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

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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

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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.