directly from the time–evolution of Wigner function. This leads to an infinite hierarchy of equations in which the evolu-

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tion of the n th-order moment depends upon the spatial derivative of the $(n + 1)$ th moment [22, 23]. In general, there is no closure relation for this hierarchy. However, we show that in the presence of an environment the hierarchy can be rapidly truncated to include only second-order cumulant terms. Further, this truncation becomes exact in the classic limit.

Theoretical Development

QUANTUM MODE COUPLING EQUATIONS

To begin, we write the density matrix, $\rho(x, y)$, in terms of relative variables, $q = (x + y)/2$ and $z = (x - y)$, corresponding to diagonal and off-diagonal matrix elements. In this relative coordinate frame,

$$\rho(q, z) = \psi(x + y/2)\psi^*(x - y/2). \quad (1)$$

In what follows, we will derive a hierarchy of equations of motion for a particle and its hydrodynamic moments. These moments are defined in terms of the Taylor expansion coefficients of $\rho(q, z)$ in the z -direction [22, 23]:

$$\rho(q, z) = \sum_n \frac{z^n}{n!} (\partial_z^n \rho(q, z))_{z=0}. \quad (2)$$

Because ρ can also be written in terms of the Wigner distribution

$$\rho(q, z) = \int_{-\infty}^{\infty} W(p, q) e^{ipz/\hbar} dp, \quad (3)$$

the n th term in the Taylor expansion is related to the n th moment of the corresponding momentum distribution given by $W(p, q)$:

$$(\partial_z^n \rho(q, z))_{z=0} = \left(\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} p^n W(p, q) dp. \quad (4)$$

Thus, the Taylor series can be recast as an expansion in terms of the momentum moments of the Wigner function.

$$\rho(q, z) = \sum_n \frac{z^n}{n!} \left(\frac{i}{\hbar}\right)^n \rho_n \quad (5)$$

Moreover, the time-evolution of these moments can be generated from the time-evolution of the Wigner function [22]:

$$\partial_t W(p, q) = \{H, W\} + QW, \quad (6)$$

where QW represents a inhomogeneous quantum mechanical addition to the Liouville equation for a classic phase-space distribution.

$$Q = \sum_{k=1}^{\infty} \left(\frac{\hbar}{2i}\right)^{2k} \frac{1}{(2k+1)!} \frac{\partial^{2k+1} V(q)}{\partial q^{2k+1}} \frac{\partial^{2k+1}}{\partial p^{2k+1}}. \quad (7)$$

The method of moments [24] provides a straightforward procedure for determining the evolution of the momentum moments. Thus, multiplying both sides of Eq. (6) by p^n and integrating over just momentum we can easily find [22]

$$\begin{aligned} \partial_t \rho_n = & -\frac{1}{m} \partial_q \rho_{n+1} - \sum_{k=0}^{(n-1)/2} \left(\frac{\hbar}{2i}\right)^{2k} \\ & \times \binom{n}{2k+1} \frac{\partial^{2k+1} V(q)}{\partial q^{2k+1}} \rho_{n-(2k+1)}, \end{aligned} \quad (8)$$

where $\binom{n}{m}$ is the binomial coefficient. Working through the first few equations of motion, one finds

$$\partial_t \rho_0 = -\left(\frac{\partial_q \rho_1}{m}\right), \quad (9)$$

$$\partial_t \rho_1 = -(\rho_0 V'(q)) - \frac{\partial_q \rho_2}{m}, \quad (10)$$

$$\partial_t \rho_2 = -2\rho_1 V'(q) - \frac{\partial_q \rho_3}{m}, \quad (11)$$

$$\partial_t \rho_3 = -3\rho_2 V'(q) + \frac{\hbar^2}{4} \rho_0 V^{(3)}(q) - \frac{\partial_q \rho_4}{m}, \quad (12)$$

and so forth.

The first few terms in this hierarchy carry obvious physical interpretations. For example, Eq. (9) is the continuity equation because we can write $\rho_1 = p(q)\rho_0/m$ as the current density, $j(q)$, and $\rho_0 = \rho(q)$ is the probability density at a given point, q . What we have is an *infinite* hierarchy of equations with the evolution of each moment depending upon the next higher moment. To use this description, we would have to develop a series of approximations to trun-

cate the hierarchy or limit ourselves to potential surfaces that can be described (at least locally) by low-order polynomials. Moreover, the equations are nonlocal because they involve spatial derivatives. If we discretize the spatial grid, then nonlocality enters through the coupling between the moments at one point with the next higher moments at the neighboring points. The origin of this nonlocality can be traced to the kinetic energy term in the Hamiltonian—much like the origins of the quantum potential in the dBB description. Numerical implementation of this approach as it stands would be extremely sensitive to rapid variations in higher-level moments. Consequently, the long-time stability would be compromised by potentially undamped oscillations in the highest-order moments. We need to be able to incorporate the influence of higher moments into the dynamics of the particle.

Faced with this, we turn to a cumulant generating procedure, using

$$G(q, z) = \log \rho(q, z) \quad (13)$$

to generate the *connected* terms in the momentum distribution via

$$\rho_n^{(c)} = \left. \frac{\partial^n G}{\partial z^n} \right|_{z=0}. \quad (14)$$

Using this definition, it is straightforward to compute the momentum cumulants and their time derivatives.

Because $G(q, z)$ is a complex function, we can perform a Taylor series expansion about $z = 0$:

$$G(q, z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \left(g^{(n)}(q) + \frac{i}{\hbar} S^{(n)}(q) \right). \quad (15)$$

A series expansion of ρ about $z = 0$ yields

$$\begin{aligned} \rho(q, z) = \rho(q) & \left(1 + \frac{iS'(0)z}{\hbar} + \frac{1}{2} \left(-\left(\frac{S'(0)^2}{\hbar^2} \right) + g''(0) \right) \right. \\ & \times z^2 + \frac{i}{6\hbar^3} (-S'(0)^3 + \hbar^2(3S'(0)g^{(2)}(0) \\ & \left. + S^{(3)}(0))z^3 + \mathcal{O}(z^4) \right). \quad (16) \end{aligned}$$

Comparing Eq. (16) term by term with Eq. (2) yields for the first momentum moments expressed in

terms of the momentum cumulants. The first few of these read

$$\rho_0 = \rho(q), \quad (17)$$

$$\rho_1 = p(q)\rho(q), \quad (18)$$

$$\rho_2 = \rho(q)(p(q)^2 - \hbar^2 g^{(2)}(q)), \quad (19)$$

$$\rho_3 = \rho(q)(p(q)^3 - 3\hbar^2 p(q)g^{(2)}(q) - \hbar^2 S^{(3)}(q)), \quad (20)$$

where $S^{(n)}(q) = (\partial_z^n S)_{z=0}$ and $g^{(n)}(q) = (\partial_z^n g)_{z=0}$ denote the derivatives of S and g with respect to z . The first term [Eq. (17)] is obviously the probability density at the point q . In the next term, we identify $p(q) = (\partial_z S)_{z=0} = S^{(1)}(q)$ as the canonical momentum of a particle at point q [11],¹ thereby relating ρ_1 to the current density at a given point. The third term, ρ_2 in Eq. (19), is related to the kinetic energy density at q , $T(q) = \rho_2/2m$. This can be decomposed into two terms, the first associated with the actual motion of the particle, $T_{\text{motion}} = \rho(q)p^2(q)/2m$ along the trajectory $m\dot{q} = p(q)$ and a second related to the “localization” energy determined by coherence length of the quantum particle.

We can also derive physical meaning from in the cumulants. For example, the second cumulant, $g^{(2)}$, can be written as

$$g^{(2)}(q) = -\frac{1}{\hbar^2} \left(\frac{\rho_2(q)}{\rho_0(q)} - \left(\frac{\rho_1(q)}{\rho_0(q)} \right)^2 \right). \quad (21)$$

Thus, $g^{(2)}$ represents the fluctuations in the kinetic energy when the system is in the state, $|q\rangle$. The total time derivative is then

$$-\hbar^2 d_t g^{(2)} = \frac{1}{\rho(q)} d_t \rho_2 - \left(\frac{\rho_2}{\rho(q)} \right) \frac{1}{\rho(q)} d_t \rho(q) - 2p(q) d_t p(q). \quad (22)$$

We can now derive the Lagrangian equations of motion for the moments in terms of the cumulants. The first term is the continuity equation:

$$d_t \rho_0 = -\frac{\rho_0}{m} \frac{\partial p(q)}{\partial q}. \quad (23)$$

¹Note that this is similar to the definition of momentum along the diagonal we gave in Ref. [11] with the sign change coming about due a slight difference in the definition of the off-diagonal and diagonal coordinates. Here: $z = x - y$ and $q = (x + y)/2$ and in Ref. [11]: $z = (y - x)/\sqrt{2}$ and $q = (x + y)/\sqrt{2}$.

The second term gives the equations of motion for the Lagrangian particles:

$$\begin{aligned} d_t p &= -\frac{\partial V}{\partial q} + \frac{\hbar^2}{m\rho_0} \frac{\partial}{\partial q} (g^{(2)}\rho_0) \\ &= -\frac{\partial V}{\partial q} + \frac{\hbar^2}{m} \left(\frac{\partial g^{(2)}}{\partial q} + g^{(2)} \frac{1}{\rho_0} \frac{\partial \rho_0}{\partial q} \right). \end{aligned} \quad (24)$$

The last term on the right side of Eq. (24) is the quantum force, now written solely in terms of the second momentum cumulant and the density at a given point, q . The first term in the quantum force

depends upon the local curvature of the density matrix in the z direction and how that curvature changes with respect to q . For a postdecoherent system, where the density matrix has been approximately diagonalized due to its interaction with an environment, $g^{(2)}$ is constant in time and is expected to show little variation with respect to q . The second term is an *osmotic force* [26] and depends upon the local shape of the density matrix about a given trajectory.

To complete our derivation of the equations of motion, we can use Eqs. (23) and (24) to write the time derivatives of the cumulants as

$$\begin{aligned} d_t g^{(0)} &= -\frac{1}{m} (\partial_q S^{(1)} + S^{(1)} \partial_q g^{(0)}) \\ d_t S^{(1)} &= -V' + \frac{\hbar^2}{m} (\partial_q g^{(2)} + g^{(2)} \partial_q g^{(0)}) \\ d_t g^{(2)} &= -\frac{1}{m} (\partial_q S^{(3)} + S^{(3)} \partial_q g^{(0)}) - \frac{2}{m} g^{(2)} \partial_q S^{(1)} \\ d_t S^{(3)} &= -\frac{1}{4} V^{(3)} - \frac{3}{m} S^{(3)} \partial_q S^{(1)} + \frac{\hbar^2}{m} (g^{(4)} \partial_q g^{(0)} + 3g^{(2)} \partial_q g^{(2)} + \partial_q g^{(4)}) \\ &\vdots \\ d_t Q_{\text{even } n}^{(n)} &= -\frac{1}{m} \partial_q Q^{(n+1)} - \frac{1}{m} \sum_{k=0}^{n-1} \binom{n}{k} Q^{(n-2k+1)} \partial_q Q^{(k)} \\ d_t Q_{\text{odd } n}^{(n)} &= -\frac{1}{2^{n-1}} V^{(n)} + \frac{\hbar}{m} \partial_q Q^{(n+1)} - \frac{\hbar}{m} \sum_{k=0}^{n-1} (-1)^k \hbar^{1+(-1)^k} \binom{n}{k} Q^{(n-k+1)} \partial_q Q^{(k)}, \end{aligned}$$

where $Q^{(n)}$ represents $g^{(n)}$ when n is even and $S^{(n)}$ when n is odd. For comparison, let us consider the case of a coherent state in a harmonic oscillator well. Here, $g^{(2)} = -m\omega/2\hbar$, resulting in a quantum force

$$F_Q = m\omega^2(q - q(t)), \quad (25)$$

where $q(t) = q_0 \cos(\omega t)$ is the trajectory followed by the center of the Gaussian. Thus, for an arbitrary trajectory

$$\dot{p}(t) = -m\omega^2 q_0 \cos(\omega t), \quad (26)$$

$$\dot{q}(t) = p(t)/m. \quad (27)$$

Plots of these trajectories are shown in Figure 1 and we note immediately that these are identical to the Bohm trajectories for this system [3, 13].

For a stationary system, the potential force and the quantum force must be in balance, so again

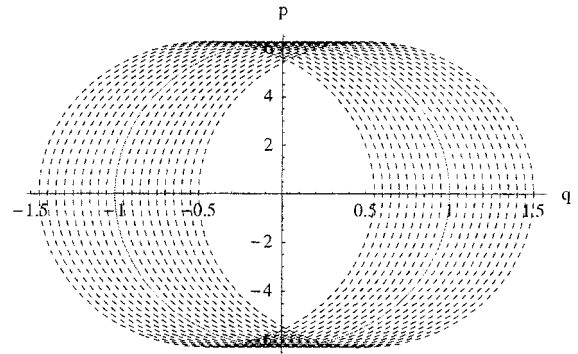


FIGURE 1. Coherent state trajectories for a harmonic oscillator. The solid curve corresponds to the trajectory followed by the peak of the coherent state.

assuming that decoherence is rapid relative to relaxation we can ignore the curvature force and require

$$-\frac{\partial V}{\partial q} + \frac{\hbar^2}{m} g^{(2)} \frac{\partial \log \rho_0}{\partial q} = 0. \quad (28)$$

At thermal equilibrium, where the quantum density matrix can be approximated via the classic density matrix,

$$\log \rho_0(q) = \frac{m}{g^{(2)} \hbar^2} V = -V(q)/kT. \quad (29)$$

Thus, at thermal equilibrium, we have a classic limit estimate for $g^{(2)}$;

$$g^{(2)} = -\frac{mkT}{\hbar^2} \quad (30)$$

Thus, we can formulate a simple semiclassical formalism for incorporating rudimentary quantum mechanical effects such as barrier penetration and zero-point motion by running an ensemble of trajectories where the motion of the particles is given by

$$d_t p_{sc} = -\frac{\partial V}{\partial q} - kT \left(\frac{\partial \log \rho_0}{\partial q} \right). \quad (31)$$

Thus, the system and particles become stationary when $\log \rho_0 = -V/kT$. This may seem like a circular tautology, but it points out the significant role that the quantum force plays in the dynamics of the particles. As shown in the next section, similar equations arise when the system is placed in contact with a thermal bath.

In essence, this analysis provides a more generalized description of quantum dynamics than the original Bohmian description. From a computational viewpoint, these equations are considerably simpler to implement because the quantum force involves only log-derivative of the density, as opposed to third-derivative of $\sqrt{\rho_0}$ as in the original dBB equations of motion:

$$F_Q^{(dBB)} = \frac{\hbar^2}{2m} \frac{\partial}{\partial q} \frac{1}{\sqrt{\rho_0}} \nabla_q^2 \sqrt{\rho_0}. \quad (32)$$

The mode equations introduced and described here should not exhibit the same instabilities near nodes

as encountered in previous quantum trajectory methods. Moreover, as we have indicated, one can make a rapid-decoherence approximation and obtain equations of motion for thermal trajectories in an arbitrary system.

Dissipative Systems

The theory of dissipative quantum systems reaches across broad areas of physics and the literature is vast. Model systems include nonadiabatic electronic relaxation and proton transfer in biomolecules. In each area, the question is how does a bath of oscillators influence the dynamics of a few important degrees of freedom, such as a tagged oscillator, a spin state, or an excess electron. For a classic system, coupling to a thermal bath causes an initial displacement from equilibrium to relax back to equilibrium at a rate depending upon the power spectrum of the coupling between the system and the bath and the temperature of the bath (population relaxation). For a quantum system, interaction between the system and the bath causes the system's wave function to lose phase information as well, that is, a coherent superposition state evolves into a statistical mixed state as a function of time due to its contact with the bath. The information in the phase is lost to the bath as the system "decoheres."

Quantum decoherence is a central issue in the theory of measurement. It has also received considerable attention in conjunction with macroscopic quantum systems, such as SQUIDS, quantum computing, coherent control theory, and the emergence of time in quantum cosmology. Moreover, it appears to play a central role in nonadiabatic transition rates between electronic states in molecules by reducing or increasing the transition rate depending upon the particular system. It is also an important consideration in the design and implementation of quantum control and quantum computing schemes, where the inevitable contact with an external environment destroys the quantum superposition states in the *qubit* logic elements and thus prevents the qu-puter from functioning as expected.

For a classic system, the motion of a Brownian particle is well known and can be described phenomenologically at least by the Langevin equation:

$$m\ddot{q} + \gamma\dot{q} + V'(q) = F(t), \quad (33)$$

where $F(t)$ is a fluctuating force that is assumed to have zero mean $\langle F(t) \rangle = 0$. In the case where the environment retains no memory of its previous interaction with the system, the correlation function for the random force is given by

$$\langle F(t)F(0) \rangle = 2\gamma kT\delta(t). \quad (34)$$

If we consider the distribution of all possible trajectories, one is led to the Kramer–Moyal equation:

$$\begin{aligned} \frac{\partial P(q, p, t)}{\partial t} = & -\frac{\partial}{\partial q}(pP) + \frac{\partial}{\partial p}(V'P) \\ & + \frac{\eta}{m} \frac{\partial}{\partial p}(pP) + D \frac{\partial^2}{\partial p^2} P, \end{aligned} \quad (35)$$

where $D = \gamma kT/m^2$ is the diffusion constant. Because no Hamiltonian or Lagrangian description is possible for systems with dissipation, standard quantization procedures fail. However, a perhaps overly naive approach using the correspondence principle leads to a master equation of the form

$$i \frac{\partial \rho}{\partial t} = [H, \rho] + \frac{\gamma}{2} [x, \{p, \rho\}] - i\Lambda [x, [x, \rho]], \quad (36)$$

which is the Caldeira–Leggett master equation obtained using a path-integral description of a particle coupled to a bath of harmonic oscillators. Here, η is the viscosity, $\gamma = \eta/m$ is the kinetic energy relaxation rate, and $\Lambda = \gamma mkT$ is the localization or decoherence rate. This equation is not completely adequate because it does not preserve the positivity of the density matrix. Nonetheless, it does provide a reasonable description at high-temperature where kT is greater than the level spacing of the system in the absence of the coupling to the environment. The first term in the CL equation gives the unitary evolution of the system in the absence of the environment. The second two introduce nonunitary evolution and are responsible for dissipation and decoherence, respectively. Taking the Fourier transform yields the time–evolution of the Wigner function.

$$\frac{\partial W}{\partial t} = (\{H, W\} + QW + \gamma \partial_p(pW) + \Lambda \partial_p^2 W). \quad (37)$$

Consequently, the nonunitary part of the evolution of the moments is determined by the following integrals:

$$\begin{aligned} \gamma \int_{-\infty}^{\infty} p^n \frac{\partial}{\partial p}(pW) dp &= \gamma \int_{-\infty}^{\infty} (p^{n+1}W_p + p^n W) dp \\ &= -n\gamma \rho_n \end{aligned} \quad (38)$$

and

$$\Lambda \int_{-\infty}^{\infty} p^n \frac{\partial^2}{\partial p^2} W dp = 2!\Lambda \binom{n}{2} \rho_{n-2}. \quad (39)$$

Thus, the nonunitary contribution to the n th moment reads [23]

$$d_t^{(n)} \rho_n = n(-\gamma \rho_n + \Lambda \rho_{n-2}). \quad (40)$$

The continuity equation is unaffected so as to preserve norm and the momentum term picks up a friction term:

$$d_t p = -\frac{\partial V}{\partial q} + \frac{\hbar^2}{m\rho_0} \frac{\partial}{\partial q}(g^{(2)}\rho_0) - \gamma p. \quad (41)$$

Taking the classic limit of $\hbar \rightarrow 0$ yields the Ehrenfest relations for a particle approaching thermal equilibrium:

$$\begin{aligned} d_t q(t) &= p(q)/m \\ d_t p(q) &= -\langle \partial_q V \rangle - \gamma p(t). \end{aligned} \quad (42)$$

Decoherence enters in at the second term:

$$\begin{aligned} d_t^{(nu)} \rho_2 &= -2(\gamma \rho_2 - \Lambda \rho_0) \\ &= -2(\gamma(p(q)^2 - \hbar^2 g^{(2)}(q)) - \Lambda)\rho(q) \\ &= -2 \frac{\eta}{m} (p(q)^2 - \hbar^2 g^{(2)}(q) - mkT)\rho(q) \end{aligned} \quad (43)$$

and corresponds to relaxation of the total kinetic energy (including the curvature term) to its thermal equilibrium value.

Armed with the time derivatives of the first few moments, we can readily evaluate the dissipative/nonunitary part of the time evolution of $g^{(2)}$. Substituting Eqs. (43) and (42) into Eq. (41) above and

keeping only the dissipative parts yields a relaxation equation,

$$\left. \frac{dg^{(2)}}{dt} \right|_{\text{relax}} = -2\gamma g^{(2)} - \frac{\Lambda}{\hbar^2}, \quad (44)$$

which is trivial to solve

$$g_{\text{relax}}^{(2)}(t) = -\frac{mkT}{\hbar^2} + e^{-\gamma t} g^{(2)}(0). \quad (45)$$

Clearly, as $t \rightarrow \infty$ we recover the ansatz we made above and hence the classic statistical distribution. What is totally surprising is the absence of an explicit temperature dependence on the relaxation rate of $g^{(2)}$ under this approximation. Here, the rate constant for $g^{(2)}$ is simply γ , the rate at which the kinetic energy relaxes to its thermal equilibrium expectation value. Quantum decoherence, which is associated with the relaxation of the off-diagonal elements of the density matrix, is expected to have a relaxation rate proportional to the localization rate, Λ , and hence carry an explicit temperature dependency. Clearly, further investigations into the nature of decoherence in the context of these mode-coupling equations is warranted.

The time-evolution for the modes can be easily calculated for the relaxation of a Gaussian density matrix in a harmonic well [11]. In this particular case, in fact, only $p(q)$ and $g^{(2)}$ appear because the relaxing density matrix retains its Gaussian form. In Figures 2 and 3, we have plotted $g^{(2)}$ and the root mean square (RMS) deviation of the population

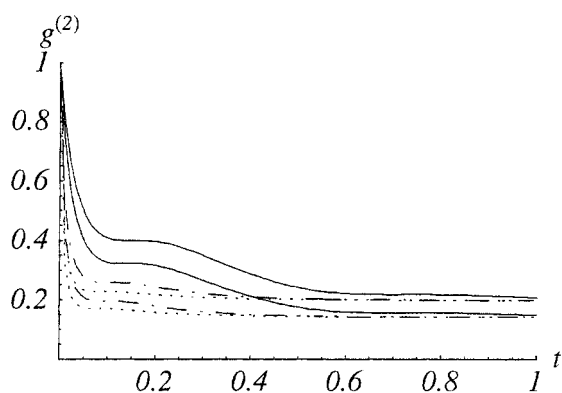


FIGURE 2. Relaxation of $g^{(2)}$ cumulant for a Gaussian density matrix in a harmonic well for two different temperatures. The various curves correspond to underdamped (solid), overdamped ($\cdot\cdot\cdot$), and critically ($-\cdot-\cdot-$) damped cases.

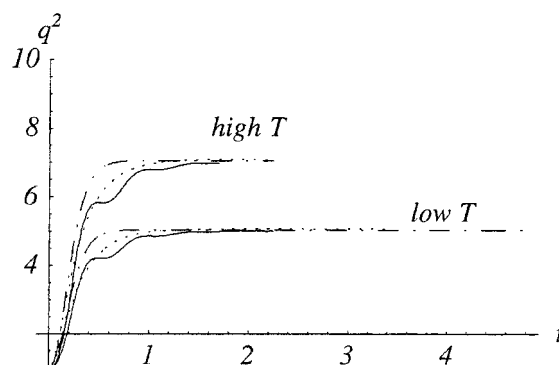


FIGURE 3. Relaxation of the mean-square deviation of the width of the density matrix about its mean value for a Gaussian density matrix in a harmonic well for two different temperatures. The various curves correspond to underdamped (solid), overdamped ($\cdot\cdot\cdot$), and critically ($-\cdot-\cdot-$) damped cases.

about its mean for the overdamped, underdamped, and critically damped cases at two temperatures ($T_{\text{high}} = 5\hbar\omega/2kT$ and $T_{\text{low}} = 3\hbar\omega/2kT$). Figure 2 shows the expected rapid relaxation of the momentum cumulant to its equilibrium value. Thus, the process of decoherence can be interpreted as the relaxation of the kinetic energy fluctuations to their equilibrium values. The mechanical component of the relaxation process occurs on a slower time-scale, entirely governed by the friction coefficient, γ , independent of the temperature. On the other hand, the relaxation rate of $g^{(2)}$ is temperature dependent. Lastly, in Figure 4 we show the linear entropy of the Gaussian system via

$$S = -\text{Tr}(\rho \log \rho).$$

Discussion

In this article, we laid the formal groundwork for the development of a novel hydrodynamic method for propagating the quantum density matrix based upon its momentum cumulants and moments. While we have not presented any explicit numerical calculations based upon this method, this is certainly the direction in which we are headed and the procedure is exact and should be readily implemented. As noted above, the procedure has certain distinct advantages over the Bohmian formulation in that the basic equations of motion involve low-order derivatives of the probability density, the momentum field, and its associated moments. As usual, there is no such thing as a free lunch. The

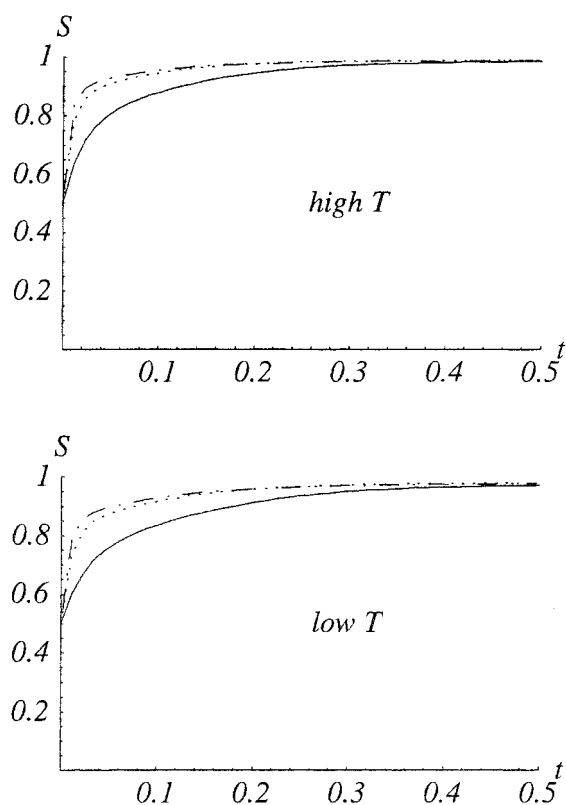


FIGURE 4. Linear entropy evolution for tagged oscillator for high- and low-temperature cases.

price we pay is that we have a hierarchy of moments, which is not closed. However, in the presence of dissipation, all of the modes are damped and only the second cumulant, $g^{(2)}$, has a nonzero equilibrium value in the high-temperature limit.

Using this approach, one can develop systematic quantum/classic schemes that incorporate quantum nonlocality and kinetic energy fluctuations into the classic equations of motion. For example, the classic/thermal limiting equations of motion, Eq. (31), one can incorporate “kinetic” or activated tunneling dynamics into a classic calculation.

Finally, the mode analysis procedure may be useful in reconstructing the quantum density matrix and wave function from experimental data, as originally suggested by Johansen [22]. Indeed, various experimental and theoretical schemes [29] for doing this have been proposed using homodyne tomology [30] to reconstruct the quantum state of the radiation field and material particles. What we have shown here is that the cumulants can be written easily in terms of the moments, allowing one to reconstruct the Wigner distribution or the density matrix using a relatively few number of connected

terms; and, once the effects of the environment are considered and decoherence occurs the second-order term in the cumulant expansion of the momentum space distribution will rapidly dominate.

This approach also points the way toward systematically incorporating quantum effects such as a dynamic tunneling and zero-point motion into multidimensional classic MD or Monte-Carlo simulations. The method we envision entails discretizing the classic phase space into cells, computing the moments from the classic distribution, and using the moments to provide an auxiliary quantum potential to propagate a swarm of trajectories.

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