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On the linear potential hill

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By explicitly solving the Schrödinger equation for a particle encountering a linear potential hill ($V = 0$, $x < 0$; $V = V_0 x/a$, $0 < x < a$; $V = V_0$, $x > a$), we obtain corrections to the quantum ($a \rightarrow 0$) and classical ($a \rightarrow \infty$) limits for the transmission coefficient, demonstrating the influence of the range a over which the potential rises.

A standard offering in undergraduate courses on quantum mechanics,¹ one which highlights the difference between classical and quantum physics, is the transmission of a particle across a potential step. It is probably the first illustration which the student encounters of the profound effect caused by the wavelike nature of matter: despite the fact that the particle has enough energy to overcome the step, one is surprised to find that the transmission coefficient is less than unity—a result at total variance with classical expectations since it runs contrary to everyone's normal experience (e.g., a ball with sufficient energy rolling up a hill, etc.). The basic explanation for the quantum effect—and this is not emphasized nearly enough in the standard texts—does not actually lie in the magnitude of the potential change but in the range, say a , over which the change occurs; only if a is smaller than the de Broglie wavelength $\gamma = 2\pi/k$ of the incoming particle do we expect the standard quantum answer; on the other hand, for $ka \gg 1$ we anticipate the classical, macroscopic answer of total transmission, a limit which can of course be recovered by applying well-known semiclassical WKB methods¹ to the Schrödinger equation, because the potential is then slowly varying.

In this note we would like to demonstrate the influence of ka on the transmission factor by treating the problem of the linear potential hill,

$$\begin{aligned} V &= 0, & x < 0 \\ &= V_0 x/a, & 0 < x < a \\ &= V_0, & x > a. \end{aligned} \quad (1)$$

This exercise has the advantage of being completely soluble in terms of well tabulated (Airy) functions. Though we feel sure that many people must have addressed themselves to this example in the course of their undergraduate teaching, we are not aware of the details having been exhibited anywhere in the literature²; we have undertaken to do so in this article, hoping it will interest the keen student of quantum mechanics. Specifically, we shall determine analytically the corrections to the limiting situations ($ka \gg 1$ and $ka \ll 1$) in appropriate powers of ka . Obviously, a computer could provide the total link between the two regions of a large and a small.

FORMAL SOLUTION

In the Schrödinger equation, for a particle of energy $E > V_0$, make the usual substitutions $\hbar^2 k^2/2m = E$ and $\hbar^2 k_0^2/2m = E - V_0$, where k and k_0 are the wave numbers to the left and right of the hill potential (1). Thus

$$\psi'' + k^2 \psi = 0, \quad x < 0;$$

$$\psi'' + k_0^2 \psi = 0, \quad x > a.$$

In the region of the hill, $0 < x < a$,

$$\psi'' + [k^2 - (k^2 - k_0^2)x/a] \psi = 0,$$

it is appropriate to change variable to

$$\begin{aligned} Z &= [(k^2 - k_0^2)/a]^{1/3} x - [ak^3/(k^2 - k_0^2)]^{2/3} \\ &= (2mV_0 a^2/\hbar^2)^{1/3} (x/a - E/V_0) \end{aligned} \quad (2)$$

in order to cast the differential equation into standard (Airy) form

$$d^2\psi/dZ^2 - Z\psi = 0. \quad (3)$$

Note that Z is negative in the region of interest.

The appropriate solutions for left incoming waves are

$$\begin{aligned} \psi &= e^{ikx} + re^{-ikx}, \quad x < 0 \\ &= \alpha \text{Ai}(Z) + \beta \text{Bi}(Z), \quad 0 < x < a \\ &= te^{ik_0(x-a)}, \quad x > a \end{aligned} \quad (4)$$

and the continuity relations for ψ and ψ' give

$$\begin{aligned} 1 + r &= \alpha \text{Ai}(Z_0) + \beta \text{Bi}(Z_0), \\ i(1 - r) &= (-Z_0)^{1/3} [\alpha \text{Ai}'(Z_0) + \beta \text{Bi}'(Z_0)], \\ t &= \alpha \text{Ai}(Z_a) + \beta \text{Bi}(Z_a), \\ it &= (-Z_a)^{1/3} [\alpha \text{Ai}'(Z_a) + \beta \text{Bi}'(Z_a)]. \end{aligned} \quad (5)$$

Above, Ai and Bi are the two (linearly independent) Airy function solutions³ of (3) and

$$\begin{aligned} Z_0 &= Z(x=0) = -[ak^3/(k^2 - k_0^2)]^{2/3} = -[kaE/V_0]^{2/3} \\ Z_a &= Z(x=a) = -[ak_0^3/(k^2 - k_0^2)]^{2/3} \\ &= -[k_0 a(E/V_0 - 1)]^{2/3}. \end{aligned} \quad (6)$$

It is an elementary algebraic exercise to determine the reflexion r and transmission amplitude t from (5):

$$Dt = 2i/\pi(-Z_a)^{1/2}, \quad (7a)$$

$$\begin{aligned} Dr &= [\text{Ai}(Z_0) + i \text{Ai}'(Z_0)(-Z_0)^{-1/2}][\text{Bi}(Z_a) \\ &\quad + i \text{Bi}'(Z_a)(-Z_a)^{-1/2}] - [\text{Bi}(Z_0) + i \text{Bi}'(Z_0) \\ &\quad \times (-Z_0)^{-1/2}][\text{Ai}(Z_a) + i \text{Ai}'(Z_a)(-Z_a)^{-1/2}], \end{aligned} \quad (7b)$$

$$\begin{aligned} D &\equiv [\text{Ai}(Z_0) - i \text{Ai}'(Z_0)(-Z_0)^{-1/2}][\text{Bi}(Z_a) \\ &\quad + i \text{Bi}'(Z_a)(-Z_a)^{-1/2}] - [\text{Bi}(Z_0) - i \text{Bi}'(Z_0)(-Z_0)^{-1/2}] \\ &\quad \times [\text{Ai}(Z_a) + i \text{Ai}'(Z_a)(-Z_a)^{-1/2}], \end{aligned} \quad (7c)$$

upon using the Wronskian $\text{Ai Bi}' - \text{Ai}' \text{Bi} = 1/\pi$. It is

straightforward to check that the reflexion and transmission coefficients

$$R = |r|^2, \quad T = |t|^2 k_0/k = |t|^2 (Z_a/Z_0)^{1/2}, \quad (8)$$

satisfy flux conservation, $R + T = 1$.

From this point onwards there is nothing left to do but look up the properties and tables³ of Airy functions in order to determine R and T . A simple computer program could easily accomplish this.

ANALYTICAL EXPRESSIONS NEAR THE CLASSICAL AND QUANTUM LIMITS

We prefer, however, to display asymptotic expressions in the classical ($ka \gg 1$) and quantum ($ka \ll 1$) limits which show the deviations from the standard textbook answers for finite a . For this we require the series expansions:

$$\text{Ai}(Z) = c_1 f(Z) - c_2 g(Z), \\ \text{Bi}(Z) = 3^{1/2} [c_1 f(Z) + c_2 g(Z)], \quad (9a)$$

with

$$c_1 c_2 = 1/2\pi^{3/2} \quad (9b)$$

and

$$f(Z) = 1 + Z^3/6 + O(Z^6), \\ g(Z) = Z + Z^4/12 + O(Z^7) \quad (9c)$$

useful when $Z \ll 1$, i.e., $ka \ll 1$. We also need the asymptotic expansions for $Z \gg 1$ ($ka \gg 1$),

$$\text{Ai}(-Z) \sim \pi^{-1/2} Z^{-1/4} [\sin(\zeta + \pi/4)F(Z) - \cos(\zeta + \pi/4)B(Z)],$$

$$\text{Bi}(-Z) \sim \pi^{-1/2} Z^{-1/4} [\cos(\zeta + \pi/4)F(Z) + \sin(\zeta + \pi/4)G(Z)],$$

$$\text{Ai}'(-Z) \sim -\pi^{-1/2} Z^{1/4} [\cos(\zeta + \pi/4)\bar{F}(Z) + \sin(\zeta + \pi/4)\bar{G}(Z)],$$

$$\text{Bi}'(-Z) \sim \pi^{-1/2} Z^{1/4} [\sin(\zeta + \pi/4)\bar{F}(Z) - \cos(\zeta + \pi/4)\bar{G}(Z)], \quad (10a)$$

where

$$\zeta = 2Z^{3/2}/3 \quad (10b)$$

and

$$F(Z) = 1 - 385/4608Z^3 + O(Z^{-6}), \\ G(Z) = 5/48Z^{3/2} + O(Z^{-9/2}), \\ \bar{F}(Z) = 1 + 455/4608Z^3 + O(Z^{-6}), \\ \bar{G}(Z) = -7/48Z^{3/2} + O(Z^{-9/2}). \quad (10c)$$

The first limit of interest, $ka \ll 1$, corresponds to a steep potential hill. Both Z_0 and Z_a are small here for finite E , and we can substitute expansions (10) in (7). One finds

$$\pi D \simeq \frac{\sqrt{-Z_a} + \sqrt{-Z_0}}{\sqrt{Z_0 Z_a}} [1/2(Z_a - Z_0) \\ \times (\sqrt{-Z_a} + \sqrt{-Z_0}) \\ + i\{1 + 1/6(Z_a - Z_0)^2(Z_0 + Z_a - \sqrt{Z_0 Z_a})\}]$$

giving

$$T \simeq \frac{4(Z_0 Z_a)^{1/2}}{(\sqrt{-Z_0} + \sqrt{-Z_a})^2} |1 + 1/12(Z_a - Z_0)^2 \\ \times (\sqrt{-Z_a} - \sqrt{-Z_0})^2|^2 \\ = \frac{4kk_0}{(k + k_0)^2} [1 + 1/12a^2(k - k_0)^2 + O(ka)^4]. \quad (11)$$

Notice how the transmission coefficient is *enhanced* by the finite width a of the hill.⁴

The second, classical, limit for a shallow hill has $a \rightarrow \infty$ with k and k_0 finite; this means taking Z_a and Z_0 to $-\infty$. Going through the same rigmarole, one finds

$$\pi D = \frac{2ie^{i(\delta_a - \delta_0)}}{(Z_0 Z_a)^{1/4}} \\ \times \left(1 + \frac{i}{72}(\delta_a^{-1} - \delta_0^{-1}) + \frac{35}{10368}(\delta_a^{-1} - \delta_0^{-1})^2 \right. \\ \left. - \frac{i}{72}(\delta_0 \delta_a)^{-1} \sin(\delta_0 - \delta_a) e^{i(\delta_0 - \delta_a)} + O(\delta^{-4})\right)$$

where $\delta_i = 2/3(-Z_i)^{3/2}$. One easily computes

$$T = 1 - (1/64)[\{(-Z_0)^{-3/2} - (-Z_a)^{-3/2}\}^2 \\ + 4 \sin^2(\delta_0 - \delta_a)(Z_0 Z_a)^{-3/2} + O(Z^{-6})] \\ = 1 + (1/64)(Z_0^3 + Z_a^3) + O(Z^{-6}), \quad \text{upon averaging } \sin^2 \delta, \\ = 1 - \frac{(k^2 - k_0^2)^2}{64a^2}(k^{-6} + k_0^{-6}) + O((ka)^{-4}). \quad (12)$$

Here one sees that transmission is *lowered*⁵ by the finite range a , as expected.

There is one final limit which can be treated analytically which has $Z_0 \rightarrow \infty$ and $Z_a \rightarrow 0$ simultaneously. In this situation we must have $ka \rightarrow \infty$ and $k_0 a$ finite, which corresponds to a particle that can barely creep over a shallow hill. Here we have a formulas (9) and (10). Without going through the obvious details again, we shall quote the answers in leading order:

$$D = 2\pi^{-1/2}(-Z_0)^{-1/4} [c_2(-Z_a)^{-1/2} e^{-i(\delta_0 - 5\pi/6)} \\ + c_1 e^{-i(\delta_0 - 2\pi/3)}] + O(Z_a^{3/2}, Z_0^{-3/2})$$

or

$$T \simeq (-Z_a)^{1/2} / \pi c_2^2 \simeq 4.76 k_0 a (ka)^{-2/3}. \quad (13)$$

Thus when the de Broglie wavelength of the transmitted wave is comparable with the range of the potential rise, we are still far from the classical situation of full transmission.⁶

DISCUSSION

We believe that the model and the results which we have obtained for it are characteristic of more general *physical* potentials which undergo smooth rises from $V = 0$ to $V = V_0$. That is, the finite physical extent of the potential increase results in an enhancement of the quantum-mechanical transmission factor [by terms of order (ka)], or equivalently a diminution of the classical unit transmission factor [by terms of order $(k_0 a)^{-2}$]. In practice, of course, we should be concerned with incoming wave packets, not plane waves. What our results show is that, for a rather steep hill, there is a sizeable increase in transmission for the Fourier components having incoming k of order $1/a$ or less; while for the opposite case of a shallow hill, it is the same Fourier components which are relevant for depressing the

classical transmission coefficient below 1. The detailed answers obviously depend on the detailed composition of the wave packet and the shape of the potential.²

This investigation was prompted by Dr. D. Websdale who questioned the relevance of standard textbook presentations of the potential step in the context of ordinary macroscopic situations, and was interested to see how the transition from the classical to the quantum limit can be exhibited most simply at one stroke.

¹See, for instance, A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. I.

²The only reference we have been able to locate where a comparable example is treated is the book by I. I. Goldman, V. D. Krivchenkov, V. I.

Kogan, and V. M. Galitskii, *Problems in Quantum Mechanics* (Info-search Ltd., London, 1960). These authors consider the potential $V(x) = V_0[1 + e^{-2\pi x/a}]^{-1}$ and work out the transmission factor to be $T = (\sinh ak)(\sinh ak_0)/\sinh^2 \frac{1}{2}a(k + k_0)$ where k and k_0 refer to the wave numbers as $x \rightarrow -\infty$ and $x \rightarrow \infty$ respectively. It is amusing to compare the limiting values of this formula with our example and results (11), (12), and (13): one finds that it is the corrections to the classical answer $T = 1$ which are most sensitive to the detailed *shape* of the potential rise.

³M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

⁴The potential of Ref. 2 yields the same answer to this order.

⁵The same effect is apparent in the potential of Ref. 2, although the answer, $T = 1 - (e^{-ak} - e^{-ak_0})^2 + \dots$, is rather different.

⁶Again Ref. 2 supports this statement, although it specifically yields $T = 2k_0a$, instead of (13).

AAPT MEETINGS

A reminder of dates: AAPT winter meeting in San Francisco, January 23-26, 1978
Summer meeting in London, Ontario June 14-16, 1978.