CONTINUITY OF Ψ AND Ψ' FOR A DISCONTINUOUS POTENTIAL

6. Consider a potential $V(x)$ having a finite discontinuity at $x = x_0$ (Fig. I

the interval $(x_0-d,\ x_0+d)$, by replacing $V(x)$ by the line segment shown in the

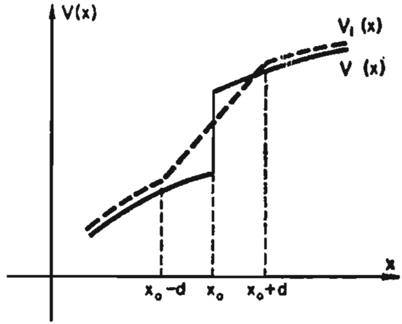


FIG. II.16.

one obtains a continuous potential $V_1(x)$. The Schrödinger equation then becomes

$$\psi_1''(x)+\frac{2m}{\hbar^2}(E-V_1(x))\,\psi_1(x) = 0,$$

whence

$$(\psi_1')_{x_0+d}-(\psi_1')_{x_0-d} = \frac{2m}{\hbar^2}\int\limits_{x_0-d}^{x_0+d}(V_1(x)-E)\,\psi_1(x)\,dx.$$

$$\int_{x_0-d}^{x_0+d} \frac{d}{dx}\left(\frac{d\Psi}{dx}\right) dx = \left.\frac{d\Psi}{dx}\right|_{x_0+d} - \left.\frac{d\Psi}{dx}\right|_{x_0-d}$$

F

shrink $d \to 0$ and note that since $V_1(x)$ is continuous and we assume for the moment that ψ is also continuous.

Then

$$\lim_{d \to 0} \int_{x_0-d}^{x_0+d} \left(V_1(x) - E \right) \psi(x)\, dx \to 0$$

Thus ψ' is continuous

How about ψ?

Integrate Schroedinger eq. w.r.t. x (between x_a and x) $\bar{\omega}$ x_a arbitrary value.

$$-\frac{\hbar^2}{2m} \frac{d}{dx} \psi(x) = -\frac{\hbar^2}{2m} \left.\frac{d\psi}{dx}\right|_{x=x_a} + \int_{x_a}^{x} \left(E - V(x')\right) \psi(x')\, dx'$$

Now integrate this equation over the dis-continuity at x_0

$$-\frac{\hbar^2}{2m}\left(\psi\Big|_{x_0+d} - \psi\Big|_{x_0-d} \right) = +\frac{\hbar^2}{2m} \int_{x_0-d}^{x_0+d} \underbrace{\left.\frac{d\psi}{dx}\right|_{x=x_a}}_{\text{constant}} dx$$

$$+ \int_{x_0-d}^{x_0+d} \left[\int_{x_a}^{x} \left(E - V(x')\right) \psi(x')\, dx' \right] dx$$

Both integrals $\to 0$ as $d \to 0$ $\Rightarrow$ $\psi(x)$ continuous.

4. *The Potential Step.* Next in order of increasing complexity is the potential step $V(x) = V_0\eta(x)$ as shown in Figure 6.3. There is no physically acceptable solution for $E < 0$ because of the general theorem that E can never be less than the absolute minimum of $V(x)$. Classically this is obvious. But, as the examples of the harmonic oscillator and the free particle have already shown us, it is also true in quantum mechanics despite the possibility of penetration

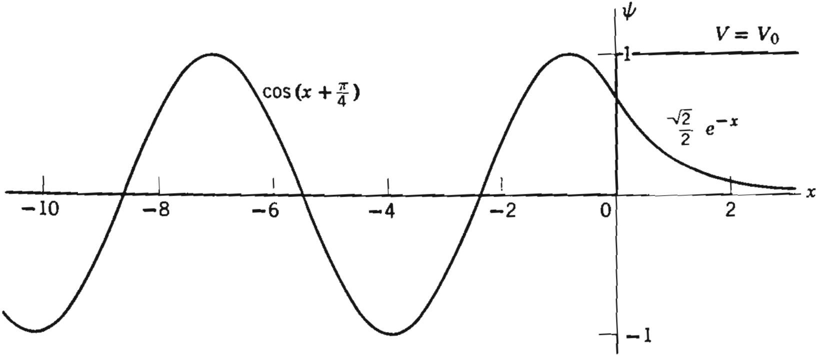


Figure 6.3. Eigenfunction for the potential step $V(x) = V_0\eta(x)$ corresponding to an energy $E = V_0/2$.

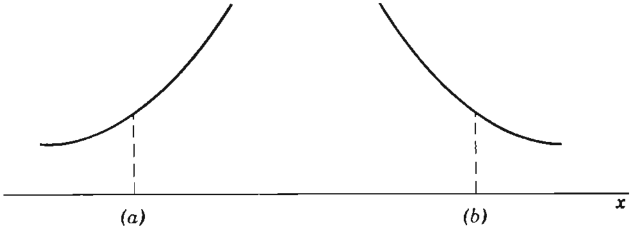


Figure 6.4. Shape of the wave function in the nonclassical region.

into classically inaccessible regions. We can prove the theorem by considering the real solutions of the Schrödinger equation (see Exercise 4.7)

$$-\frac{\hbar^2}{2\mu}\psi'' + [V(x) - E]\psi = 0$$

If $V(x) > E$ for *all* x, ψ'' has the same sign as ψ. Hence, if ψ is positive at some point x, the wave function has one of the two shapes shown in Figure 6.4, depending on whether the slope is positive or negative. In Figure 6.4*a* ψ can never bend down to be finite as $x \to \infty$. In Figure 6.4*b* ψ diverges as $x \to -\infty$. Hence, there must always be some region where $E > V(x)$ and where the particle could be found classically.

Now we consider the potential step with $0 < E < V_0$. Classically a particle of this energy, if it were incident from the left, would move freely until reflected at the potential step. Conservation of energy requires it to turn around, changing the sign of its momentum.

The Schrödinger equation has the solution

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x < 0) \\ Ce^{-\kappa x} & (x > 0) \end{cases} \tag{6.31}$$

Here

$$\hbar k = \sqrt{2\mu E} \qquad \hbar\kappa = \sqrt{2\mu(V_0 - E)}$$

The second linearly independent solution for $x > 0$, $e^{\kappa x}$, has been omitted because it is in conflict with the boundary condition that ψ remain finite as $x \to \infty$. Since one of the two linearly independent solutions is excluded, the stationary states for $E < V_0$ are nondegenerate.[5]

By matching the wave function and its slope at the discontinuity of the potential, $x = 0$, we have

$$A + B = C$$
$$ik(A - B) = -\kappa C$$

[5] See Chapter 5, Footnote 4.

or

$$\frac{B}{A} = \frac{ik + \kappa}{ik - \kappa} = e^{i\alpha} \qquad (\alpha\text{: real})$$
$$\frac{C}{A} = \frac{2ik}{ik - \kappa} = 1 + e^{i\alpha} \tag{6.32}$$

Substituting these values into (6.31), we obtain

$B = Ae^{i\alpha}$
$\therefore |B|^2 = |A|^2$

$$\psi = \begin{cases} 2Ae^{i\alpha/2}\cos\left(kx - \dfrac{\alpha}{2}\right) & (x < 0) \\ 2Ae^{i\alpha/2}\cos\dfrac{\alpha}{2}\, e^{-\kappa x} & (x > 0) \end{cases} \tag{6.33}$$

in agreement with the remark made in Section 5 of Chapter 4 that the wave function in the case of no degeneracy is real except for an arbitrary constant factor. Hence, a graph may be drawn of such a wave function (Figure 6.3). The classical turning point ($x = 0$) is a point of inflection of the wave function. The oscillatory and the exponential portions can be joined smoothly at $x = 0$ for all values of E between 0 and V_0: the energy spectrum is continuous.

draw picture

The solution (6.31) can be given a straightforward interpretation. It represents a plane wave incident from the left with an amplitude A and a reflected wave which propagates toward the left with an amplitude B. According to (6.32), $|A|^2 = |B|^2$; hence the reflection is *total*. Although ψ has a finite value in the region to the right of the potential step, there is no permanent penetration. A wave packet which is a superposition of eigenfunctions (6.31) could be constructed to represent a particle incident from the left. This packet would move classically, being reflected at the wall and giving again a vanishing probability of finding the particle in the region of positive x after the wave packet has receded.

$S = \frac{\hbar k}{m}(|A|^2 - |B|^2)$
$\Rightarrow S = 0$
no net momentum in the wave

These remarks can perhaps be better understood if we observe that for one-dimensional motion the conservation of probability leads to particularly transparent consequences. For a stationary state (4.2) reduces to $dj/dx = 0$. Hence, the current density

$\frac{\partial \rho}{\partial t} + \frac{d}{dx} S = 0$
for ρ ind of t

$$j = \frac{\hbar}{2\mu i}\left[\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right] \tag{6.34}$$

$\frac{dS}{dx} = 0$
$S = \text{const.}$

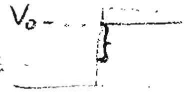
has the same value at all points x. j, when calculated with the wave function (6.33), is seen to vanish, as it does for any essentially real wave function. Hence, there is no net current anywhere at all. To the left of the potential step the relation $|A|^2 = |B|^2$ insures that incident and reflected probability currents cancel one another. If there is no current, there is no net momentum in ~~it~~

$e^{i\alpha}$ is a p
α is x independent

$\psi(x) \sim e^{-\kappa x}$ $x > 0$

$\Delta x \sim \frac{1}{\kappa}$

$\Delta p > \hbar$



state (6.31). In order to observe the particle in the exponential tail, it must be localized within a distance of order $\Delta x \simeq 1/\kappa$. Hence, its momentum must be uncertain by

inequality ⇒ energy into classical region

$$\Delta p > \hbar/\Delta x \simeq \hbar\kappa = \sqrt{2\mu(V_0 - E)}$$

The particle of energy E can thus be located in the nonclassical region only if it is given an energy $V_0 - E$, sufficient to raise it into the classically allowed region.

The case of an infinitely high potential barrier ($V_0 \to \infty$ or $\kappa \to \infty$) deserves special attention. From (6.31) it follows that in this limiting case $\psi(x) \to 0$ in the region under the barrier, no matter what value the coefficient C may have. According to (6.32), the joining conditions for the wave function at $x = 0$ now reduce formally to

$$\lim_{\kappa\to\infty} \frac{B}{A} = -1, \qquad \lim_{\kappa\to\infty} \frac{C}{A} = 0$$

or $A + B = 0$ and $C = 0$ as $V_0 \to \infty$. These equations show that at a point where the potential makes an infinite jump the wave function must vanish, whereas its slope may jump discontinuously from a finite value $2ikA$ to zero.[6]

→ break

discuss Goethe

We next examine the quantum mechanics of a particle which encounters the potential step in one dimension with an energy $E > V_0$. Classically this particle passes the potential step with altered velocity but no change of direction. The particle could be incident either from the right or from the left. The solutions of the Schrödinger equation are now oscillatory in both regions; hence, to each value of the energy correspond two linearly independent, degenerate eigenfunctions. For the physical interpretation their explicit construction is best accomplished by specializing the general solution:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x < 0) \\ Ce^{ik_1x} + De^{-ik_1x} & (x > 0) \end{cases} \tag{6.35}$$

go back to previous t-dep wave to see this

where $\hbar k = \sqrt{2\mu E}$ and $\hbar k_1 = \sqrt{2\mu(E - V_0)}$. Two useful particular solutions are obtained by setting $D = 0$, or $A = 0$. The first of these represents a wave incident from the left. Reflection occurs at the potential step, but there is also transmission to the right. The second particular solution represents incidence and transmission from right to left and reflection toward the right.

We consider here only the first case ($D = 0$). The remaining constants are related by the condition for smooth joining at $x = 0$,

$$A + B = C \qquad \text{and} \qquad k(A - B) = k_1 C$$

[6] The discontinuity of the slope is not in conflict with the condition of smooth joining derived for *finite* jumps of the potential.

from which we solve

$$\frac{B}{A} = \frac{k - k_1}{k + k_1} \quad \text{and} \quad \frac{C}{A} = \frac{2k}{k + k_1} \tag{6.36}$$

The current density is again constant, but its value is no longer zero. Instead,

$$j = \frac{\hbar k}{\mu}(|A|^2 - |B|^2) \qquad (x < 0)$$

$$j = \frac{\hbar k_1}{\mu}|C|^2 \qquad (x > 0)$$

The equality of these values is assured by (6.36). We thus have

$$\frac{|B|^2}{|A|^2} + \frac{k_1}{k}\frac{|C|^2}{|A|^2} = 1 \tag{6.37}$$

In analogy to optics the first term in this sum is called the *reflection coefficient*, the second is the *transmission coefficient*. We have

$$R = \frac{|B|^2}{|A|^2} = \frac{(k - k_1)^2}{(k + k_1)^2} \tag{6.38}$$

$$T = \frac{k_1}{k}\frac{|C|^2}{|A|^2} = \frac{4kk_1}{(k + k_1)^2} \tag{6.39}$$

Equation (6.37) assures us that $R + T = 1$. R and T depend only on the ratio E/V_0.

For a wave packet incident from the left the presence of reflection means that the wave packet may, when it arrives at the potential step, split into two parts, provided that its average energy is close to V_0. This splitting up of the wave packet is a distinctly nonclassical effect which affords an argument against the early attempts to interpret the wave function as measuring the matter (or charge) density of the particle which it accompanies. For the splitting up of the wave packet would then imply a physical breakup of the particle, and this would be very difficult to reconcile with the facts of observation. After all, electrons and other particles are always found as complete entities with the same distinct properties. On the other hand, there is no contradiction between the splitting up of a wave packet and the probability interpretation of the wave function.

Exercise 6.5. Show that the coefficients for reflection and transmission at a potential step are the same for a wave incident from the right as for a wave incident from the left.

Problem 22. Scattering at a symmetric potential barrier

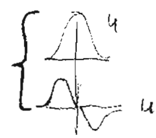
A current of particles of energy E strikes a potential barrier $V(x)$ restricted to the region $-a \leqq x \leqq +a$. The potential is supposed to be an even function of x:

$$V(x) = V(-x). \tag{22.1}$$

The amplitudes of backward and forward scattered waves shall be determined in terms of the logarithmic derivatives of the wave function at $x = \pm a$.

Solution. The symmetry condition (22.1) has the important consequence that for every energy E there exists a solution of the Schrödinger equation of even parity,

$$u_+(x) = u_+(-x); \qquad u'_+(x) = -u'_+(-x), \tag{22.2a}$$



and a solution of odd parity,

$$u_-(x) = -u_-(-x); \qquad u'_-(x) = u'_-(-x). \tag{22.2b}$$

Since both are, of course, linearly independent of one another, the general solution will be any linear combination of them. The two partial solutions u_+ and u_- may be determined inside the interval $-a \leq x \leq +a$, in the worst case by numerical procedures starting from $x=0$ with

$$u_+(0) = 1; \qquad u'_+(0) = 0$$

and

$$u_-(0) = 0; \qquad u'_-(0) = 1$$

in an arbitrary normalization of these two basic solutions. Thus we can compute their logarithmic derivatives at $x=a$ which we shall write for convenience in a dimensionless form

$$a u'_+(a)/u_+(a) = L_+; \qquad a u'_-(a)/u_-(a) = L_- \tag{22.3}$$

independent of their respective normalizations. The logarithmic derivatives $a u'_\pm(-a)/u_\pm(-a)$ at $x=-a$ then follow from (22.2) to be $-L_+$ and $-L_-$.

The solution, corresponding to a wave of unit amplitude incident from the left, can be written

$$u(x) = \begin{cases} e^{ikx} + B e^{-ikx}, & -\infty < x \leq -a, \\ C_1 u_+(x) + C_2 u_-(x), & -a \leq x \leq +a, \\ (1+F) e^{ikx}, & +a \leq x < +\infty. \end{cases} \tag{22.4}$$

$D = 1+F$

if ψ nondegenerate $\psi(x) = c\,\psi(-x) = c\,(c\,\psi(x)) = c^2 \psi(x)$

$\therefore \; c = \pm 1$

Continuity of $u(x)$ and $u'(x)$ at $x = \pm a$ yields four conditions, viz.

at $(-a)$

$$e^{-ika} + B e^{ika} = \quad C_1 u_+(a) - C_2 u_-(a), \tag{22.5a}$$

$$ik(e^{-ika} - B e^{ika}) = -C_1 u'_+(a) + C_2 u'_-(a), \tag{22.5b}$$

at (a)

$$(1+F) e^{ika} = \quad C_1 u_+(a) + C_2 u_-(a), \tag{22.5c}$$

$$ik(1+F) e^{ika} = \quad C_1 u'_+(a) + C_2 u'_-(a). \tag{22.5d}$$

The sum of (22.5a) and (22.5c) gives $2C_1 u_+(a)$ and the difference of (22.5b) and (22.5d) $2C_1 u'_+(a)$. The ratio of both is

$$L_+ = ika \frac{-e^{-ika} + (1+F+B)e^{ika}}{e^{-ika} + (1+F+B)e^{ika}}. \tag{22.6a}$$

By the same procedure, with opposite signs, we find

$$L_- = ika \frac{e^{-ika} + (1+F-B)e^{ika}}{-e^{-ika} + (1+F-B)e^{ika}}. \tag{22.6b}$$

Solving (22.6a, b) with respect to $1+F \pm B$ and using the abbreviation

$$ka = q \tag{22.7}$$

we finally arrive at the amplitude relations

$$B = -\frac{1}{2} e^{-2iq} \left[\frac{L_+ + iq}{L_+ - iq} + \frac{L_- + iq}{L_- - iq} \right] \tag{22.8a}$$

and

$$1 + F = -\frac{1}{2} e^{-2iq} \left[\frac{L_+ + iq}{L_+ - iq} - \frac{L_- + iq}{L_- - iq} \right]. \tag{22.8b}$$

According to the equation of continuity, we expect the sum of reflected and transmitted intensities to be equal to the incident one. Indeed, from (22.8a, b) there follow the formulae

$$|B|^2 = \frac{(L_+ L_- + q^2)^2}{(L_+ L_- + q^2)^2 + q^2 (L_+ - L_-)^2} \tag{22.9a}$$

and

$$|1+F|^2 = \frac{q^2 (L_+ - L_-)^2}{(L_+ L_- + q^2)^2 + q^2 (L_+ - L_-)^2}. \tag{22.9b}$$

They evidently satisfy the expected relation

$$|B|^2 + |1+F|^2 = 1. \tag{22.10}$$

The problem of determining the scattering amplitudes in forward and backward directions has thus been reduced to finding the logarithmic derivatives (22.3) at $x=a$ of the even and the odd parity wave functions. This cannot, of course, be accomplished as long as no special form of the potential (22.1) has been introduced.

In contradistinction to Problem 21, we no longer have $B=F$. Forward scattering prevails if

$$q|L_+ - L_-| > |L_+ L_- + q^2|,$$

backward scattering in the opposite case.

Problem 23. Reflection at a rectangular barrier

The general formulae derived in Problem 22 shall be applied to a potential barrier with

$$\frac{2m}{\hbar^2} V = k_0^2 \quad \text{in } |x| \leq a, \tag{23.1}$$

and $V=0$ elsewhere. The transmittance of the barrier shall be determined.

Solution. Inside the barrier, the Schrödinger equation becomes

$$u'' + (k^2 - k_0^2) u = 0. \tag{23.2}$$

There are, therefore, solutions of different type for a kinetic energy below ($k<k_0$) and above ($k>k_0$) threshold. We begin with the first case and write

$$k_0^2 - k^2 = \varkappa^2; \qquad u'' - \varkappa^2 u = 0. \tag{23.3}$$

Then the even solution is

$$u_+(x) = \cosh \varkappa x; \qquad u_+(0) = 1; \qquad u'_+(0) = 0 \tag{23.4 a}$$

and the odd solution

$$u_-(x) = \frac{1}{\varkappa} \sinh \varkappa x; \qquad u_-(0) = 0; \qquad u'_-(0) = 1. \tag{23.4 b}$$

Hence,

$$L_+ = a u'_+(a)/u_+(a) = \varkappa a \tanh \varkappa a; \tag{23.5 a}$$

$$L_- = a u'_-(a)/u_-(a) = \varkappa a \coth \varkappa a. \tag{23.5 b}$$

The transmittance of the barrier then follows from (22.9 b) by elementary reshaping:

$$T \equiv |1+F|^2 = \frac{1}{1 + \left(\dfrac{k_0^2}{2k\varkappa}\right)^2 \sinh^2 2\varkappa a} \tag{23.6}$$

whereas the reflectance, according to (22.10), is given by

$$R \equiv |B|^2 = 1 - T. \tag{23.7}$$

In classical mechanics, the whole flux arriving from the left side would be reflected at the barrier so that $|B|^2 = 1$ and $|1+F|^2 = 0$. This happens, according to Eq. (23.6) if, and only if, $\varkappa a \to \infty$, i.e. if there is a very great „potential mountain" above the energy level of the particles, the transparency of the barrier will become very small though still finite ("tunnel effect"). The transmittance of the barrier may then be written approximately

$$T = \frac{16 k^2 \varkappa^2}{k_0^4} e^{-4\varkappa a}, \tag{23.8}$$

its order of magnitude being mainly determined by the exponential factor.

The exponent

$$4\varkappa a = 2 \int_{-a}^{+a} dx \sqrt{\frac{2m}{\hbar^2}(V - E)}$$

will be generalized to this integral form for any potential $V(x)$, below (cf. Problem 116).

If, on the other hand, the kinetic energy exceeds the height of the barrier, the quantity $\varkappa$ defined by (23.3) becomes imaginary. With the abbreviation

$$K^2 = k^2 - k_0^2 = -\varkappa^2 \tag{23.9}$$

we may then write, instead of (23.6),

$U = \frac{\hbar^2 k_0^2}{2m}$

$$T = \frac{1}{1 + \left(\frac{k_0^2}{2kK}\right)^2 \sin^2 2Ka}. \tag{23.10}$$

Though in classical mechanics there should be $T = 1$ and $R = 0$ at these energies, the transparency following from (23.10) shows maxima of $T = 1$ only at $2Ka = n\pi$ $(n = 1, 2, 3, \ldots)$. Between these there are minima in the neighbourhood of $2Ka = (n + \frac{1}{2})\pi$ which lie the closer to $T = 1$ the smaller the factor in front of the sine in (23.10), i.e. the higher the energy above threshold.

The general behaviour of T as a function of the energy (in units of the threshold height, say, U) is shown in Fig. 5 where T has been drawn as a function of E/U for the example $2k_0 a = 3\pi$. The wave function has been explained in Fig. 6 where $|u|^2$ has been drawn vs. x. On the right-hand side of the barrier we simply have $|u|^2 = |1+F|^2$, i.e. constant,

wavefunctions in the barrier are sin, cos – they interfere
for $2Ka = n\pi$ $(n = 1, 2, ..)$ No $n=0$ (no oscillation for $K=0$)

$K = \phi$

whereas on its left there is interference of the incident with the reflected wave. Fig. 6 shows this feature for $k^2 = \varkappa^2 = \frac{1}{2}k_0^2$ and different widths of the barrier. The broader the latter, the smaller is the intensity transmitted and the more pronounced the interference phenomena become.

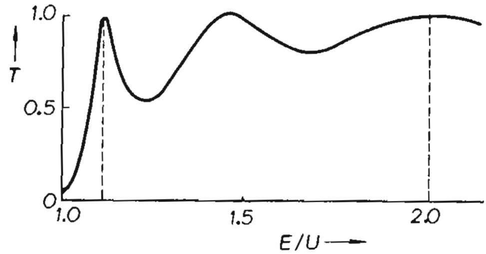


Fig. 5. Transmittance of potential barrier for $E > U$ in dependence upon energy

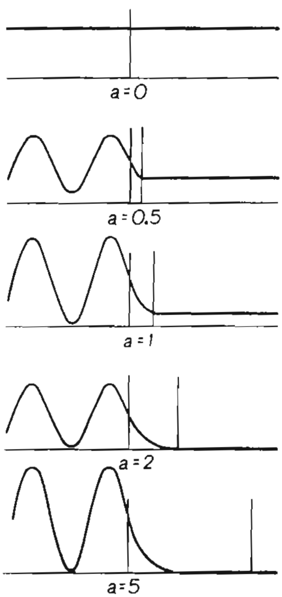


Fig. 6. Probability density $|u|^2$ in the current falling upon the barrier from the left, in the case $E < U$. The two vertical lines mark the width a of the barrier. The waves on the left are caused by interference between incident and reflected beams

Problem 24. Inversion of reflection

Let a potential threshold $V(x)>0$ in the interval $0<x<a$ form an obstacle to a wave incident from the left $(x<0)$. It shall be proved that the coefficient of reflection is the same when the wave falls on the obstacle from the right $(x>a)$, whatever the potential shape.

Solution. Let $u(x)$ and $v(x)$ be two real and independent solutions of the Schrödinger equation in the interval $0<x<a$ with the Wronskian

$$uv'-vu'=1\,. \tag{24.1}$$

The wave function in the case of the wave incident from the left is then of the form[2]

$$\psi=\left\{\begin{array}{ll} e^{ikx}+Re^{-ikx}, & x<0,\\ Au(x)+Bv(x), & 0<x<a,\\ Ce^{ik(x-a)}, & a<x \end{array}\right\} \tag{24.2}$$

and the conditions for continuity of ψ and ψ' at $x=0$ and $x=a$ are

$$\left.\begin{array}{l} 1+R\;=Au(0)\;+Bv(0),\\ ik(1-R)=Au'(0)+Bv'(0),\\ Au(a)\;+Bv(a)\;=C,\\ Au'(a)+Bv'(a)=ikC. \end{array}\right\} \tag{24.3}$$

From the last pair of equations, making use of (24.1), we find

$$\left.\begin{array}{l} A=\;\;\,C[v'(a)-ikv(a)],\\ B=-C[u'(a)-iku(a)]. \end{array}\right\} \tag{24.4}$$

Putting these expressions for A and B into the first pair of the Eqs. (24.3) we get

$$1+R=(p_{0a}-iq)C;\qquad 1-R=(p_{a0}-ir)C \tag{24.5}$$

with the abbreviations

$$\left.\begin{array}{l} p_{0a}=u(0)v'(a)-v(0)u'(a),\\ p_{a0}=u(a)v'(0)-v(a)u'(0),\\ q=k[u(0)v(a)-v(0)u(a)],\\ r=\dfrac{1}{k}[u'(0)v'(a)-v'(0)u'(a)]. \end{array}\right\} \tag{24.6}$$

From (24.5) we finally find

$$R=\frac{(p_{0a}-p_{a0})-i(q-r)}{(p_{0a}+p_{a0})-i(q+r)}, \tag{24.7}$$

[2] We write ψ for the space part of the wave function in this problem since u is used in another sense.

and the reflection coefficient becomes

$$|R|^2 = \frac{(p_{0a}-p_{a0})^2+(q-r)^2}{(p_{0a}+p_{a0})^2+(q+r)^2}. \tag{24.8}$$

Now take the opposite case with the wave incident from the right-hand side. The wave function (24.2) has then to be replaced by

$$\tilde\psi = \begin{cases} \tilde C e^{-ikx}, & x<0, \\ \tilde A u(x)+\tilde B v(x), & 0<x<a, \\ e^{-ik(x-a)}+\tilde R e^{ik(x-a)}, & a<x. \end{cases} \tag{24.9}$$

The conditions of continuity run as follows:

$$\left.\begin{aligned} 1+\tilde R &= \tilde A u(a)+\tilde B v(a), \\ -ik(1-\tilde R) &= \tilde A u'(a)+\tilde B v'(a), \\ \tilde A u(0)+\tilde B v(0) &= \tilde C, \\ \tilde A u'(0)+\tilde B v'(0) &= -ik\tilde C. \end{aligned}\right\} \tag{24.10}$$

They have the same structure as Eqs. (24.3) from which they can be obtained by exchanging the two arguments $x=0$ and $x=a$ and replacing k by $-k$. This transformation, applied to (24.6) renders

$$p_{0a}\to p_{a0}; \quad p_{a0}\to p_{0a}; \quad q\to q; \quad r\to r, \tag{24.11}$$

i. e. the only difference in the final formulae (24.7) and (24.8) occurs by exchanging p_{0a} and p_{a0}. Therefore, since (24.8) is symmetrical in p_{0a} and p_{a0}, the reflection coefficient

$$|\tilde R|^2 = |R|^2 \tag{24.12}$$

is the same for waves incident from both sides, as was to be proved. This does not, however, hold for R, Eq. (24.7) which, written as a ratio $R=\alpha/\beta$ of two complex numbers α and β according to (24.7) is transformed into $\tilde R = -\alpha^*/\beta$.

Problem 25. Rectangular potential hole

For a rectangular potential hole

$$V(x) = \begin{cases} -U & |x|<a, \\ 0 & \text{elsewhere} \end{cases} \tag{25.1}$$

the bound-state solutions and their eigenvalues shall be determined.

Solution. Since for states of positive energy the general behaviour can be gathered without difficulty from the preceding problem, it suffices to discuss negative energies, i. e. bound states.

$$-\frac{\hbar^2}{2m}u'' \mp \frac{\hbar^2}{2m}k_0^2 u = -\frac{\hbar^2}{2m}\kappa^2 u$$

$$u'' + (k_0^2 \mp \kappa^2)u = 0$$

$$u'' + k^2 u = 0 \qquad u=\cos kx \quad u' = -k\sin kx \quad u'' = -k^2\cos kx \checkmark$$

The potential is invariai
so that the solutions have
Putting

$$E = -\frac{\hbar^2\kappa^2}{2m};$$

these solutions are

even:

$$u_+(x) = \begin{cases} A_+\cos \\ A_+\cos \end{cases}$$

$$u_+(-x) = u_+(x),$$

$$1/A_+^2 = \frac{1}{k}[ka+$$

odd:

$$u_-(x) = \begin{cases} \\ \end{cases}$$

$$u_-(-x) = -$$

$$1/A_-^2 = \frac{1}{k}$$

Here the amplitudes inside
adjusted to make $u(a)$ conti
been calculated from the cor

Continuity of u' at $x=a$ ad

even: $-k$

or

t

odd: k c

or

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The potential is invariant with respect to inversion, $V(x)=V(-x)$, so that the solutions have either even or odd parity (cf. Problem 20). Putting

$$E=-\frac{\hbar^2\varkappa^2}{2m};\qquad U=\frac{\hbar^2 k_0^2}{2m};\qquad k^2=k_0^2-\varkappa^2 \tag{25.2}$$

these solutions are

take [0,a] side

even:

$$\left.\begin{aligned} u_+(x)&=\begin{cases}A_+\cos kx, & 0\le x\le a,\\ A_+\cos ka\,e^{\varkappa(a-x)}, & x>a,\end{cases}\\ u_+(-x)&=u_+(x),\\ 1/A_+^2&=\frac{1}{k}\left[ka+\sin ka\cos ka\right]+\frac{1}{\varkappa}\cos^2 ka;\end{aligned}\right\} \tag{25.3e}$$

odd:

$$\left.\begin{aligned} u_-(x)&=\begin{cases}A_-\sin kx, & 0\le x\le a,\\ A_-\sin ka\,e^{\varkappa(a-x)}, & x>a,\end{cases}\\ u_-(-x)&=-u_-(x),\\ 1/A_-^2&=\frac{1}{k}\left[ka-\sin ka\cos ka\right]+\frac{1}{\varkappa}\sin^2 ka.\end{aligned}\right\} \tag{25.3o}$$

Here the amplitudes inside and outside the potential hole have been adjusted to make $u(a)$ continuous. The normalization constants have been calculated from the condition

$$\int_{-\infty}^{+\infty} dx\,|u|^2=1. \qquad = 2\left[\int_0^a dx|u|^2+\int_a^\infty dx|u|^2\right]$$

Continuity of u' at $x=a$ adds another relation, viz.

same + and −
since $|u_-(x)|^2$
$=|-u_-(-x)|^2$
$=+|u_-(-x)|^2$

even: $$-k\sin ka=-\varkappa\cos ka$$

or

$$\tan ka=\frac{\varkappa}{k}; \tag{25.4e}$$

odd: $$k\cos ka=-\varkappa\sin ka$$

or

$$\text{tan}\ \cot ka=-\frac{k}{\varkappa}. \tag{25.4o}$$

Using (25.4) and (25.2), we can recast the normalization expressions so that we obtain the same equation

$$1/A_{\pm}^2 = a + \frac{1}{\varkappa} \tag{25.5}$$

for both cases.

In order to find the eigenvalues from (25.4), we replace $\varkappa$ on the right-hand side according to (25.2) and introduce the abbreviation

$$C = k_0 a . \tag{25.6}$$

We thus obtain

even: $$\tan ka = \frac{\sqrt{C^2-(ka)^2}}{ka} ; \tag{25.7e}$$

odd: $$\tan ka = -\frac{ka}{\sqrt{C^2-(ka)^2}} . \tag{25.7o}$$

For a given potential, C is a constant determining the size of the hole ($C^2 \propto U a^2$), and Eqs. (25.7e, o) can be used to find all values of ka and thus of the energy

$-\varkappa^2 = -k_0^2 \left[\frac{k_0^2 - k^2}{k_0^2} \right] = k^2 - k_0^2$

$$E = -U\left[1-\left(\frac{ka}{C}\right)^2\right] \tag{25.8}$$

compatible with the size of the hole.

Fig. 7 shows the function $\tan ka$ vs. ka as well as the expressions on the right-hand side of (25.7e) and (25.7o). The solution of these eigenvalue equations is obtained from the intersection of the curves of

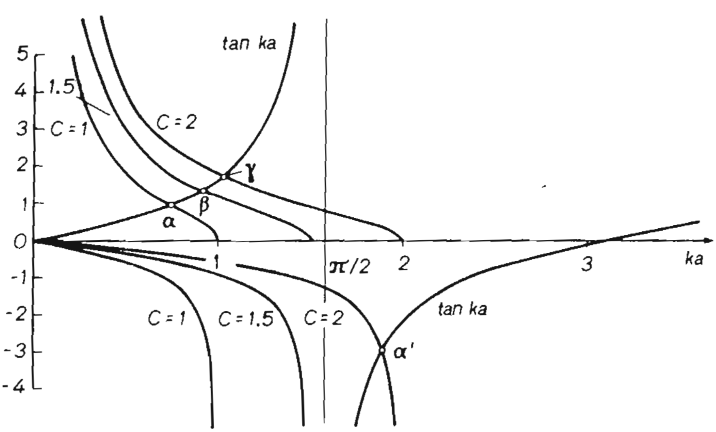
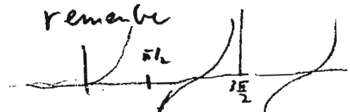
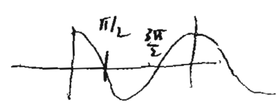


Fig. 7. Graphical solution of Eqs. (25.7e, o). The line $\tan ka$ intersects the curves which represent the right-hand sides for different values of the size parameter C. Curves at positive ordinates for even, at negative ones for odd parity

where are two even states remember





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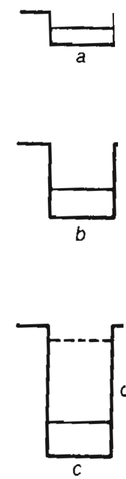

Fig. 8a—f. E
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($E_\gamma < E_\beta$), b
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are shown i

the last two with the tangent line. These curves, of course, still depend on the size parameter C. Starting with $C=1$, e. g., we have the intersection denoted by α in the even, and no intersection at all in the odd case. A hole of this size therefore contains no more than one eigenstate with even parity. In Fig. 8a the hole has been drawn with its eigen-

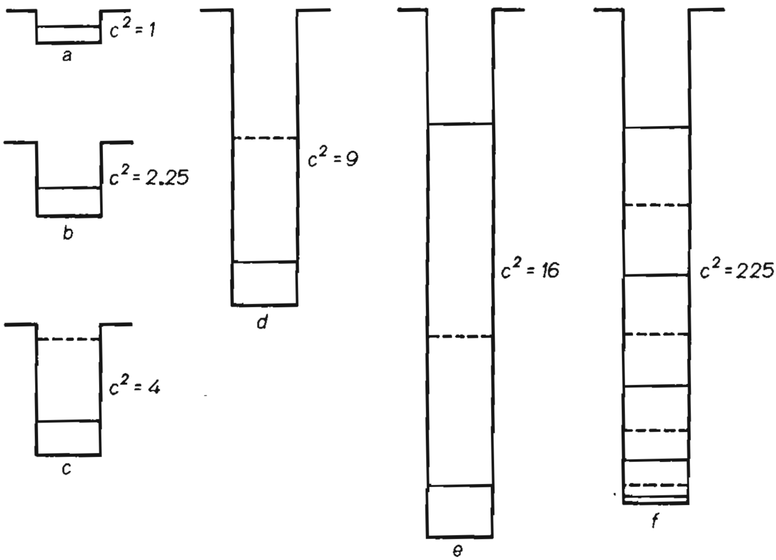


Fig. 8a—f. Energy levels in potential holes of different sizes determined by the size parameter C. Full lines even, broken lines odd parity

value. For a bigger hole, $C=1.5$, the intersection in Fig. 7 occurs at the point β; again we have only one even-parity state (Fig. 8b), and $E_\beta < E_\alpha$ because $(ka)_\beta > (ka)_\alpha$. If we further increase the size, taking e. g. $C=2$, the intersection γ leads to the lowest even-parity state $(E_\gamma < E_\beta)$, but an odd-parity state is now added corresponding to the intersection at α' (cf. Fig. 8c). Further increase gives a growing "capacity" for eigenstates to the hole (Figs. 8d, e, f), the number of states growing linearly with C and forming an alternate series of even and odd states. The eigenfunctions follow the general rule that, the more zeros they have, the higher they lie in the energy scale. The four lowest states are shown in Fig. 9 for $C=5$.

In classical mechanics, the particle might oscillate with any energy between the two walls at $x = \pm a$ bounding the hole. Outside, it would have negative kinetic energy so that these regions would be inaccessible. In quantum mechanics, this condition becomes less rigorous. The probability of finding the particle inside the hole, P_i, is less than unity:

$$P_i = \int_{-a}^{+a} dx|u|^2 = 1 - \frac{k^2}{k_0^2(1+\varkappa a)}, \tag{25.9}$$

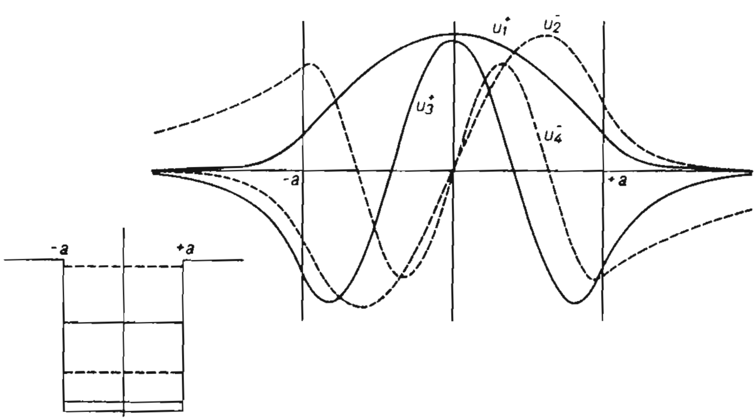


Fig. 9. Energy levels and eigenfunctions for $C=5$. Full lines even, broken lines odd parity

so that there remains a finite probability that it will stay outside. For any interval outside, this probability decreases exponentially as $e^{-2\varkappa(|x|-a)}$ with increasing distance $|x|-a$ from the hole.

Problem 26. Rectangular potential hole between two walls

The solutions of the Schrödinger equation shall be determined for the potential drawn in Fig. 10. Special consideration shall be given to the limit $l \to 0$ for the states of positive energy.

Solution. We begin with a brief discussion of the "bound" states, $E<0$. Using again the symbols k^2, k_0^2, and $\varkappa^2$ defined in (25.2) and normalizing so that

$$\int_{-l}^{+l} dx|u|^2 = 1,$$

we may write the wave functions as follows:

even parity:

$$u_+ = \begin{cases} A_+ \cos kx, & 0 \le x \le a, \\ A_+ \dfrac{\cos ka}{\sinh \varkappa(l-a)} \sinh \varkappa(l-x), & a < x \le l, \end{cases}$$

$$1/A_+^2 = \frac{1}{k}[ka + \sin ka \cos ka] + \frac{\cos^2 ka}{\varkappa}\left[\coth \varkappa(l-a) - \frac{\varkappa(l-a)}{\sinh^2 \varkappa(l-a)}\right] \tag{26.1e}$$

odd parity:

$$u_- = \begin{cases} A_- \sin kx, & 0 \le x \le a, \\ A_- \dfrac{\sin ka}{\sinh \varkappa(l-a)} \sinh \varkappa(l-x), & a < x \leqq l, \end{cases}$$

$$1/A_-^2 = \frac{1}{k}[ka - \sin ka \cos ka] + \frac{\sin^2 ka}{\varkappa}\left[\coth \varkappa(l-a) - \frac{\varkappa(l-a)}{\sinh^2 \varkappa(l-a)}\right]. \tag{26.1o}$$

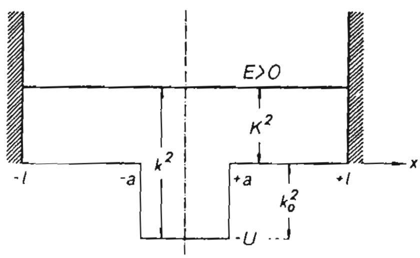


Fig. 10. Potential of Problem 26

Here again, as in Problem 25, $u(a)$ is made continuous, but continuity of $u'(a)$ imposes another condition in either case, viz. for

even parity: $$\tan ka = \frac{\varkappa}{k} \coth \varkappa(l-a), \tag{26.2e}$$

odd parity: $$\tan ka = -\frac{k}{\varkappa} \tanh \varkappa(l-a) \tag{26.2o}$$

elementary relation $s=\rho v_0$; for $x \lessgtr x_0$ we find $s \lessgtr \rho v_0$, and this is reasonable because at a point $x<x_0$ $(x>x_0)$ there have arrived at the time t those parts of the packet whose velocity is smaller (bigger) than v_0.

It may finally be mentioned that the normalization condition $\int dx\,\rho=1$ holds for all times, thus reflecting the conservation of matter.

Problem 18. Standing wave

A particle is included between two impenetrable potential walls at $x=-a$ and $x=+a$. (The walls idealize a strong repulsion of the particle when it approaches these boundaries.) The eigenstates shall be determined and discussed.

Solution. We have

$$\psi(x,t)=u(x)\,e^{-i\frac{E}{\hbar}t} \tag{18.1}$$

for stationary states. The space function $u(x)$ satisfies the Schrödinger equation

$$u''+k^2u=0 \tag{18.2}$$

with

$$k^2=\frac{2mE}{\hbar^2}; \tag{18.3}$$

thence follows its most general form

$$u(x)=A\,e^{ikx}+B\,e^{-ikx}. \tag{18.4}$$

Finally, the potential walls are imposing boundary conditions

$$u(a)=0; \qquad u(-a)=0 \tag{18.5}$$

which, combined with the normalization condition

$$\int_{-a}^{+a} dx\,|u(x)|^2=1, \tag{18.6}$$

permit the complete determination of the eigenfunctions, always excepting the constant phase factor which remains free in quantum mechanics.

From (18.5) put into (18.4), we find two homogeneous linear equations for A and B,

$$A\,e^{ika}+B\,e^{-ika}=0,$$
$$A\,e^{-ika}+B\,e^{ika}=0,$$

permitting a non-zero solution only for vanishing determinant:

$$\begin{vmatrix} e^{ika} & e^{-ika} \\ e^{-ika} & e^{ika} \end{vmatrix} = 0 \quad \text{or} \quad \sin 2ka = 0. \tag{18.7}$$

This *eigenvalue condition* is satisfied only for the eigenvalues of k,

$$k_n = \frac{\pi}{2a} n, \qquad n = \pm 1, \pm 2, \pm 3, \ldots \tag{18.8}$$

The value $k=0$, also satisfying (18.7), can be excluded since it contradicts the normalization condition (18.6). The eigenvalues of the energy follow from (18.3) and (18.8):

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2}{8ma^2} n^2. \tag{18.9}$$

From (18.8) we have

$$e^{ik_n a} = e^{i\frac{\pi}{2}n} = i^n$$

so that

$$B = (-1)^{n+1} A.$$

If n is an odd integer, $B = A$ and the normalized eigenfunctions are

$$u_n^+(x) = a^{-\frac{1}{2}} \cos k_n x = a^{-\frac{1}{2}} \cos \frac{\pi n x}{2a}, \qquad n = \pm 1, \pm 3, \ldots \tag{18.10a}$$

If n is an even integer, $B = -A$ and we have

$$u_n^-(x) = a^{-\frac{1}{2}} \sin k_n x = a^{-\frac{1}{2}} \sin \frac{\pi n x}{2a}, \qquad n = \pm 2, \pm 4, \ldots \tag{18.10b}$$

Since u_n, apart from an irrelevant sign in (18.10b), does not depend upon the sign of n, we can ignore negative values of n so that e.g. the four lowest states become

$$\left.\begin{array}{lll} n=1, & E_1 = \dfrac{\hbar^2 \pi^2}{8ma^2}, & u_1^+ = a^{-\frac{1}{2}} \cos \dfrac{\pi x}{2a}, \\[2ex] n=2, & E_2 = 4E_1, & u_2^- = a^{-\frac{1}{2}} \sin \dfrac{\pi x}{a}, \\[2ex] n=3, & E_3 = 9E_1, & u_3^+ = a^{-\frac{1}{2}} \cos \dfrac{3\pi x}{2a}, \\[2ex] n=4, & E_4 = 16E_1, & u_4^- = a^{-\frac{1}{2}} \sin \dfrac{2\pi x}{a}. \end{array}\right\} \tag{18.11}$$

It should be noted that the eigenfunctions are alternate symmetric (n odd) and antisymmetric (n even) with respect to reflection at the origin. This property is called the *parity* of the state; in the case of symmetry we speak of positive, in the opposite case of negative parity. The plus and minus signs (u_n^+, u_n^-) refer to this property.

The first four eigenfunctions have been drawn in Fig. 1.

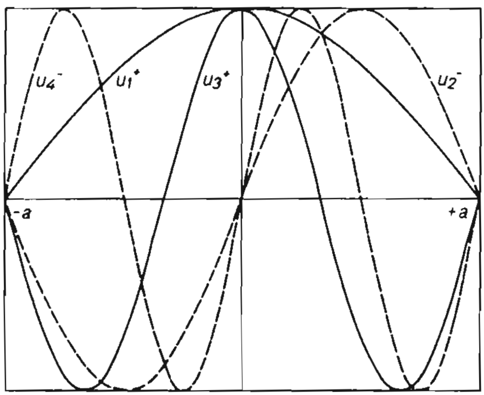


Fig. 1. The first four eigenfunctions of the one-dimensional potential well

Since the space part of the eigenfunctions is real, there can exist no resulting flux in any state. This is a consequence of $|A|=|B|$ in Eq. (18.4), cf. the discussion in Problem 16: The A wave and B wave in (18.4) contribute opposite currents and momenta. The eigenfunctions of the hamiltonian belonging to sharp energy values therefore are not eigenfunctions of the momentum operator

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x}.$$

Indeed, differentiation of the functions (18.10a, b) does not reproduce them but exchanges cosine with sine solutions. The expectation value, however, of the momentum can be computed according to

$$\langle n|p|n\rangle = \frac{\hbar}{i}\int_{-a}^{+a} dx\, u_n(x)\frac{\partial}{\partial x}u_n(x).$$

Since the integrand is an odd function of x, this integral vanishes for all states: $\langle n|p|n\rangle = 0$, in accordance with the vanishing flux.

NB. The mathematical problem is very much the same as the classical one of the vibrating string, the only difference being that here eigenvalues of the energy and there eigenvalues of the frequency follow the quadratic law (18.9). The classical vibration energy has no analogue, however, in the quantum mechanical problem since it derives from the possible excitation of the string vibration to arbitrary amplitudes, whereas the amplitudes of our wave functions are fixed by the normalization condition (18.6), i. e. by the fact that the particle number is one.

Problem 19. Opaque division wall

In the preceding problem an opaque wall of infinitely small width but infinitely large height shall be introduced at $x=0$ and its effect upon the eigenstates investigated.

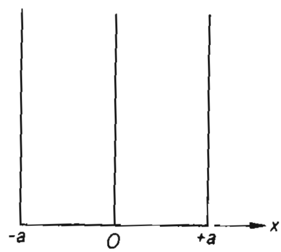


Fig. 2. Potential well with opaque wall

Solution. The opaque wall dividing the whole region into two equal parts may be obtained by idealization of a barrier of finite width 2ε (between $x=-\varepsilon$ and $x=+\varepsilon$) and height V_0. We introduce the abbreviations

$$\frac{2mE}{\hbar^2}=k^2; \quad \frac{2m}{\hbar^2}(V_0-E)=\varkappa^2, \tag{19.1}$$

then we have a total of four boundary conditions at this barrier, viz. continuity of $u(x)$ and $u'(x)$ at $x=\pm\varepsilon$, besides the two boundary conditions $u(\pm a)=0$. Satisfying the latter two and writing the solution in real form, we have

$$u=\left\{\begin{array}{ll} A_1 \sin k(x+a) & -a \leq x \leq -\varepsilon, \\ B e^{-\varkappa x}+C e^{\varkappa x} & -\varepsilon \leq x \leq +\varepsilon, \\ A_2 \sin k(x-a) & +\varepsilon \leq x \leq +a. \end{array}\right\} \tag{19.2}$$

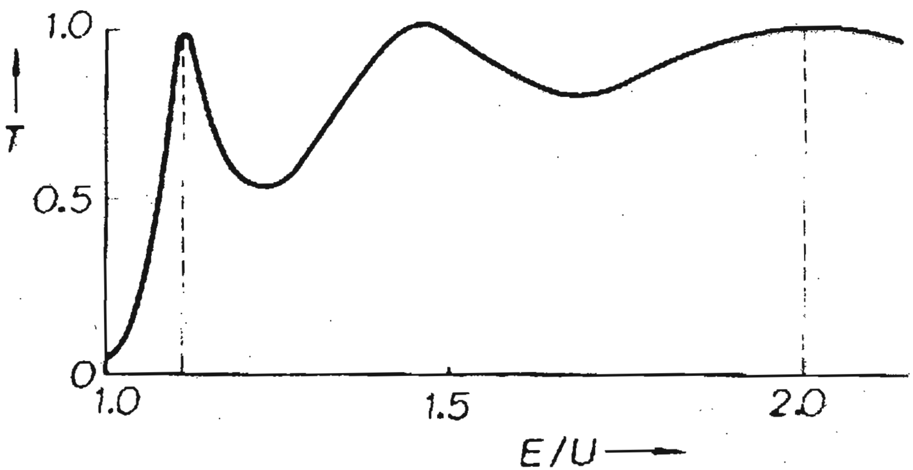


Fig. 5. Transmittance of potential barrier for $E > U$ in dependence upon energy

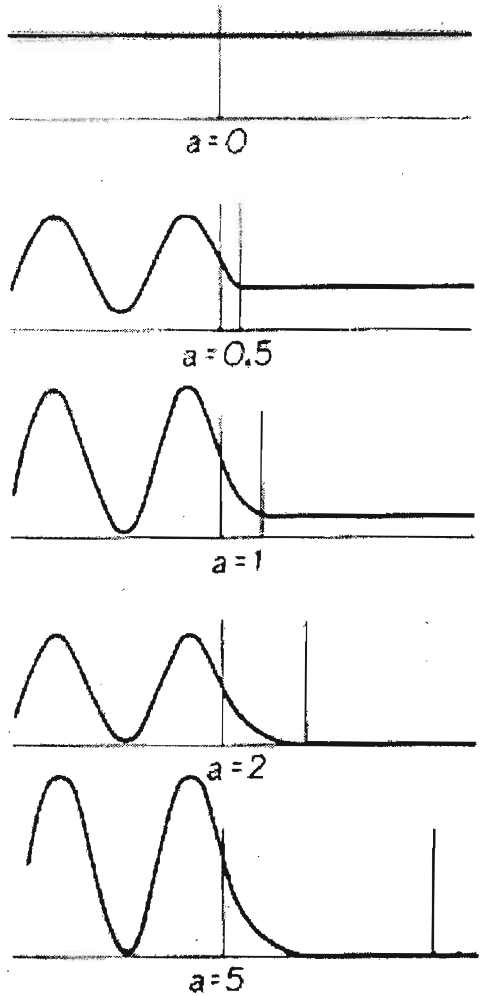
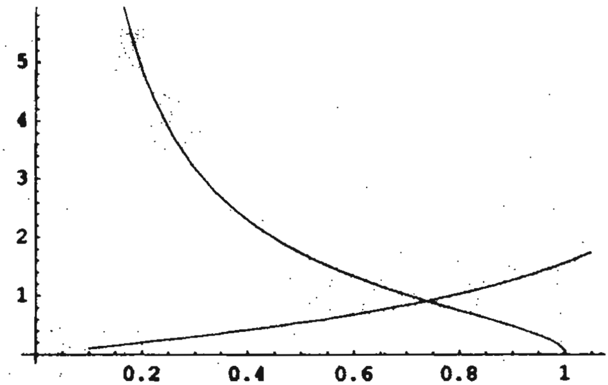


Fig. 6. Probability density $|u|^2$ in the current falling upon the barrier from the left, in the case $E < U$. The two vertical lines mark the width a of the barrier. The waves on the left are caused by interference between incident and reflected beams

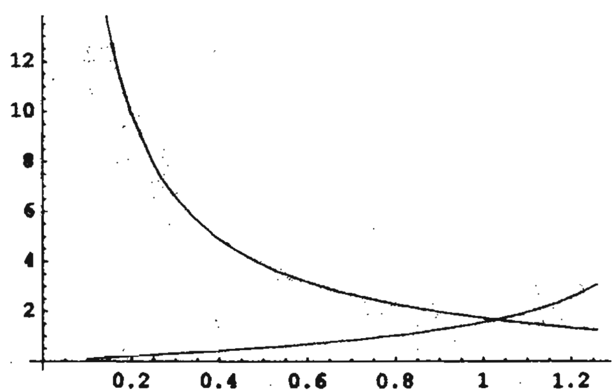
```
f1 := Tan[ka]
f2 := Sqrt[1^2 - ka^2] / ka
Plot[{f1, f2}, {ka, 0.1, Pi / 3}]
```




```
In[40]:= FindRoot[f1 == f2, {ka, 0.7}]

Out[40]= {ka → 0.739085}
```

```
f2 := Sqrt[2^2 - ka^2] / ka
Plot[{f1, f2}, {ka, 0.1, Pi / 2.5}]
```




```
In[53]:= FindRoot[f1 == f2, {ka, 0.7}]

Out[53]= {ka → 1.02987}
```

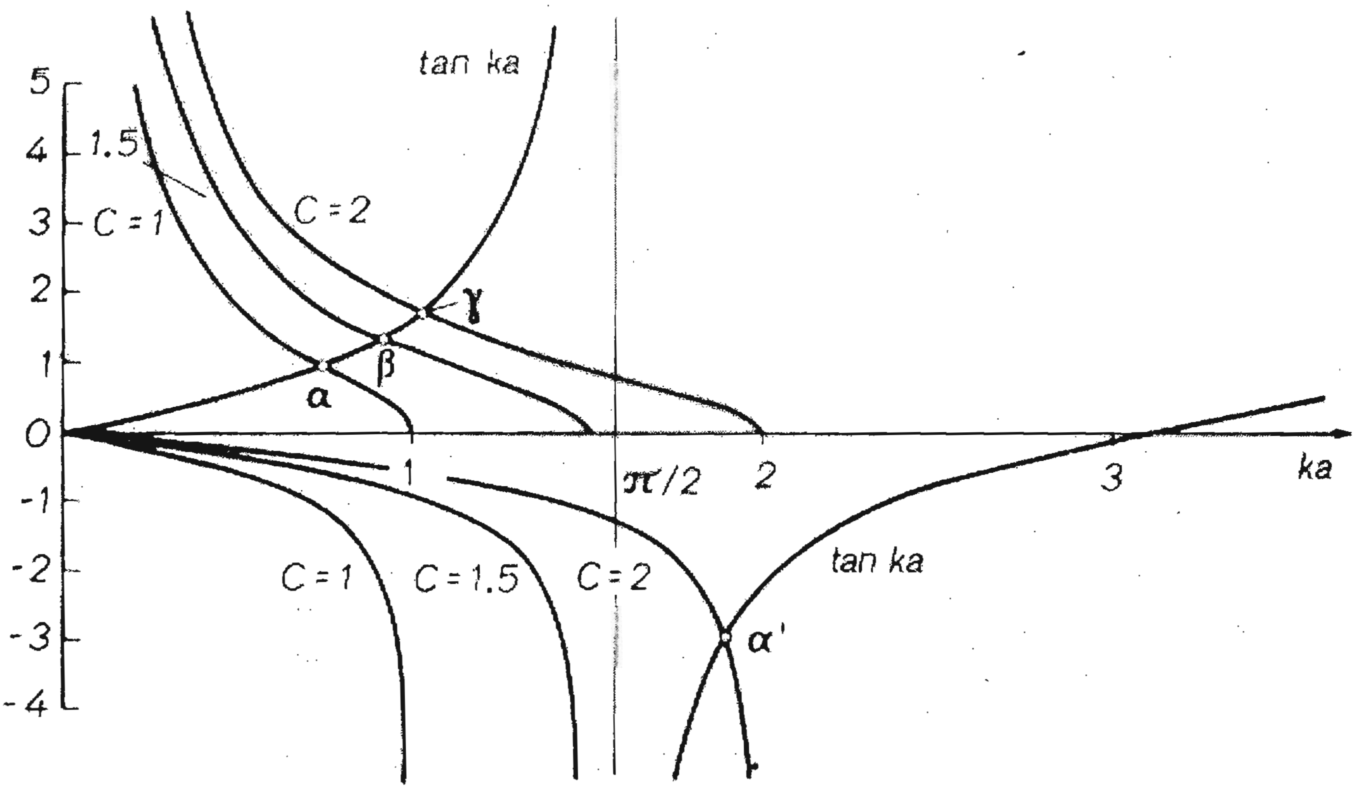


Fig. 7. Graphical solution of Eqs. (25.7e, o). The line $\tan ka$ intersects the curves which represent the right-hand sides for different values of the size parameter C. Curves at positive ordinates for even, at negative ones for odd parity

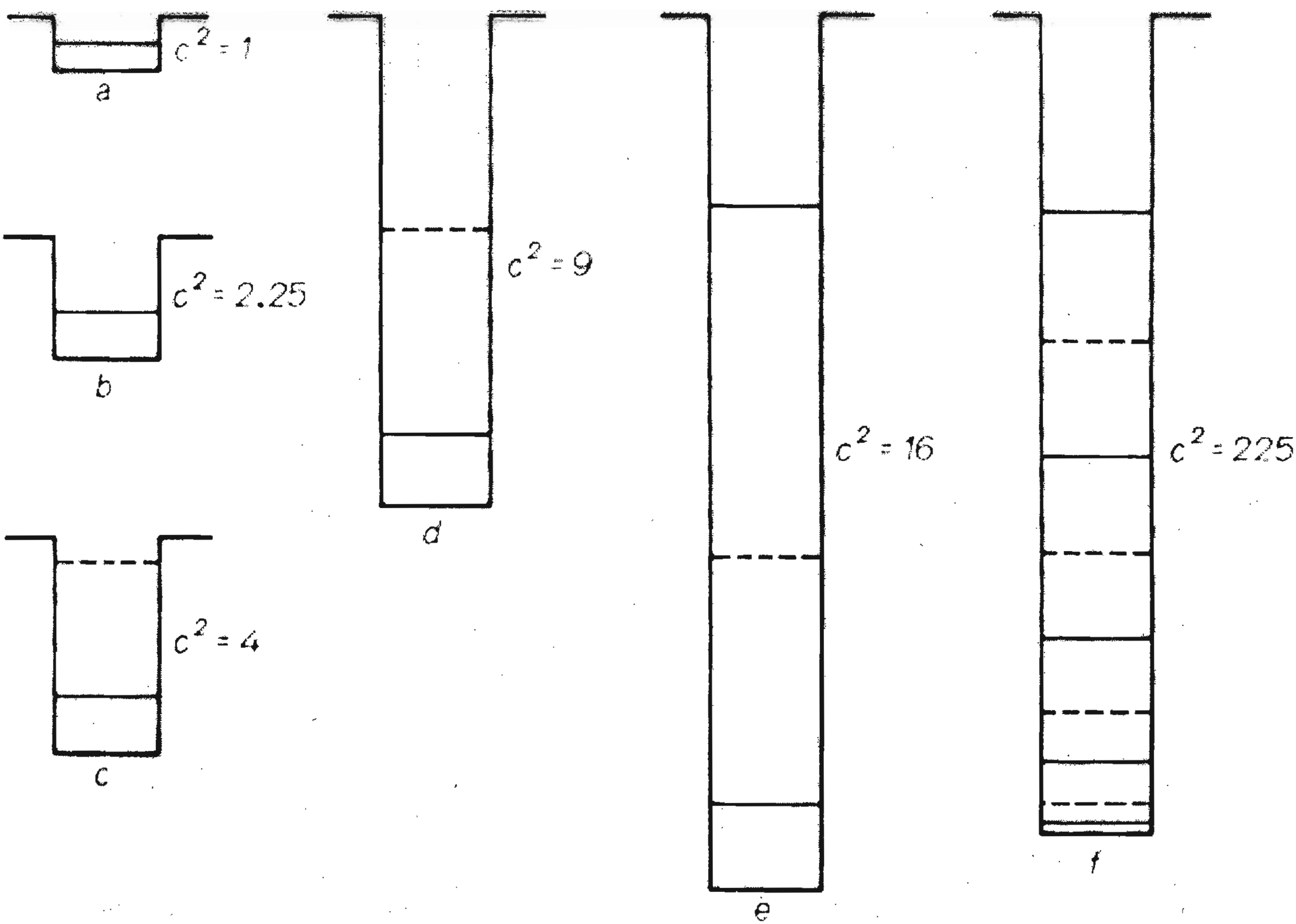


Fig. 8a–f. Energy levels in potential holes of different sizes determined by the size parameter C. Full lines even, broken lines odd parity

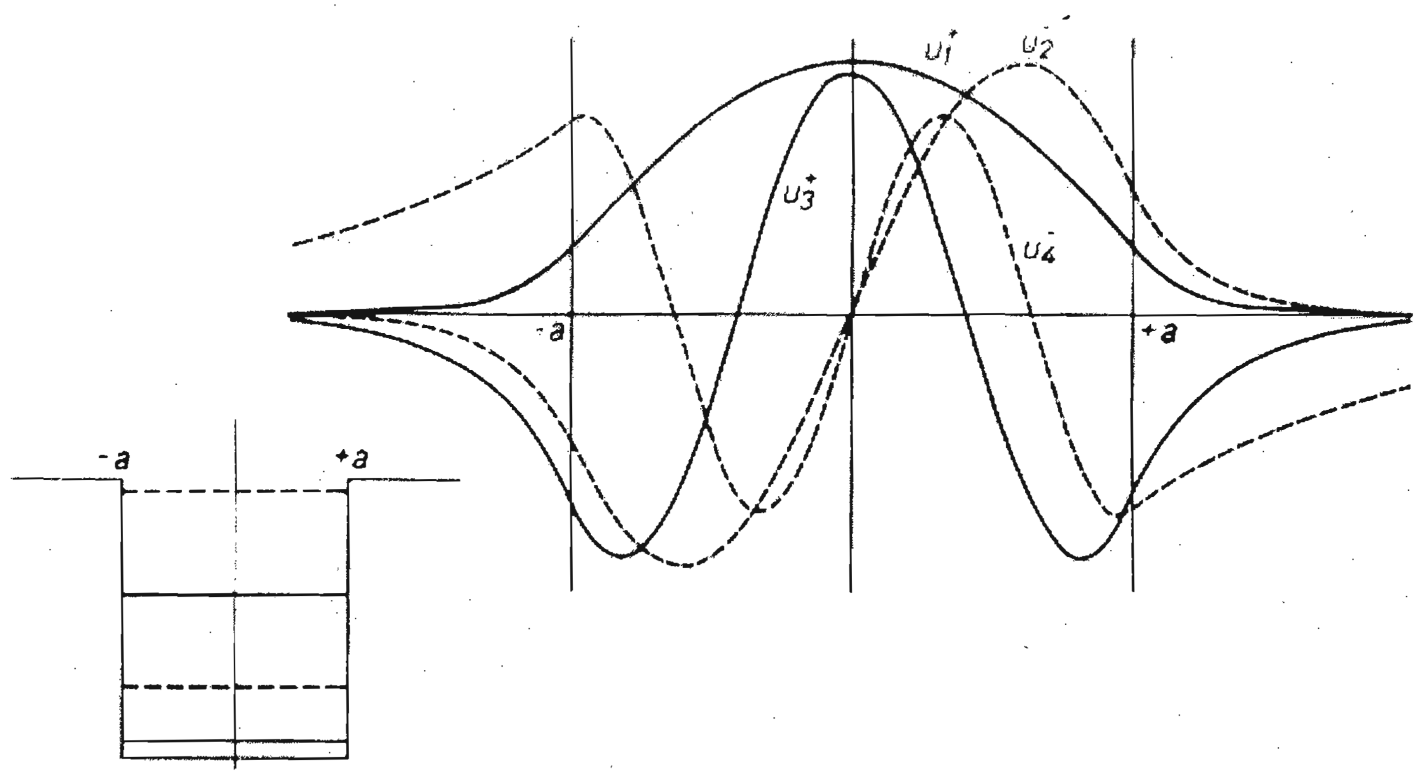


Fig. 9. Energy levels and eigenfunctions for $C = 5$. Full lines even, broken lines odd parity

```
In[55]:= sn[n_, x_] = Sqrt[2 / L] * Sin[n * Pi * x / L]
         Integrate[sn[n, x] * sn[m, x], {x, 0, L}]
```

Out[55]= $\sqrt{2}\,\sqrt{\frac{1}{L}}\ \mathrm{Sin}\left[\frac{n\,\pi\,x}{L}\right]$

Out[56]= $\dfrac{2\left(\frac{L\,\mathrm{Sin}[(m-n)\,\pi]}{2\,(m-n)\,\pi}-\frac{L\,\mathrm{Sin}[(m+n)\,\pi]}{2\,(m+n)\,\pi}\right)}{L}$

```
In[57]:= Simplify[%]
```

Out[57]= $\dfrac{2\,n\,\mathrm{Cos}[n\,\pi]\ \mathrm{Sin}[m\,\pi]-2\,m\,\mathrm{Cos}[m\,\pi]\ \mathrm{Sin}[n\,\pi]}{m^2\,\pi-n^2\,\pi}$

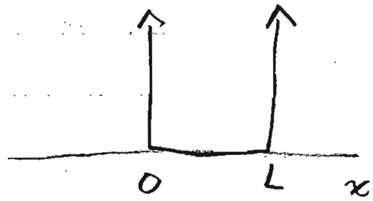
```
In[58]:= Integrate[sn[n, x] * sn[n, x], {x, 0, L}]
```

Out[58]= $\dfrac{2\left(\frac{L}{2}-\frac{L\,\mathrm{Sin}[2\,n\,\pi]}{4\,n\,\pi}\right)}{L}$

```
In[59]:= Simplify[%]
```

Out[59]= $1-\dfrac{\mathrm{Sin}[2\,n\,\pi]}{2\,n\,\pi}$

For an infinitely deep square well $(0, L)$



$$-\frac{d^2\psi}{dx^2} = \frac{2mE}{\hbar^2}\psi$$

In the middle have free particle. The bc is special—
$\psi(0) = \psi(L) = 0$

$$\psi(x) = A \sin \frac{\sqrt{2mE}}{\hbar} x \qquad \text{where } \frac{\sqrt{2mE}}{\hbar} L = n\pi \quad n = 1, 2, \ldots$$

$$E = n^2 \frac{\hbar^2 \pi^2}{2mL^2}$$

$$\int \psi_n^*(x)\,\psi_n\,dx = A^2 \int_0^L \sin^2 \frac{\sqrt{2mE_n}}{\hbar} x\,dx = A^2 \int_0^L \sin^2 \frac{n\pi x}{L}\,dx = A^2 \frac{L}{2}$$

$$A = \sqrt{2/L}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

Orthonormality

$$\int_0^L \psi_m^*(x)\,\psi_n(x) = \delta_{nm} \equiv \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$ Math result

completeness — represent any $\psi(x)$ as such a series
$$\psi(x) = \sum_n a_n \psi_n(x)$$

For these eigenfunctions its clear because of Fourier series analysis.
But, it is a general concept. Though needs to be proven case-by-case

What are the a_n's? Easy to get (N.B. switch $n \to m$ explain)

$$\int_0^L dx\, \psi_n^*(x)\, \psi(x) = \sum_m a_m \int_0^L dx\, \psi_n^*(x)\, \psi_m(x) = \sum_m a_m \delta_{nm} = a_n$$

$$\boxed{\therefore\ a_n = \int_0^L dx\, \psi_n^*(x)\, \psi(x)}$$

<u>closure</u> relation (N.B. switch $x \to x'$ explain)

$$\psi(x) = \sum_n a_n \psi_n(x) = \sum_n \int_0^L dx'\, \psi_n^*(x')\, \psi_n(x)\, \psi(x')$$

$$= \int_0^L \psi(x') \left[\sum_n \psi_n^*(x')\, \psi_n(x) \right] dx'$$

How can this give $\psi(x)$? Only way is that

$$\sum_n \psi_n^*(x')\, \psi_n(x) = \delta(x-x').$$

If so, $\psi(x) = \int_0^L \psi(x')\, \delta(x-x')\, dx' = \psi(x)$

The closure relation is $\boxed{\delta(x-x') = \sum_n \psi_n^*(x')\, \psi_n(x)}$

If a set of functions is complete, there will be a closure relation.

Note that the $\psi_n(x)$ are eigenfunctions of the energy operator $\hat{H}$

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\hat{H}\psi_n = E_n\psi_n$$

The eigenfunctions are ψ_n, the eigenvalues are E_n.

A general solution of the time dependent S equation is (remember our separation of variables, where the separation constant is the same for both x and t dependent differential equations)

$$\Psi(x,t) = \sum_n a_n(t)\,\psi_n(x)$$

where $a_n(t) = e^{-iE_nt/\hbar}\,a_n(0)$

If $a_n(0) = \delta_{nm}$, say, then

$$\Psi(t) = \sum_n e^{-iE_nt/\hbar}\,\delta_{nm}\,\psi_n(x) = e^{-iE_mt/\hbar}\,\psi_m(x)$$

$\rho(x,t) = \Psi^*(t)\Psi(t) = \psi_m^*(x)\,\psi_m(x)$ is time independent, If a particle is in a definite quantum state ($a_n(0) = \delta_{nm}$) it is always there. This is the meaning of a <u>stationary state</u>

Let's say that $a_1(0) = \frac{\sqrt{2}}{2}$ $\quad a_2(0) = \frac{\sqrt{2}}{2}$

$$\int dx\,\Psi^*(x,0)\,\Psi(x,0) = \int dx\,\left(a_1^*(0)\,\psi_1^*(x) + a_2^*(0)\,\psi_2^*(x)\right)\left(a_1(0)\,\psi_1(x) + a_2(0)\,\psi_2(x)\right)$$

$$= |a_1(0)|^2 \int dx\, \psi_1^*(x)\psi_1(x) + |a_2(0)|^2 \int dx\, \psi_2^*(x)\psi_2(x)$$
$$+ a_1^*(0)\, a_2(0) \int dx\, \psi_1^*(x)\psi_2(x) + a_1(0)\, a_2^*(0) \int dx\, \psi_2^*(x)\psi_1(x)$$

use orthonormality.

$$= \tfrac{1}{2} + \tfrac{1}{2} = 1$$

$$\psi^*(x,t)\,\psi(x,t) = \left(\frac{\sqrt{2}}{2} e^{+iE_1 t/\hbar}\psi_1^*(x) + \frac{\sqrt{2}}{2} e^{+iE_2 t/\hbar}\psi_2^*(x)\right)$$
$$\otimes \left(\frac{\sqrt{2}}{2} e^{-iE_1 t/\hbar}\psi_1(x) + \frac{\sqrt{2}}{2} e^{-iE_2 t/\hbar}\psi_2(x)\right)$$

$$= \tfrac{1}{2}\psi_1^*(x)\psi_1(x) + \tfrac{1}{2}\psi_2^*(x)\psi_2(x) + \tfrac{1}{2} e^{-i(E_1-E_2)t/\hbar}\psi_1(x)\psi_2^*(x)$$
$$+ \tfrac{1}{2} e^{+i(E_1-E_2)t/\hbar}\psi_1^*(x)\psi_2(x)$$

since $\psi_1(x) = \sin \pi x/L$ $\quad \psi_2(x) = \sin 2\pi x/L$ are real

$\rho(x,t) =$
$$\psi^*(x,t)\psi(x,t) = \tfrac{1}{2}\sin^2\left(\frac{\pi x}{L}\right) + \tfrac{1}{2}\sin^2\left(\frac{2\pi x}{L}\right) + \cos\left(\frac{(E_2-E_1)t}{\hbar}\right)\sin\frac{\pi x}{L}\sin\frac{2\pi x}{L}$$

Thus $\rho(x,t)$ is time dependent - superposition of different energy states is not a stationary state,

Energy representation

The state of this system for the infinite square well is given by $\psi(x,t) = \sum a_n(t)\,\psi_n(x)$

Instead of giving $\psi(x,t)$, if we give the coefficient list $a_n(t)$ $\quad n = 1, 2, \ldots$

we will also specify the state.

This is a very powerful idea

Since the $a_n(t) = e^{-iE_n t/\hbar} a_n(0)$ are obtained from

$$\hat{H}\,\psi_n(x) = E_n\,\psi_n(x),$$

we say that we are working in the
<u>Energy</u> <u>representation</u>

We can organize the $a_n(t)$ coeff. into a vector – a column vector

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \equiv \text{state } \underline{\underline{\text{vector}}}$$

($n = 1, 2, 3, .. \infty$ so need to be careful!)

Along with this vector is a row vector
$(a_1^* \; a_2^* \ldots)$

Using row – column multiplication of vectors (inner (dot) product)

$$(a_1^* \; a_2^* \; \ldots)\,(a_1 \; a_2 \ldots)^T = \sum_n |a_n|^2$$

Using our expression for $a_n(t)$

$$= \sum \left[\int \psi_n^*(x)\,\psi(x,t)\,dx\right]^* \left[\int \psi_n^*(x')\,\psi(x',t)\,dx'\right]$$

$$= \int dx \int dx' \underbrace{\left[\sum_n \psi_n^*(x)\,\psi_n(x')\right]}_{\delta(x-x')} \psi^*(x',t)\,\psi(x,t)$$

$$= \int dx \int dx'\,\delta(x-x')\,\psi^*(x',t)\,\psi(x,t) = \int dx\,|\psi(x,t)|^2 = 1.$$

$$\boxed{\therefore \quad \sum_n |a_n|^2(t) = 1}$$

The probability interpretation of QM says that $|a_n(t)|^2$ gives the prob. of observing the system to have energy E_n when the energy is measured. Why? Well, if we evaluate the following —

$$\int \Psi^*(x,t)\, \hat{H}\, \Psi(x,t)\, dx \;\equiv\; \langle \hat{H} \rangle$$ ← expectation value of the energy operator

we get

$$\int \sum_n a_n(t)\, \psi_n^*(x)\; \hat{H} \sum_{n'} a_{n'}(t)\, \psi_{n'}(x)\; dx$$

$$= \int \sum_n a_n(t)\, \psi_n^*(x) \sum_{n'} a_{n'} E_{n'}\, \psi_{n'}(x)\, dx$$

$$= \sum_n \sum_{n'} a_n(t)\, a_{n'}(t)\, E_{n'} \int \underbrace{\psi_n^*(x)\; \psi_{n'}(x)\, dx}_{\delta_{nn'}}$$

$$= \sum_{n=1}^{\infty} |a_n(t)|^2 E_n \;=\; \langle \hat{H} \rangle$$

That says that the energy is split into a superposition of probabilities for each possible E_n value —

N.B. since the E_n are discrete, for this particle in an infinite well, we get a $\sum_n$ – but an INFINITE sum. If we did the finite well, we would get a finite sum of over n of the bound states (the ones we worked out) but also an integral over the continuum of non-bound states.

Matrix Mechanics

Lets pose the question as to how $x\Psi(x,t)$ looks in the energy representation.

$$x\Psi(x,t) = \sum_n x\, a_n \psi_n(x)$$

consider $f_n(x) \equiv x\psi_n(x)$. Since we have Fourier theorem we know that

number, not a function

$$f_n(x) = \sum_m x_n^m \psi_m(x) \quad \text{i.e. we know } f(x) = \sum_m x_m \psi_m(x)$$

So, just need another label. But, organize as a matrix,

$$f_n(x) = \sum_m x_{mn} \psi_m(x)$$

what are x_{nm} - get the usual way! ASK CLASS

$$x_{mn} = \int_0^L \psi_m^*(x)\, x\, \psi_n(x)\, dx$$

easy integrals to do explicitly - but the numbers are not the point here.

$$x\psi_n(x) = \sum_m x_n^m \psi_m(x)$$

$$\int \psi_\ell^*(x)\, x\, \psi_n(x) = \sum_m x_n^m \int dx\, \psi_\ell^*(x)\psi_m(x) = x_n^\ell = x_{\ell n}$$

Now lets rewrite $x\Psi(x,t)$ as

$$x\Psi(x,t) = \sum_n a_n \sum_m x_{mn} \psi_m(x)$$

$$= \sum_m \left(\sum_n x_{mn} a_n \right) \psi_m(x)$$

and set

$$a_m' \equiv \sum_n x_{mn} a_n$$

$$x\Psi(x,t) = \sum_m a_m' \psi_m(x)$$

This means that in energy representation multiplication of x is represented as matrix multiplication.

$$\begin{pmatrix} a_1' \\ a_2' \\ \vdots \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & x_{3} & \cdots \\ x_{21} & x_{22} & \cdots & \\ \vdots & & & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

In general the matrices representing observables in QM are Hermitian — $x_{mn} = (x_{nm})^* \equiv x^*_{mn}$ — complex conjugate transpose.