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Time evolution of Wigner function in dissipative quantum systems using entangled trajectory molecular dynamics

Lifei Wang[1,*], Yan Wang[2], Qin Zhang[1], Haibo Sun[1] and Juan Zhao[1]

[1] *School of Science, Shandong Jiaotong University, Jinan 250357, China*
[2] *Department of Computer and Information Science, Southwest Forestry College, Kunming 650224, China*

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Abstract. The dissipative quantum systems are treated using Klein-Kramers equation, combined with the Gaussian kernel trajectory ensemble, for time evolution of Wigner function $\rho_w(q,p,t)$ in phase space. The entangled trajectory molecular dynamics approach is used to obtain trajectory solutions for the Klein-Kramers equation with three models: free particle, damped harmonic oscillator and metastable potential. It is found that the performance of semiclassical Wigner propagation is effectively for the relaxation of damped harmonic oscillator and dissipative decay of a metastable state. In addition, the energy of trajectory ensemble decays faster with smaller friction value and changes slightly with variable temperature parameters.

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Key words: Klein-Kramers equation, Wigner function, entangled trajectory molecular dynamics.

1 Introduction

The description of quantum mechanics via phase space distributions developed by Wigner [1] is a seminal work for the formulation of semiclassical quantum motion equations. Since then Wigner distribution function has been a standard tool for establishing the quantum classical correspondence [2–4], and has a wide range of applications in material science and quantum optics as well as quantum computing [5–7]. Wigner function is termed as a quasi-probability distribution, as it may become negative in some regions of phase space even for nonnegative initial conditions. For a closed quantum system with a

*Corresponding author. *Email address:* wanglf@sdjtu.edu.cn (L.-F. Wang)

potential $V(\mathbf{q})$, the time evolution of Wigner function is governed by the quantum Liouville equation equivalent to the Schrödinger equation,

$$\frac{\partial \rho_w(\mathbf{q},\mathbf{p};t)}{\partial t} = -\sum_{k=1}^{n} \frac{p_k}{m} \frac{\partial \rho_w(\mathbf{q},\mathbf{p};t)}{\partial q_k} + \int d\xi J(\mathbf{q},\xi-\mathbf{p})\rho_w(\mathbf{q},\xi;t), \tag{1}$$

where

$$J(\mathbf{q},\xi) = \frac{i}{2^n \pi^n \hbar^{n+1}} \int d\mathbf{z} \left[U\left(\mathbf{q}+\frac{\mathbf{z}}{2}\right) - U\left(\mathbf{q}-\frac{\mathbf{z}}{2}\right) \right] e^{-\frac{i}{\hbar}\mathbf{z}\cdot\xi}. \tag{2}$$

Recently Martens and coworkers have proposed an entangled trajectory molecular dynamics method of solving the quantum Liouville equation in the context of Wigner formalism [8–12]. The entangled trajectory ensemble evolves as a unified whole by spatial and momentum partial derivatives of Wigner distribution in equations of motion. The theory of open quantum systems plays a major role in quantum physics since perfect isolation of quantum systems is impossible [13]. Quantum Markov processes represent the simplest case of the dynamics of open systems. An appropriate equation of motion for a Markovian system in phase space is Klein-Kramers equation [14–17], which describes the deterministic evolution of Wigner function $\rho_w(\mathbf{q},\mathbf{p},t)$,

$$\frac{\partial \rho_w}{\partial t} = -\frac{\mathbf{p}}{m}\frac{\partial \rho_w}{\partial \mathbf{q}} + U'(\mathbf{q})\frac{\partial \rho_w}{\partial \mathbf{p}} + \gamma_0 \frac{\partial}{\partial \mathbf{p}}\left(\mathbf{p} + mk_B T \frac{\partial}{\partial \mathbf{p}}\right)\rho_w, \tag{3}$$

where the first of the two terms involving the friction coefficient γ_0 is the dissipative term and the second acts to smooth out momentum diffusion in the distribution function. Several analytical and numerical approaches have been developed to solve this partial differential equation or research the characteristics of its solutions [18, 19]. Entangled trajectory approaches to quantum dynamics in phase space have become the subject of many recent studies. The ensemble of trajectories in phase space is sampled from an initial distribution $\rho_w(\mathbf{q},\mathbf{p},0)$, and the evolving time-dependent density $\rho_w(\mathbf{q},\mathbf{p},t)$ is obtained by solving the Klein-Kramers equation.

The entangled trajectory molecular dynamics (ETMD) approach has been extensively studied for closed quantum systems in our previous work [20–24], while the average energy of trajectory ensemble keeps a constant with time evolution. Particularly, we have vividly interpreted the quantum tunneling phenomenon for closed systems based on the Wigner-Liouville formulation of quantum physics. Here we show in detail how to solve the semiclassical master equation for quantum open systems.

The structure of this paper is organized as follows. In Sec. 2, we present the theoretical approach to pave a way for subsequential analysis on quantum open systems. In Sec. 3, numerical analysis on three models are discussed with physical pictures. The paper is ended up with conclusion in Sec. 4.

2 Theory

Wigner showed that quantum mechanics can be reformulated in phase space $(\mathbf{q},\mathbf{p})$ with quasi-probability distribution [1]

$$\rho_w(\mathbf{q},\mathbf{p};t)=\left(\frac{1}{2\pi\hbar}\right)^n\int d\mathbf{y}\,\psi^*(\mathbf{q}+\mathbf{y}/2;t)\,\psi(\mathbf{q}-\mathbf{y}/2;t)e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{y}}, \tag{4}$$

where all integrals are from $-\infty$ to $+\infty$ unless otherwise mentioned. Particularly, markovian master equations of dissipation systems in Wigner's formulation can be described by the Klein-Kramers equation. Since the phase space trace of Wigner function is conserved $\mathrm{Tr}\rho_w=\int\rho_w d\mathbf{q}d\mathbf{p}=1$, the trajectory ensemble obeying the continuity equation,

$$\frac{\partial\rho_w}{\partial t}+\nabla\cdot\mathbf{j}=0, \tag{5}$$

where $\mathbf{j}=(\mathbf{j}_q,\mathbf{j}_p)$ and $\nabla=(\frac{\partial}{\partial\mathbf{q}},\frac{\partial}{\partial\mathbf{p}})$ are the current vector and gradient operator in phase space, respectively. The N trajectories $\{q_k,p_k\}$ $(k=1,2,...,N)$ of the ensemble are propagated by integrating the set of coupled differential equations

$$\begin{aligned}\dot{q}_k&=\frac{p_k}{m},\\ \dot{p}_k&=-U'(q_k)-\gamma_0 p_k-\gamma_0 m k_B T\frac{1}{\rho_w(q_k,p_k)}\frac{\partial\rho_w(q_k,p_k)}{\partial p}.\end{aligned} \tag{6}$$

Many approaches to the problem of constructing a smooth (positive) distribution from a finite set of sampled points have been developed. The distribution ρ is represented in terms of N trajectories $\{q_k,p_k\}$ $(k=1,2,...,N)$.

$$\rho_w(q,p,t)=\frac{1}{N}\sum_{k=1}^{N}\delta(q-q_k(t))\delta(p-p_k(t)). \tag{7}$$

We employ the kernel density estimation [25–27] method to fit $\rho_w(q,p,t)$ in Eq. (6) in every step of the propagation. For two-dimensional Gaussian kernel can be expressed as

$$\phi(q,p)=\frac{1}{2\pi h^2\sigma_q\sigma_p}\exp\left(-\frac{q^2}{2h^2\sigma_q^2}-\frac{p^2}{2h^2\sigma_p^2}\right), \tag{8}$$

where the width parameters of D dimensional data sets are determined by $h=(4/N(D+2))^{1/(D+4)}$. Then the continuous distribution $\rho(q,p,t)$ is given by

$$\rho_w(q,p,t)=\frac{1}{N}\sum_{k=1}^{N}\phi(q-q_k(t),p-p_k(t)). \tag{9}$$

The initial state is set as a Gaussian wave packet,

$$\Psi^0(q,0)=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\exp(ip_0q)\exp\left(-\frac{m\omega}{2\hbar}(q-q_0)^2\right). \tag{10}$$

And it corresponds to the ground state of a harmonic oscillator with mass m and frequency ω, where q_0 and p_0 are the initial mean position and mean momentum, respectively. And the corresponding Wigner distribution is,

$$\rho_w^0(q,p,0)=\frac{1}{\pi\hbar}\exp\left(-\frac{(q-q_0)^2}{2\sigma_q^2}-\frac{(p-p_0)^2}{2\sigma_p^2}\right), \tag{11}$$

where $\sigma_q=\sqrt{\hbar/(2m\omega)}$ and $\sigma_p=\sqrt{\hbar m\omega/2}$. We choose $m=200.0$, $\omega=0.005$, and have the same width of position and momentum $\sigma_q=\sigma_p$.

3 Numerical results

3.1 Free particle

The trajectory ensemble equations for a free particle model can be described as follows,

$$\begin{aligned}\dot{q}_k&=\frac{p_k}{m},\\ \dot{p}_k&=0.0.\end{aligned} \tag{12}$$

In Fig. 1, we show four phase space snapshots of the evolving trajectory ensemble for the free particle model. The initial distribution is shown in the frame labeled $t=0$, with same width of position and momentum. The contour of Wigner distribution with quantity 0.03 is also shown. It is found that the contour line with initial circle boundary changes to an elliptic shape with time evolution. And the width of the position distribution becomes wider, but the momentum width keeps invariant. The Wigner distribution function at four time steps are shown in Fig. 2. During the time interval, the motion along p is nearly frozen. However the spatial distribution becomes widely with time evolution, and the Wigner distribution changes largely at the density maps. Obviously, the energy of trajectory ensemble keeps a constant with time evolution in Fig. 3.

3.2 Damped harmonic oscillator

The effect of dissipation on a nonlinear quantum system is a problem of fundamental interest. For simplicity, we discuss the well-understood problem of the damped harmonic oscillator. And we believe the results illustrate this simple prototype model might expect in more complicated systems. The potential of the harmonic oscillator is given by

$$U(q)=\frac{1}{2}m\omega^2q^2. \tag{13}$$

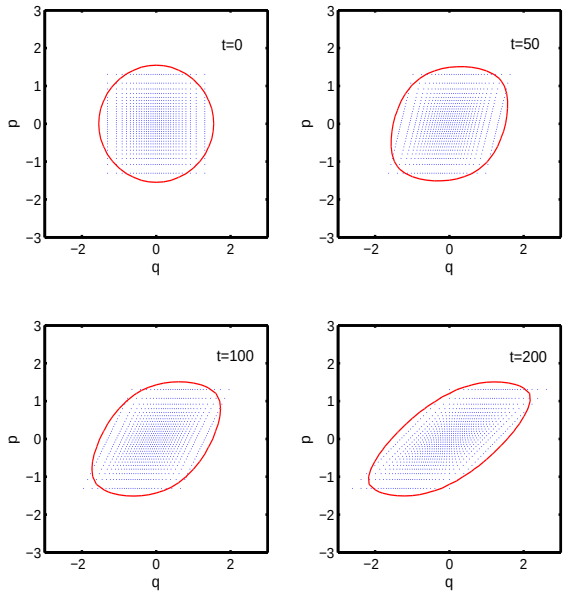

Figure 1: (Color online) Snapshots of trajectory ensemble and contour plot of the Wigner distribution evolution of the free particle model with initial mean position and momentum $q_0 = 0.0$ and $p_0 = 0.0$.

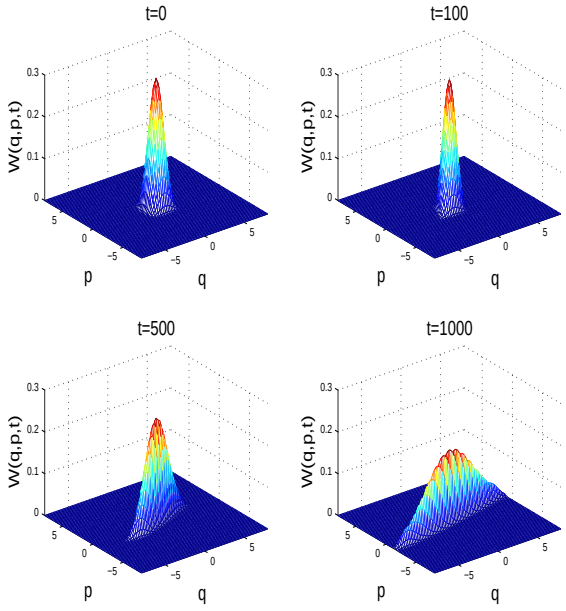

Figure 2: (Color online) Density maps at four time steps for the free particle model.

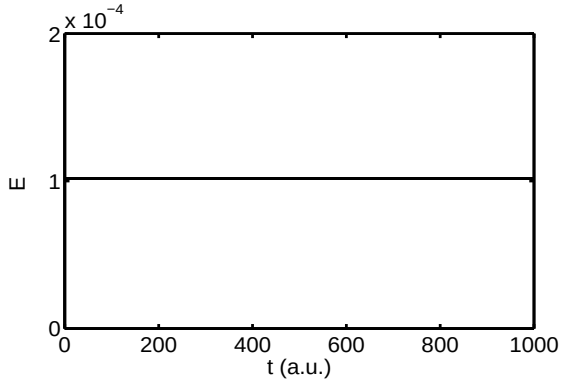

Figure 3: Energy of free particle with time evolution.

And the initial phase space distribution obeys the Klein-Kramers equation which relaxes to a Maxwell-Boltzmann distribution

$$\rho_{eq} = Z\exp[-H/(k_B T)], \tag{14}$$

where

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2. \tag{15}$$

And the explicitly expression of the Maxwell-Boltzmann distribution

$$\rho_{eq} = Z\exp\left[-\frac{p^2}{2mk_B T} - \frac{m\omega^2 q^2}{2k_B T}\right]. \tag{16}$$

According to initial Wigner distribution, we got the bath temperature in this simulation work

$$k_B T = \sigma_p^2/m. \tag{17}$$

Then the entangled trajectory ensemble for the damped harmonic oscillator are propagated by integrating the set of coupled differential equations

$$\begin{aligned}
&\dot{q}_k = \frac{p_k}{m}, \\
&\dot{p}_k = -m\omega^2 q_k - \gamma_0 p_k - \frac{\gamma_0}{h^2}\sum_{j=1}^{N}\frac{(p_k - p_j)\phi(q_k - q_j, p_k - p_j)}{\phi(q_k - q_j, p_k - p_j)}.
\end{aligned} \tag{18}$$

In Fig. 4, we show four phase space snapshots of an evolving ensemble for the case $\gamma_0 = 0.5$, with the temperature bath $k_B T = \sigma_p^2/m = 0.0025$. The initial Winger distribution is taken to be centered at $q_0 = 3.03$ and $p_0 = 0.0$. It is shown that the momentum distribution relaxes to the final distribution rapidly. And the spatial relaxation to the bottom of the harmonic oscillator ($q_0 = 0.0$) needs longer times than the momentum relaxation. The contour of Wigner distribution with quantity 0.03 is also shown, which shown that the contour line keeps circle shape. The evolution of the Wigner distribution is illustrated in

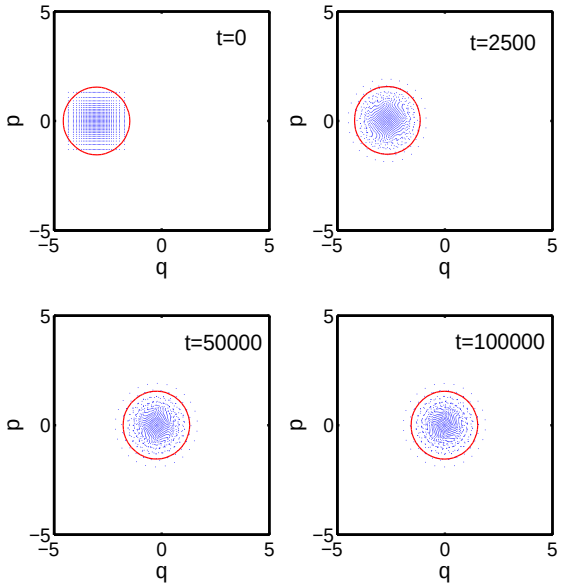

Figure 4: (Color online) Damped harmonic oscillator phase space snapshots of the evolving trajectory ensemble for the case of $\gamma_0=0.5$. The initial distribution is shown in the frame labeled $t=0$. Three subsequent snapshots are shown at $t=2500$, 50000, 100000. The ensemble has relaxed to a thermal Gaussian final distribution at the bottom of the harmonic well. The contour of Wigner distribution function with quantity 0.03 are also shown.

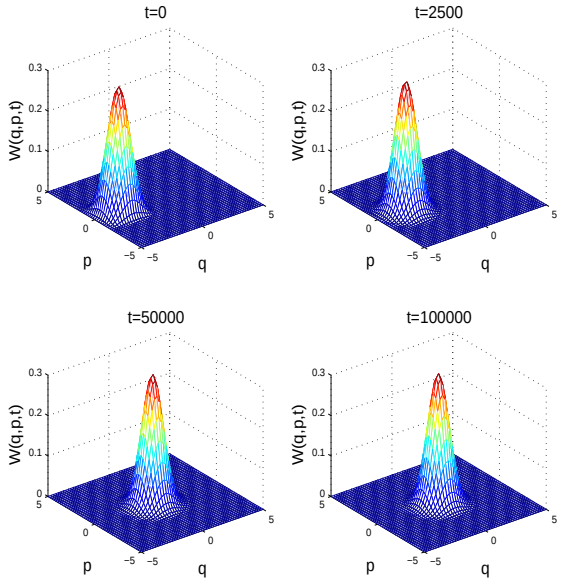

Figure 5: (Color online) Evolution of the Wigner distribution function $\rho_w(q,p,t)$ for the damped harmonic oscillator with $\gamma_0=0.5$. The initial distribution is shown in the frame labeled $t=0$. Three subsequent snapshots are shown at $t=2500$, 50000, 100000. The ensemble has relaxed to a thermal Gaussian final distribution at the bottom of the harmonic well.

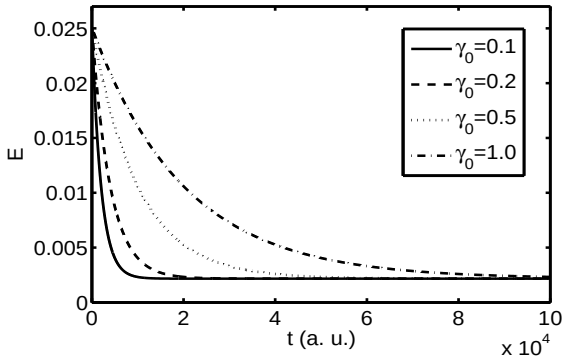

Figure 6: Energy decay of a displaced harmonic oscillator in a thermal bath with different friction values γ_0.

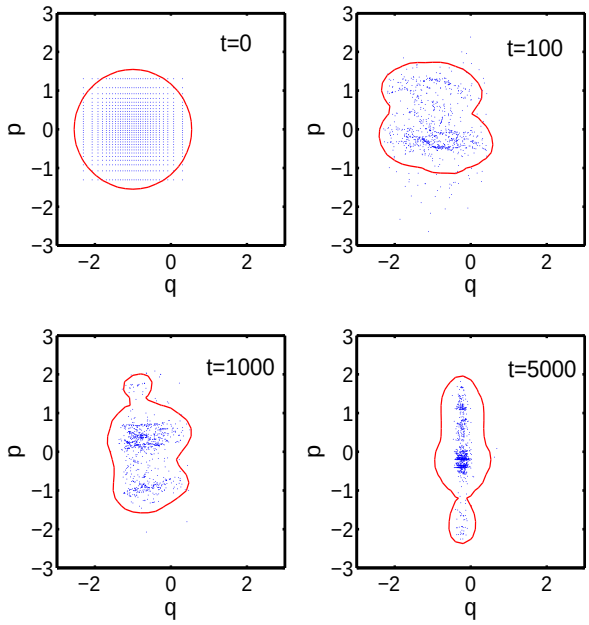

Figure 7: (color online) Snapshots of a trajectory ensemble evolving for the trajectory ensemble in a metastable potential with initial center $q_0 = -1.0$ and $p_0 = 0.0$ at four different times: t=0, 100, 1000, 5000. The contour of Wigner distribution function with quantity 0.03 are also shown.

more detail in Fig. 5. It is shown that the distribution with initial center $q_0 = 3.03$ and $p_0 = 0.0$ propagated to $q_0 = 0.0$ and $p_0 = 0.0$ with time evolution. The zero point energy of the harmonic oscillator is $E_0 = \hbar\omega/2 = 0.0025$. The initial energy is $E = 10E_0 = 0.025$. The energy decay of the damped harmonic oscillator with several values of γ_0 is shown

in Fig. 6. It is shown that the energy decays to the zero point energy with several friction values. In addition, the rate of energy decay is faster as the friction γ_0 is small.

3.3 Metastable potential

In this study, a different metastable potential of the form

$$U(q)=\alpha q^2-\beta q^3, \tag{19}$$

with the parameter values $\alpha=0.1$ and $\beta=0.06$ [28]. These values were chosen to ensure that there is little probability of escape from the well when the interaction with the bath is turned off. This potential has a minimum at $q=0.0$ and a barrier height of $V^*=0.0412$ at $q=1.1111$. Initially, the distribution of minimum uncertainty is centered at (0,0) in phase space. The entangled trajectory ensemble for the metastable potential is propagated by integrating the set of coupled differential equations

$$\begin{aligned}\dot{q}_k&=\frac{p_k}{m},\\ \dot{p}_k&=-2\alpha q_k+3\beta q_k^2-\gamma_0 p_k-\frac{\gamma_0 m k_B T}{h^2\sigma_p^2}\sum_{j=1}^{N}\frac{(p_k-p_j)\phi(q_k-q_j,p_k-p_j)}{\phi(q_k-q_j,p_k-p_j)}.\end{aligned} \tag{20}$$

Four snapshots of the evolving trajectory ensembles in the phase space with parameters $\gamma_0=5.0$ and $k_BT=0.0025$ are shown in Fig. 7. The initial ensemble snapshot centered in the $q_0=-1.0$ and $p_0=0.0$ with energy 0.2740. The contour plot of the initial Wigner distribution function with quantity 0.03 are shown. It is found that the shape of the contour changes largely from the initial circle. It is shown that no particle can escape to right of the barrier height $(q=1.1111)$ under the entangled trajectory molecular dynamics method with time evolution due to strongly damped value $\gamma_0=5.0$ and the entangled trajectory ensemble. The initial energy of trajectory is higher than the barrier height, the energy decay with both the friction and energy interactions between trajectory ensemble. The trajectory ensemble propagates as a unified whole, so the trajectory initial energy is higher than the barrier cannot escape from the well due to being hindered by the small initial energy of trajectories. And the corresponding Winger distribution function evolves are shown in the Fig. 8. We found the center of distribution propagates to the $q_0=0.0$ and $p_0=0.0$ with time evolution. The energy decay of the trajectory ensemble is shown in Fig. 9. The center of momentum distribution are set to zero, and three position center are $q_0=-0.8,-1.0$, and -1.5 respectively. Three different initial energies decay to nearly zero with time evolution due to this high friction value. In addition, the energy decay of the trajectory ensemble with three different friction and temperature values are show in Fig. 10. It is found that the energy of trajectory ensemble decays faster with smaller friction value due to weak friction. However, the energy decay changes slightly even when the temperature is increased ten times. It is demonstrated that the friction parameter is more effective than the thermal bath in this metastable potential.

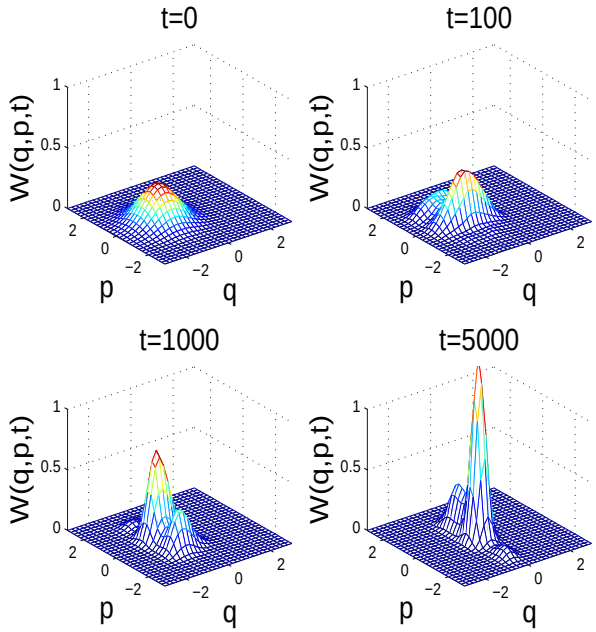

Figure 8: (color online) Evolution of the Wigner distribution function $\rho_w(q,p,t)$ for the metastable potential with γ_0=5.0. The initial distribution is shown in the frame labeled t=0. Three subsequent snapshots are shown at t=100, 1000, 5000. The ensemble has relaxed to a thermal Gaussian final distribution at the bottom of the harmonic well.

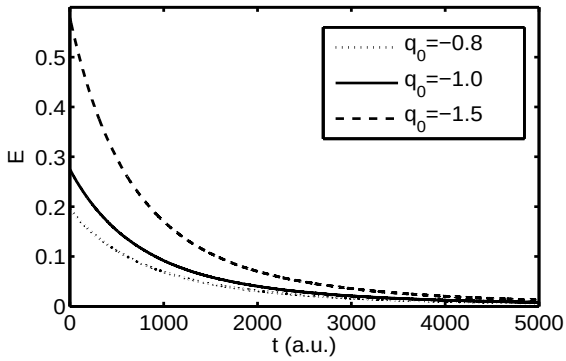

Figure 9: Energy decay of the trajectory ensemble in the metastable potential with a constant thermal bath for three different initial center.

4 Conclusion

In this paper, we extend the entangled trajectory molecular dynamics approach to solve the Klein-Kramers equation for simple models of dissipative systems. Wigner distribu-

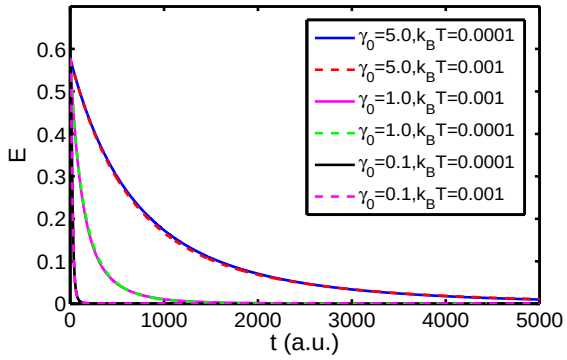

Figure 10: Energy decay of the trajectory ensemble in the metastable potential with three different friction and temperature values.

tion of the damped oscillator propagated to the bottom of the oscillator potential and the energy of corresponding trajectory ensemble decayed to the zero point energy. For high friction of the metastable potential, nearly all trajectories under the ETMD method are trapped by the potential well. This phenomena can be explained in terms of the entangled trajectory molecular dynamics. The trajectory ensemble propagates as a unified whole and concomitant energy exchanges along with the time evolution. The initial energy of trajectory is higher than the barrier height cannot cross the barrier due to the both the friction and entangled trajectory ensemble reasons. We believe the entangled trajectory molecular dynamics method can be used to research more complicated quantum diffusion systems.

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References

[1] E. P. Wigner, Phys. Rev. **40**(1932) 749.
[2] A. O. Bolivar, *Quantum-Classical Correspondence: Dynamical Quantization and the Classical Limit* (Spinger, Berlin, 2004).
[3] S. Haroche and J. M. Raimond, *Exploring the Quantum: Atoms, Cavities and Photons*, (Oxford:Oxford University Press, 2006).
[4] D. J. Bondar , R. Cabrera , D. V. Zhdanov, and H. A. Rabitz, Phys. Rev. A. **88**(2013) 052108.
[5] V. Veitch, C. Ferrie , D. Gross , and J. Emerson, New J. Phys. **14**(2012) 113011.
[6] A. Mari and J. Eisert, Phys. Rev. Lett. **109**(2012) 230503.
[7] V. Veitch, N. Wiebe , C. Ferrie, and J. Emerson, New J. Phys. **15**(2013) 013037.
[8] A.Donoso and C. C. Martens, Phys. Rev. Lett. **87**(2001) 223202.

[9] A. Donoso and C. C. Martens, Int. J. Quantum. Chem. **90**(2002) 1348.
[10] A. Donoso , Y. Zheng, and C. C. Martens, J. Chem. Phys. **119** (2003) 5010.
[11] C. C. Martens , A. Donoso, and Y. Zheng, *Quantum Trajectories in Phase Space*. In Quantum trajectories; Chattsaraj P K Ed, (CRC Press, 2011).
[12] B. L. Hyland and C. C. Martens, Theor. Chem. Acc, **133**(2014) 1536.
[13] H. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*, (Oxford: Oxford University Press, 2002).
[14] C. W. Gardiner, *Handbook of Stochastic Methods*, (Springer-Verlag, Berlin, 1983).
[15] H. Risken, *The Fokker-Planck Equation*, Springer-Verlag, Berlin, 1996).
[16] S. Chandrasekhar, Rev. Mod. Phys., **21**(1949) 383.
[17] H. A. Kramers, Physica Utrecht, **7**(1940) 284.
[18] M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys., **17**(1945) 323.
[19] D. J. Tannor and D. Kohen, J. Chem. Phys., **100**(1994) 4932.
[20] A. Wang , Y. Zheng , C. C. Martens, and W. Ren, Phys. Chem. Chem. Phys. **11**(2009) 1588.
[21] L. Wang, and Y. Zheng, Chem. Phys. Lett. **563**(2013) 112.
[22] L. Wang , C. C. Martens, and Y. Zheng, J. Chem. Phys. **137**(2012) 034113 .
[23] F. Xu and Y. Zheng, Acta Phys. Sin. **62**(2013) 213401.
[24] L. Wang , F. Xu, and Y. Zheng, J. At. Mol. Sci. **5**(2014) 21.
[25] A. Donoso and C. C. Martens, J. Chem. Phys. **116**(2002) 10598.
[26] B. W. Silverman, *Density Estimation for Statistics and Data Analysis* (Chapman and Hall, London, 1986).
[27] K. Fukunaga, *Introduction to Statistical Pattern Recognition*, (Academic, San Diego, 1990).
[28] C. J. Trahan and R. R. Wyatt, J. Chem. Phys., **119**(2003) 7017.