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Transmission through an inverted biharmonic oscillator potential

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Abstract. The exact penetrability for an inverted biharmonic oscillator potential is calculated and compared with that obtained from the WKB method.

A recent addition to the collection of exactly solvable models in one dimension is the biharmonic oscillator, quantum solutions for which were considered by Gettys and Graben (1975). The purpose of this paper is to consider the problem of the penetration of a particle encountering an inverted biharmonic potential barrier.

The potential corresponding to an inverted biharmonic oscillator potential is given by

$$V(\mathbf{x}) = \begin{cases} V_0 - \frac{1}{2}m\omega_1^2 x^2, & x < 0 \text{ (region I)} \end{cases}$$
(1*a*)

$$V_0 - \frac{1}{2}m\omega_2^2 x^2, \qquad x > 0 \quad (region II)$$
 (1b)

where V_0 is the height of the potential and ω_1 and ω_2 are the oscillator frequencies in regions I and II respectively.

The Schrödinger equation can be reduced to the standard form:

$$\frac{d^2\Psi}{dy^2} + (\frac{1}{4}y^2 - \alpha)\Psi = 0$$
(2)

with the following substitutions:

$$u = \left(\frac{2m\omega_1}{\hbar}\right)^{1/2}, \qquad \alpha_1 = \frac{V_0 - E}{\hbar\omega_1} \qquad (\text{region I}) \tag{3a}$$

$$v = \left(\frac{2m\omega_2}{\hbar}\right)^{1/2}, \qquad \alpha_2 = \frac{V_0 - E}{\hbar\omega_2} \qquad (region II)$$
(3b)

solutions for which can be sought in terms of Weber's parabolic cylinder functions (Abramowitz and Stegun 1965). A study of the asymptotic behaviour of the parabolic cylinder functions for large values of positive and negative x will facilitate the choice of proper wavefunctions. In region I, $E^*(\alpha_1, -u)$ would represent the incident wave and the reflected component would be given by $E(\alpha_1, -u)$. In region II however, there should be wave packets moving to the right only and accordingly we will have the function $E(\alpha_2, v)$.

Here the function $E(\alpha, x)$ is the complex linear combination

$$E(\alpha, x) = k^{-1/2} W(\alpha, x) + i k^{1/2} W(\alpha, -x)$$
(4a)

of the fundamental parabolic function $W(\alpha, x)$ (Abramowitz and Stegun 1965); the quantity k is defined by

$$k = (1 + e^{2\pi\alpha})^{1/2} - e^{\pi\alpha}.$$
 (4b)

By observing that the probability current should be conserved at all values of x, we obtain the following relation for the penetrability:

$$P = \left(\frac{\omega_2}{\omega_1}\right)^{1/2} \left|\frac{T}{A}\right|^2.$$
(5*a*)

The amplitude ratio |T/A| is obtained by matching the wavefunction and their derivatives with respect to x at x = 0.

The expression for penetrability in equation (5a) can be simplified to read

$$P = 4G^{-1}(\omega_1\omega_2)^{1/2}[(1+e^{2\pi\alpha_1})(1+e^{2\pi\alpha_2})]^{-1/2}$$
(5b)

where G is given by

$$G = \omega_1^{1/2} \left| \frac{\Gamma(\frac{3}{4} + \frac{1}{2}i\alpha_1)\Gamma(\frac{1}{4} + \frac{1}{2}i\alpha_2)}{\Gamma(\frac{1}{4} + \frac{1}{2}i\alpha_1)\Gamma(\frac{3}{4} + \frac{1}{2}i\alpha_2)} \right|^{1/2} + \omega_2^{1/2} \left| \frac{\Gamma(\frac{3}{4} + \frac{1}{2}i\alpha_2)\Gamma(\frac{1}{4} + \frac{1}{2}i\alpha_1)}{\Gamma(\frac{1}{4} + \frac{1}{2}i\alpha_2)\Gamma(\frac{3}{4} + \frac{1}{2}i\alpha_1)} \right|^{1/2}.$$
(5c)

The penetrability in equation (5b) is invariant under an interchange of ω_1 and ω_2 . In some special cases, equation (5b) for penetrability can be simplified to give revealing results. We discuss them below.

Case 1. If we put u = v then $\alpha_1 = \alpha_2 = \alpha$ and we obtain $G = 4\omega$ whence the penetrability is given by

$$P = \{1 + \exp[2\pi (V_0 - E)/\hbar\omega]\}^{-1}$$
(6)

which is the Hill-Wheeler expression (Hill and Wheeler 1953) for the penetration of an inverted harmonic oscillator potential. Note that if we put $V_0 = E$, P = 0.5 irrespective of the value ω .

Case 2. At $V_0 = E$, we have $\alpha_1 = \alpha_2 = 0$ in which case

$$G = (\omega_1^{1/2} + \omega_2^{1/2})^2$$

and the penetrability is given by

$$P = 2\left[\left(\frac{\omega_2}{\omega_1}\right)^{1/4} + \left(\frac{\omega_1}{\omega_2}\right)^{1/4}\right]^{-2}.$$
(7)

This formula enables us to study the departure of the penetrability function for an inverted biharmonic oscillator barrier from that of an inverted harmonic oscillator barrier.

Case 3. If in equation (5b), the factor 1 can be neglected in comparison with the exponentials, which would correspond to the case of a tall and thick barrier, the

penetrability would then be given by

$$P = 4G^{-1}(\omega_1\omega_2)^{1/2} \exp\left[-V_0(1-\xi)\left(\frac{1}{\hbar\omega_1} + \frac{1}{\hbar\omega_2}\right)\right]$$
(8)

where $\xi = E/V_0$.

Now, G is a slowly varying function of V_0 , with the result that for a given value of ξ , the exponential factor dominates the behaviour of P.

For smoothly varying potentials the transmission coefficient in the WKB method is given by the formula (Froman and Froman 1965)

$$P \simeq \begin{cases} [1 + \exp(2K)]^{-1}, & E < V_0 \end{cases}$$
(9a)

$$\int \left[1 + \exp(-2|K|) \right]^{-1}, \qquad E > V_0$$
(9b)

where K is given by

$$K = \int_{a}^{b} \left(\frac{2m}{\hbar^{2}}(V(x) - E)\right)^{1/2} \mathrm{d}x.$$
 (9c)

Here a and b are the classical turning points. Strictly speaking, the use of equations (9a) and (9b) to obtain the transmission coefficient for the inverted biharmonic oscillator potential is not fully justified, because the potential is not smooth at x = 0. However, for purposes of comparison if we take the validity of equations (9a) and (9b) as granted, the integration is straightforward and one obtains

$$K = \frac{\pi (V_0 - E)}{2\hbar} \left(\frac{1}{\omega_1} + \frac{1}{\omega_2} \right). \tag{9d}$$

It is seen from equation (9d) that ω_1 and ω_2 can be interchanged, to give the same value of penetrability as in equations (9a) and (9b).

A comparison between the exact and WKB penetrabilities is made in figure 1, which gives the behaviour of the penetrability functions of equations (5) and (9) respectively as



Figure 1. Exact (full curves) and WKB (chain curves) penetrabilities for an inverted biharmonic oscillator barrier as a function of ξ . (a) $V_0 = 1.0$, $\hbar\omega_1 = 1.0$, $\hbar\omega_2 = 2.0$; (b) $V_0 = 1.0$, $\hbar\omega_1 = 1.0$, $\hbar\omega_2 = 5.0$.

a function of ξ for some typical values of V_0 , $\hbar\omega_1$ and $\hbar\omega_2$. It is evident from the figures that the penetrability obtained from WKB methods agree with the exact results only at low values of the incident energies. The exact transmission coefficient reaches the value one at large values of ξ . For given values of V_0 and $\hbar\omega_1$ the approach to one is faster for lower values of $\hbar\omega_2$.

The departure of the transmission coefficient for the inverted biharmonic barrier from that of an inverted harmonic barrier is best studied at $\xi = 1.0$. A plot of the penetrability given by equation (7) against the ratio (ω_2/ω_1) for $\xi = 1.0$ is shown in figure 2. The maximum value of the penetrability is 0.5 at $\omega_1 = \omega_2$ and falls off on either side of $(\omega_2/\omega_1) = 1$.



Figure 2. Exact penetrability for the inverted biharmonic oscillator barrier as a function of the ratio (ω_2/ω_1) for $\xi = 1.0$.

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