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APPLICATION OF SUPERSYMMETRY TO DOUBLE WELL PROBLEMS

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ABSTRACT

Employing the method of supersymmetric quantum mechanics, we propose a highly accurate and rapidly converging perturbative scheme to compute the energy splitting between the ground state and the first excited state of an asymmetric double well.

In a double-well potential, quantum mechanical tunneling generates an energy split $\delta E \equiv E_1 - E_0$ between the ground state and the first excited state. This purely quantum effect is obviously of great relevance to many branches of physics and chemistry and hence has been studied from various angles since the early days of quantum mechanics. The relevance of supersymmetric quantum mechanics (SUSY-QM)[1] to this problem stems from the following observations: For 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 $V_-(x)$, and hence the calculation of δE becomes much more tractable in the $V_+(x)$ sector.

In this talk, I will present the results of our recent analysis regarding the applicability of SUSY-QM to the case of asymmetric double well. 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 non-trivial problem of deep wells, this perturbative expansion is highly convergent and improves substantially upon the semi-classical analyses.

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. $E_n^+ = E_{n+1}^-$, where $E_n^\pm$ are eigenvalues of $V_\pm(x)$.

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The two Hamiltonians H_- and H_+ can be written (with units $\hbar = 2m = 1$) respectively as A^+A and AA^+, where

$$A = \left(\frac{d}{dx} + W(x)\right), \quad A^+ = \left(-\frac{d}{dx} + W(x)\right). \tag{1}$$

Here, $W(x) \equiv -\frac{\psi_0'^{(-)}}{\psi_0^{(-)}}$, is the so called superpotential and $\psi_0^{(-)}$ is the ground state wavefunction of H_-. A specific example of an asymmetric double well which we will consider in detail corresponds to the simple choice of a ground state wavefunction which is the sum of two Gaussians centered at $\pm x_0$, $\psi_0^{(-)} = e^{-(x+x_0)^2} + e^{-a(x-x_0)^2}$, which leads to the potential

$$V_-(x) \quad = \left(\frac{[-2a + 4a^2(x - x_0)^2]e^{-a(x-x_0)^2} + [-2 + 4(x + x_0)^2]e^{-(x+x_0)^2}}{e^{-(x+x_0)^2} + e^{-a(x-x_0)^2}}\right). \tag{2}$$

In Fig. 1, we have plotted $V_-(x)$ for various values of the asymmetry parameter a.

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, thanks to supersymmetry, happens to be the same as the ground state energy of the potential $V_+(x)$.

From the ground state wavefunction $\psi_0^{(-)}$ of H_-, we can construct a well defined normalizable function $\phi(x)$ given by

$$\phi(x) = \frac{\int_x^\infty \left(\psi_0^{(-)}(y)\right)^2 dy}{2I_+\psi_0^{(-)}(x)} \text{ for } x > 0; \text{ and } \frac{\int_{-\infty}^x \left(\psi_0^{(-)}(y)\right)^2 dy}{2I_-\psi_0^{(-)}(x)} \text{ for } x < 0,$$

with $I_\pm = \pm\left[\int_0^{\pm\infty} \left(\psi_0^{(-)}(y)\right)^2 dy\right]$. It is easy to show that $\phi(x)$ thus constructed is a zero energy normalizable eigenfunction of the singular Hamiltonian H_0 given by

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

and hence the ground state energy of H_+ turns out to be the expectation value of the term within braces. For the purpose of computation of this expectation value, we follow a very convergent perturbation expansion scheme, the so-called logarithmic perturbation theory[2] which gives excellent result, and the first order expression is given by

$$E^{(1)} \quad = \quad \frac{1}{4}\left[\frac{1}{I_+} + \frac{1}{I_-}\right] \frac{1}{\int_{-\infty}^{\infty} \phi^2(x)dx}. \tag{3}$$

To be brief, we are not presenting higher order corrections, computations of which are fairly straight forward.

To test the accuracy of our scheme, we compare our perturbative results with those obtained from standard WKB method[3], and also with numerical results obtained by solving the Schrödinger equation using fourth order Runge-Kutta method for the potential in Eq. (2). 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.

In Fig. 2, we plot δE calculated by different methods against the asymmetry parameter a, keeping x_0 fixed at 2.0. 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. We also note that, for very asymmetric cases ($a \approx .4$), SUSY-QM approach provides results that are again, in excellent agreement with the numerical solution. However, as we have stated before, 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.

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2. T. Imbo and U. Sukhatme, Am. J. Phys. **52**, 140 (1984), and references therein.
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Fig. 1. The potential $V_-(x)$ (Eq. 2) parameter a.
Fig. 2. A plot of δE vs. a for $x_0 = 2.0$.

FIG. 1

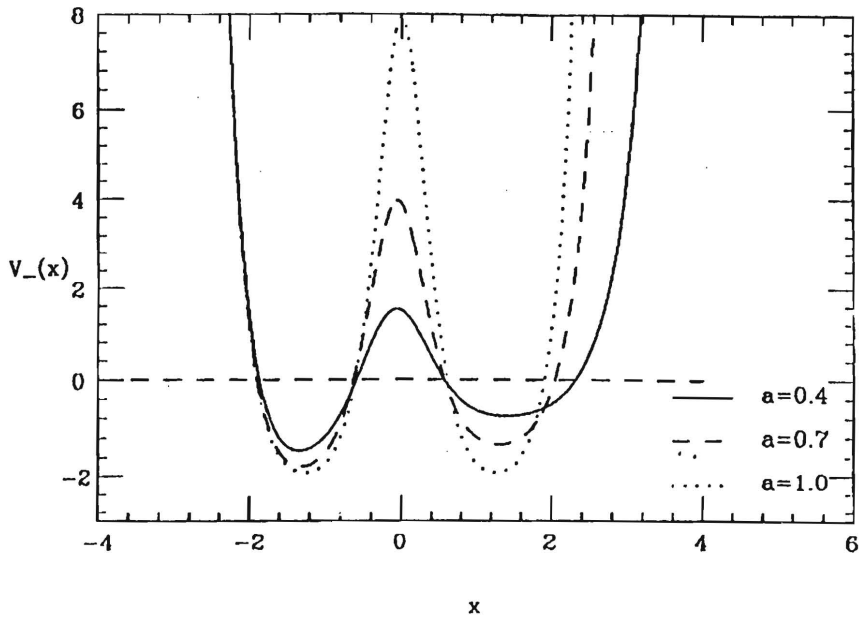
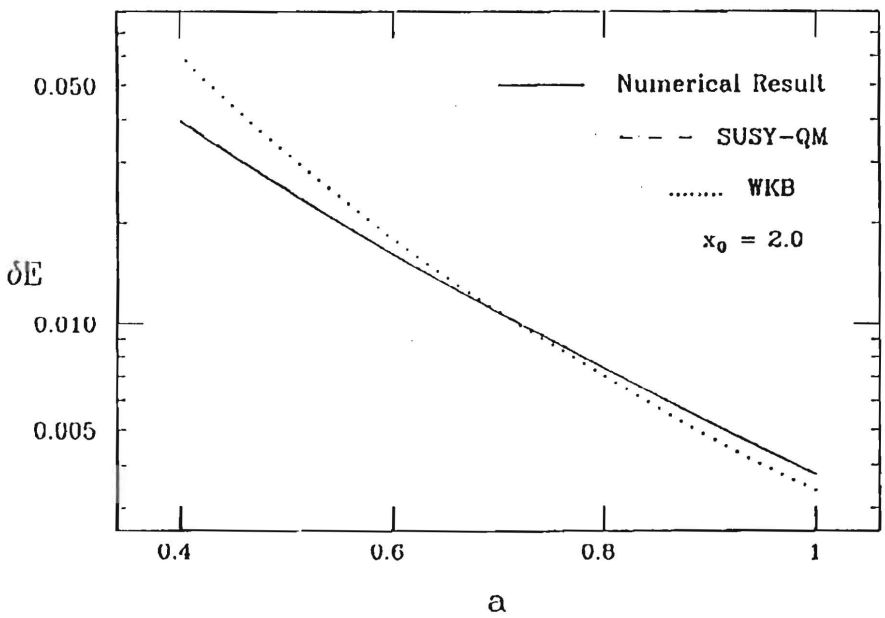

8
6
4
2
0
-2
V_(x)
-4
-2
0
2
4
6
x
a=0.4
a=0.7
a=1.0

FIG. 2


0.050
0.010
0.005
δE
0.4
0.6
0.8
1
a
Numerical Result
SUSY-QM
WKB
x0 = 2.0