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Localization or tunneling in asymmetric double-well potentials



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ABSTRACT

An asymmetric double-well potential is considered, assuming that the wells are parabolic around the minima. The WKB wave function of a given energy is constructed inside the barrier between the wells. By matching the WKB function to the exact wave functions of the parabolic wells on both sides of the barrier, for two almost degenerate states, we find a quantization condition for the energy levels which reproduces the known energy splitting formula between the two states. For the other low-lying non-degenerate states, we show that the eigenfunction should be primarily localized in one of the wells with negligible magnitude in the other. Using Dekker's method (Dekker, 1987), the present analysis generalizes earlier results for weakly biased double-well potentials to systems with arbitrary asymmetry.

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1. Introduction

Quantum tunneling has been of continuing interest since the advent of quantum mechanics, and the inversion of an ammonia molecule and proton tunneling are well-known examples of microscopic quantum tunneling which may be described by one-dimensional models (see, e.g., Refs. [1–3]). For a one-dimensional symmetric double-well potential of two wells being sufficiently separated and deep, the lower energy eigenvalues are closely bunched in pairs, to give rise to tunneling dynamics for a wave packet initially localized in one of the wells with the energy of approximately one of the eigenvalues (see, e.g., Ref. [4]). It has then been well-known that, upon adding a small asymmetry to a symmetric potential, the two states that started out as tunneling states in the symmetric case correspond increasingly to states localized in one well or the other, to quench the tunneling motion [1–3]. Further, it is known that, for an asymmetric potential, if there exist two states which are almost degenerate then tunneling dynamics take place for a localized wave packet made up of those states [5], and the analytic expression for the energy splitting between the states is given in Ref. [6].

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In addition to microscopic quantum tunneling, a recent breakthrough makes it possible to realize macroscopic quantum tunneling in a superconducting quantum interference device with Josephson junctions where numerous microscopic degrees of freedom are tied together to form a collective dynamical variable (see, e.g., Refs. [6–8]), and, for the system of the transmon Hamiltonian of a cosine potential, the analytic expression for the energy splitting between the nearly degenerate even and odd eigenstates is given when the amplitude of the potential is large [8]. In obtaining the expression for the splitting [8] that could exactly reproduce the rigorous mathematical expression for the widths of the low-lying energy bands of the associated Mathieu equation (see Refs. [7.9–11]), a WKB wave function is normalized to be matched in a forbidden region of one of the wells onto a normalized eigenfunction of an harmonic oscillator centered at the minimum of the well: this normalization corrects the underestimate for a low-lying state that the method described in Ref. [12] may give. Then, the tight bonding approximation for a periodic system is applied based on the normalized WKB wave functions [8]. For an asymmetric double-well potential, while the analytic expression for the energy splitting between pairwise degenerate left and right states is succinctly given in Ref. [6], before applying the Lifshitz-Herring approximation for the expression, it is necessary to normalize the WKB wave function by matching it onto a normalized eigenfunction of a harmonic oscillator in a forbidden region between the wells [4,6,13].

Instead of using an approximation with the normalized WKB functions, by assuming that the two wells are parabolic with an angular frequency ω_0 , Dekker in Ref. [14] first shows that the consistency condition which comes from that a WKB function should match onto the exact solutions on both sides of the potential barrier determines the energy splitting between the pair of the lowest eigenvalues, when a small bias is added to a symmetric double-well potential. Further, he shows, if the bias increases, the ground state becomes almost localized in the deeper of the two wells, implying that the tunneling motion is quenched. In Ref. [13], a similar analysis is carried out for the pairs of the low-lying states of an asymmetric potential assuming that the difference of the minima is close to a multiple of $\hbar\omega_0$. Indeed, in the region where the potential is quadratic(parabolic), the exact wave function is described by the parabolic cylinder function, and thus the wave function in its asymptotic expansion could have an additional leading term aside from that of a Hermite–Gaussian wave function of a harmonic oscillator [15], which makes Dekker's method work.

In this article, we will consider an asymmetric double-well potential for which the separation between the two wells is large, assuming that the two wells are parabolic with angular frequencies ω_L and ω_R around the minima of the left-hand and right-hand wells, respectively. In the case that there exist two almost degenerate eigenstates, through the systematic application of Dekker's method, we arrive at a quantization condition for the eigenvalues which is a refined version of that found in a semiclassical analysis without the assumption of parabolicity [16,17]. We further analyze this quantization condition, to find the energy splitting formula given in Ref. [6]. For a low-lying non-degenerate eigenstate, however, as a leading term in the asymptotic expansion of the wave function is dominant over that of the Hermite–Gaussian wave function in one of the wells, we only have an equation which shows that the eigenstate has negligible magnitude in the well and is primarily localized in the other. We also include the two-level approach which amounts to the method used in Ref. [6], not only to provide the explicit form of the normalized WKB function (see, e.g., Refs. [13,18]) but also to supplement the validity of Dekker's method in the vanishing limit of the energy splitting where the wave function is accurately described by the Hermite–Gaussian functions.

This paper is organized as follows: In Section 2, using Dekker's method, we find the quantization condition and the energy splitting formula for the two almost degenerate eigenstates. For a low-lying non-degenerate eigenstate, an equation which shows the localization of the state is given. Particular attention is paid on the validity of the method. In Section 3, the two-level approximation is used to re-obtain the energy splitting formula. In Section 4, we give some concluding remarks.

2. A WKB wave function and the quantization condition

We assume that the double-well potential V(x) has quadratic minima at $x = a_L$ and at $x = a_R$ with angular frequencies ω_L and ω_R , respectively (see Fig. 1). For the eigenfunction $\psi(x)$ corresponding to

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