Effect of Anharmonicity on the WKB Energy Splitting in a Double Well Potential

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Abstract

We investigate the effect of anharmonicity on the WKB approximation in a double well potential. By incorporating the anharmonic perturbation into the WKB energy splitting formula we show that the WKB approximation can be greatly improved in the region over which the tunneling is appreciable. We also observe that the usual WKB results can be obtained from our formalism as a limiting case in which the two potential minima are far apart.
It is well known that quantum tunneling leads to a splitting of degenerate energy levels in a symmetrical two-well potential. There are three approaches to the calculation of this energy splitting: the WKB approximation, the instanton method, and numerical calculation. From the comparison of the results from the WKB and instanton methods with those of numerical calculations, it was shown that the instanton method is better than the WKB approximation [1], because the WKB method is generally believed to have inherent errors associated with the connection formula [2]. The modified-barrier [3] and modified-well [4] formalisms have been proposed for the improvement of the WKB approximation. Recently the authors in Ref. [5] have shown that a careful account of the phase changes in connection formula improves the accuracy of the WKB wave function.

In this letter we propose another formalism whereby the energy splitting within the WKB approximation becomes consistent with the instanton result. Unlike many of the WKB formalisms, the present work incorporates the anharmonicity into the WKB formalism, which gives a more realistic model, and hence more improved energy splitting result. In other words, the incorporation of anharmonicity results in a level shift due to the perturbation in each well.

Consider a particle of mass \( m \) in a one-dimensional symmetrical two-well potential

\[
V(x) = \frac{m\omega^2}{8a^2} (x - a)^2 (x + a)^2,
\]

where \( \omega \) is the angular frequency in each well when the two wells are far apart, and \( \pm a \) are the positions of the two potential minima. For a tunneling to occur the separation between the two minima should be large enough so that the height of the barrier \( \frac{m\omega^2a^2}{8} \) is higher than the lowest energy level in each well. In the limit \( a \to \infty \), the potential is divided into two independent harmonic oscillator potentials in which the lowest energies are the same and given by \( E_0 = \frac{1}{2}\hbar\omega \). When these two harmonic oscillator potentials approach each other, they become an anharmonic potential, so that the lowest energies are no longer \( E_0 \) because of the anharmonic perturbation.

To evaluate the lowest perturbation energies we expand \( V(x) \) around each minima \( \pm a \).
Since the potential is symmetric, we consider one of either positions. For the minimum at $x = a$ we have

$$V(x) = \frac{m\omega^2}{2}(x-a)^2 \left[ 1 + \frac{x-a}{a} + \frac{3(x-a)^2}{a^2} \right]. \quad (2)$$

Following a standard perturbation theory it is straightforward to show that the perturbation energy to second order correction is

$$E = E_0 \left[ 1 + \epsilon(\eta) \right], \quad (3)$$

where $\epsilon(\eta)$ is defined as

$$\epsilon(\eta) = \frac{\eta^2}{16}(25 - 189\eta^2),$$

and we have introduced a dimensionless parameter

$$\eta = \sqrt{\frac{\hbar}{m\omega a^2}}$$

which is small for large $a$. We see that the first term in Eq.(3) corresponds to the lowest energy of the unperturbed harmonic potential and $\epsilon(\eta)$ is the correction term which was ignored in the previous studies. In the following, we demonstrate that this correction term plays an important role in the improvement of the WKB approximation.

Using Eq.(3) we write the WKB level splitting formula as

$$\Delta E_{WKB} = \frac{2\hbar}{T} e^{-S}, \quad (4)$$

where

$$S = \frac{1}{\hbar} \int_{-\alpha}^{\alpha} \sqrt{2m(V(x) - E)} \, dx,$$

$$T = \int_{\alpha}^{\gamma} \frac{\sqrt{2m}}{\sqrt{E - V(x)}} \, dx, \quad (5)$$

and $\pm \alpha$, $\pm \gamma$ are the four classical turning points (Fig. 1) corresponding to the perturbed energy $E$. $\alpha$ and $\gamma$ can be expressed in terms of $\epsilon(\eta)$, respectively, as

$$\alpha = a\sqrt{1 - 2\eta\sqrt{1 + \epsilon(\eta)}}, \quad \gamma = a\sqrt{1 + 2\eta\sqrt{1 + \epsilon(\eta)}}. \quad (6)$$
Since we are interested in the region with large values of $a$, the elliptic integrals in Eq.(5) can be performed asymptotically for small $\eta$. Keeping only the dominant terms in $\eta$, we obtain the WKB energy splitting

$$\Delta E_{WKB} \approx \left[ \frac{\hbar \omega}{\pi \eta} e^{\frac{a}{3 \eta^2}} \right] \delta(\eta),$$

where $\delta(\eta)$ is defined as

$$\delta(\eta) = \frac{1}{\sqrt{1 + \epsilon(\eta)}} \exp \left[ \frac{\epsilon(\eta)}{2} - \epsilon(\eta) \ln \left( \frac{\eta \sqrt{1 + \epsilon(\eta)}}{4} \right) \right].$$

Comparing this with the instanton result \cite{7}

$$\Delta E_{in} = \frac{4 \hbar \omega}{\sqrt{\pi \eta}} e^{\frac{-2}{3 \eta^2}},$$

we find that

$$\frac{\Delta E_{WKB}}{\Delta E_{in}} = \sqrt{\frac{e}{\pi}} \delta(\eta).$$

In the limit that the two potential minima are completely separated, which implies $\eta \rightarrow 0$, we see from Eq.(8) that $\delta(\eta) \rightarrow 1$. In this regime the Eq.(9) reduces to

$$\frac{\Delta E_{WKB}^{(0)}}{\Delta E_{in}} = \sqrt{\frac{e}{\pi}},$$

where $\Delta E_{WKB}^{(0)}$ is the WKB energy splitting obtained without considering the anharmonicity effect. The ratios in Eqs. (9) and (10) as a function of dimensionless parameter $\eta$ are shown in Fig.2. Note that, in the range of an appreciable tunneling probability (e.g., $0.1 \leq \eta \leq 0.15$), the WKB result obtained from the present formalism is arbitrarily close to the instanton result.

A few comments are addressed in the following. Eq.(10) agrees well with the results of Refs.[1,2] in which the difference between the WKB approximation and the instanton method is claimed to be attributed to the errors introduced by the WKB connection formula. We note here that they \cite{1,2} obtained the energy splitting in the limit $a \rightarrow \infty$, which corresponds to zero tunneling probability and is not allowed in the calculation of the energy splitting due
to tunneling. In order for the tunneling probability not to vanish, thus, the two potential wells should not be far apart. In this case, the coupled potential wells are simulated as an anharmonic potential more realistically than two idealized harmonic potentials which was assumed in their calculations. Our result shown in Eq.(7), which includes the effect of anharmonicity, is based on the formalism that includes the region where the tunneling probability is appreciable. As we can see in Table I, within the range of the occurrence of a considerable tunneling, significant improvement in the usual WKB approximation can be achieved by the incorporation of the anharmonicity.

In summary, we suggest a more realistic formalism with anharmonicity included than the previous ones only with ideal harmonicity. While the results from Refs.[1,2] are valid only in the limiting case of $a \to \infty$, our approach is applicable to the broader range of the separation between two wells, over which the tunneling amplitude is conspicuous. Moreover, in this region, our formalism greatly improves the usual WKB methods, and the WKB energy splitting obtained from this formalism is shown to be in good agreement with that from the instanton method. Taking the limit $a \to \infty$ of our result, we found that our expression reduces to the previous one as shown in Eq.(10) [2]. Whereas it was only conjectured in Ref. [2] that the modification factor $\sqrt{\frac{e^{\pi}}{\pi}}$ may come from the connection formula of the WKB approximation, we, here, obtained that factor through the analytical method with anharmonicity incorporated.

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FIGURES

FIG. 1. One dimensional anharmonic double well potential. $E$ is the perturbation energy to second order and $\pm \alpha, \pm \gamma$ are the classical turning points corresponding to $E$.

FIG. 2. The ratios in (9) and (10) as a function of $\eta$ are plotted. The region of large $\eta$ has been excluded in this plot because the two equations (9) and (10) are asymptotic expressions for small $\eta$. In the limit $\eta \to 0$ (that is, $a \to \infty$) the two plots exactly agree with each other.
TABLE I. A comparison between $\Delta E_{WKB}$ and $\Delta E_{in}$ within the range of $0.1 \leq \eta \leq 0.15$.

| $\eta$      | $\frac{\Delta E_{WKB}}{\Delta E_{in}}$ |
|-------------|----------------------------------------|
| 0.1         | 0.98104                                |
| 0.121       | 0.99870                                |
| 0.122513    | 1.00000                                |
| 0.123       | 1.00042                                |
| 0.125       | 1.00214                                |
| 0.127       | 1.00386                                |
| 0.13        | 1.00644                                |
| 0.15        | 1.02349                                |
Fig. 1
Fig. 2

\[
\frac{\Delta E_{\text{WKB}}}{\Delta E_{\text{in}}}, \quad \frac{\Delta E^{(0)}_{\text{WKB}}}{\Delta E_{\text{in}}}
\]