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Quantum dynamics in double-well system with polychromatic perturbation using entangled trajectory molecular dynamics method

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Abstract. We investigate quantum dynamics in a double-well system subject to time-dependent perturbation with some incommensurate frequencies using entangled trajectory molecular dynamics method. We first compare time evolution of energy of the driven system with two mode perturbation under classical dynamics with one under quantum dynamics, it is found that quantum dynamics obeys Ehrenfest's theorem and it shows our results obtain from entangled trajectory molecular dynamics method are correct and accurate. Quantum coherence suppresses trajectory which initial energy is higher than barrier to get over it, this process is named coherent destruction of tunneling (CDT). We show this interesting phenomenon through showing entangled trajectory and corresponding classical trajectory in phase space and discuss their energy fluctuation with time. Furthermore, we discuss quantum dynamics with different frequency mode perturbation from the perspective of autocorrelation evolution, classical chaos brings remarkable influence on quantum-mechanical phenomena.

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Key words: Entangled trajectory molecular dynamics method, Coherent destruction of tunneling, Classical chaos.

1 Introduction

Quantum dynamics process in a double-well system with a periodically oscillating external field has been one of the subjects of long-lasting interest in diverse branches of physics and chemistry [1]. In particular, the coherent destruction of tunneling (CDT) which is an interesting phenomenon originally discovered by Grossmann has attracted

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much attention [2–4]. CDT phenomenon displays coherent control of quantum dynamics via a periodically oscillating external field, it has potential application in quantum motor and quantum-information processing and is very useful to understand much fundamental time-dependent processes [5, 6]. Even weak chaos can bring huge effect on quantum dynamics, Igarashi investigated classical chaos effect on dynamical behavior in driven quantum double-well systems numerically and showed chaos-assisted tunneling [7–9]. Recently, we study chaos-assisted tunneling of driven double-well system uses a new method named entangled trajectory molecular dynamics method (ETMD) and show this quantum phenomenon vividly with the help of entangled trajectories in phase space [10].

Entangled trajectory molecular dynamics method is an effective improvement to classical dynamics molecular method [10,13–18], it includes quantum effect during dynamics process at the cost of statistical independence of trajectories. ETMD not only can be used as a numerical method to solve the quantum Liouville equation, but also can show quantum underline dynamics process through showing entangled trajectories in phase space. A lot of works show ETMD method is an effective tool to deal with quantum dynamics of small molecular system, such as: capturing quantum tunneling effect [13–15, 19, 20], calculating photodissociation crosssection of water in its first absorption band [16], and autocorrelation function [21]. Most of these works used ETMD method used Wigner function which is well-known quantum phase space distribution function can be negative even the initial is positive anywhere to describe the evolution of the system. ETMD needs a positive definited ansatz approximation to fit the relationship between trajectories and distribution function, this approximation makes ETMD method based on Wigner presentation miss some important information about quantum dynamics, such as can not describe quantum interference phenomenon accurately [22]. For avoiding it, we use Husimi function which is positive anywhere to study quantum dynamics process in double-well system with polychromatic perturbation.

In the present paper, we study quantum dynamical behaviors in double well system with polychromatic perturbation using ETMD method based on Husimi presentation. Different from other similar works, we not only give some numerical calculation results, but also show quantum underline dynamics process through showing entangled trajectories in phase space. Firstly, we indirectly demonstrate ETMD method is a correct and accurate tool to deal with quantum driven system through checking the evolution of energy, the accord with Ehrenfest's theorem shows our numerical calculation is reasonable and precisely. The core of this paper is show coherent destruction of tunneling phenomenon with entangled trajectory and compare to classical one, we show the evolution of quantum coherence in this interesting case. At the end, we discuss quantum dynamics with different frequency mode perturbation from the perspective of autocorrelation evolution, the classical dynamics of some frequency mode perturbation shows chaotic behavior, chaos brings remarkable influence on quantum-mechanical phenomena.

The structure of this paper is as follows. In Section 2, we describe the basic theoretical formalism of the entangled trajectory molecular dynamics method based on Husimi representation and the model of double-well system with polychromatic perturbation. In