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Gaussian wavepacket dynamics and quantum tunneling in asymmetric double-well systems

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HIGHLIGHTS

- We have studied dynamics of Gaussian wavepacket in asymmetric double-well systems.
- Time-dependent tunneling probability is calculated as a function of the asymmetry.
- Resonant tunneling is not realized for motion starting from the lower minimum of the well.
- Narrower Gaussian wavepacket is less vulnerable to the asymmetry.
- The uncertainty product in the resonant tunneling state is calculated.

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ABSTRACT

We have studied dynamical properties and quantum tunneling in asymmetric double-well (DW) systems, by solving Schrödinger's equation with the use of two kinds of spectral methods for initially squeezed Gaussian wavepackets. Time dependences of wavefunction, averages of position and momentum, the auto-correlation function, an uncertainty product and the tunneling probability have been calculated. Our calculations have shown that (i) the tunneling probability is considerably reduced by a potential asymmetry ΔU, (ii) a resonant tunneling with $|\Delta U| \simeq \kappa\hbar\omega$ is realized for motion starting from the upper minimum of asymmetric potential wells, but not for motion from lower minimum ($\kappa = 0, 1, 2, \ldots$; ω: oscillator frequency at minima), (iii) the reduction of the tunneling probability by an asymmetry is less significant for the Gaussian wavepacket with narrower width, and (iv) the uncertainty product $\langle\delta x^2\rangle\langle\delta p^2\rangle$ in the resonant tunneling state is larger than that in the non-resonant tunneling state. The item (ii) is in contrast with the earlier study [D. Mugnai, A. Ranfagni, M. Montagna, O. Pilla, G. Viliani, M. Cetica, Phys. Rev. A 38 (1988) 2182] which showed the symmetric result for motion starting from upper and lower minima.

1. Introduction

Double-well (DW) systems have been extensively studied in a wide range of fields including physics, chemistry and biology (for a recent review on DW systems, see Ref. [1]). Quantum tunneling is one of the most fascinating phenomena in DW systems [2]. Many experimental and theoretical studies have been made on the tunneling of a quantum particle in DW systems. Quantum tunneling of a particle is possible from one-side well to the other-side well through a classically forbidden region. Well-known old examples of DW systems include an inversion of ammonia molecules. In recent years, there has been an advance in the experimental study on macroscopic quantum tunneling such as a Josephson junction and Bose–Einstein condensation in a double trap.

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A DW potential does not have to be symmetric and it may be asymmetric in general. In many experiments, the asymmetry of the DW potential can be changed by modifying external parameters. However, most theoretical studies have been made for symmetric DW systems, and asymmetric systems have received less theoretical attention than symmetric ones [3–8]. This is because solving an asymmetric DW system is more difficult than a symmetric one. Theoretical studies on asymmetric DW systems have been made based on various approximate methods like the WKB for simplified artificial DW potentials which are analytically tractable but not realistic [2]. By using such DW potentials, Weiner and Tse [3], and Nieto et al. [4] showed that although the tunneling probability is significantly reduced by the potential asymmetry, it is enhanced when the asymmetry meets the resonance condition. Mugnai et al. [5] studied the fractal nature of the trajectory in asymmetric DW systems. By using WKB, Song [6] studied an asymmetric DW system where the difference of the potential minima is close to a multiple of $\hbar\omega$ (harmonic frequency in the wells). Rastelli [7] obtained a semi-classical formula for the tunneling amplitude in asymmetric DW systems with the use of the WKB method. Conventional theories for DW systems have adopted the two-level approximation where the initial state in one-dimensional system is assumed to be given by $\Psi(x,0) = [\Psi_0(x) - \Psi_1(x)]/\sqrt{2}$, $\Psi_\nu(x)$ denoting the νth ($\nu = 0, 1$) eigenfunction. In order to discuss the tunneling probability in asymmetric DW systems, Cordes and Das [8] proposed a generalized two-level approximation: a related discussion will be given in Section 4.

For a study on the dynamics of wavepacket or tunneling in DW systems, it is necessary to solve the time-dependent Schödinger equation subject to appropriate initial and boundary conditions [9]. In the past when quantum mechanics was born, it was very difficult to numerically solve the time-dependent Schödinger equation even for a simple potential except for a harmonic oscillator (HO) potential. One had to develop approximation methods applicable to simple tractable DW models although they are not necessarily realistic. In recent years, however, there have been significant developments in computers and their software. It is now possible for us to solve the time-dependent Schrödinger equation with sufficient accuracy, by using convenient packages such as MATHEMATICA, MATLAB and Maple.

The purpose of the present study is to numerically study dynamics of Gaussian wavepackets and to examine the effect of the asymmetry on quantum tunneling in asymmetric DW systems. Quite recently it has been pointed out that a potential asymmetry of a DW system has significant effects on its specific heat [10]. We expect that it is the case also for dynamical properties of DW systems. We will solve the time-dependent Schödinger equation by the spectral method for a given squeezed Gaussian wavepacket [11,12], adopting the realistic quartic DW potential. In order to investigate the influence of the initial state on dynamical properties, we adopt two squeezed Gaussian wavepackets with different parameters.

The paper is organized as follows. In Section 2, we will briefly mention the model and calculation method employed in our study [13]. In solving the time-dependent Schrödinger equation, we have adopted the two kinds of spectral method A (Eq. (16)) and spectral method B (Eq. (22)) with energy matrix elements evaluated for a finite size N_m (= 30). By using the spectral method A, we have calculated time-dependences of the magnitude of wavefunction, expectation values of position and momentum, the auto-correlation function, the uncertainty product and the tunneling probability, whose results are reported in Section 3. In Section 4 the tunneling probability is discussed with the use of the spectral method B. We discuss also wavepacket dynamics when the Gaussian wavepacket starts from near the top of the DW potential. Section 5 is devoted to our conclusion.

2. Adopted model and calculation method

2.1. Asymmetric double-well systems

We assume a quantum DW system whose Hamiltonian is given by

$$H = \frac{p^2}{2m} + U(x) = H_0 + V(x), \tag{1}$$

where

$$U(x) = C\ (x^2 - x_s^2)^2 - d\left(\frac{x^3}{3} - x_s^2 x\right), \quad \left(C = \frac{m\omega^2}{8x_s^2}\right) \tag{2}$$

$$H_0 = \frac{p^2}{2m} + U_0(x), \tag{3}$$

$$U_0(x) = \frac{m\omega^2 x^2}{2}, \tag{4}$$

$$V(x) = U(x) - U_0(x). \tag{5}$$

Here m, x and p express mass, position and momentum, respectively, of a particle, $U(x)$ denotes the DW potential with a degree of the asymmetry d, H_0 signifies the Hamiltonian for an HO potential $U_0(x)$ with the oscillator frequency ω, and $V(x)$ stands for a perturbing potential to H_0. The asymmetric DW potential $U(x)$ has locally stable minima at $x = \pm x_s$ and an