Supersymmetry and tunneling in an asymmetric double well

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The techniques of supersymmetric quantum mechanics are applied to the calculation of the energy difference between the ground state and the first excited state of an asymmetric double well. This splitting, originating from the tunneling effect, is computed via a systematic, rapidly converging perturbation expansion. Perturbative calculations to any order can be easily carried out using a logarithmic perturbation theory. Our approach yields substantially better results than alternative widely used semiclassical analyses.

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I. INTRODUCTION

In a double-well potential, a classical particle can remain indefinitely in the neighborhood of a higher local minimum that is separated by a barrier from a lower minimum, provided the kinetic energy of the particle is less than the height of the barrier. However, a quantum-mechanical particle with its wave function initially localized in the higher minimum has a finite probability of being found in the lower minimum due to tunneling through the potential barrier. This purely quantum-mechanical effect is of great relevance to many branches of physics and chemistry [1–4]. Of particular interest in this problem is the energy difference $\delta E \equiv E_1 - E_0$, having its origin in this tunneling phenomenon. Recently Bernstein and Brown [4] and Boyanovsky, Willey, and Holman [5] have computed δE using supersymmetric quantum mechanics (SUSY-QM) and the path-integral formalism, respectively. (Readers interested in the path-integral approach to the tunneling can find details in Coleman [6], Callan and Coleman [7], and references therein.) The relevance of SUSY-QM to this problem stems from the following observation. Given any potential $V_-(x)$, with the ground state adjusted to have zero energy, SUSY-QM allows one to construct a partner potential $V_+(x)$ with exactly the same energy eigenvalues except for the ground state, which remains unpaired. Often it is considerably easier to determine the ground state of $V_+(x)$ rather than the first excited state of $V_-(x)$, as was the case in Ref. [4]. In such cases one can profitably use $V_+(x)$ instead of $V_-(x)$ to determine δE. In this paper, we carefully reanalyze the applicability of the techniques of SUSY-QM. In particular, it is shown that the calculation of δE, which originates from a non-perturbative tunneling effect in the potential $V_-(x)$, can be converted to a fully quantum-mechanical, perturbative problem in the partner potential $V_+(x)$. Furthermore, for the nontrivial problem of deep wells, this perturbative expansion is highly convergent and improves substantially upon the semiclassical methods. This has to be contrasted with the variational approach of Ref. [4], where the perturbation correction to the leading term was substantial.

In Sec. II, we briefly review the formalism of supersymmetric quantum mechanics; for a more detailed description the reader is referred to Ref. [8]. In Sec. III, we calculate the energy splitting via SUSY-QM. One way to determine this splitting of the energy levels is to solve the Schrödinger differential equation numerically. However, that becomes increasingly difficult and less reliable as the barrier gets higher and the splitting gets smaller. The SUSY-QM based approach described in this paper gives an extremely reliable and accurate determination of the energy splitting. In fact, the reliability increases for smaller splitting. We compare our SUSY-QM results with numerically computed values, and with those coming from a recent semiclassical analysis [5].

II. SUPERSYMMETRIC QUANTUM MECHANICS

For a quantum-mechanical problem with a potential $V_-(x)$, supersymmetry allows one to construct a partner potential $V_+(x)$ whose energy eigenvalues E_n^+ are in one to one correspondence with the excited states of $V_-(x)$, i.e., $E_{n-1}^+ = E_n^-$, where E_n^- are eigenvalues of $V_-(x)$ and n is a positive integer (i.e., $n \in Z_+$). In the arena of SUSY-QM, it is customary to describe $V_-(x)$ in terms of its ground-state wave function. Hence, let us assume that the wave function $\psi_0^{(-)} \equiv \psi_0$ of $V_-(x)$ is known, and the corresponding ground-state energy E_0^- has been adjusted to be zero. The relevant Schrödinger equation is given by

$$H_-\psi_0(x) \equiv \left[-\frac{d^2}{dx^2} + V_-(x)\right]\psi_0 = 0 \ , \tag{1}$$

and we are using units with $\hbar=2m=1$. The above Hamiltonian can also be written in terms of the ground-state wave function $\psi_0(x)$ as

$$H_- = \left[-\frac{d^2}{dx^2} + \frac{\psi_0''}{\psi_0} \right], \tag{2}$$

where ψ_0'' represents the second spatial derivative of the wave function. We now define two operators

$$A = \left[\frac{d}{dx} - \frac{\psi_0'}{\psi_0} \right], \quad A^\dagger = \left[-\frac{d}{dx} - \frac{\psi_0'}{\psi_0} \right]. \tag{3}$$

In terms of A and $A^\dagger$, the Hamiltonian H_- is simply given by $A^\dagger A$. However, one can define another operator $H_+ \equiv A A^\dagger = -d^2/dx^2 + V_+(x)$, where

$$V_+(x) = V_-(x) - 2\frac{d}{dx}\left[\frac{\psi_0'}{\psi_0} \right] = -V_-(x) + 2\left[\frac{\psi_0'}{\psi_0} \right]^2 .$$

By construction, H_+ is a Hermitian and positive semidefinite operator. The potentials $V_-(x)$ and $V_+(x)$ are known as supersymmetric partners. We shall show shortly that they have the same eigenvalues except for the ground-state energy E_0^-. The superpotential $W(x)$ is related to ψ_0 by $W(x) = -\psi_0'/\psi_0$ or equivalently $\psi_0(x) = \exp[-\int^x W(x')dx']$. Operators A and $A^\dagger$ can now be written as

$$A = \left[\frac{d}{dx} + W(x) \right], \quad A^\dagger = \left[-\frac{d}{dx} + W(x) \right], \tag{4}$$

and the potentials $V_-(x)$ and $V_+(x)$ are given by

$$V_\pm = W^2(x) \pm W'(x), \quad W'(x) = \frac{dW}{dx} . \tag{5}$$

The commutator $[A, A^\dagger]$ is equal to $2W'(x)$.

Now we shall explicitly show the correspondence between E_n^- and E_{n-1}^+. Let us denote the eigenfunctions of $H_\pm$ that correspond to eigenvalues $E_n^\pm$, by $\psi_n^{(\pm)}$. One discovers that for $n \neq 0$,

$$\begin{aligned} H_+(A\psi_n^{(-)}) &= AA^\dagger(A\psi_n^{(-)}) = A(A^\dagger A\psi_n^{(-)}) \\ &= AH_-(\psi_n^{(-)}) = E_n^-(A\psi_n^{(-)}) , \end{aligned} \tag{6}$$

and thus for positive integral values of n, $A\psi_n^{(-)}$ is an eigenfunction of H_+, and we shall call it the supersymmetric partner state of $\psi_n^{(-)}$. Since the ground state of $V_-(x)$ does not have a SUSY partner ($A\psi_0^{(-)}=0$), one finds $E_{n-1}^+ = E_n^-$, where $n \in Z_+$. Thus, if the eigenvalues and the eigenfunctions of H_- were known, one automatically learns the eigenvalues and the eigenfunctions of, what in general is, a completely different Hamiltonian H_+.

III. CALCULATION OF THE ENERGY DIFFERENCE

In a potential with a symmetric double-well structure, eigenstates with energy substantially below the peak of the barrier, necessarily occur in pairs with small energy splitting. This splitting of energy levels gets smaller as the barrier increases. The same is also true for asymmetric double wells, provided the deviation from the symmetry is small. In low-energy studies the splitting between lowest two states play a dominant role. in the rest of this section, we will evaluate this energy splitting for an asymmetric well using SUSY-QM and compare with results obtained from the WKB formalism of Boyanovsky, Willey, and Holman [5] and with the numerical values resulting from solving the Schrödinger equation directly. We will extend the formalism developed by Keung, Kovacs, and Sukhatme [9] for finding the energy difference for symmetric double wells. The tunneling probability in an asymmetric double well has also been used to compute the rate of a chemical reaction in Ref. [11].

In order to use the SUSY-QM method one needs to know the ground-state wave function $\psi_0^{(-)}$. A specific example of an asymmetric double well which we will consider in detail corresponds to a ground-state wave function which is the sum of two Gaussians centered at $\pm x_0$,

$$\psi_0^{(-)} = e^{-(x+x_0)^2} + e^{-a(x-x_0)^2} . \tag{7}$$

The positive parameter a is a measure of the asymmetry, and $a=1$ corresponds to a symmetric wave function. The corresponding superpotential and potential are given by

$$W(x) = -\frac{\psi_0'^{(-)}(x)}{\psi_0^{(-)}(x)} = \left[\frac{-2a(x-x_0)e^{-a(x-x_0)^2} + 2(x+x_0)e^{-(x+x_0)^2}}{e^{-(x+x_0)^2} + e^{-a(x-x_0)^2}} \right]$$

and

$$V_-(x) = \frac{\psi_0''^{(-)}(x)}{\psi_0^{(-)}(x)} = \left[\frac{[-2a+4a^2(x-x_0)^2]e^{-a(x-x_0)^2} + [-2+4(x+x_0)^2]e^{-(x+x_0)^2}}{e^{-(x+x_0)^2} + e^{-a(x-x_0)^2}} \right],$$

respectively.

In Fig. 1, we have plotted $V_-(x)$ for various values of the asymmetry parameter a. For $a=1$, they reduce to the symmetric case treated in Ref. [9], i.e.,

$$W(x) = 2[x - x_0\tanh(2xx_0)]$$

and

$$V_-(x) = 4[x - x_0\tanh(2xx_0)]^2 - 2[1 - 2x_0^2\operatorname{sech}^2(2xx_0)] .$$

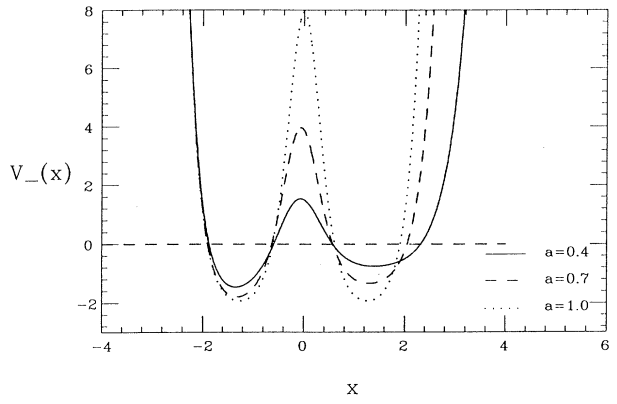

FIG. 1. This set of graphs depicts the form of $V_-(x)$ for three different values of the asymmetry parameter a. These potentials correspond to the ground-state wave functions given in Eq. (7).

Increasing x_0 increases the height of the barrier, and also increases the distance between valleys.

To find δE, since the ground-state energy of $V_-(x)$ is zero, we have to determine the energy of the first excited state of $V_-(x)$, and that, due to supersymmetry, happens to be the same as the ground-state energy of the potential $V_+(x)$. Frequently, it is easier to determine numerically the ground-state energy of $V_+(x)$ than the first excited state of $V_-(x)$ [4].

From the ground-state wave function $\psi_0^{(-)}$ of H_-, we can generate a function $1/\psi_0^{(-)}$ that solves the Schrödinger equation for H_+ with an eigenvalue zero; i.e., $H_+(1/\psi_0^{(-)})=0$. However, $1/\psi_0^{(-)}$ is not a normalizable function since $1/\psi_0^{(-)}\to\infty$ as $|x|\to\infty$. But from this function, one can construct a normalizable function $\phi(x)$,

$$\phi(x)=\frac{\int_x^\infty[\psi_0^{(-)}(y)]^2dy}{2I_+\psi_0^{(-)}(x)} \quad \text{for } x>0$$
$$=\frac{\int_{-\infty}^x[\psi_0^{(-)}(y)]^2dy}{2I_-\psi_0^{(-)}(x)} \quad \text{for } x<0\ , \tag{8}$$

with $I_\pm$ given by

$$I_-=\left[\int_{-\infty}^0[\psi_0^{(-)}(y)]^2dy\right]\ ,$$
$$I_+=\left[\int_0^\infty[\psi_0^{(-)}(y)]^2dy\right]\ , \tag{9}$$

respectively. The function $\phi(x)$ is well defined for all values of x. It is easy to see that $\phi(x)$ is continuous at $x=0$ with a value $\phi(0)=1/2\psi_0^{(-)}(0)$. One can easily show $H_+\phi(x)=0$ for $x\neq 0$. However, $\phi(x)$ is also not an eigenfunction of H_+, as its derivative has a discontinuity at the origin; the discontinuity is given by

$$\phi'|_{+\epsilon}-\phi'|_{-\epsilon}=-\frac{\psi_0^{(-)}(0)}{2}\left[\frac{1}{I_+}+\frac{1}{I_-}\right]\ . \tag{10}$$

However, $\phi(x)$ can be viewed as the ground-state wave function of the singular Hamiltonian H_0 given by

$$H_0=H_+-[\psi_0^{(-)}(0)]^2\left[\frac{1}{I_+}+\frac{1}{I_-}\right]\delta(x)\ ,$$

which allows eigenfunctions with discontinuous derivative owing to the presence of the δ-function term. Equivalently, one can write

$$H_+=H_0+\delta H$$
$$=H_0+[\psi_0^{(-)}(0)]^2\left[\frac{1}{I_+}+\frac{1}{I_-}\right]\delta(x)\ , \tag{11}$$

and hence the ground-state eigenvalue and the eigenfunction of H_+ can be determined perturbatively by considering $[\psi_0^{(-)}(0)]^2[1/I_++1/I_-]\delta(x)$ as a perturbation on the unperturbed Hamiltonian H_0. Here we should like to point out that $\psi_0^{(-)}(0)$ plays the role of a small expansion parameter of this problem. This is an especially good choice for a symmetric double-well potential with a high barrier since the value of $\psi_0(0)$ is very small. For the asymmetric case, there is nothing particularly special about the origin and the discontinuity of $\phi(x)$ described in Eq. (10) can be chosen at another point, say $x=\bar{x}$. If $\bar{x}$ is chosen at the peak of the barrier (where $\psi_0^{(-)}$ has a very small value); the perturbation expansion converges even more rapidly. All the equations in this paper have been written with the choice $\bar{x}=0$, but a generalization to an arbitrary value of $\bar{x}$ is straightforward.

The first-order correction to the energy is

$$E^{(1)}=\frac{\int_{-\infty}^\infty\phi(x)(\delta H)\phi(x)dx}{\int_{-\infty}^\infty\phi^2(x)dx}$$
$$=\frac{\int_{-\infty}^\infty\phi(x)[\psi_0^{(-)}(0)]^2\left[\frac{1}{I_+}+\frac{1}{I_-}\right]\delta(x)\phi(x)dx}{\int_{-\infty}^\infty\phi^2(x)dx}$$
$$=\frac{1}{4}\left[\frac{1}{I_+}+\frac{1}{I_-}\right]\frac{1}{\int_{-\infty}^\infty\phi^2(x)dx}\ . \tag{12}$$

Higher-order corrections can be computed using the familiar Rayleigh-Schrödinger perturbation expansion, but this involves summations over all intermediate unperturbed eigenstates, which in general are not known. A much simpler alternative approach is to use logarithmic perturbation theory [10], which only requires knowledge of the unperturbed ground-state wave function. The second-order correction to the energy is given by

$$E^{(2)}=-\left[\int_{-\infty}^0dx\left[\frac{E^{(1)}\int_{-\infty}^x\phi^2(y)dy}{\phi(x)}\right]^2\right.$$
$$\left.+\int_0^\infty dx\left[\frac{E^{(1)}\int_x^\infty\phi^2(y)dy}{\phi(x)}\right]^2\right]\ , \tag{13}$$

and the second-order corrected δE is given by $E^{(1)}+E^{(2)}$. Similarly, even higher-order corrections can be readily computed.

As mentioned before, an alternative analytic approach

for computing δE is the WKB method. Reference [5] is one of the most recent references on this formalism. It gives the following expression for the energy difference δE:

$$\delta E = \frac{2}{T_1}[(\delta W)^2 + e^{-2W_2}]^{1/2}, \tag{14}$$

where

$$T_1 = \int_{x_1}^{x_2} dx[E - V_-(x)]^{-1/2},$$
$$W_2 = \int_{x_2}^{x_3} dx[V_-(x) - E]^{1/2},$$

and δW is equal to $W_3 - W_1$. W_1 and W_3 are themselves given by

$$W_1 = \int_{x_1}^{x_2} dx[E - V_-(x)]^{1/2},$$
$$W_3 = \int_{x_3}^{x_4} dx[E - V_-(x)]^{1/2}. \tag{15}$$

The limits of integrations x_1, x_2, x_3, and $x_4 (x_1 < x_2 < x_3 < x_4)$ are roots of the equation $[E - V_-(x)] = 0$. In general, four classical turning points are to be expected for double-well potentials.

To check the performance of the SUSY-QM and WKB methods, we also computed δE by solving Schrödinger equation numerically using the fourth-order Runge-Kutta method. This was done for the specific example of Eq. (7). We call it the numerical result of Fig. 2. We also calculated δE using WKB method, and in Fig. 2, plotted all three values of δE [obtained from Eqs. (13), (14), and from the numerical solution], as functions of x_0 for $a = 0.4$. We find that, as x_0 increases the barrier gets higher, and the SUSY-QM generated result for δE approaches extremely close to the numerical answer and it is better than the WKB value for all values of x_0. In Fig. 2, for $x_0 > 1.5$ the SUSY-QM generated result agrees so well with the numerical result that their graphs practically fuse with each other. In Figs. 3(a) and 3(b), we plot δE calculated by different methods against the asymmetry parameter a, keeping x_0 fixed at the values of 1.2 and 2.0, respectively. It is worth mentioning that in Fig. 3(a) our approximation is poorer for the asymmetric well as compared with the symmetric one. This is to be expected as the perturbation parameter $[\psi_0^{(-)}(0)]^2$ in Eq. (11) has a smaller value in the first case (I_+ and I_- are not very sensitive to the values of x_0). This is due to the fact that as the asymmetry parameter a decreases from the symmetric value of $a = 1.0$ (for a fixed x_0), the barrier height gets smaller and this increases the value of the wavefunction at the origin (see Fig. 1). Lastly, Figs. 3(a) and 3(b) indicate that this method works better for larger x_0. This is also to be expected and can be easily understood by looking at the simpler case of the symmetric well. The perturbation parameter $[\psi_0^{(-)}(0)]^2 = 4e^{-2x_0^2}$ is smaller for larger values of x_0 and explains the faster convergence. We find that results based on the WKB method deviate much faster from the numerical solution as the asymmetry parameter is decreased ($a = 1$ is the symmetric case) than SUSY-QM generated answer. Again we find that, for almost symmetric situation the SUSY-QM generated output agrees extremely well with the numerical result. We also note that, for very asymmetric cases ($a \approx 0.4$), the SUSY-QM approach provides results that are again, in excellent agreement with the numerical solu-

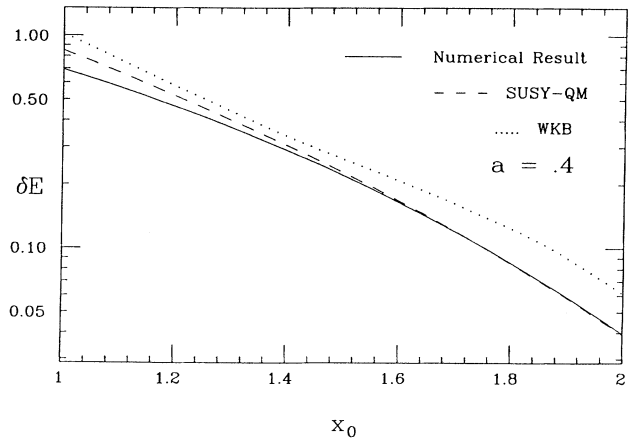

FIG. 2. A plot of the energy splitting δE vs x_0 for the asymmetry parameter $a = 0.4$.

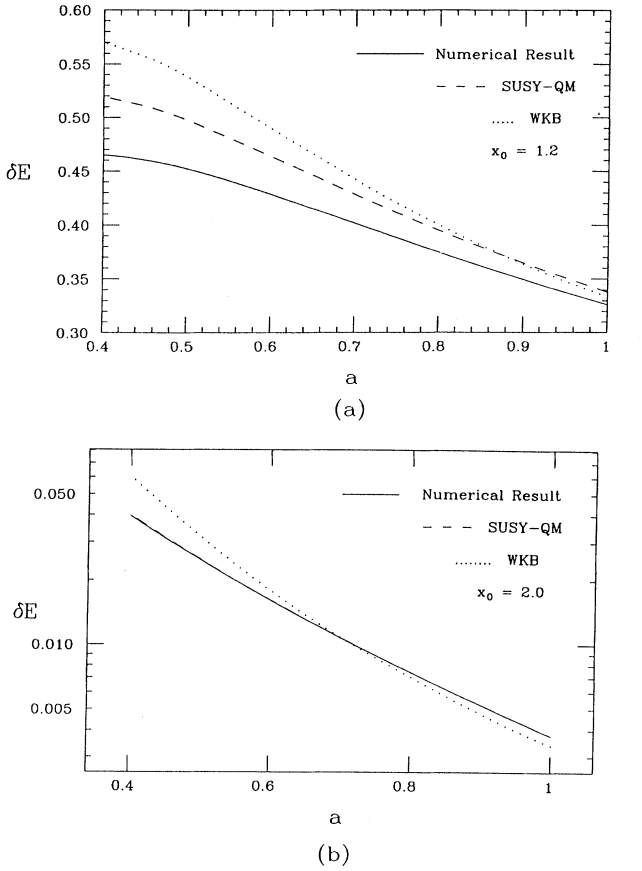

FIG. 3. A plot of δE vs a for (a) $x_0 = 1.2$ and (b) $x_0 = 2.0$.

tion. However, as we have stated before, a supersymmetry based approach is much easier than solving the Schrödinger equation with an extremely small eigenvalue lying very close to the ground state with vanishing energy.

IV. CONCLUSION

In this paper, we have shown how the idea of supersymmetric quantum mechanics can be profitably exploited to calculate the splitting of two lowest levels of an asymmetric double well. Interestingly, this nonperturbative problem in the potential $V_-(x)$, becomes a perturbative problem in $V_+(x)$ with a δ-function perturbation. The logarithmic perturbation method used in the text gave a rapidly converging series for δE.

This is a fully quantum-mechanical analysis, and can be easily carried out to any desired level of accuracy using logarithmic perturbation theory. We find that this method works very well in giving the energy splitting δE, even for exceedingly asymmetric double wells. The perturbation series converges especially rapidly when the potential barrier is high.

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