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Entangled trajectories based on Wigner function with negative values

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Abstract. Wigner function is a fundamental method to study the connection between quantum and classical system. Since negative value can be accepted by Wigner function even from a positive initial condition, they are various issues existing in corresponding interpretation as well as the development of numerical methods. We present the entangled trajectories based on the Wigner distributions with negative values.

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Key words: Entangled trajectory, Wigner function.

1 Introduction

Wigner function can reveal the deep insights between quantum system and classical world. It has the similar form compared with classical probability distribution which can be integrated over the whole phase space to obtain unit. However, negative values of Wigner function indicate that such a function can only be regarded as quasi-probability distribution. Such a characteristic cause many issues when we want to propagate Wigner function in a general form. Meanwhile, negative values, illustrated in Fig. 1, for instance, also make the distinctions between quantum and classical trajectories in the phase space. We choose a special case to propagate Wigner function precisely by eigenvalues and then analysis the natures of the entangled trajectories in detail.

2 Wigner function and Liouville equation

Here we only consider one dimensional case since multi-dimensional can be easily expanded. As a solution from time-dependent Schrödinger equation, $\Psi(x)$ can be used to

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construct Wigner function as follows:

$$\rho^w(q,p;t) = \frac{1}{2\pi\hbar}\int \Psi^*(q+x/2,t)\Psi(q-x/2,t)e^{(ipx/\hbar)}dx. \tag{1}$$

Combined with the time-dependent Schrödinger equation, we can obtain the quantum Liouville equation

$$\frac{\partial\rho^w}{\partial t} = -\frac{p}{m}\frac{\partial\rho^w}{\partial q} + \int J(q,\xi-p)\rho^w(q,\xi)d\xi, \tag{2}$$

where

$$J(q,\xi) = \frac{i}{2\pi\hbar^2}\int_{-\infty}^{\infty}[V(q+y/2)-V(q-y/2)]e^{(-iz\xi/\hbar)}dz. \tag{3}$$

Similar as a probability distribution, we can impose the continuity condition as

$$\frac{\partial\rho^w}{\partial t} = -\vec{\nabla}\cdot\vec{j}, \tag{4}$$

where $\vec{j} = (j_q, j_p)$ is the current vector in phase space and $\vec{\nabla} = (\partial/\partial q, \partial/\partial p)$is the gradient operator. The current is as follows

$$\vec{\nabla}\cdot\vec{j} = \frac{\partial}{\partial q}(\frac{p}{m}\rho^w) - \int_{-\infty}^{\infty} J(q,\xi-p)\rho^w(q,\xi,t)d\xi, \tag{5}$$

with

$$j_q = \frac{p}{m}\rho^w, \tag{6}$$

$$j_p = -\int_{-\infty}^{\infty}\Theta(q,\xi-p)\rho^w(q,\xi,t)d\xi, \tag{7}$$

and

$$\Theta(q,\eta) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}[V(q+y/2)-V(q-y/2)]\frac{e^{-i\imath\eta y/\hbar}}{y}dy. \tag{8}$$

Since we can link the current density to density as well as velocity field in phase space by $\vec{j} = \rho^w\vec{v}$, we can finally deduce the equation of motion for the entangled trajectories as [1]

$$\dot{q} = \frac{p}{m}, \tag{9}$$
$$\dot{p} = \frac{1}{\rho^w}\int_{-\infty}^{\infty}\Theta(q,p-\xi)\rho^w(q,\xi)d\xi.$$

We can use the above formula to realize the time evolution of the entangled trajectories.

3 Wigner function evolution by eigenvalue

We study a special case where the particle is experiencing a one-dimensional attractive potential, $V=-e^{-x^2/2\sigma^2}$. Thus the Schrödinger equation becomes

$$H\Psi(x)=\left\{-\frac{1}{2}\frac{d^2}{dx^2}-e^{x^2/2\sigma^2}\right\}\Psi(x). \tag{10}$$

Here we set $\hbar=1$. Then we can expand the wave function by a set of Gaussian functions with different widths, which means

$$\Psi(x)=\sum_{n=1}^{n_{max}} a_n\psi_n(s), \tag{11}$$

where the basis function is

$$\psi_n(x)=\frac{e^{-x^2/2\beta_n^2}}{(\sqrt{\pi}\beta_n)^{1/2}}, \tag{12}$$

and $\beta_n=\sqrt{n}\beta_0$. Such method used to propagate Wigner function have been discussed by Wong [2] and here we only give main results without deduction. Notice that the normalized basis is not orthogonal, then we can obtain

$$B_{nm}=\langle n|m\rangle=\sqrt{\frac{2\beta_n\beta_m}{\beta_n^2+\beta_m^2}}, \tag{13}$$

as the matrix element of overlap matrix B. Based on properties of Gaussian function, we further construct eigenvalue equation as

$$(T+V)a=EBa, \tag{14}$$

where T is the matrix for kinetic term, with elements

$$T_{nm}=\left\langle n\left|-\frac{1}{2}\frac{d^2}{dx^2}\right|m\right\rangle=\frac{1}{2}\sqrt{\frac{2\beta_n\beta_m}{\beta_n^2+\beta_m^2}}\frac{1}{\beta_n^2+\beta_m^2}. \tag{15}$$

V is the matrix for potential, then

$$V_{nm}=\langle n|-e^{-x^2/2\sigma^2}|m\rangle=-\sqrt{\frac{2\beta_n\beta_m}{\beta_n^2+\beta_m^2}\frac{\sigma^2}{\beta_{nm}^2+\sigma^2}}, \tag{16}$$

where $\beta_{nm}^2=\frac{\beta_n^2\beta_m^2}{\beta_n^2+\beta_m^2}$. Then the eigenvalues can ba obtained by solving Eq. 14 by invert matrix B to the left side. Our initial state can be set as

$$\Phi(x,t=0)=\sum_\lambda b_\lambda\Psi_\lambda(x). \tag{17}$$

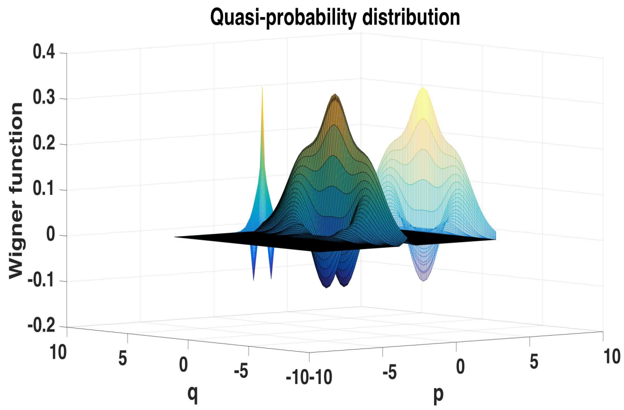

Figure 1: Initial Wigner function.

where b_λ is amplitudes of eigenstates $\Psi_\lambda(x)$, which need to be normalized by $\int dx|\Psi_\lambda(x)|^2 = 1$. Time dependent wave function turns to be

$$\Phi(x,t=0)=\sum_\lambda b_\lambda e^{-iE_\lambda t}\Psi_\lambda(x). \tag{18}$$

According to the definition and after doing several integral, we can construct Wigner function as

$$\rho^w(q,p,t)=\frac{1}{2\pi}\sum_{nm}c_n(t)c_m^*(t)\rho_{nm}^w(xp), \tag{19}$$

where

$$c_n(t)=\sum_\lambda b_\lambda e^{iE_\lambda t}a_{\lambda n}, \tag{20}$$

$$\rho_{nm}^w(xp)=2\sqrt{\frac{2\beta_n\beta_m}{\beta_n^2+\beta_m^2}}e^{-\nu_{nm}}, \tag{21}$$

$$\nu_{nm}=\frac{(\beta_n^2+\beta_m^2)(x^2-\mu_{nm}^2/4)}{2\beta_n^2\beta_m^2}, \tag{22}$$

$$\mu_{nm}=4\frac{\beta_n^2\beta_m^2}{\beta_n^2+\beta_m^2}\left[x\left(\frac{1}{2\beta_n^2}-\frac{1}{2\beta_m^2}\right)+ip\right]. \tag{23}$$

Then using Eq. 19, we can obtain Wigner function at any time. In our calculation, we set $\sigma=3$, $n_{max}=50$, $\beta_0=1$, $b_\lambda=1/\sqrt{2}$, and pick two lowest real eigenvalues, $E_0=-0.844$ and $E_1=-0.3147$, respectively.

4 Results and discussion

By the accurate time evolution of Wigner function, we can study the behavior of quantum trajectories based on Eq. 9, starting from the initial condition selected in the phase space.

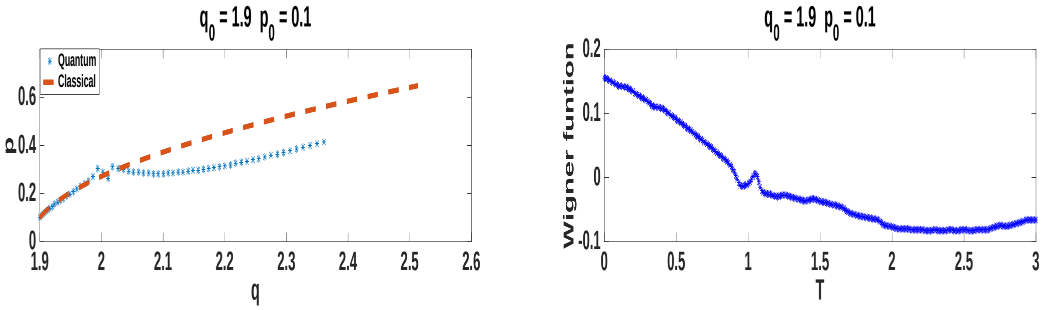

Figure 2: Wigner function starts from positive value.

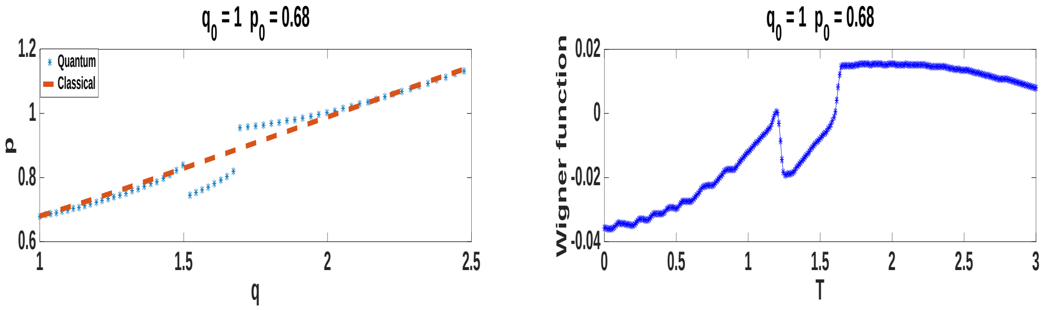

Figure 3: Wigner function starts from negative value.

Energy of out initial state is $(E_0+E_1)/\sqrt{2}=0.8193$, which should also correspond to the initial energy of our classical system. We pick 4 different initial points sharing the same energy in the phase space, locating at (1.9,0.1), (1,0.67), (1.5,0.45), (−1.8,0.24) as (q_0,p_0). Wigner functions $\rho^w(q(t),p(t))$ are illustrated correspondingly. Fig. 2 starts from a point where Wigner function is positive and the first stage of the quantum trajectories matches the classical one pretty well before Wigner function turns to zeros. A fluctuating behavior can be observed in both graphs when Wigner function is approximately zero, which will cause singularity according to Eq. 9. Afterwards quantum trajectory deviates from the classical one. Similar phenomena occur in Fig. 3 and even more obvious in Fig. 4 with a zero Wigner function at the beginning. Fig. 5 give us a chance to witness the fact that a stronger quantum effect can separate quantum and classical trajectories even the Winer function is far from zero point. The wave packet starts from $q_0=-1.8$ and move towards the center of potential, which means quantum effect plays an increasingly important role. When $q>-1.72$, quantum trajectory starts deviating from the classical one remarkably. Such effect can be explained by the series expansion of Eq. 9,

$$\dot{p}=-V'(q)+\frac{\hbar^2}{24}V'''(q)\frac{1}{\rho^w}\frac{\partial^2\rho^w}{\partial p^2}+\cdots \tag{24}$$

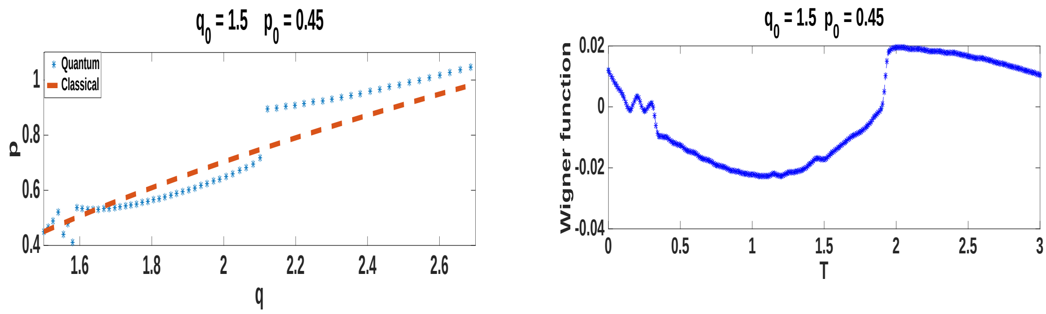

Figure 4: Wigner function starts from zero.

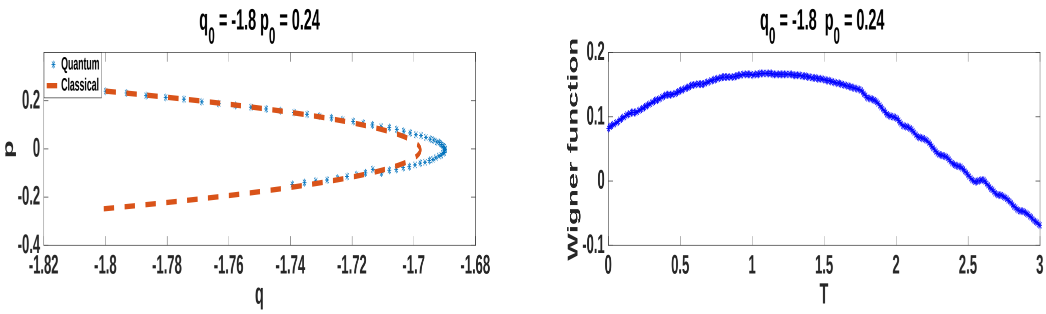

Figure 5: Quantum effect causes separation.

The first term on the right side is as same as the term in classical equation of motion. However, quantum effect accounts for higher order terms which are also the explanation for our results in Fig. 5.

5 Conclusion

We used eigenvalue method to propagate Wigner function accurately and then we use equation of motion, deducted from quantum Liouville equation, to study quantum trajectories in the phase space. Based on the analysis above, we figure out that when quantum effect is not strong and Wigner function is far from zero, quantum trajectory will be similar to the classical one. However, quantum trajectory will definitely fluctuate or even jump when the corresponding Wigner function approaches zero. Thus the property that Wigner function can have negative values must play a profound role in the gap between quantum and classical world since zero points can not be avoided during the evolution.

There are still various interesting problems with respect to Wigner function and quantum trajectories. The most significant one should be developing a general numerical technique to realize the time evolution of Wigner function. There are several attempts, for instance, ETMD [1] can be effective when we tackle certain cases even though the negative values have to be abandoned, which means deep and fascinating physics insights might not be captured. Further study will also cover realms concerning entanglement entropy [3] formed by Wigner function, and even we can study entanglements between distinct quantum trajectories by the definition of trajectory's entropy.

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References

[1] A. Wang, Y. Zheng, C. C. Martens, and W. Ren, Phys. Chem. Chem. Phys. 11(2009), 1588-94.
[2] C.-Y. Wong, J. Optics B5 (2003) S420.
[3] G. Manfredi, M. R. Feix, Phys. Rev. E 62(2000) 4665.