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Quantum tunneling dynamics in symmetrical driven double well system based on Husimi representation

Feng Xu [a,*], Liangjun Zhai [b], Yujun Zheng [c]

[a] School of Physics and Telecommunication Engineering, Shaanxi University of Technology, Hanzhong 723001, China
[b] The School of Mathematics and Physics, Jiangsu University of Technology, Changzhou 213001, China
[c] School of Physics, Shandong University, Jinan 250100, China

HIGHLIGHTS

- Three different physical mechanisms of tunneling process have been shown, chaotic behavior of entangled trajectories enhances quantum tunneling process.
- Chaotic behavior of entangled trajectories enhances quantum tunneling process.
- Quantum coherence suppresses quantum wave packet tunneling.

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ABSTRACT

In present study, the quantum tunneling process in symmetrical driven double-well system is studied by using the entangled trajectory molecular dynamics method based on the Husimi representation. Quantum tunneling dynamics show three different physical mechanisms vary with the amplitude and frequency of driven force: reposeful tunneling, chaos-assisted tunneling, oscillatory tunneling. Different form other methods, quantum underline dynamics process are explored by showing entangled trajectory in the phase space. We show chaotic behavior of entangled trajectories in the phase space, and the quantum tunneling process is vividly shown by comparing entangled trajectory with the classical trajectory with the same initial state. Furthermore, we discuss the effect of symmetry breaking on the potential to the quantum dynamical process, quantum tunneling probability will be remarkably reduced by breaking potential's symmetry. Finally, the suppression of quantum wave packet tunneling under strong force is presented.

1. Introduction

In the study of quantum physics, quantum dynamical processes in driven systems is always an interesting and important subject. In particular, the tunneling dynamics of driven system have attracted much attention [1,2]. As a purely quantum phenomenon, tunneling plays an important role in many physical, chemical and biological processes. Quantum dynamical tunneling process has been presented unambiguous in bound states by Davis and Heller [3]. The tunneling dynamics with a time-periodic driving field was usually used to study the control of quantum tunneling process, and many interesting phenomena have been found, such as the chaos-assisted tunneling [4–6], the resonance assisted tunneling [7], the photon-assisted tunneling [8,9] and the coherent destruction of tunneling [10,11]. The chaos-assisted tunneling is caused by an

* Corresponding author.
E-mail addresses: xufengxlx@snut.edu.cn (F. Xu), yzheng@sdu.edu.cn (Y. Zheng).

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intermediate state which resides in a classic chaotic region in the phase space. The tunneling frequency is enhanced by several order of magnitude because of the classical chaos, which have been experimentally observed recently in various systems. The coherent destruction of tunneling is quite opposite to the chaos-assisted tunneling, the tunneling between the wells can be completely suppressed by choosing appropriate parameters of driven force. The control of quantum tunneling has important significance in both the understanding and application of quantum physics. Recently, the quantum dynamical behavior in oscillatory driven system has been numerically studied [12–18], and it is shown that the time-dependent transition probability for an initially localized wave packet between the wells showed two types of motion: coherent and incoherent motion. Hai and coworkers investigated the coherent control of quantum tunneling for a single particle in driven systems [19], whose results could be useful for the experiments of controlling single-particle tunneling.

Some semiclassical methods based on trajectory has been used as an effective tool to deal with quantum dynamics process [20–22]. Atom–Diatom collision based on complex classical dynamics method first introduced by W.H. Miller [20]. The semiclassical method based on Husimi function was expand by S. Adachi. The tunneling phenomenon in non-integrable system first studied based on semiclassical method by Shudo and his co-workers [21]. Quantum maps for time continuous systems based on semiclassical method has been developed by Takahashi and Ikeda [22]. Entangled trajectory molecular dynamics method (ETMD) is an new developed semiclassical method based on quantum phase space theory [23–30]. It not only can be used as a powerful tool to numerically solve the quantum Liouville equation, but also reveal quantum underline dynamical process through showing entangled trajectories in phase space. Compared to classical molecular dynamics method, ETMD method get quantum effect in the evolution and need lesser trajectories to get convergent results [26,31]. Another key point of ETMD is that the computational time cost increase with the number of degrees of freedom is linearly (not exponential form) [32]. Some important works have been done using ETMD method in many fields of physics, such as capturing quantum tunneling effect in quantum dynamics [23–25,31,32], calculating photodissociation cross section of water [26], and autocorrelation function [33]. The ETMD method used in the previous works were mostly based on Wigner representation, which could be negative anywhere even the initial state is positive. However, ETMD method based on Wigner representation could not get the negative part of Wigner function because it needs to use a positive definited ansatz approximation. Therefore, some important information about quantum dynamics would be missed. For example, it cannot describe quantum interference phenomenon accurately [34]. To avoid this problem, the ETMD method based on the Husimi representation could be an alternative suggestion, since the Husimi representation is positive at all time,the accuracy based on Husimi representation has been demonstrated [24]. Some previous works on the tunneling for a driven system also based on Husimi representation [35–37].

In present work, the quantum tunneling dynamical process in the symmetrical driven double-well system is studied using the ETMD method based on the Husimi representation. Besides the usual numerical calculation results, the quantum underline dynamics processes are also presented through showing the entangled trajectories in the phase space. Based on the numerical calculation, the relations between the amplitude and frequency of driven force and quantum tunneling dynamical process is investigated. It is shown that the quantum tunneling probability will increase with the enhancement of driven force for a non-resonance frequency. However, when the driven force is strong enough, quantum tunneling dynamics show different behaviors. There are three types quantum tunneling for the strongly driven force with same amplitude: reposeful tunneling for the low frequency, chaos-assisted tunneling for the moderate frequency, and oscillatory tunneling for the high frequency. To characterize the physical picture of the quantum tunneling process, the corresponding classical trajectories with the same initial states of entangled trajectories are also displayed in the phase space. Since the symmetry of potential has a great effect on quantum dynamics, quantum tunneling probability with asymmetry and symmetry potential is presented. It is shown that quantum tunneling probability will remarkably reduce by breaking the symmetry of potential surface. In the end, quantum dynamical tunneling process under strong force is showed, the wave packet will be suppressed in the left well for a while in this case.

The structure of this paper is as follows. In Section 2, the basic theoretical formalism of the ETMD method based on Husimi representation and the model of symmetrical driven double-well system are presented. In Section 3, the quantum tunneling probability are calculated to show the dependence of tunneling dynamics on the amplitude and frequency of the driven force. A visual physical picture of entangled trajectories and corresponding classical ones are displayed together with their energy evolution. The properties of quantum tunneling process with respect to the symmetry of the potential are investigated. We discuss quantum dynamical behavior under strong force in the end. Some conclusions are drawn in Section 4. Atomic units are used throughout the paper unless noted and $\hbar = 1$ is used in our calculations.

2. Theory

2.1. ETMD based on Husimi representation

In quantum phase space theory, the state of a system can be described by the quantum probability distribution function, which is the same as a wavefunction. The most famous quantum probability distribution function is Wigner function, which is first introduced by Wigner in the derivation of quantum correction terms to the Boltzmann formula. The definition of quantum probability distribution functions are not uniqueness, another often used quantum probability distribution function is the Husimi function, which is nonnegative in any way, and can get by smooth Wigner distribution with a Gaussian wave packet. The Husimi distribution behaves most regularly and has the simplest and smoothest structure in phase space,