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Quantum mechanical penetration through multiple barriers

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Abstract. We illustrate the interesting results of particle penetration through multiple potential barriers with the use of rectangular barriers. We show that complete transmission is possible through any number of barriers even at energies well below the barrier top. The tedious algebra is much simplified through the use of Pauli matrices.

1. Introduction

The study of particle penetration through single potential barriers is a standard exercise in introductory quantum mechanics courses (Merzbacher 1970). For energies well below the barrier top there is a finite, though very small, penetration probability which increases monotonically as the energy is increased to the value equal to the top of the barrier, there onwards it oscillates with decreasing amplitude and asymptotically reaches unity. With the recent discovery of double-humped (and triple-humped) barriers in nuclear fission studies (Gai *et al* 1969, Crammer and Nix 1970, Brack *et al* 1972) understanding of penetration through multiple barriers has become important. The results obtained with realistic potentials are very surprising at first sight (Bhandari 1976). Below the barrier top, the transmission probability (T) is not a monotonically increasing function of energy, but shows some resonance-like peaks which could, in some cases, be as high as $T=1$.

In this paper we illustrate this phenomenon of complete transmission through multiple barriers with the help of rectangular barriers. We follow very closely the notations of Merzbacher (1970).

2. Mathematical details

Consider a potential barrier of height V and width $2a$ centred at the origin (figure 1(a)). The wavefunction to the left of the barrier is given by

$$\psi(x)=A_1\,e^{ikx}+B_1\,e^{-ikx} \qquad \text{for } x<-a, \tag{1}$$

and to the right of the barrier by:

$$\psi(x)=A_2\,e^{ikx}+B_2\,e^{-ikx} \qquad \text{for } x>a, \tag{2}$$

where $k^2=2mE/\hbar^2$. From now on we use units such that $2m/\hbar^2=1$. Also we define q through $q^2=V-E$. Then we obtain the following relation between the coefficients

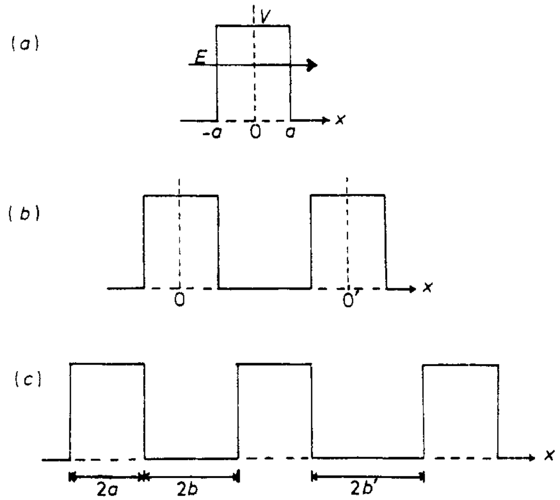

Figure 1. (*a*) A single rectangular potential barrier; (*b*) two equal barriers separated by a well of width $2b$; (*c*) three equal barriers separated by two asymmetric wells.

A_1, B_1 and A_2, B_2:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \tag{3}$$

where

$$\begin{aligned} M_{11} &= M_{22}^* = (\cosh 2qa + \tfrac{1}{2}\mathrm{i}\epsilon \sinh 2qa)\,\mathrm{e}^{2\mathrm{i}ka} \\ M_{12} &= M_{21}^* = \tfrac{1}{2}\mathrm{i}\eta \sinh 2qa \\ \det(M) &= 1. \end{aligned} \tag{4}$$

Here

$$\epsilon = \frac{q}{k} - \frac{k}{q} \quad \text{and} \quad \eta = \frac{q}{k} + \frac{k}{q}. \tag{5}$$

Noting that $B_2 = 0$ for a beam incident from the left, we get the transmission coefficient for $E < V$ as

$$T = |M_{11}|^{-2} = (1 + \tfrac{1}{4}\eta^2 \sinh^2 2qa)^{-1}. \tag{6}$$

Above the top of the barrier ($E > V$) we have

$$T = (1 + \tfrac{1}{4}\epsilon'^2 \sin^2 2q'a)^{-1} \tag{7}$$

with

$$q'^2 = E - V \quad \text{and} \quad \epsilon' = \frac{q'}{k} - \frac{k}{q'}. \tag{8}$$

Now we shall consider the case of two identical barriers separated by a well of width $2b$ (figure 1(*b*)). Let us introduce new coordinates with origin O′ at the centre of the second barrier. Then, for the penetration through the second barrier equations

(3)–(5) are valid if the wavefunctions are written in the new coordinate system. That is:

$$\begin{aligned} \psi(x') &= A'_2\, e^{ikx'} + B'_2\, e^{-ikx'} \qquad \text{for } a < x < a+2b \\ \psi(x') &= A'_3\, e^{ikx'} + B'_3\, e^{-ikx'} \qquad \text{for } x > 3a+2b. \end{aligned} \tag{9}$$

Then we have

$$\begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix} = M \begin{pmatrix} A'_3 \\ B'_3 \end{pmatrix}, \tag{10}$$

with M given by equation (4). The relation between A_2, B_2 and A'_2, B'_2 of equations (2) and (9) can be seen to be

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = N \begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix}$$

where

$$N = \begin{pmatrix} e^{-2ik(a+b)} & 0 \\ 0 & e^{2ik(a+b)} \end{pmatrix}. \tag{11}$$

Now we can write the final relation between the incident and transmitted amplitudes through

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = MNM \begin{pmatrix} A'_3 \\ B'_3 \end{pmatrix}. \tag{12}$$

With suitable notation, this result can be extended to any number of barriers

$$\begin{pmatrix} A \\ B \end{pmatrix} = MNMNM \ldots \begin{pmatrix} A' \\ B' \end{pmatrix}. \tag{13}$$

Hence the problem of multiple barriers needs only the efficient handling of the transfer matrices M and N. It is convenient to define a new matrix

$$S = N^{1/2} M N^{1/2} \tag{14}$$

with

$$\begin{aligned} S_{11} &= S^*_{22} = (\cosh 2qa + \tfrac{1}{2} i\epsilon \sinh 2qa)\, e^{-2ikb} \\ S_{12} &= S^*_{21} = \tfrac{1}{2} i\eta \sinh 2qa \end{aligned} \tag{15}$$

so that equation (13) becomes

$$\begin{pmatrix} A \\ B \end{pmatrix} = N^{-1/2} S^n N^{-1/2} \begin{pmatrix} A' \\ B' \end{pmatrix}. \tag{16}$$

Now, we write S as a linear combination of the unit matrix and the three Pauli matrices

$$S = s_0 I + s_1\sigma_1 + s_2\sigma_2 + s_3\sigma_3 \tag{17}$$

$$\begin{aligned} s_0 &= \cosh 2qa \cos 2kb + \tfrac{1}{2}\epsilon \sinh 2qa \sin 2kb \\ s_1 &= 0 \\ s_2 &= -\tfrac{1}{2}\eta \sinh 2qa \\ s_3 &= -i(\cosh 2qa \sin 2kb - \tfrac{1}{2}\epsilon \sinh 2qa \cos 2kb) \end{aligned} \tag{18}$$

and

$$s_0^2 = 1 + s_2^2 + s_3^2.$$

Then we have

$$S^n = P + Q(s_2\sigma_2 + s_3\sigma_3) \tag{19}$$

where

$$\begin{aligned} P &= s_0^n + {}^nc_2 s_0^{n-2}(s_2^2+s_3^2) + {}^nc_4 s_0^{n-4}(s_2^2+s_3^2)^2 + \dots \\ Q &= {}^nc_1 s_0^{n-1} + {}^nc_3 s_0^{n-3}(s_2^2+s_3^2) + {}^nc_5 s_0^{n-5}(s_2^2+s_3^2)^2 + \dots . \end{aligned} \tag{20}$$

Similarly we can expand $N^{-1/2} = c_0 I + c_3\sigma_3$. However, since we are interested only in the transmission coefficient and not in the phases of the incident and transmitted beams we can write

$$T = |(S^n)_{11}|^{-2} = (P^2 - Q^2 s_3^2)^{-1}$$

which, on using condition (18) and noting that $P^2 = 1 + Q^2(s_0^2 - 1)$, reduces to

$$T = (1 + Q^2 s_2^2)^{-1}. \tag{21}$$

3. Symmetric double and triple barriers

Now, we study the double and triple barriers in detail. For the double barrier the transmission coefficient is given by

$$T = (1 + 4s_0^2 s_2^2)^{-1}, \tag{22}$$

where s_2 is a monotonically increasing function of k (for $E < V$), but s_0 is an oscillating function. Total transmission ($T = 1$) is obtained when $s_0 = 0$, i.e.,

$$\cot 2kb = -\tfrac{1}{2}\epsilon \tanh 2qa. \tag{23}$$

This equation is to be solved graphically or numerically. It can be seen that for E well below the barrier top V, q is large and we have $2kb \approx n\pi$, which shows that the transmission resonances are located at energies corresponding to the bound states in the potential well between the barriers. A plot of ln T against k is shown in figure 2 for a typical choice of $V = 40$ and $2a = 2b = 1$. Above the barrier top also there are unit peaks in T coming for such values of the energies for which either s_0 or s_2 $(= -\tfrac{1}{2}\epsilon' \sin 2q'a)$ vanishes. In order to estimate the width of the transmission resonances, we write equation (21) as

$$T = [1 + (\alpha^2 - 1)4\alpha^2 \cos^2\beta]^{-1} \tag{24}$$

with

$$\begin{aligned} \alpha^2 &= 1 + \tfrac{1}{4}\eta^2 \sinh^2 2qa \\ \beta &= \tan^{-1}(\tfrac{1}{2}\epsilon \tanh 2qa) - 2kb. \end{aligned} \tag{25}$$

$T = 1$ if $\beta = (n + \tfrac{1}{2})\pi$. Since α is a smoothly varying function, it can be shown that for low lying resonances the halfwidth is given by

$$\Delta k = (4b\alpha^2)^{-1}. \tag{26}$$

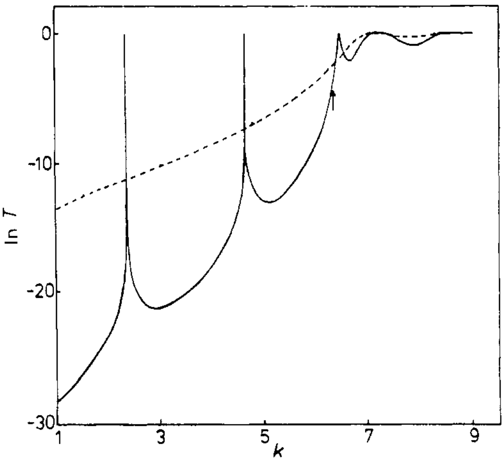

Figure 2. Ln T against k for $V = 40$, $2a = 2b = 1$. The full curve is for double barrier and the broken curve for single barrier. The arrow indicates the points at which $E = V$.

The estimated widths for the two resonances of figure 2 are of the order of $1{\cdot}2\times10^{-5}$ and $5{\cdot}3\times10^{-4}$ respectively.

In the case of symmetric triple barriers we have

$$T = [1 + s_2^2(4s_0^2 - 1)^2]^{-1}. \tag{27}$$

Again, as before, the unit transmission peaks occur if,

$$s_0 = \pm\tfrac{1}{2} \qquad \text{or} \qquad \cos\beta = \pm 1/(2\alpha). \tag{28}$$

Thus we have some closely spaced pairs of unit peaks of very small width. Again, in analogy with the double barriers, we could associate them with the bound states of a double potential well. A plot of T for the triple barrier is shown in figure 3 (along with the cube of transmission probability for a single barrier, for comparison). The separation between the peaks is given by

$$\delta k = (4b\alpha)^{-1}. \tag{29}$$

For the first and second doublets in figure 3 the separation is 3×10^{-3} and $1{\cdot}8\times10^{-2}$ respectively. The halfwidth of the peaks is obtained as

$$\Delta k = (8b\alpha^2)^{-1}. \tag{30}$$

The double peaks are so narrow and close that they cannot be seen separately in the figure; so a magnified picture of the second resonance is shown as an inset.

Above the barrier top the curve shows more double peaks and, in addition, there is another class of unit peaks coming from the condition $s_2 = 0$. The superposition of closely lying three unit peaks makes the curve look as if it has a broad plateau. (In figure 3, the superposing peaks are at $k = 7{\cdot}06$, $7{\cdot}12$, $7{\cdot}43$ and later at $10{\cdot}5$, $11{\cdot}34$, $11{\cdot}5$ and so on.) It may be noted that, in the case of symmetric barriers, all the peaks have unit magnitude. For $E < V$, we have peaks at $k = 2{\cdot}371$, $2{\cdot}374$, $4{\cdot}628$ and $4{\cdot}6465$.

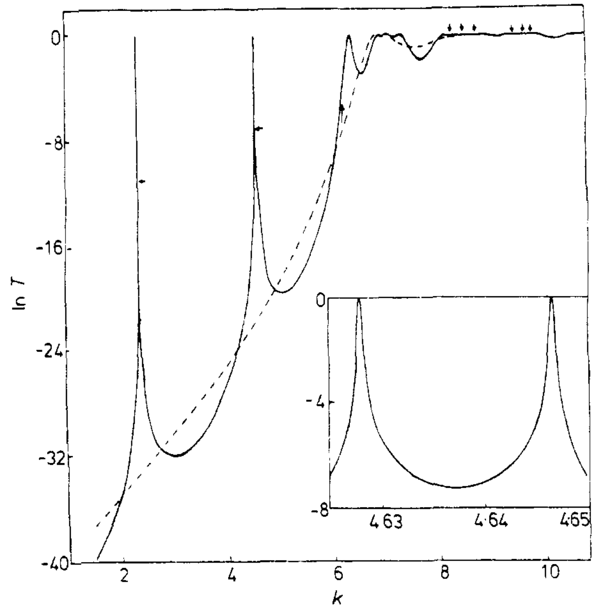

Figure 3. Full curve, ln T against k for symmetric triple barrier; broken curve, $\ln(T)^3$ against k for single barrier. The inset is an enlarged picture of the second doublet. The arrows to the left indicate the minima between the double peaks. The arrows pointing down show shallow peaks between broad maxima.

Generalisation of these results to any number of barriers is straightforward. For n barriers we expect resonances each consisting of $(n-1)$ very closely spaced unit peaks (for $E < V$) and flattening out above the barrier.

4. Triple barrier with asymmetric wells

The problem of penetration of particles through a triple barrier with two asymmetric wells (figure 1(c)) can be handled in a similar manner. We obtain

$$T^{-1} = A + B \sin 2\delta + C \sin^2 \delta, \tag{31}$$

where

$$\begin{aligned} A &= 1 + (\alpha^2 - 1)(4\alpha^2 \cos^2 \beta - 1)^2 \\ B &= -2\alpha^2 \sin 2\beta(\alpha^2 - 1)(4\alpha^2 \cos^2 \beta - 1) \\ C &= -8\alpha^2 \cos^2 \beta(\alpha^2 - 1)(4\alpha^2 \cos^2 \beta - 2\alpha^2 - 1) \\ \delta &= 2k(b' - b). \end{aligned} \tag{32}$$

One obtains peaks at energies corresponding to the bound states of either of the wells. No doublets are observed and the peaks are not of unit magnitude (except when they correspond to bound states in both the wells—this can happen when k corresponds to a bound state in one of the wells and b' satisfies the condition $\delta = \pm n\pi$).

Figure 4 shows a plot of T against k for the case $V = 40$, $2a = 2b = 1$ and $2b' = 0{\cdot}8$. The peaks at $k = 2{\cdot}3725$ and $4{\cdot}637$ correspond to bound states in the first well and those at $k = 2{\cdot}7864$ and $5{\cdot}3415$ correspond to the bound states in the second well.

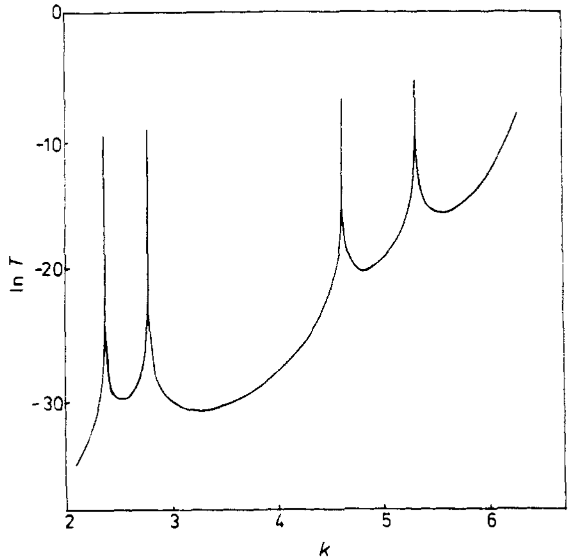

Figure 4. Ln T against k for the asymmetric case. $V = 40$, $2a = 2b = 1$; $2b' = 0{\cdot}8$.

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