Chapter 8

Barriers and Wells

The quantum mechanical nature of matter has some surpising consequences

The behaviors seen in realistic experiments and applications can be illustrated in highly simplified systems which contains one - dimensional potentials with sharp edges

General Discussions

Time - dependent Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \qquad (A)$$

$V(x)$ is assumed to be real and independent of time.

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \underset{V(x)}{\overset{\shortparallel}{V^*(x)}}\psi^* \qquad (B)$$

$\psi^* \cdot (A) - \psi \cdot (B)$

$$\Rightarrow \quad i\hbar\left[\psi^* \frac{\partial}{\partial t}\psi + \psi \frac{\partial}{\partial t}\psi^*\right] = -\frac{\hbar^2}{2m}\left[\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x}\right]$$

$$\frac{\partial}{\partial t}\psi^*\psi = \frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2}\psi - \frac{\hbar^2}{2m}\psi^*\frac{\partial^2 \psi}{\partial x^2}\right)$$

$$= -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right]\right.$$

Define the probability flux $S(x,t) = \frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)$

$$\Rightarrow \quad \frac{\partial}{\partial t}P(x,t) + \frac{\partial}{\partial x}S(x,t) = 0$$

[Going to three dimensional case

$$\frac{\partial}{\partial t}P(\vec{r},t) + \nabla\cdot\vec{S}(\vec{r},t) = 0 \qquad (C)$$

$$\vec{S}(\vec{r},t) = \frac{\hbar}{2im}\left[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \nabla\psi^*(\vec{r},t)\psi(\vec{r},t)\right)$$

It is similar to the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\vec{j} = 0 \quad \leftrightarrow \quad \text{conseration of charge}$$

Equation (C) $\rightarrow$ conservation of probability.]

$$\frac{\partial}{\partial t}\int_a^b dx\, P(x,t) = -\int_a^b dx \frac{\partial}{\partial x} S(x,t)$$

$$= S(a,t) - S(b,t)$$

$\Rightarrow$ $S(x,t) \rightarrow$ probability flux.
(probability / time cross point x)

Remark: (C) is a consequence of $V(x)$ is real.

When $V(x)$ is independent of time $\rightarrow$ seperation of variable method can be used.

$$\psi(x,t) = \psi_E(x)\, e^{-iEt/\hbar} = \psi_E(x)\, e^{-\omega t}$$

with

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_E(x) + V(x)\,\psi_E(x) = E\,\psi_E(x)$$

$\psi_E(x) \equiv \psi(x)$ — time independent Schrodinger equation.

Requirements for acceptible solutions

(i) $\psi(x)$ is square integrable* — for unbound motion, we shall discuss this point further

(ii) (a) $\psi(x)$ must be finite
(b) $\psi(x)$ must be continuous
(c) $\frac{d\psi(x)}{dx}$ must be finite
(d) $\frac{d\psi(x)}{dx}$ must be continuous

(a), (c) follows from the requirement that $P(x,t)$, $S(x,t)$ are well-defined

(b) follows from requirement (c)

Requirement (d) $\leftrightarrow$ Schrodinger equation

Time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

$$\Rightarrow \frac{d^2}{dx^2}\psi(x) = \frac{m}{\hbar^2}[V(x)-E]\,\psi(x)$$

Integrate the above equation from $a-\epsilon$ to $a+\epsilon$

$$\left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon}\frac{2m}{\hbar^2}[V(x)-E]\,\psi(x)\,dx$$

$\longrightarrow 0$ as $\epsilon \rightarrow 0$
if V is finite

Note: If potential V has an infinite discontinuity, then the right-hand side may or may not vanish

Example $\quad V(x) = V_0 \delta(x-a)$

$$\Rightarrow \quad \left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon} \frac{2m}{\hbar^2}\left[V_0 \delta(x-a) - E\right]\psi(x)\,dx$$

$$= \frac{2m}{\hbar^2} V_0 \psi(a)$$

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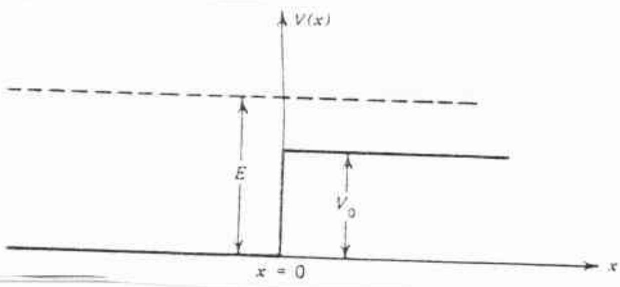
The Potential Step

$E > V_0 > 0$

$$V(x) = \begin{cases} 0 & \text{for } x<0 \\ V_0 & \text{for } x>0 \end{cases}$$



The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1 = E\psi_1 \quad \text{in I } (x<0)$$

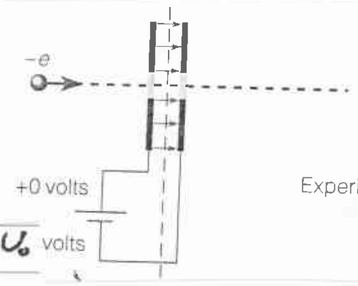
$$\Rightarrow \frac{d^2}{dx^2}\psi_1 = -\frac{2mE}{\hbar^2}\psi_1 = -k_1^2\psi_1$$

$$k_1 = \sqrt{2mE}/\hbar$$

$$\Rightarrow \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_1(x,t) = \psi_1 e^{-i\omega t}$$

$$= A\underbrace{e^{ik_1x - i\omega t}}_{\text{incident plane wave}} + B\underbrace{e^{-ik_1x - i\omega t}}_{\text{reflected plane wave}}$$



Experimental setup

$V_0 = eU_0$

Experimental setup

The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2(x) = E\psi_2(x) \quad \text{in II } (x>0)$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_2 = -\frac{2m}{\hbar^2}(E-V_0)\psi_2 = -k_2^2\psi_2$$

$$k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$\Rightarrow \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

$D = 0$ (no new potential to reflect the wave from the right)

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x<0 \\ \psi_2(x) = Ce^{ik_2x}, & x>0 \end{cases}$$

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Continuity equation at $x=0$

$$\psi_1(x=0) = \psi_2(x=0) \quad \Rightarrow \quad A+B=C$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \quad \Rightarrow \quad k_1(A-B) = k_2 C$$

$$\Rightarrow \quad B = \frac{k_1-k_2}{k_1+k_2} A$$

$$C = \frac{2k_1}{k_1+k_2} A$$

$$\Rightarrow \quad \psi(x) = \begin{cases} A e^{ik_1x} + A\dfrac{k_1-k_2}{k_1+k_2} e^{-ik_1x} & x<0 \\ A\dfrac{2k_1}{k_1+k_2} e^{ik_2x} & x \geq 0 \end{cases}$$

$$\psi(x,t) = \psi(x) e^{-i\omega t}$$

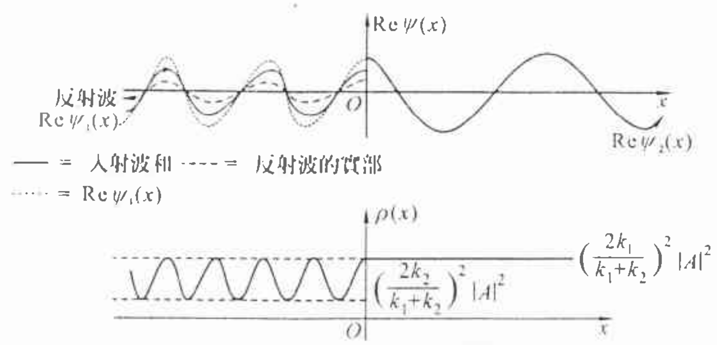
$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

$$= \begin{cases} \dfrac{4}{(k_1+k_2)^2} |A|^2 (k_1\cos k_1x - ik_2\sin k_1x)(k_1\cos k_1x + ik_2 \sin k_1 x) & [x \leq 0] \\ \dfrac{2k_1}{(k_1+k_2)^2} |A|^2 & x \geq 0 \end{cases}$$

$\rho(x,t)$ is positive definite and independent of time.

$$\rho_I(x) = \frac{4|A|^2}{(k_1+k_2)^2}(k_1^2\cos^2 k_1x + k_2^2 \sin^2 k_1 x)$$

$$\rho_{II}(x) = \frac{4k_1^2}{(k_1+k_2)^2}|A|^2$$



$$\rho(x<0) = \frac{4|A|^2}{(k_1+k_2)^2}(k_1^2\cos^2 k_1x + k_2^2\sin^2 k_1x) \qquad \rho(x \geq 0) = \frac{4k_1^2}{(k_1+k_2)^2}|A|^2$$

$\psi(x)$= 能量本徵函數, $\rho(x)$= 概率密度

Reflection Coefficient and Transmission Coefficient

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

$R \downarrow$ reflection coefficient

$$= \frac{\left(\frac{k_1-k_2}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{ik_1x}\frac{d}{dx}e^{-ik_1x} - e^{-ik_1x}\frac{d}{dx}e^{ik_1x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

$$= \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \left\{\frac{1-\sqrt{1-\frac{V_0}{E}}}{1+\sqrt{1-\frac{V_0}{E}}}\right\}^2$$

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

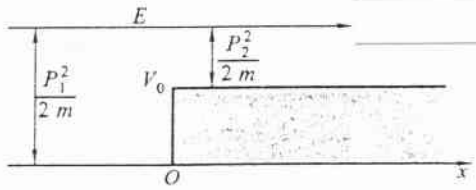
$$= \frac{\left(\frac{2k_1}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{-ik_2x}\frac{d}{dx}e^{ik_2x} - e^{ik_2x}\frac{d}{dx}e^{-ik_2x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

$$= \frac{4k_1k_2}{(k_1+k_2)^2}$$

Remarks

- For classical mechanics, when $E > V_0$, the particle only change its momentum at $x = 0$

  $R \neq 0$, the presence of reflected wave, is due to the wave property of particle
  $\downarrow$
  quantum effect.



- Probability density $\rho(x)$ is real, positive-definite.
  $\rho(x)\,dx \sim$ probability of finding the particle in the interval dx

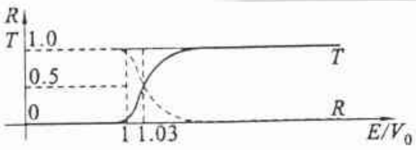
- $\rho(x,t)$ is independent of time
  Probability conservation

$$\frac{\partial S}{\partial x} + \frac{\partial \rho}{\partial t} = 0$$

$\Rightarrow$ $S(x)$ is a constant

Furthermore, $R + T = 0$

can be seen from the following figure
(R, T are plotted as a function of $\frac{V_0}{E}$)



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$E < V_0$

In region (I)

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

In region (II)

Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2 + V_0\psi_2 = E\psi_2$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_2 = \frac{2m(V_0-E)}{\hbar^2}\psi_2 = k_2^2\psi_2$$

$$k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\Rightarrow \psi_2(x) = Ce^{k_2x} + De^{-k_2x}$$

cannot increase exponentially as $x \to \infty$

$\Rightarrow C = 0$

$$\Rightarrow \psi_2(x) = De^{-k_2x}$$

Continuity equation at $x = 0$

$$\psi_1(x=0) = \psi_2(x=0) \quad \Rightarrow \quad A + B = D$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \quad \Rightarrow \quad ik_1(A-B) = -k_2D$$

$$\Rightarrow A = \frac{D}{2}\left(1 + \frac{ik_2}{k_1}\right)$$

$$B = \frac{D}{2}\left(1 - \frac{ik_2}{k_1}\right)$$

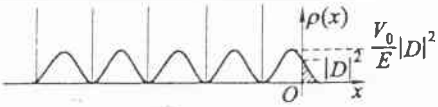
$$\Rightarrow \psi(x,t) = \psi(x)e^{-i\omega t}$$

$$= \begin{cases} \left(D\cos k_1x - D\frac{k_2}{k_1}\sin\frac{k_2}{k_1}\sin k_1x\right)e^{-i\omega t} & x<0 \\ De^{-k_2x}e^{-i\omega t} & x>0 \end{cases}$$

$$\rho(x,t) = \begin{cases} |D|^2\left(\cos k_1x - \frac{k_2}{k}\sin k_1x\right)^2 & x<0 \\ |D|^2e^{-2k_2x} & x>0 \end{cases}$$

$\rho(x,t)$ is independent of time, positive-definite

The $\rho(x)$ can be plotted



Penetrating depth.

$$\rho(x>0) = |D|^2 e^{-2k_2 x}$$

The particle can penerate into $x>0$ region (classically forbidden region)

The penetrating depth

$$\Delta x = \frac{1}{2k_2} \sim \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0-E)}}$$

$$\Delta p \sim \frac{\hbar}{\Delta x} = \sqrt{2m(V_0-E)}$$

$$\Rightarrow \quad \Delta E \sim \frac{(\Delta p)^2}{2m} = V_0 - E$$

↳ the energy deficit

Reflection coefficient

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

$$= \frac{\frac{1}{4}|D|^2\left(1+\frac{ik_2}{k_1}\right)\left(1-\frac{ik_2}{k_1}\right)}{\frac{1}{4}|D|^2\left(1-\frac{ik_2}{k_1}\right)\left(1+\frac{ik_2}{k_1}\right)} = 1$$

Transmission coefficient

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

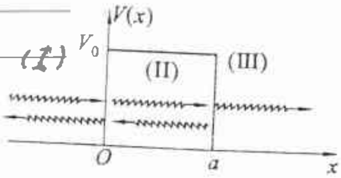
$$\text{Transmitted probability flux} = \frac{\hbar}{2im}|D|^2\left(e^{-k_2x}\frac{d}{dx}e^{-k_2x} - e^{-k_2x}\frac{d}{dx}e^{-k_2x}\right)$$

$= 0$

$$\Rightarrow \quad T = 0 \quad \Rightarrow \quad T + R = 1$$

Furthermore $S = 0$ for all x

The Potential Barrier



$$V(x) = \begin{cases} V_0 & 0 \le x \le a \\ 0 & x < 0 \ , \ x > a \end{cases}$$

$E < V_0$

Region I

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1$$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

Region II

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2$$

$$\psi_2(x) = Fe^{-k_2x} + Ge^{k_2x}$$

$$k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Region III

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_3}{dx^2} = E\psi_3$$

$$\psi_3(x) = Ce^{ik_3x} + De^{-ik_3x}$$

$$k_3 = \frac{\sqrt{2mE}}{\hbar} = k_1$$

Tunneling problem
$\downarrow$
Incident wave is partially reflected and partially transmitted.

[Note, only the origin is shifted between the two figures]

In classical mechanics, the particle cannot be transmitted.

A particle may transmit through a potential barrier is due to the wave property of particle
$\downarrow$
quantum effect

[Furthermore, a "whole" particle (electron) is transmitted with probability, related to T

This quantum effect is known as tunneling phenomena.

Matching the boundary condition at $x=0$ and $x=a$.

$\psi_1(x=0) = \psi_2(x=0)$ $\qquad$ $A+B=F+G$

$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0}$ $\qquad$ $ik_1(A-B) = k_2(G-F)$

$\psi_2(x=a) = \psi_3(x=a)$ $\qquad$ $Ge^{k_2 a} + Fe^{-k_2 a} = Ce^{ik_1 a}$

$\left(\frac{d\psi_2}{dx}\right)_{x=a} = \left(\frac{d\psi_3}{dx}\right)_{x=a}$ $\qquad$ $k_2(Ge^{k_2 a} - Fe^{-k_2 a}) = ik_1 C e^{ik_1 a}$

There are 5 unknowns (A, B, G, F, C) and 4 equations

$\Rightarrow$ A, B, G, F can be solved in terms of C.

$$A = c\left\{\cosh(k_2 a) + i\frac{k_2^2 - k_1^2}{2k_1k_2}\sinh(k_2 a)\right\}e^{ik_1 a}$$

$$B = -i\left(c\frac{k_1^2+k_2^2}{2k_1k_2}\sinh k_2 a\right)e^{ik_1 a}$$

$$F = \frac{c}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(k_2+k_1)a}$$

$$G = \frac{c}{2}\left(1+i\frac{k_1}{k_2}\right)e^{(-k_2+ik_1)a}$$

$\psi(x,t)$ is given (up to a constant C)

$$\psi_1(x,t) = \psi_1(x)e^{-i\omega t} = ic\frac{k_1^2+k_2^2}{2k_1k_2}\sinh(k_2 a)\left(e^{ik_1x+\omega t)}\right.$$
$$\left.+e^{i(k_1x-\omega t)}\right)e^{ik_1 a} + c\left(\cosh k_2 a + i\frac{k_2}{k_1}\sinh(k_2 a)\right)e^{ik_1 a}\, e^{i(k_1x-\omega t)}$$

$$\psi_2(x,t) = \psi_2(x)e^{-i\omega t}$$
$$= c\left\{\cosh[k_2(x-a)] + i\frac{k_1}{k_2}\sinh[k_2(x-a)]\right\}e^{i(k_1a-\omega t)}$$

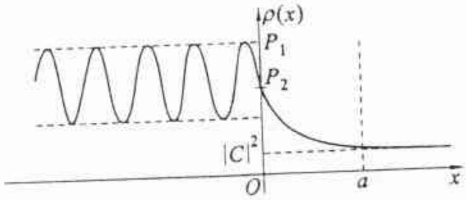
$$\psi_3(x,t) = \psi_3(x)e^{-i\omega t} = Ce^{i(k_1x-\omega t)}$$

Using $\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$, $\rho(x,t)$ can be calculated.

$\downarrow$

$\rho(x,t)$ is positive definite and independent of time.

$\rho(x,t) = \rho(x)$



The most interesting quantity for tunneling problem is the transmission coefficent T

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

$$= \frac{\left|\frac{\hbar}{2im}\left\{e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right\}\right| |C|^2}{\left|\frac{\hbar}{2im}\left\{e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right\}\right| |A|^2}$$

$$= \frac{\frac{\hbar k_1}{m}|C|^2}{\frac{\hbar k_1}{m}|A|^2} = \frac{|C|^2}{|A|^2}$$

$$\Rightarrow T = \left[\cosh^2(k_2a) + \frac{1}{4}\left(\frac{k_2^2-k_1^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}$$

$$= \left[1 + (\sinh^2(k_2a))\left(1 + \frac{1}{4}\frac{(k_2^2-k_1^2)^2}{k_1^2k_2^2}\right)\right]^{-1}$$

$$= \left[1 + \frac{\sinh^2 k_2a}{4\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\right]^{-1} = \left[1 + \frac{(e^{k_2a} - e^{-k_2a})^2}{16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\right]^{-1}$$

$$= \left[1 + \frac{e^{2k_2a}(1 - 2e^{-2k_2a} + e^{-4k_2a})}{16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\right]^{-1}$$

T is a function of E, V_0 and a.

$\downarrow$

This is the fundamental equation for discussing the tunneling problem.

If $k_2a \gg 1$, then

$$T \sim \left[\frac{e^{2k_2a}}{16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\right]^{-1} = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2k_2a}$$

$$= 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\sqrt{2m(V_0-E)}\,a/\hbar}$$

Usually, the exponential is the dominating factor.

Potential barrier with $E > V_0$ can be carried out with the same method. (with appropriate changes in region II

$$R = \frac{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar}a\right]}{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar}a + 4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)\right.}$$

$$T = \frac{4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)}{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar} + 4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)\right.}$$

Although the reflection and transmission probabilities are in general non-zero, the numerator of the reflection probability involve a sine. When the sine is zero, there is no reflection

$\downarrow$

resonant transmission.

The condition is

$$\frac{\sqrt{2m(E-V_0)}}{\hbar}a = \underbrace{n}_{\text{integer}}\pi \quad \Longrightarrow \quad E = V_0 + \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Compare with the formula in the textbook (where the detail has not been worked out)

$k_2 a \gg 1$

$$T \cong \left[\frac{1}{4}\left(\frac{k_2^2+k_1^2}{k_1 k_2}\right)^2 \frac{1}{4} e^{2k_2 a}\right]^{-1}$$

$$= \frac{16\, k_1^2 k_2^2}{k_1^2+k_2^2} e^{-2k_2 a}$$

[$\cosh k_2 a \sim \sinh k_2 a \sim \frac{1}{2} e^{k_2 a}$ as $ka \gg 1$]

With the identification

	our notation	notation of the textbook
	k_1	k
	k_2	κ
width	a	$2a$
	T	$\lvert T\rvert^2$

$\Rightarrow$ we recover the equation (8-18)

$$T = \frac{16\, k^2 \kappa^2}{k^2+\kappa^2} e^{-4\kappa a}$$

[Our notation follow that of 林清涼 "近代物理" I 第十章]

In general, the barriers that encounter in physical phenomena are not square

$\Rightarrow$ we want to obtain an approximate expession for the transmission coefficient $|T|^2$ through irregular barrier

Proper way: WKB method will not be discussed here

still an approximate method

The most important factor $e^{-4\kappa a} = e^{-2\kappa(2a)}$ ← width

Other factors are slowly varying compared with this factor

For a square barrier

$$\ln|T|^2 = -2\kappa(2a) + 2\ln\underbrace{\frac{2(ka)(\kappa a)}{(ka)^2+(\kappa a)^2}}_{\text{will neglect this term}}$$

Approximate a smooth barrier by a juxaposition of square potential barrier (See the following figure

$$\ln|T|^2 = \sum_{\substack{\text{partial}\\ \text{barrier}}} \ln|T_{\substack{\text{partial}\\ \text{barrier}}}|^2$$

$$\simeq -2\sum \underbrace{\Delta x}_{\substack{\text{width of}\\ \text{the barrier}}} \underbrace{\langle\kappa\rangle}_{\substack{\text{average } \kappa \text{ in}\\ \text{the inverval}}}$$

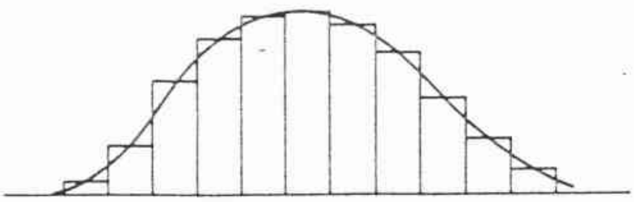
$$\simeq -2\int dx \sqrt{\frac{2m}{\hbar^2}[V(x)-E]}$$

$$\Rightarrow |T|^2 \simeq e^{-2\int dx\sqrt{\frac{2m}{\hbar^2}[V(x)-E]}}$$

The equation requires for each partial barrier $2\Delta x \cdot \kappa \gg 1$

$\Rightarrow$ (i) the above approximation is poor near the turning point (i.e., $V(x)=E \Rightarrow \kappa = 0$)

(ii) $V(x)$ must be smooth so that one can approximate a curved barrier by a stack of sufficient large width square barrier

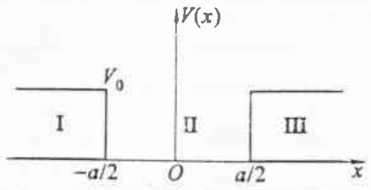


Approximation of smooth barrier by a juxtaposition of square potential barriers.

Potential Well

We have already discussed the problem of infinite potential well.

In this section, we shall discuss the finite potential well problem.



$E < V_0$

Region I

$x < -\frac{a}{2}$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi_1(x) = E\psi_1(x)$$

$$\Rightarrow \psi_1(x) = Ce^{k_1 x} + De^{-k_1 x}$$

$$k_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

The wave function is finite at $x = -\infty$

$\Rightarrow D = 0$

Region II

$-\frac{a}{2} < x < \frac{a}{2}$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2(x) = E\psi_2(x)$$

$$\Rightarrow \psi_2(x) = A'e^{ik_2 x} + B'e^{-ik_2 x}$$

$$= A\sin k_2 x + B\cos k_2 x$$

$$k_2 = \frac{\sqrt{2mE}}{\hbar}$$

we use sin and cos because we want to take advantage of the symmetry property

Region III

$\frac{a}{2} < x$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi_3(x) = E\psi_3(x)$$

$$\Rightarrow \psi_3(x) = Fe^{k_1 x} + Ge^{-k_1 x}$$

The wave function must be finite at $x = \infty$

$\Rightarrow F = 0$

$$\psi(x) = \begin{cases} \psi_1(x) = Ce^{k_1 x} & x < -\frac{a}{2} \\ \psi_2(x) = A\sin k_2 x + B\cos k_2 x & -\frac{a}{2} < x < \frac{a}{2} \\ \psi_3(x) = Ge^{-k_1 x} & \frac{a}{2} < x \end{cases}$$

Symmetry of the potential

$$V(x) = V(-x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

Let $x \to -x$ (we just rename our variable

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(-x) + V(-x)\psi(-x) = E\psi(-x)$$

With $V(x) = V(-x)$, the equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(-x) + V(x)\psi(-x) = E\psi(-x)$$

If $\psi(x)$ is eigenfunction of the Schrodinger equation with eigenvalue E, then $\psi(-x)$ is also an eigenfunction of the same Schrodinger equation with the same eigenvalue E.

From superposition principle

$$\psi_{\substack{\text{even}\\ \text{odd}}}(x) = \frac{1}{\sqrt{2}}\left(\psi(x) \pm \psi(-x)\right)$$

are also eigenfunctions of the Schrodinger equation with eigenvalue E

$$\psi_{\text{even}}(x) = \psi_{\text{even}}(-x)$$

$$\psi_{\text{odd}}(x) = -\psi_{\text{odd}}(-x)$$

$\Rightarrow$ With $V(x) = V(-x)$, we can solve the problem by looking for even, odd eigenfunction.

Even solution

$$\psi_1(x) = C e^{k_1 x} \qquad x < -\frac{a}{2}$$

$$\psi_2(x) = B\cos k_2 x \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$$\psi_3(x) = C e^{-k_1 x} \qquad x > \frac{a}{2}$$

Matching the boundary condition at $x = -\frac{a}{2}$

$$\psi_1\left(x = -\frac{a}{2}\right) = \psi_2\left(x = -\frac{a}{2}\right)$$

$$B\cos\frac{k_2 a}{2} = C e^{-k_1\frac{a}{2}}$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=-\frac{a}{2}} = \left(\frac{d\psi_2}{dx}\right)_{x=-\frac{a}{2}}$$

$$-Bk_2 \sin\left(k_2\left(\frac{-a}{2}\right)\right) = Ck_1 e^{k_1\left(-\frac{a}{2}\right)}$$

$$\Rightarrow \quad k_2 \tan k_2 a = k_1$$

Compare our notation with that used in the textbook

Our notation	Notation of the textbook
k_2	q
k_1	$\varkappa$

We recover the equation (8-35) of the textbook, i.e.,

$$q \tan qa = \kappa \qquad \text{(A)}$$

· With V_0, a given, (A) is an equation for E

$\downarrow$

only certain values of E will satisfy (A)

$\downarrow$

only discrete energies are allowed.

· The boundary conditions at $x = \frac{a}{2}$, can be shown, are satified automatically

· Equation (A) is solved graphically

From Equation (A), we have

$$\sqrt{\frac{2mE}{\hbar}} \tan \sqrt{\frac{mEa^2}{2\hbar^2}} = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

Eigenvalue of E can be found by solving above equation.

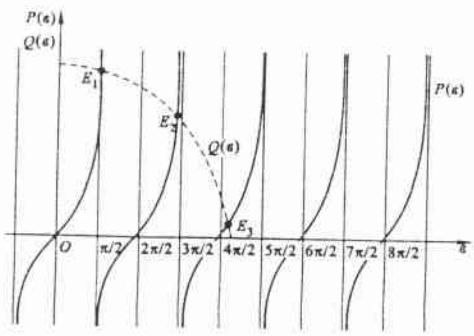
Analytic solutions are difficult to find, we usually solved it using graphic method, i.e., plot LHS, RHS as function of E. The intersection $\Rightarrow$ eigenvalues of E

Define $\epsilon = \sqrt{\frac{mEa^2}{2\hbar^2}}$

Equation (A) becomes $\underbrace{\epsilon \tan \epsilon}_{P(\epsilon)} = \underbrace{\sqrt{\frac{mV_0a^2}{2\hbar^2} - \epsilon^2}}_{Q(\epsilon)}$

$$Q(\epsilon) = \sqrt{\frac{mV_0a^2}{2\hbar^2} - \epsilon^2} \Rightarrow Q^2 + \epsilon^2 = \frac{mV_0a^2}{2\hbar^2}$$

(a circle when Q is plotted against ϵ.



The energy eigenvalues: $\underset{\substack{\parallel \\ E_{e0}}}{E_{even,0}}, \underset{\substack{\parallel \\ E_{e1}}}{E_{even,1}}, \cdots$ can be found.

Odd solution.

$\psi_1(x) = Ce^{k_1 x}$ $\qquad x < -\frac{a}{2}$

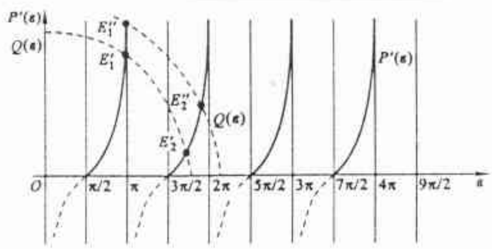
$\psi_2(x) = A \sin k_2 x$ $\qquad -\frac{a}{2} < x < \frac{a}{2}$

$\psi_3(x) = -Ce^{-k_1 x}$ $\qquad x > \frac{a}{2}$

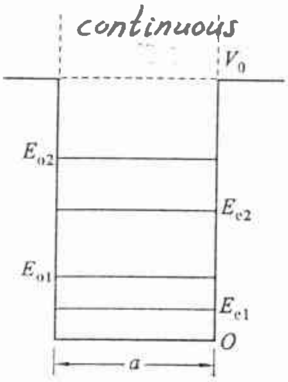
$k_2 \cot \frac{k_2 a}{2} = -k_1$ (from matching the boundary conditions)

$$\Rightarrow \sqrt{\frac{2mE}{\hbar^2}} \cot \sqrt{\frac{mEa^2}{2\hbar^2}} = -\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

Again, graphic method can be used to find E_{o1}, E_{o2}, ...



From these calculation, we find the energy spectrum of this finite square well problem.

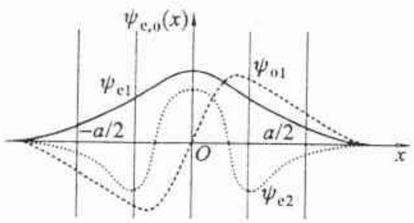


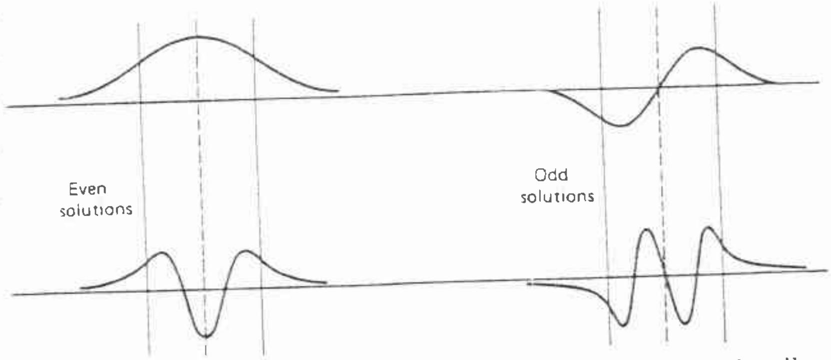
With eigenvalue E given, the wave function is now determined

· k_1, k_2 are known

· the only free parameter is C, can be determined through normalization.

The wave functions (eigenfunctions) corresponding to the first few lowest eigenvalues (energy) E_{e1}, E_{e2}, E_{o1}, E_{o2} are given in the following figure.





Solutions for discrete spectrum in attractive potential well.

The more nodes, the higher are the energies of the bound states.

This can be understood as follows

- $p \propto \frac{d\psi}{dx}$

  $\downarrow$

  roughly speaking, the more a wave function wiggles, the higher is the average value of the slope, and accordingly the higher is the average kinetic energy

- The sign of the slope is not important, since the kinetic energy involves the square of the momentum.

Single and Double δ-Function Potential

Single δ-Function Potential

$V(x) = -V_0\,\delta(x)$ $\qquad$ $V_0 > 0$ → attractive potential

The Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) - V_0\,\delta(x)\,u(x) = E\,u(x)$$

$$\Rightarrow \frac{d^2}{dx^2}u(x) + \frac{2mE}{\hbar^2}u(x) = -\frac{2mV_0}{\hbar^2}\delta(x) = -\lambda\,\delta(x)$$

$$\lambda \equiv \frac{2mV_0}{\hbar^2}$$

$E<0$ $\qquad$ $\frac{d^2u}{dx^2} - \kappa^2 u(x) = 0$ for $x \neq 0$

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

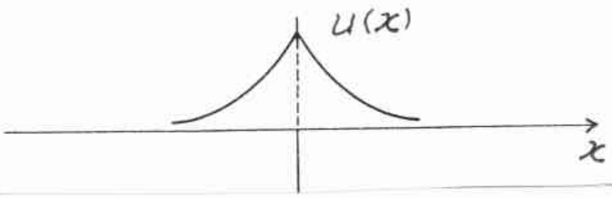
$u(x) = Ae^{-\kappa x} + A'e^{\kappa x}$ $\qquad$ for $x>0$

$A' = 0$ required by normalization condition

$u(x) = Be^{\kappa x} + B'e^{-\kappa x}$ $\qquad$ for $x<0$

$B' = 0$ required by normalization condition

The wave function must be continuous at $x=0 \Rightarrow A = B$



The derivative of the wave function has a discontinuity at $x=0$

$$\left(\frac{du}{dx}\right)_{x=0^+} - \left(\frac{du}{dx}\right)_{x=0^-} = -\lambda u(0)$$

$$-\kappa A - \kappa a = -\lambda A$$

$$\Rightarrow \kappa = \frac{\lambda}{2} \quad \Rightarrow \quad \frac{\lambda^2}{4} = \frac{2m|E|}{\hbar^2}$$

$\Rightarrow$ only at $|E| = \frac{\hbar^2\lambda^2}{8m}$ there exists solution

Normalization $|A|^2 \left[\int_0^\infty e^{-2\kappa x} dx + \int_{-\infty}^0 e^{2\kappa x} dx \right] = 1$

$\Rightarrow |A|^2 \frac{1}{2\kappa} \cdot 2 = 1 \Rightarrow |A|^2 = \kappa$

$\Rightarrow A = \frac{1}{\sqrt{\kappa}}$

Double δ - Function Potential

$V(x) = -V_0\,\delta(x+a) - V_0\,\delta(x-a)$

$V(-x) = V(x)$, the potential is symmetric under $x \to -x$.
The solution should be either even or odd
We shall discuss the case, $E < 0$

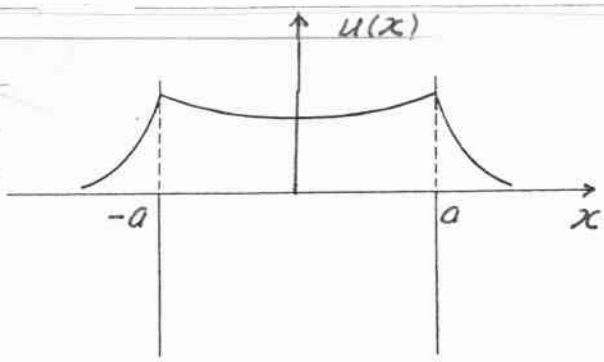
Even solution.

We are looking for the eigenvalue of the problem, we may leave the overall normalization to be open.

$u(x) = e^{-\kappa x}$ for $x > a$ ($e^{\kappa x}$ term is absent due to normalization requirement)

$u(x) = A\cosh \kappa x$ for $a > x > -a$ (originally, it is a linear combination of $e^{\kappa x}$ and $e^{-\kappa x}$, even solution requirement makes it possible to write it as $\cosh \kappa x$)

$u(x) = e^{\kappa x}$ for $x < -a$ (from even solution requirement)



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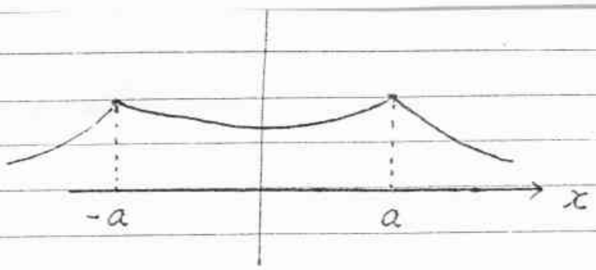


Wave function is continuous at $x = a$

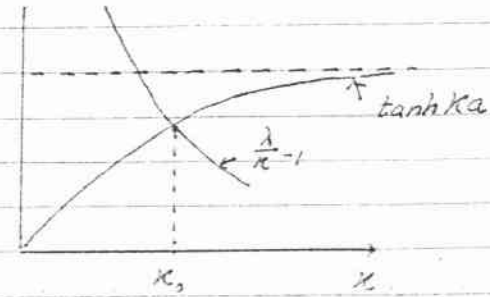
$$e^{-\kappa a} = A \cosh \kappa a$$

Derivative of the wave function has a discontinuity at $x = a$

$$-\kappa e^{-\kappa a} - \kappa A \sinh \kappa a = -\lambda \underbrace{e^{-\kappa a}}_{u(a)} \qquad \lambda = \frac{2mV_0}{\hbar^2}$$

Due to symmetry requirement, the boundary condition at $x = -a$ will give no new result.

$$\Rightarrow \quad \tanh \kappa a = \frac{\lambda}{\kappa} - 1 \quad \text{eigenvalue equation}$$



$$\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}$$

$\kappa_0 \rightarrow$ eigenvalue of energy

Discussion

$\tanh \kappa a > 0 \qquad \frac{\lambda}{\kappa_0} - 1 > 0 \Rightarrow \lambda > \kappa_0$

$\tanh \kappa a < 1 \qquad \frac{\lambda}{\kappa_0} - 1 < 1 \Rightarrow \frac{\lambda}{2} < \kappa_0$

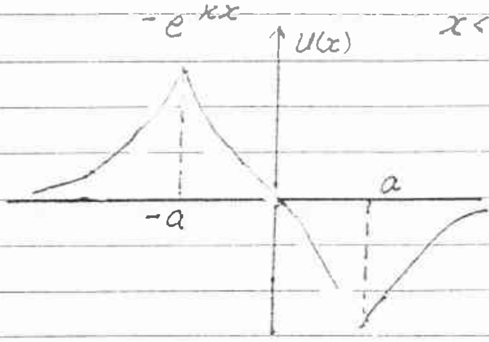
$\Rightarrow \quad \lambda > \kappa_0 > \frac{\lambda}{2} \qquad \kappa = \frac{\lambda}{2}$ for single δ function

Energy of the double well is a larger negative number than that of a single δ function potential with the same strength

In real world: an electron bound to two nuclei seperated by a small distance (similar to a double δ-function potential) will have lower energy than bound to a single nuclei (similar to a single δ-function potential)

Odd solution

$$U(x) = \begin{cases} e^{-\kappa x} & x > a \\ A\sinh \kappa x & a > x > -a \\ -e^{\kappa x} & x < -a \end{cases}$$



Boundary condition at $x = a$

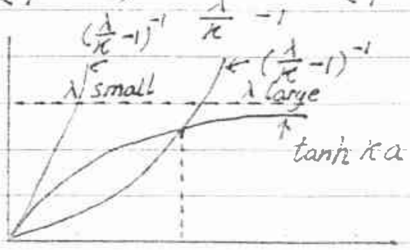
$$A \sinh \kappa a = e^{-\kappa a}$$

$$-\kappa e^{-\kappa a} - \kappa a \cosh \kappa a = -\lambda e^{-\kappa a}$$

$$\Rightarrow \quad \coth \kappa a = \frac{\lambda}{\kappa} - 1 \qquad \Rightarrow \quad \tanh \kappa a = \frac{1}{\left(\frac{\lambda}{\kappa} - 1\right)}$$

$$\tanh \kappa a > 0 \quad \Rightarrow \quad \frac{\lambda}{\kappa} - 1 > 0 \quad \Rightarrow \quad \frac{\lambda}{\kappa} > 1 \quad \Rightarrow \quad \lambda > \kappa$$

$$\tanh \kappa a < 1 \quad \Rightarrow \quad \frac{1}{\frac{\lambda}{\kappa} - 1} < 1 \quad \Rightarrow \quad 1 < \frac{\lambda}{\kappa} - 1 \quad \Rightarrow \quad \kappa < \frac{\lambda}{2}$$



⇒ The odd solution, if there is a bound state, is less strongly bound than the even solution.
The wave function, which has to go through zero, is forced to be steep because the wells, and thus can only accommodate to a less rapidly falling exponential
Depending on the size of λ, there may or may not exist an odd bound state.

Supplement 4-B

Tunneling in Nuclear Physics

Tunneling is important in nuclear physics. Nuclei are very complicated objects, but under certain circumstances it is appropriate to view nucleons as independent particles occupying levels in a potential well. With this picture in mind, the decay of a nucleus into an α-particle (a He nucleus with $Z = 2$) and a daughter nucleus can be described as the tunneling of an α-particle through a barrier caused by the Coulomb potential between the daughter and the α-particle (Fig. 4B-1). The α-particle is not viewed as being in a bound state: if it were, the nucleus could not decay. Rather, the α-particle is taken to have positive energy, and its escape is only inhibited by the existence of the barrier.[1]

If we write

$$|T|^2 = e^{-G} \tag{4B-1}$$

then

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{1/2} \int_R^b dr \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r} - E} \tag{4B-2}$$

where R is the nuclear radius[2] and b is the turning point, determined by the vanishing of the integrand (4B-2); Z_1 is the charge of the daughter nucleus, and Z_2 ($= 2$ here) is the charge of the particle being emitted. The integral can be done exactly

$$\int_R^b dr\left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} = \sqrt{b}\left[\cos^{-1}\left(\frac{R}{b}\right)^{1/2} - \left(\frac{R}{b} - \frac{R^2}{b^2}\right)^{1/2}\right] \tag{4B-3}$$

At low energies (relative to the height of the Coulomb barrier at $r = R$), we have $b \gg R$, and then

$$G = \frac{2}{\hbar}\left(\frac{2mZ_1Z_2e^2b}{4\pi\varepsilon_0}\right)^{1/2}\left[\frac{\pi}{2} \sqrt{\frac{R}{b}}\right] \tag{4B-4}$$

with $b = Z_1Z_2e^2/4\pi\varepsilon_0E$. If we write for the α-particle energy $E = mv^2/2$, where v is its final velocity, then

$$G = \frac{2\pi Z_1Z_2e^2}{4\pi\varepsilon_0\hbar v} = 2\pi\alpha Z_1Z_2\left(\frac{c}{v}\right) \tag{4B-5}$$

[1] If you find it difficult to imagine why a repulsion would keep two objects from separating, think of the inverse process, α capture. It is clear that the barrier will tend to keep the α-particle out.

[2] In fact, early estimations of the nuclear radius came from the study of α-decay. Nowadays one uses the size of the charge distribution as measured by scattering electrons off nuclei to get nuclear radii. It is not clear that the two should be expected to give exactly the same answer.

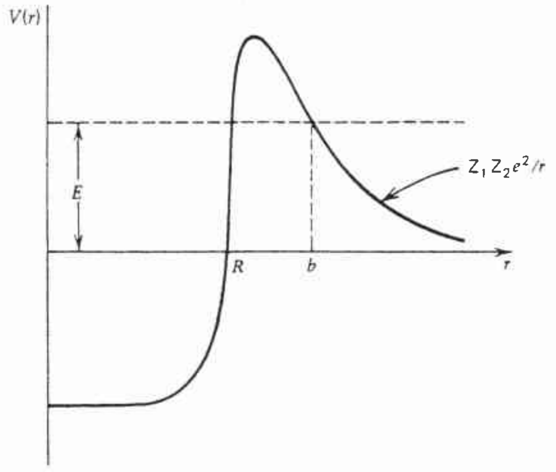


Figure 4B-1 Potential barrier for α decay.

The time taken for an α-particle to get out of the nucleus may be estimated as follows: the probability of getting through the barrier on a single encounter is e^{-G}. Thus the number of encounters needed to get through is $n \simeq e^G$. The time between encounters is of the order of $2R/v$, where R is again the nuclear radius, and v is the α velocity inside the nucleus. Thus the lifetime is

$$\tau \simeq \frac{2R}{v} e^G \tag{4B-6}$$

The velocity of the α inside the nucleus is a rather fuzzy concept, and the whole picture is very classical, so that the factor in front of the e^G cannot really be predicted without a much more adequate theory. Our considerations do give us an order of magnitude for it. For a 1-MeV α-particle,

$$v = \sqrt{\frac{2E}{m}} = c\sqrt{\frac{2E}{mc^2}} = 3 \times 10^8 \sqrt{\frac{2}{4 \times 940}} \simeq 7.0 \times 10^6 \text{ m/s}$$

so that one predicts, for low energy α's, the straight-line plot

$$\log_{10} \frac{1}{\tau} \simeq \text{const} - 1.73 \frac{Z_1}{\sqrt{E(\text{MeV})}} \tag{4B-7}$$

with the constant in front of the order of magnitude 27–28 when τ is measured in years instead of seconds. A large collection of data shows that a good fit to the lifetime data is obtained with the formula

$$\log_{10} \frac{1}{\tau} = C_2 - C_1 \frac{Z_1}{\sqrt{E}} \tag{4B-8}$$

Here $C_1 = 1.61$ and C_2 lying between 55 and 62. The exponential part of the fit differs slightly from our derivation, but given the simplicity of our model, the agreement has to be rated as good.

For larger α energies, the G factor depends on R, and with $R = r_0 A^{1/3}$, one finds that r_0 is a constant—that is, that the notion of a Coulomb barrier taking over the role of the potential beyond the nuclear radius has some validity. Again, simple qualitative considerations explain the data.

Supplement 4-C

Periodic Potentials

Metals generally have a crystalline structure; that is, the ions are arranged in a way that exhibits a spatial periodicity. In our one-dimensional discussion of this topic, we will see that this periodicity has two effects on the motion of the free electrons in the metal. One is that for a perfect *lattice*—that is, for ions spaced equally—the *electron propagates without reflection*; the other is that there are restrictions on the energies allowed for the electrons; that is, *there are allowed and forbidden energy "bands."*

We begin with a discussion of the consequences of perfect periodicity.

The periodicity will be built into the potential, for which we require that

$$V(x + a) = V(x) \tag{4C-1}$$

Since the kinetic energy term $-(\hbar^2/2m)(d^2/dx^2)$ is unaltered by the change $x \rightarrow x + a$, the whole *Hamiltonian is invariant under displacements by a.* For the case of zero potential, when the solution corresponding to a given energy $E = \hbar^2k^2/2m$ is

$$\psi(x) = e^{ikx} \tag{4C-2}$$

the displacement yields

$$\psi(x + a) = e^{ik(x+a)} = e^{ika}\psi(x) \tag{4C-3}$$

that is, the original solution multiplied by a phase factor, so that

$$|\psi(x + a)|^2 = |\psi(x)|^2 \tag{4C-4}$$

The observables will therefore be the same at x as at $x + a$; that is, we cannot tell whether we are at x or at $x + a$. In our example we shall also insist that $\psi(x)$ and $\psi(x + a)$ differ only by a phase factor, which need not, however, be of the form e^{ika}.

We digress briefly to discuss this requirement more formally. The invariance of the Hamiltonian under a displacement $x \rightarrow x + a$ can be treated formally as follows. Let D_a be an operator whose rule of operation is that

$$D_a f(x) = f(x + a) \tag{4C-5}$$

The invariance implies that

$$[H, D_a] = 0 \tag{4C-6}$$

We can find the eigenvalues of this operator by noting that

$$D_a\psi(x) = \lambda_a\psi(x) \tag{4C-7}$$

together with

$$D_{-a}D_a f(x) = D_aD_{-a} f(x) = f(x) \tag{4C-8}$$

implies that $\lambda_a\lambda_{-a} = 1$. This then implies that λ_a must be of the form e^{iqa}. Here q must be real, because if q had an imaginary part, a succession of displacements by a would make the wave function larger and larger with each displacement in one or the other direction.

Consider now a simultaneous eigenfunction of H and D_a, and define

$$u(x) = e^{-iqx}\psi(x) \tag{4C-9}$$

Then, using the fact that $\lambda_a = e^{iqa}$, we get

$$D_a u(x) = e^{-iq(x+a)}D_a\psi(x) = e^{-iq(x+a)}e^{iqa}\psi(x) = e^{-iqx}\psi(x) = u(x) \tag{4C-10}$$

This means that $u(x)$ is a periodic function obeying $u(x + a) = u(x)$. The upshot is that a function which is a simultaneous eigenfunction of H and D_a must be of the form

$$\psi(x) = e^{iqx}u(x) \tag{4C-11}$$

with $u(x)$ periodic. This result is known as *Bloch's Theorem.*

For a free particle $q = k$, the wave number corresponds to the energy E. More generally, the relation between q and k is more complicated. In any case, it is clear that (4C-4) holds, so that the net flux is unchanged as we go from x to $x + a$, and by extension to $x + na$. This means that an electron propagates without a change in flux.

Let us consider a series of ions in a line, with their centers located at $x = na$. To avoid having to deal with *end effects*, we assume that there are N ions placed on a very large ring, so that $n = 1$ and $n = N + 1$ are the same site. We will assume that the most loosely bound electrons—the ones that are viewed as "free"—are still sufficiently strongly bound to the ions that their wave functions do not overlap more than one or two nearest neighbors. We may now ask: What is the effect of this overlap on the energies of the electrons?

To answer this question, we consider first a classical analogy. We represent the electrons at the different sites by simple harmonic oscillators, all oscillating with the same angular frequency ω. In the absence of any coupling between the oscillators, we have the equation of motion

$$\frac{d^2x_n}{dt^2} = -\omega^2 x_n \qquad (n = 0, 1, 2, \ldots) \tag{4C-12}$$

If the harmonic oscillators are coupled to their nearest neighbors, then the equation is changed to

$$\frac{d^2x_n}{dt^2} = -\omega^2 x_n - K[(x_n - x_{n-1}) + (x_n - x_{n+1})] \tag{4C-13}$$

To solve this we write down a trial solution

$$x_n = A_n \cos \Omega t \tag{4C-14}$$

When this is substituted into (4C-13), we get

$$(\omega^2 - \Omega^2)A_n = -K(2A_n - A_{n-1} - A_{n+1}) \tag{4C-15}$$

This is known as a *difference equation*. We solve it by a trial solution. Let us assume that

$$A_n = L^n \tag{4C-16}$$

The identification of the sites at $n = 1$ and $N + 1$ implies $A_1 = A_{N+1}$ so that $L^N = 1$. This means that

$$L = e^{2\pi ir/N} \qquad r = 0, 1, 2, \ldots, (N - 1) \tag{4C-17}$$

The equation for the frequency Ω now yields

$$\omega^2 - \Omega^2 = -2K\left(1 - \cos\frac{2\pi r}{N}\right) = -4K \sin^2\frac{\pi r}{N}$$

The result

$$\Omega^2 = \omega^2 + 4K \sin^2\frac{\pi r}{N} \tag{4C-18}$$

shows that the frequencies, which, without coupling are all ω—that is, are *N-fold degenerate* (which corresponds to all the pendulums moving together)—are now spread over a range from ω to $\sqrt{\omega^2 + 4K}$. For large N there are many such frequencies, and they can be said to form a *band*. If we think of electrons as undergoing harmonic oscillations about their central locations, we can translate the above into a statement that in the absence of neighbors, all electron energies are degenerate, and the interaction with neighboring atoms spreads the energy values. We can, of course, have several fundamental frequencies $\omega_1, \omega_2, \ldots$, and different couplings to their neighbors, with strengths $K_1, K_2, \ldots$, which will then give rise to several bands that may or may not overlap.

The spreading of the frequencies is the same effect as the spreading of the energy levels of the most loosely bound electrons. For atoms far apart, with spacing larger than the exponential fall-off of the wave functions, all the energies are the same so that we have an N-fold degenerate single energy. Because the atoms are not so far apart, there is some coupling between nearest neighbors, and the energy levels spread. The classical analogy is suggestive, but not exact, since for the quantum case levels are pushed up as well as down, whereas all the frequencies above, lie above ω. Later we solve the Kronig-Penney model in which the potential takes the form

$$V(x) = \frac{\hbar^2}{2m}\frac{\lambda}{a}\sum_{-\infty}^{\infty}\delta(x - na) \tag{4C-19}$$

The solution can be shown to lead to a condition on q, which reads

$$\cos qa = \cos ka + \frac{1}{2}\lambda\frac{\sin ka}{ka} \tag{4C-20}$$

As can be seen from Figure (4C-1), this clearly shows the energy band structure.

THE KRONIG-PENNEY MODEL

To simplify the algebra, we will take a series of repulsive delta-function potentials,

$$V(x) = \frac{\hbar^2}{2m}\frac{\lambda}{a}\sum_{n=-\infty}^{\infty}\delta(x - na) \tag{4C-21}$$

Away from the points $x = na$, the solution will be that of the free-particle equation—that is, some linear combination of $\sin kx$ and $\cos kx$ (we deal with real functions for simplicity). Let us assume that in the region R_n defined by $(n - 1)\,a \le x \le na$, we have

$$\psi(x) = A_n \sin k(x - na) + B_n \cos k(x - na) \tag{4C-22}$$

and in the region R_{n+1} defined by $na \le x \le (n + 1)\,a$ we have

$$\psi(x) = A_{n+1} \sin k[x - (n + 1)\,a] + B_{n+1} \cos k[x - (n + 1)\,a] \tag{4C-23}$$

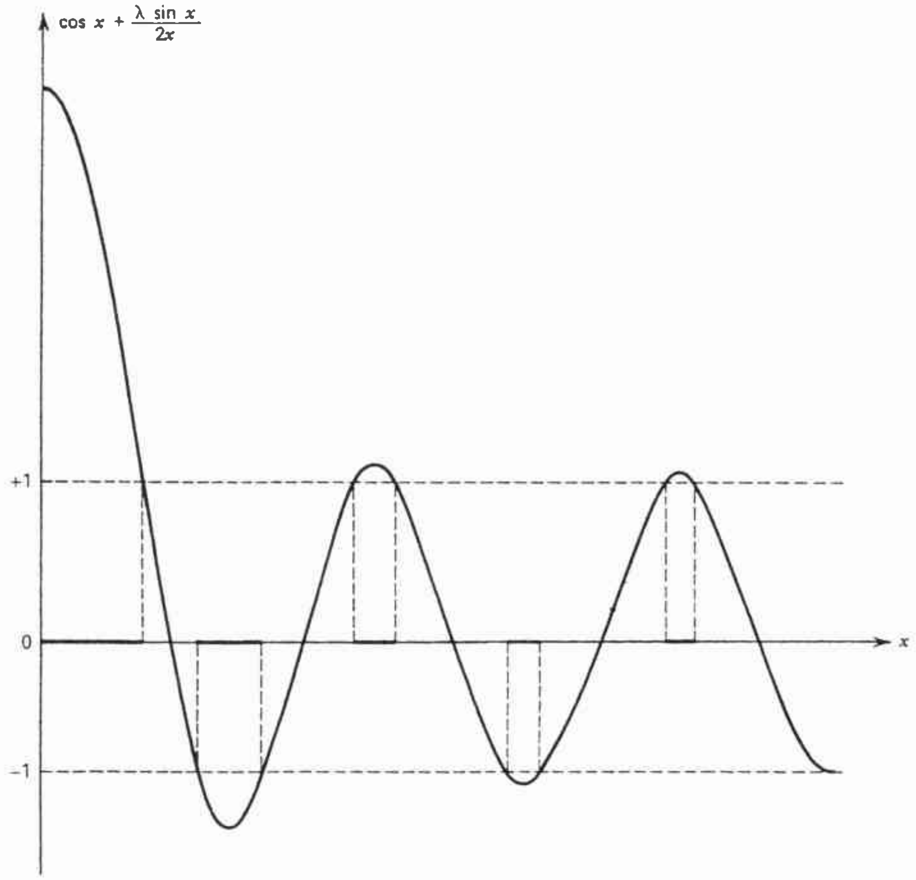


Figure 4C-1 Plot of $\cos x + (\lambda/2)(\sin x/x)$ as a function of x. The horizontal lines represent the bounds ± 1. The regions of x for which the curve lines outside the strip are forbidden.

Continuity of the wave function implies that ($x = na$)

$$-A_{n+1} \sin ka + B_{n+1} \cos ka = B_n \tag{4C-24}$$

and the discontinuity condition (4-68) here reads

$$kA_{n+1} \cos ka + kB_{n+1} \sin ka - kA_n = \frac{\lambda}{a} B_n \tag{4C-25}$$

A little manipulation yields

$$\begin{aligned} A_{n+1} &= A_n \cos ka + (g \cos ka - \sin ka) B_n \\ B_{n+1} &= (g \sin ka + \cos ka) B_n + A_n \sin ka \end{aligned} \tag{4C-26}$$

where $g = \lambda/ka$.

The requirement from Bloch's theorem that

$$\psi(x + a) = e^{iq(x+a)}u(x + a) = e^{iq(x+a)}u(x) = e^{iqa}\psi(x) \tag{4C-27}$$

implies that the wave functions in the adjacent regions R_n and R_{n+1} are related, since the wave function in (4C-22) may be written as

$$\psi(x) = A_n \sin[k((x+a)-(n+1)a] + B_n \cos k[k((x+a)-(n+1)a]$$

which is identical to that in (4C-23), provided

$$\begin{aligned} A_{n+1} &= e^{iqa} A_n \\ B_{n+1} &= e^{iqa} B_n \end{aligned} \tag{4C-28}$$

When this is inserted into the (4C-26), that is, into the conditions that the wave equation obeys the Schrödinger equation with the delta function potential, we get

$$\begin{aligned} A_n(e^{iqa} - \cos ka) &= B_n(g \cos ka - \sin ka) \\ B_n(e^{iqa} - (g \sin ka + \cos ka)) &= A_n \sin ka \end{aligned} \tag{4C-29}$$

This leads to the condition

$$(e^{iqa} - \cos ka)(e^{iqa} - (g \sin ka + \cos ka)) = \sin ka(g \cos ka - \sin ka) \tag{4C-30}$$

This may be rewritten in the form

$$e^{2iqa} - 2(\cos ka + \frac{g}{2} \sin ka)e^{iqa} + 1 = 0 \tag{4C-31}$$

This quadratic equation can be solved, and both real and imaginary parts lead to the condition

$$\cos\ qa = \cos ka + \frac{\lambda}{2}\frac{\sin ka}{ka} \tag{4C-32}$$

This is a very interesting result, because the left side is always bounded by 1; that is, there are restrictions on the possible ranges of the energy $E = \hbar^2k^2/2m$ that depend on the parameters of our "crystal." Figure 4C-1 shows a plot of the function $\cos x + \lambda \sin x/2x$ as a function of $x = ka$. The horizontal line represents the bounds on $\cos qa$, and the regions of x, for which the curve lies outside the strip, are forbidden regions. Thus there are *allowed energy bands* separated by regions that are forbidden. Note that the onset of a forbidden band corresponds to the condition

$$qa = n\pi \qquad n = \pm 1, \pm 2, \pm 3, \ldots \tag{4C-33}$$

This, however, is just the condition for Bragg reflection with normal incidence. The existence of energy gaps can be understood qualitatively. In first approximation the electrons are free, except that there will be Bragg reflection when the waves reflected from successive atoms differ in phase by an integral number of 2π—that is, when (4C-33) is satisfied. These reflections give rise to standing waves, with even and odd waves of the form $\cos \pi x/a$ and $\sin \pi x/a$, respectively. The energy levels corresponding to these standing waves are degenerate. Once the attractive interaction between the electrons and the positively charged ions at $x = ma$ (m integer) is taken into account, the even states, peaked in between, will move up in energy. Thus the energy degeneracy is split at $q = n\pi/a$, and this leads to energy gaps, as shown in Fig. 4C-1.

The Kronig-Penney model has some relevance to the theory of metals, insulators, and semiconductors if we take into account the fact (to be studied later) that energy levels occupied by electrons cannot accept more electrons. Thus a metal may have an energy band partially filled. If an external field is applied, the electrons are accelerated, and if there are momentum states available to them, the electrons will occupy the momentum states under the influence of the electric field. Insulators have completely filled bands, and an electric field cannot accelerate electrons, since there are no neighboring empty states. If the electric field is strong enough, the electrons can "jump" across a forbidden energy gap and go into an empty allowed energy band. This corresponds to the breakdown of an insulator. The semiconductor is an insulator with a very narrow forbidden gap. There, small changes of conditions, such as a rise in temperature, can produce the "jump" and the insulator becomes a conductor.

The band structure is of great relevance in solid state physics. Fig. 4C-2 shows three situations that can arise when energy levels are filled with electrons. We shall learn in Chapter 13 that only two electrons are allowed per energy level. In case (*a*) the electrons fill all the energy levels below the edge of the energy gap. The application of a weak electric field will have no effect on the material. The electrons near the top of the filled band cannot be accelerated. There are no levels with higher energy available to them. Materials in which this occurs are *insulators*; that is, they do not carry currents when electric fields are applied. In case (*b*) the energy levels are only partly filled. In this case the application of an electric field accelerates the electrons at the top of the stack of levels. These electrons have empty energy levels to move into, and they would accelerate indefinitely in a perfect lattice, as stated in the previous section. What keeps them from doing that is *dissipation*. The lattice is not perfect for two reasons: one is the presence of impurities, which destroys the perfect periodicity; the other is the effect of thermal agitation on the position of the ions forming the lattice, which has the same effect of destroying perfect periodicity. Materials in which the energy levels below the gaps are only partially filled are *conductors*.

The width of the gaps in the energy spectrum depends on the materials. For some insulators the gaps are quite narrow. When this happens, then at finite temperatures T, there is a calculable probability that some of the electrons are excited to the bottom of the set of energy levels above the gap. (To good approximation the probability is proportional to the Boltzmann factor $e^{-E/kT}$). These electrons can be accelerated as in a conductor, so that the application of an electric field will give rise to a current. The current is augmented by another effect: the energy levels that had been occupied by the electrons promoted to the higher energy band (called the *conduction band*) are now empty. They provide vacancies into which electrons in the lower band (called the *valence band*) can be accelerated into,

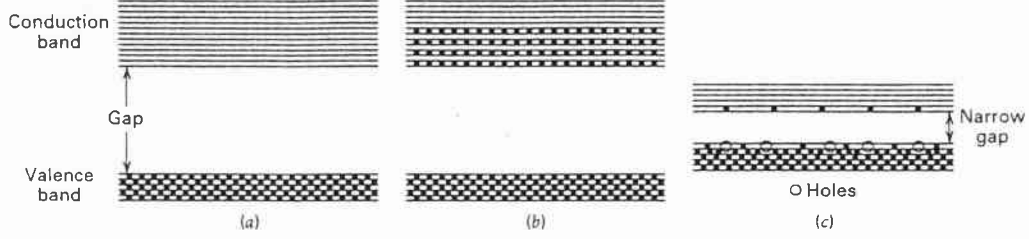


Figure 4C-2 Occupation of levels in the lowest two energy bands, separated by a gap. (*a*) Insulator has a completely filled band. Electrons cannot be accelerated into a nearby energy level. (*b*) Conductor has a half-filled band, allowing electrons to be accelerated into nearby energy levels. (*c*) In a semiconductor, thermal effects promote some electrons into a second band. These electrons can conduct electricity. The electrons leave behind them *holes* that act as positively charged particles and also conduct electricity.

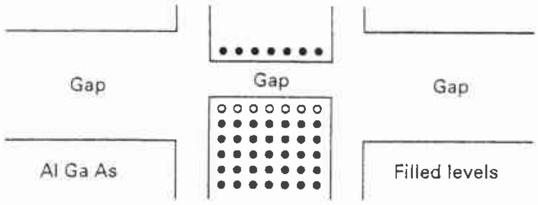


Figure 4C-3 Schematic picture of electrons and holes trapped in a well created by adjacent semiconductors with a wider gap. An example of such a heterostructure is provided by a layer of GaAs sandwiched between two layers of AlGaAs.

when an electric field is applied. These vacancies, called *holes*, propagate in the direction opposite to that of the electrons and thus add to the electric current. This is the situation shown in Fig. 4C-2(*c*).

The technology of making very thin layers of compounds of materials has improved in recent decades to such an extent that it is possible to create the analog of the infinite wells discussed in Chapter 3. Consider a "sandwich" created by two materials. The outer one has a larger energy gap than the inner one, as shown in Fig. 4C-3. The midpoints of the gaps must coincide[1] (for equilibrium reasons). The result is that both electrons and holes in the interior semiconductor cannot move out of the region between the outer semiconductors, because there are no energy levels that they can move to. Such confined regions may occur in one, two, or three dimensions. In the last case we deal with *quantum dots*. The study of the behavior of electrons in such confined regions is a very active field of research in the study of materials.

In summary, one-dimensional problems give us a very important glimpse into the physics of quantum systems in the real world of three dimensions.

[1]A brief, semiquantitative discussion of this material may be found in *Modern Physics* by J. Bernstein, P. M. Fishbane, and S. Gasiorowicz (Prentice Hall, 2000). See also Chapter 44 in *Physics for Scientists and Engineers*, (2nd Edition) by P. M. Fishbane, S. Gasiorowicz and S. T. Thornton (Prentice Hall, 1996). There are, of course, many textbooks on semiconductors, which discuss the many devices that use *bandgap engineering* in great quantitative detail. See in particular L. Solymar and D. Walsh, *Lectures on the Electrical Properties of Materials*, Oxford University Press, New York (1998).

One-dimensional potentials: potential step

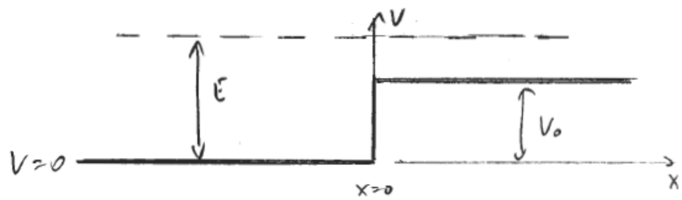


Figure I: Potential step of height V_0. The particle is incident from the left with energy E.

We analyze a time independent situation where a current of particles with a well-defined energy is incident on the barrier. The time-independent SE is

$$\hat{H}u(x) = Eu(x) \tag{15-1}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2}(x) + V(x)u(x) = Eu(x) \tag{15-2}$$

$$\frac{d^2u}{dx^2} = -\frac{2m}{\hbar^2}[E - V(x)]u(x) \tag{15-3}$$

Qualitative features of solutions for regions of constant V_1:

If $E - V_1 > 0$, the solutions are of the form $e^{\pm ik_1x}$ with $\frac{\hbar^2k^2}{2m} = E - V_1$, k_1 real.

Interpretation. $\frac{\hbar^2k^2}{2m}$ is the KE of the particle with total energy E in a region of potential V_1, the $e^{\pm ikx}$ wavefunctions correspond to particles traveling left / right.

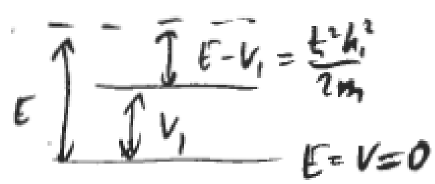


Figure II: In a region where the particle energy is greater than the (constant) potential, the solutions of the SE are plane waves $e^{\pm ikx}$, where $E - V_1 = \hbar^2k^2/2m$ is the kinetic energy of the particle in that region.

If $E - V_1 < 0$, the solutions are of the form $e^{\pm\kappa_1x}$ with $\frac{\hbar^2{\kappa_1}^2}{2m} = V_1 - E$, κ_1 real. These are damped exponentials with a decay length constant κ_1 (decay length ${\kappa_1}^{-1}$), where $\frac{\hbar^2{\kappa_1}^2}{2m} = V_1 - E$ represents the "missing" kinetic energy of the particle As $E \to V$, the decay length ${\kappa_1}^{-1}$ becomes longer and longer.

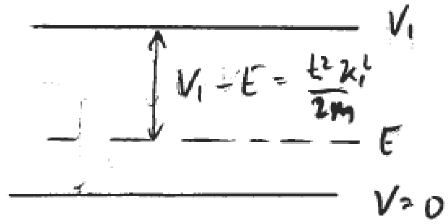


Figure III: In a region where the particle energy is less than the (constant) potential, the solutions of the SE are exponentially growing or decaying functions, $e^{\pm\kappa x}$, where $V_1 - E = \hbar^2\kappa^2/2m$ is the "missing kinetic energy" of the particle in that region.

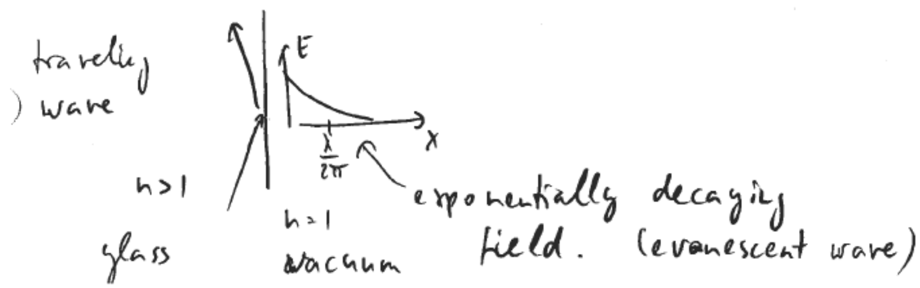


Figure IV: When a light wave experiences total internal reflection on a glass-vacuum interface, an evanescent (non-traveling, exponentially decaying wave) builds up inside the vacuum. The closer we are to the critical angle for total internal reflection, the longer the decay length of the evanescent wave. This phenomenon is analogous to a particle entering a classically forbidden region with $V_1 > E$. The less forbidden the region, the longer the decay length.

Note. There is a non-zero probability to find the particle with energy E in a "classically forbidden region" with $E < V_1$. The less the region is forbidden (the smaller $V_1 - E$), the further the particle penetrates into the forbidden region (the longer the decay length ${\kappa_1}^{-1}$). The phenomenon is similar to total internal reflection inside glass at a glass-vacuum interface.

The light field has non-zero amplitude in the "forbidden region". How do we know? Approach with a second prism. The evanescent (decaying) field existing in the vacuum is converted back into a traveling wave in the second prism.

Similarly, **a particle can tunnel through a potential barrier** even if its energy is insufficient to surpass it.

Back to potential step Assume $E > V_0$: define

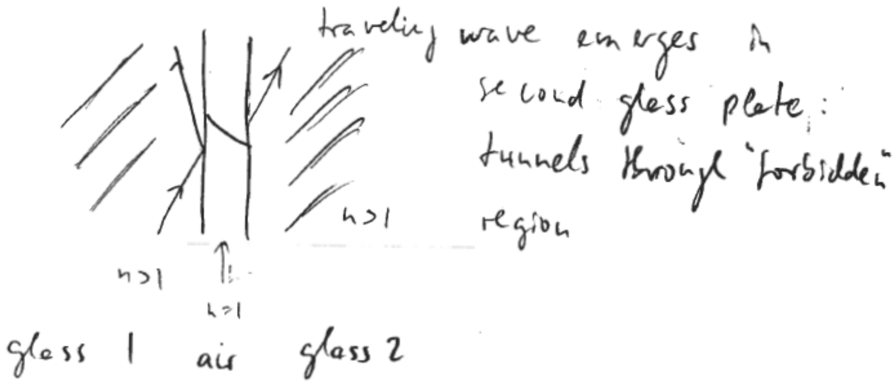


Figure V: The light field "tunneling" through the forbidden region can be detected as it emerges on the other side in a second prism.

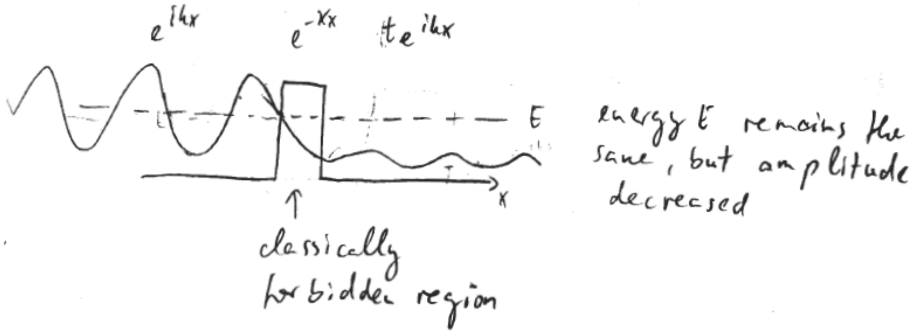


Figure VI: As a particle tunnels through a barrier and emerges from the other side, the energy E and the Broglie wavelength $2\pi/k$ remain the same. The amplitude of the emerging wave is smaller than that of the incident wave.

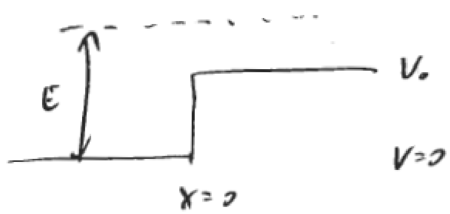


Figure VII: Potential step

$$\frac{\hbar^2 k^2}{2m} = E \qquad \text{(KE in region } x < 0) \tag{15-4}$$

$$\frac{\hbar^2 q^2}{2m} = E - V_0 \qquad \text{(KE in region } x > 0) \tag{15-5}$$

The most general solution is

$$Ae^{ikx} + Be^{-ikx} \qquad \text{in the region } x < 0 \tag{15-6}$$

$$Ce^{iqx} + De^{-iqx} \qquad \text{in the region } x > 0 \tag{15-7}$$

If we choose as the initial condition a particle incident from the left ($A \neq 0$), then the particle can be transmitted to the RHS ($C \neq 0$), or, as we shall see, partially reflected by the barrier in spite of $E > V_0$ ($B \neq 0$). However, if no particle is incident from the right then $D = 0$.

Calculate the particle current (or flux)

In region $x < 0$:

$$j_< = \frac{\hbar}{2im}\left(u^* \frac{du}{dx} - \left(\frac{du^*}{dx}\right) u\right) \tag{15-8}$$

$$= \frac{\hbar}{2im}\left[\left(A^* e^{-ikx} + B^* e^{ikx}\right)\left(ikAe^{ikx} - ikBe^{-ikx}\right) - \text{ c.c.}\right] \tag{15-9}$$

$$= \frac{\hbar k}{2m}\left[|A|^2 + AB^* e^{2ikx} - A^* B e^{-2ikx} - |B|^2 - \text{ c.c.}\right] \tag{15-10}$$

$$= \frac{\hbar k}{m}\left[|A|^2 - |B|^2\right] \quad \rightarrow \quad \text{net current for } x < 0 \tag{15-11}$$

We define the reflection amplitude $r = \frac{B}{A}$, and the reflection coefficient as $R = |r|^2 = \left|\frac{B}{A}\right|^2$.

For $x > 0$:

$$j_> = \frac{\hbar q}{m}|C|^2 \tag{15-12}$$

Continuity of wavefunction at $x = 0$:

$$\psi(x \rightarrow 0) = A + B = \psi(x \leftarrow 0) = C \tag{15-13}$$

In spite of the potential step, the derivative of the wavefunction must also be continuous:

$$\left(\frac{du}{dx}\right)_{x=\epsilon} - \left(\frac{du}{dx}\right)_{x=-\epsilon} = \int_{-\epsilon}^{\epsilon} dx \frac{d}{dx}\left(\frac{du}{dx}\right) \tag{15-14}$$

$$= -\frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon} dx[E - V(x)]u(x) = 0 \tag{15-15}$$

For future applications, we note that if the potential contains a delta function term $\lambda\delta(x - a)$, with some magnitude of the delta function λ, then the same calculation gives

$$\left(\frac{du}{dx}\right)_{x=a+\epsilon} - \left(\frac{du}{dx}\right)_{x==a-\epsilon} = \frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx \lambda \delta(x-a) u(\lambda) \tag{15-16}$$

$$= \frac{2m}{\hbar^2}\lambda u(a) \tag{15-17}$$

To summarize, we have the following rules:

Rule 1. The wavefunction u(x) is always continuous

Rule 2. The first spatial derivative of the wavefunction $\frac{du}{dx}$ is continuous if the potential does not contain δ-function like terms. (It may contain potential steps).

Rule 2.1. if the potential contains a term $\lambda\delta(x-a)$, the the first derivative $\frac{du}{dx}$ is discontinuous at $x = a$ amnd satisfies the relation

$$\left(\frac{du}{dx}\right)_{x=a+\epsilon} - \left(\frac{du}{dx}\right)_{x=a-\epsilon} = \frac{2m}{\hbar^2}\lambda u(a) \tag{15-18}$$

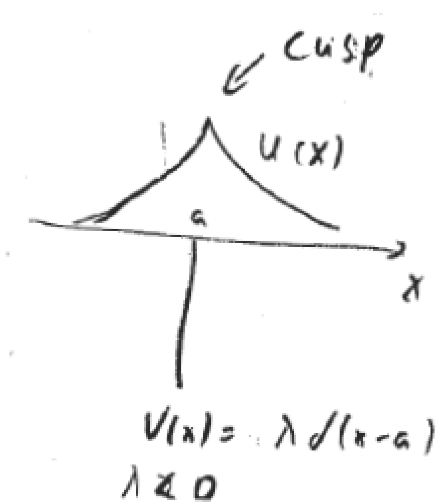


Figure VIII: A discontinuity in the slope of the wavefunction occurs at a delta function potential. The difference in wavefunction slopes is proportional to the strength of the δ potential, and to the value of the wavefunction at the cusp.

$$\text{Continuity of } \psi: \qquad A + B = C \tag{15-19}$$

$$\text{Continuity of } \psi': \qquad ik(A - B) = iqC \tag{15-20}$$

Solve for B, C in terms of A

$$C = A + B = \frac{k}{q}(A - B) \tag{15-21}$$

$$A\left(1 - \frac{k}{q}\right) = -B\left(1 + \frac{k}{q}\right) \tag{15-22}$$

$$A\frac{q-k}{q} = -B\frac{q+k}{q} \tag{15-23}$$

$$B = \frac{k-q}{k+q}A \tag{15-24}$$

$$C = A + B = A + \frac{k-q}{k+q}A = \frac{2}{k+q}A \tag{15-25}$$

Reflection amplitude
$$r = \frac{B}{A} = \frac{k-q}{k+q} \tag{15-26}$$

Transmission amplitude
$$t = \frac{C}{A} = \frac{2k}{k+q} \tag{15-27}$$

Reflection coefficient
$$|r|^2 = \left|\frac{B}{A}\right|^2 = \left(\frac{k-q}{k+q}\right)^2 \tag{15-28}$$

Transmission coefficient
$$|t|^2 = \left|\frac{C}{A}\right|^2 = \frac{4k^2}{(k+q)^2} \tag{15-29}$$

Reflection current
$$j_{\leftarrow} = \frac{\hbar k}{m}|B|^2 = \frac{\hbar k}{m}\left(\frac{k-q}{k+q}\right)^2|A|^2 \tag{15-30}$$

Transmission current
$$j_{\rightarrow, x>0} = \frac{\hbar q}{m}|C|^2 = \frac{\hbar k}{m}\frac{4kq}{(k+q)^2}{}^2|A|^2 \tag{15-31}$$

Net current for $x < 0$
$$j_{<} = \frac{\hbar k}{m}(|A|^2 - |B|^2) = \frac{\hbar k}{m}|A|^2\frac{4kq}{(k+q)^2} \tag{15-32}$$

Net current for $x > 0$
$$j_{>} = \frac{\hbar q}{m}|C|^2 = \frac{\hbar k}{m}\frac{4kq}{(k+q)^2}|A|^2 \tag{15-33}$$

The current obeys the continuity equation (see problem set)

$$\frac{\partial j}{\partial x} + \frac{\partial}{\partial t}|\psi|^2 = 0 \tag{15-34}$$

Here we are considering stationary states, $\frac{\partial}{\partial t}|\psi|^2 = 0$ (no change of probability density in time), $\Longrightarrow j = \text{const}$, current is continuous across the potential step,

$$j_{<} = j_{>}, \tag{15-35}$$

or

$$j_{\text{inc}} = j_{\rightarrow,x<0} = \frac{\hbar k}{m}|A|^2 = j_{\text{refl}} + j_{\text{trans}} \tag{15-36}$$

$$= j_{\leftarrow,x<0} + j_{\rightarrow,x>0} \tag{15-37}$$

$$= \frac{\hbar k}{m}|B|^2 + \frac{\hbar q}{m}|C|^2. \tag{15-38}$$

Note. $|r|^2 + |t|^2 \neq 1$ because the particle velocity is different for $x > 0$ from that for $x < 0$.

Discussion of results

In contrast to classical mechanics, there is some reflection at the potential step even though the energy of the particle is sufficient to surpass it. This is familiar from optics, where a step-like change in the index of refraction (e.g., air-glass interface) leads to partial reflection. The particle reflection is a consequence of the matching of the wavefunction and its derivative at the boundary. Again, this is similar to optics where the matching of th electromagnetic fields at the boundary results in a reflected field.

Note. For a very smooth change of potential (or refractive index in optics) there is not reflection. What is smooth? A change over many wavelengths. Changes of the potential over a distance l short compared to a wavelength $\lambda = \frac{2\pi}{k}$ result in reflection. Slow changes of potential over many λ do not result in reflection if particle energy exceeds barrier height.

Figure IX: A potential that varies smoothly over many de Broglie wavelengths does not produce partial reflection if the particle energy is sufficient to surpass it.

Intermediate region $l \sim \lambda$: we expect resonance phenomena (non-monotonic changes of reflection probability with particle energy). For the potential step, the reflection probability

$$|r|^2 \to 0 \qquad \text{for } k \to q \qquad (E \gg V_1), \text{and} \tag{15-39}$$

$$|r|^2 \to 1 \qquad \text{for } q \to 0 \qquad (E \gg V_1), \text{as expected.} \tag{15-40}$$

(15-41)

Interestingly, the reflection probability can be written as

$$|r|^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_1}}{\sqrt{E} + \sqrt{E - V_1}}\right)^2 \tag{15-42}$$

i.e. it does not depend explicitly on $\hbar$. However, the reflection is still inherenetly non-classical in that the potential needs to change abruptly compared to the particle's de Broglie wavelength, that depends on $\hbar$.

Solution for $E < V_0$: We define

$$\frac{\hbar^2 k^2}{2m} = E \qquad \text{(KE for } x < 0) \tag{15-43}$$

$$\frac{\hbar^2 \kappa^2}{2m} = V_0 - E \qquad \text{(“missing KE to surpass barrier”)} \tag{15-44}$$

Most general solution

$$Ae^{ikx} + Be^{-ikx} \qquad \text{for } x < 0 \tag{15-45}$$

$$Ce^{-\kappa x} + De^{\kappa x} \qquad \text{for } x > 0 \tag{15-46}$$

The $e^{+\kappa x}$ term is not normalizable, $D = 0$

We can go through the same procedure as before using the continuity of $\psi_1 \psi'$ at $x = 0$, or use the previous calculation if we set $q \to i\kappa$ ($Ce^{iqx} \to Ce^{-\kappa x}$ then). Consequently,

$$|r|^2 = \left|\frac{B}{A}\right|^2 = \left|\frac{k - i\kappa}{k + iq}\right|^2 = \frac{k^2 + \kappa^2}{k^2 + \kappa^2} = 1 \tag{15-47}$$

$$|t|^2 = \left|\frac{C}{A}\right|^2 = \left|\frac{2k}{k + i\kappa}\right|^2 = \frac{4k^2 + \kappa^2}{k^2 + \kappa^2} \neq 0 \tag{15-48}$$

(15-49)

A part of the wave penetrates the barrier, which is why the 'transmission' amplitude does not vanish. Note, however, that there is no associated particle current: Since Ce^{-kx} does not have a spatially varying phase, the particle current

$$j = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \text{ c.c.}\right) \tag{15-50}$$

vanishes for $x > 0$,

$$j_< = \frac{\hbar k}{m}(|A|^2 - |B|^2) = 0 \tag{15-51}$$

$$j_> = 0 \tag{15-52}$$

The net current is zer0 in steady-state because all particles are reflected.

Note. The reflected wave has an energy-dependent phase shift

$$r = \frac{B}{A} = \frac{k - i\kappa}{k + i\kappa} \tag{15-53}$$

$$= \frac{(k - i\kappa)^2}{k^2 + \kappa^2} \tag{15-54}$$

$$= \frac{k^2 - \kappa^2 - 2ik\kappa}{k^2 + \kappa^2} \tag{15-55}$$

$$= e^{i\phi} \tag{15-56}$$

with $\tan\phi = -\frac{2k\kappa}{k^2-\kappa^2}$

The phase shift of the wave is important in 3D scattering problems.

Can we localize the particle in the forbidden region?

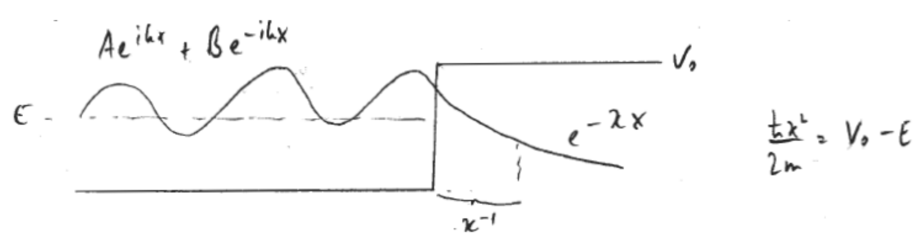


Figure X: The wavefunction for $E < V_0$ protrudes into the forbidden region $x > 0$. Can the particle be observed there?

To be sure that we have measured the particle inside the barrier, and not outside, we must measure its position at least with accuracy $\Delta x \approx \kappa^{-1}$. Then according to Heisenberg uncertainty, a momentum kick exceeding $\Delta p \geq \frac{\hbar}{\Delta x} \sim \hbar\kappa$ will be transferred onto the particle.

How much energy do we transfer?

$$\Delta E = E(p + \Delta p) - E(p) \tag{15-57}$$

$$= \frac{(p + \Delta p)^2}{2m} - \frac{p^2}{2m} \tag{15-58}$$

$$= \frac{p\Delta p}{m} + \frac{(\Delta p)^2}{2m} \tag{15-59}$$

$$p = \hbar k \tag{15-60}$$

$p\Delta p$ can be positive or negative, $(\Delta p)^2$ is always positive. the transferred energy is on average

$$\langle \Delta E \rangle = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2m(\Delta x)^2} = \frac{\hbar^2 \kappa^2}{2m} = V_0 - E \tag{15-61}$$

According to Heisenberg uncertainty, the measurement that localizes the particle inside the barrier transfers enough energy to allow the particle to be legitimately there.

Rule. A positive KE $E - V_1 > 0$ corresponds to a spatially oscillating wavefunction $e^{\pm ikx}$ with rate constant k (oscillation period $\lambda = \frac{2\pi}{k}$). A negative ("missing") KE $E - V_1 < 0$ corresponds to a spatially decaying or growing wavefunction $e^{\pm}\kappa x$ with decay rate constant κ (decay length κ^{-1}).

The "missing" KE is associated with the size of the region (κ^{-1}) that the particle occupies in the classically forbidden space.

The potential barrier: tunneling

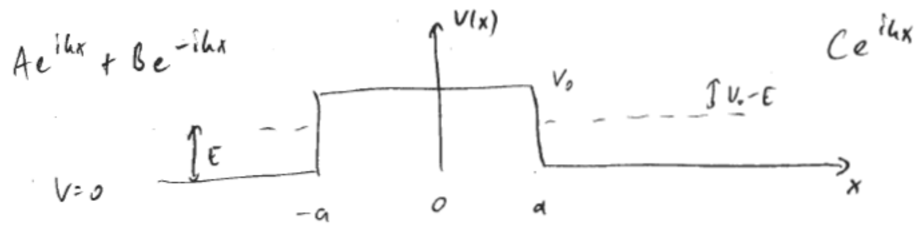


Figure I: Tunneling through a potential barrier.

Assume $E < V_0$ (classically particle is reflected). Outside barrier solutions to the SE are

$$u(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{for } x < -a, \tag{16-1}$$
$$u(x) = Ce^{ikx} \qquad \text{for } x > a, \tag{16-2}$$
$$\tag{16-3}$$

where we have omitted the term De^{-ikx} that corresponds to an incident waveform the right. Inside the barrier the SE is

$$\frac{d^2u}{dx^2}(x) = +\frac{2m}{\hbar}(V_0 - E)u(x) = \kappa^2 u(x) \tag{16-4}$$

with $\kappa^2 = \frac{2m}{\hbar^2}(V_o - E)$. As before, κ is the decay constant in the classically forbidden region (κ^{-1} is the decay length) that is associated with the "missing" KE necessary to surpass the barrier classically, $\frac{\hbar^2\kappa^2}{2m} = V_0 - E$. Consequently inside the barrier

$$u(x) = Ee^{-\kappa x} + Fe^{\kappa x}, \text{for } |x| \leq a \tag{16-5}$$

As before, we need to match the solution $u(x)$ and its derivative $u'(x)$ at the boundaries.

- At $x = -a$:

$$Ae^{-ika} + Be^{ika} = Ee^{+\kappa a} + Fe^{-\kappa a} \qquad \text{for } u \tag{16-6}$$
$$+ikAe^{-ika} - ikBe^{ika} = +\kappa Ee^{+\kappa a} + \kappa Fe^{-\kappa a} \qquad \text{for } u' \tag{16-7}$$

- At $x = a$:

$$Ce^{ika} = Ee^{-\kappa a} + Fe^{\kappa a} \qquad \text{for } u \tag{16-8}$$
$$ikAe^{ika} = -\kappa Ee^{-\kappa a} + \kappa Fe^{\kappa a} \qquad \text{for } u' \tag{16-9}$$

We are interested in the reflection amplitude $r = \frac{B}{A}$ (or the reflection probability $|r|^2 = \left|\frac{B}{A}\right|^2$) and the transmission amplitude $t = \frac{C}{A}$ (or transmission probability $|t|^2 = \left|\frac{C}{A}\right|^2$) from the barrier. Remember that $|A|^2$ determines the incident current, and is a free parameter. It is useful to divide the equation for u' by the equation for u (or alternatively, match $\frac{1}{u(x)}\frac{du}{dx} = \frac{d}{dx}(\ln u(x))$ directly. Then we write

- At $x = -a$:

$$\frac{+ikAe^{-ika} - ikBe^{+ika}}{Ae^{-ika} + Be^{ika}} = \frac{-\kappa Ee^{\kappa a} + \kappa Fe^{-\kappa a}}{Ee^{\kappa a} + Fe^{-\kappa a}} \tag{16-10}$$

- At $x = a$:

$$ik = \frac{+ikCe^{ika}}{Ce^{ika}} = \frac{-\kappa Ee^{-\kappa a} + \kappa Fe^{\kappa a}}{Ee^{-\kappa a} + Fe^{\kappa a}} \tag{16-11}$$

(matching of $\frac{d}{dx}(\ln u(x)) = \frac{1}{u(x)}\frac{du}{dx}$ at boundaries).

Now we proceed to eliminate E, F (Eq. 16-11):

$$ikEe^{-\kappa a} + ikFe^{\kappa a} = -\kappa Ee^{-\kappa a} + \kappa Fe^{\kappa a} \tag{16-12}$$

$$(\kappa + ik)Ee^{-\kappa a} = (\kappa - ik)Fe^{\kappa a} \tag{16-13}$$

$$E = \frac{\kappa - ik}{\kappa + ik}Fe^{2\kappa a} \tag{16-14}$$

Substitute into Eq. 16-10:

$$\text{RHS} = \frac{-\kappa\frac{\kappa-ik}{\kappa+ik}Fe^{3\kappa a} + \kappa Fe^{-\kappa a}}{\frac{\kappa-ik}{\kappa+ik}Fe^{3\kappa a} + Fe^{-\kappa a}} \tag{16-15}$$

$$= \frac{-\kappa(\kappa - ik)e^{+2\kappa a} + \kappa(\kappa + ik)e^{-2\kappa a}}{(\kappa - ik)e^{2\kappa a} + (\kappa + ik)e^{-2\kappa a}} \tag{16-16}$$

$$= \frac{-\kappa^2(e^{2\kappa a} - e^{-2\kappa a}) + ik\kappa(e^{2\kappa a} + e^{-2\kappa a})}{\kappa(e^{2\kappa a} + e^{-2\kappa a}) - ik(e^{2\kappa a} - e^{-2\kappa a})} \tag{16-17}$$

$$= -\frac{\kappa^2 \sinh(2\pi a) + ik\kappa \cosh(2\kappa a)}{\kappa \cosh(2\kappa a) - ik \sinh(2\kappa a)} \tag{16-18}$$

Consequently, Eq. 16-10

$$\left[+ikAe^{-ika} - ikBe^{ika}\right]\left[\kappa\cosh(2\kappa a) - ik\sinh(2\kappa a)\right] \tag{16-19}$$

$$= \left[Ae^{-ika} + Be^{ika}\right]\left[-\kappa^2\sinh(2\kappa a) + ik\kappa\cosh(2\kappa a)\right] \tag{16-20}$$

$$= Ae^{-ika}(+ik\kappa\cosh(2\kappa a) + k^2\sinh(2\kappa a) + \kappa^2\sinh(2\kappa a) - ik\kappa\cosh(2\kappa a)) \tag{16-21}$$

$$= Be^{ika}(+ik\kappa\cosh(2\kappa a) + k^2\sinh(2\kappa a) - \kappa^2\sinh(2\kappa a) + ik\kappa\cosh(2\kappa a)) \tag{16-22}$$

$$Ae^{-ika}\left[(k^2+\kappa^2)\sinh(2\kappa a)\right] = Be^{ika}\left[2ik\kappa\cosh(2\kappa a) + (k^2-\kappa^2)\sinh(2\kappa a)\right] \tag{16-23}$$

$$r = \frac{B}{A} \tag{16-24}$$

$$= e^{-2ika}\frac{(k^2+\kappa^2)\sinh(2\kappa a)}{2ik\kappa\cosh(2\kappa a) + (k^2-\kappa^2)\sinh(2\kappa a)} \tag{16-25}$$

reflection amplitude from barrier.

To calculate the transmission amplitude $\frac{C}{A}$, we use the continuity of u at $x = a$:

$$Ce^{ika} = Ee^{-\kappa a} + Fe^{+\kappa a} \tag{16-26}$$

$$= \frac{\kappa - ik}{\kappa + ik}Fe^{\kappa a} + Fe^{\kappa a} \tag{16-27}$$

$$= \frac{2\kappa}{\kappa + ik}Fe^{\kappa a} \tag{16-28}$$

We find F from the continuity of u at $x = -a$:

$$\text{RHS} = Ee^{\kappa a} + Fe^{-\kappa a} \tag{16-29}$$

$$= \frac{\kappa - ik}{\kappa + ik} Fe^{3\kappa a} + Fe^{-\kappa a} \tag{16-30}$$

$$= Fe^{\kappa a}\left[\frac{\kappa - ik}{\kappa + ik} e^{2\kappa a} + \frac{\kappa + ik}{\kappa + ik} e^{-2\kappa a}\right] \tag{16-31}$$

$$= Fe^{\kappa a} \frac{2\kappa \cosh(2\kappa a) - 2ik \sinh(2\kappa a)}{\kappa + ik} \tag{16-32}$$

$$\text{RHS} = Ae^{-ika} + Be^{ika} \tag{16-33}$$

$$= Ae^{-ika} + Ae^{-ika} \frac{(k^2 + \kappa^2)\sinh(2\kappa a)}{2ik\kappa \cosh(2\kappa a) + (k^2 - \kappa^2)\sinh(2\kappa a)} \tag{16-34}$$

$$= Ae^{-ika}\left[1 + \frac{(k^2 + \kappa^2)\sinh(2\kappa a)}{2ik\kappa \cosh(2\kappa a) + (k^2 - \kappa^2)\sinh(2\kappa a)}\right] \tag{16-35}$$

$$= Ae^{-ika} \frac{2ik\kappa \cosh(2\kappa a) + 2k^2 \sinh(2\kappa a)}{2ik\kappa \cosh(2\kappa a) + (k^2 - \kappa^2)\sinh(2\kappa a)}. \tag{16-36}$$

Then,

$$\frac{C}{A} = \frac{2\kappa}{A} \frac{F}{\kappa + ik} e^{\kappa a - ika} \tag{16-37}$$

$$= \frac{2\kappa}{A} \frac{Ae^{-2ika}}{2\kappa \cosh(2\kappa a) - 2ik \sinh(2\kappa a)} \frac{(2ik\kappa \cosh(2\kappa a) + 2k^2 \sinh(2\kappa a)}{2ik\kappa \cosh(2\kappa a) + (k^2 - \kappa^2)\sinh(2\kappa a)} \tag{16-38}$$

$$= 2\kappa e^{-2ika} ik \frac{1}{2ik\kappa \cosh(2\kappa a) + (k^2 - \kappa^2)\sinh(2\kappa a)} \tag{16-39}$$

$$= \frac{C}{A} \tag{16-40}$$

$$= e^{-2ika} \frac{2k\kappa}{2k\kappa \cosh(2\kappa a) - i(k^2 - \kappa^2)\sinh(2\kappa a)} \tag{16-41}$$

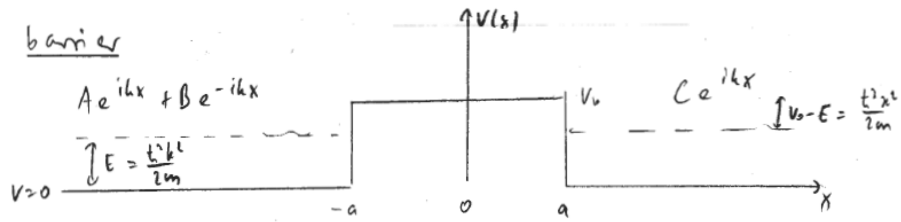


Figure II: Tunneling through the potential barrier.

Consequently, we have the **results for the barrier**

- $\frac{\hbar^2 k^2}{2m} = E$
- $\frac{\hbar^2 \kappa^2}{2m} = V_0 - E$
- $r = \frac{B}{A} = e^{-2ika} \frac{-i(k^2+\kappa^2)\sinh(2\kappa a)}{2k\kappa\cosh(2\kappa a) - i(k^2-\kappa^2)\sinh(2\kappa a)}$
- $t = \frac{C}{A} = e^{-2ika} \frac{2k\kappa}{2k\kappa\cosh(2\kappa a) - i(k^2-\kappa^2)\sinh(2\kappa a)}$

Since the energy and particle velocity are the same on both sides of the barrier, here we have $|r|^2 + |t|^2 = 1$.

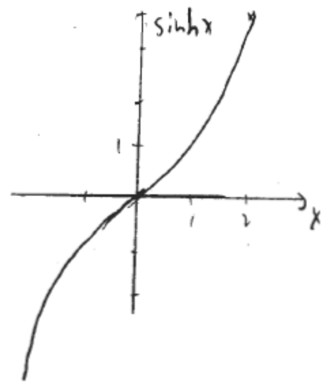


Figure III: The sinh function.

Let us look at $|t|^2$

$$|t|^2 = \frac{(2k\kappa)^2}{(2k\kappa)^2 + (k^2+\kappa^2)^2 \sinh^2(2\kappa a)} \tag{16-42}$$

where we have used $\cosh^2(x) = 1 + \sinh^2(x)$. Since, sinh is a monotonically increasing function, and $\kappa = \frac{2m}{\hbar^2}\sqrt{V_0 - E}$, the transmission is monotonically decreasing with barrier height V_0.

In the limit of small transmission, $\kappa a \gg 1$ (barrier width large compared to decay length κ^{-1}), we have $\sinh(2\kappa a) \approx \left(\frac{1}{2}e^{2\kappa a}\right)^2 = \frac{1}{4}e^{4\kappa a}$ and $|t|^2 \to \left(\frac{4k\kappa}{k^2+\kappa^2}\right)^2 e^{-4\kappa a}$. In this limit the tunneling probability falls off exponentially with barrier thickness (in units of decay length κ^{-1}).

$\to$ This exponential dependence explains the extremely wide variation in, e.g., lifetimes of unstable nuclei (μs to 10^9 years, corresponding to a variation by a factor of 10^{22}).

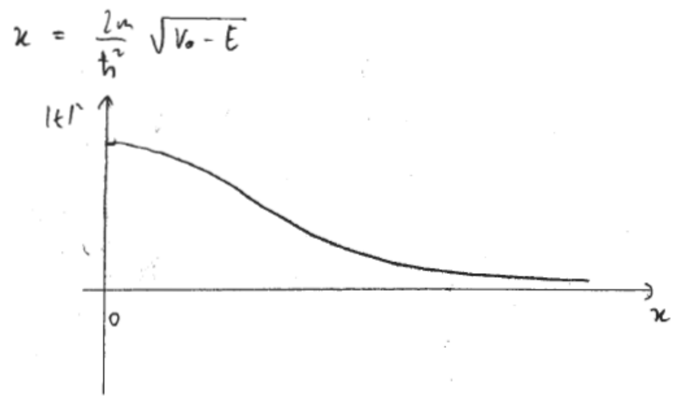


Figure IV: The transmission through the barrier as a function of decay wavevector κ.

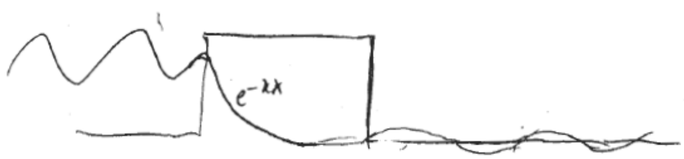


Figure V: In the limit of large barrier height or width, the transmission falls off exponentially because the wavefunction inside the barrier is dominated by the exponentially decaying term.

Potential well: resonance phenomena

We first consider scattering ($E > 0$)

$$x \leq -a : \qquad Ae^{ikx} + B^{-ikx} \tag{16-43}$$

$$-a \leq x \leq a : \qquad Ee^{+iqx} + Fe^{-iqx} \tag{16-44}$$

$$x \geq a : \qquad Ce^{ikx} \tag{16-45}$$

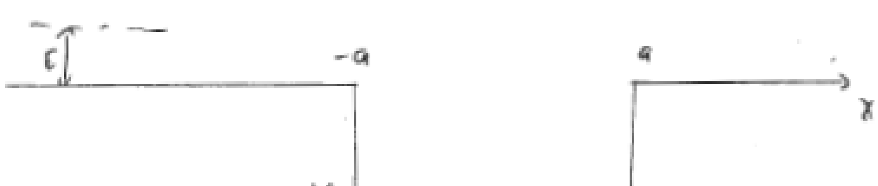


Figure VI: The potential well.

- $\frac{\hbar^2 k^2}{2m} = E$
- $\frac{\hbar^2 q^2}{2m} = V_0 + E$

Instead of going through the calculation again, we note that these equations are equivalent to those of the potential barrier (for $E < V_0$) if we replace $\kappa \to -iq$. Consequently, we obtain

$$r = ie^{-2ika}\frac{(q^2-k^2)\sin(2qa)}{2kq\cos(2qa)-i(q^2+k^2)\sin(2qa)} \tag{16-46}$$

$$t = e^{-2ika}\frac{2kq}{2kq\cos(2qa)-i(q^2+k^2)\sin(2qa)} \tag{16-47}$$

For the potential well, in contrast to tunneling through the barrier, the reflection and transmission oscillate as a function of parameter $2qa$, i.e. as a function of number of de Broglie wavelengths $\frac{2\pi}{q}$ inside the well of size a. In particular, for values

$$2q_n a = n\pi \quad \to \quad n \text{ integer} \tag{16-48}$$

$$q_n = \frac{n\pi}{2a} \tag{16-49}$$

$$\lambda_n = \frac{2\pi}{q} = \frac{4a}{n} \tag{16-50}$$

the reflection goes to zero because of destructive interference between the waves reflected at $-a$ and $+a$. This corresponds to the resonance condition for a Fabry-Perot resonator in optics. the phenomenon persists in 3D, and for electrons scattering off noble gas atoms is called a Ramsaner-Townsend resonance. A very similar phenomenon has been observed in collision of ultracold atoms, where the effective depth of the interatomic potential V_0 can be tuned with a magnetic field, there (and in nuclear collisions) it is called a Feshbach resonance).

Bound states in attractive δ-potential

What happens for negative energies $-V_0 < E < 0$ in the potential well?

We expect discrete bound states, at least if potential is sufficiently deep. Particularly simple mathematically is a limiting case where we shrink the size of the potential, simultaneously making it deeper, such that the product of depth and width is constant.

Let $V_0 \to \infty$, $\tilde{a} \to 0$ such that $\tilde{a} \cdot V_0 = \text{const} = \lambda > 0$. We then obtain the attractive delta potential $V(x) = -\lambda\delta(x)$. We are interested in bound states: $E < 0$

- Define

$$\frac{\hbar^2\kappa^2}{2m} = 0 - E = -E = |E|, \quad \kappa > 0 \tag{16-51}$$

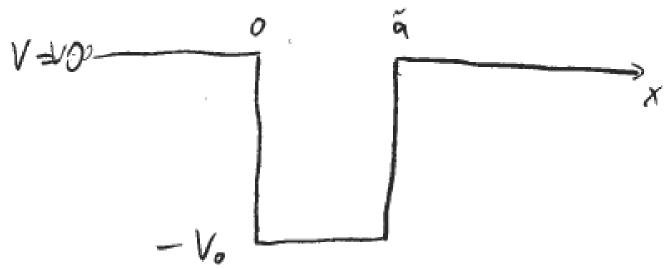


Figure VII: If the potential well is sufficiently deep or wide, it can support bound states with discrete energies $-V_0 < E < 0$.

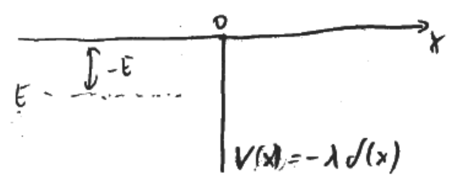


Figure VIII: Attactive delta potential.

- Solutions for $x < 0$:

$$Ae^{\kappa x} + \underbrace{\cancel{B^{-\kappa x}}}_{\text{diverges for } x \to -\infty} \tag{16-52}$$

- Solutions for $x > 0$:

$$\cancel{Ce^{\kappa x}} + D^{-\kappa x} \tag{16-53}$$

- Continuity of wavefunction at $x = 0$:

$$A = D \tag{16-54}$$

- Derivative obeys (Lecture XV)

$$u'(\epsilon) - u'(-\epsilon) = -\frac{2m}{\hbar^2}\lambda u(0) \tag{16-55}$$

$$\kappa D - \kappa A = -\frac{2m}{\hbar^2}\lambda A \tag{16-56}$$

$$-2\kappa = -\frac{2m}{\hbar^2}\lambda \tag{16-57}$$

$$\boxed{\kappa_1 = \frac{m}{\hbar^2}\lambda} \tag{16-58}$$

$$E_1 = -\frac{\hbar^2\kappa^2}{2m} = -\frac{\hbar^2 m^2}{2m\hbar^4}\lambda^2 = -\frac{m}{2\hbar^2}\lambda^2 \tag{16-59}$$

→ **Binding energy for attractive δ-function.** The δ potential supports

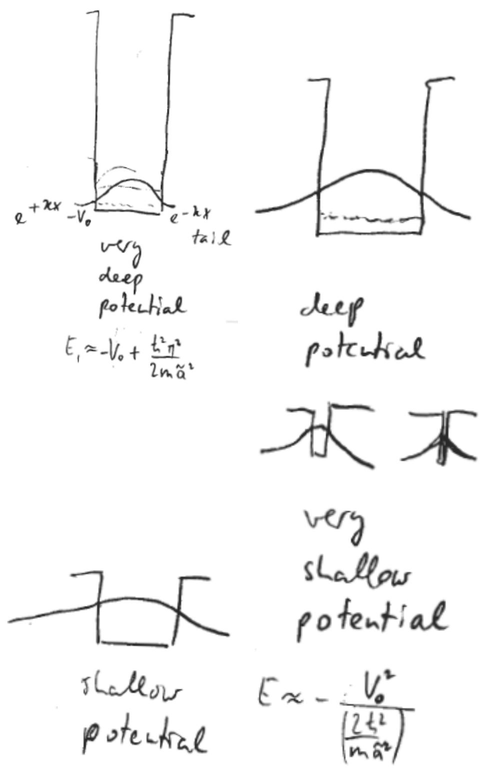


Figure IX: Comparison of bound states as the potential evolves from a very deep to a very shallow potential. In the very deep potential, like in the infinite well, the wave function oscillates sinusoidally inside the well, and decays exponentially in the forbidden region. In the very shallow potential, the wavefunction is is mostly located in the "forbidden" region outside the well.

exactly one bound state of energy $E = -\frac{m\lambda^2}{2\hbar^2}$. For a finite-size well, this result corresponds to the limiting case of a weak potential that supports only one bound state ($V_0 \ll \frac{2\hbar^2}{m\tilde{a}^2}$) with energy $E = -\frac{m\tilde{a}^2}{2\hbar^2}V_0^2$.

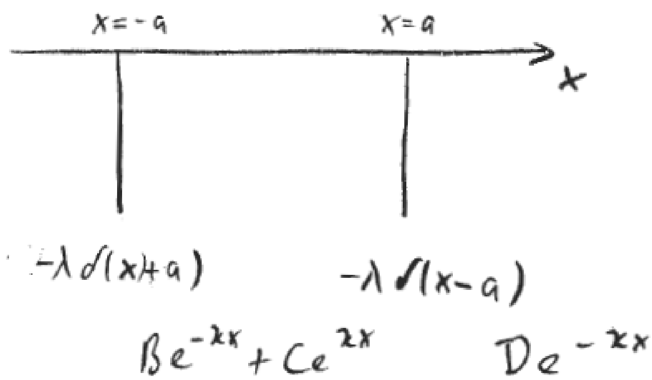


Figure X: Solutions in different regions.

Two attractive δ-potentials

We could proceed as before, or simplify slightly by making use of the fact that the potential is symmetric $x \to -x$, and therefore we expect solutions of definite parity. The even solution in the middle region is $2B\cosh(\kappa x)$, and $A = D$, which eliminates two parameters.

- Continuity of u:

$$2B\cosh(\kappa a) = Ae^{-\kappa a} \tag{16-60}$$

- Derivative:

$$-\kappa Ae^{-\kappa a} - \kappa 2B\sinh(\kappa a) = -\frac{2m}{\hbar^2}\lambda Ae^{-\kappa a} \tag{16-61}$$

$$\left(\frac{2m}{\hbar^2}\lambda - \kappa\right)Ae^{-\kappa a} = 2\kappa B\sinh(\kappa a) \tag{16-62}$$

$$\left(\frac{2m}{\hbar^2}\lambda - \kappa\right)2B\cosh(\kappa a) = 2\kappa B\sinh(\kappa a) \tag{16-63}$$

$$\frac{2ma}{\hbar^2\kappa a}\lambda - 1 = \tanh(\kappa a) \tag{16-64}$$

There is always exactly one solution of the eigenvalue equation (16-64) for even parity. From the figure we see that for the bound state $\kappa a < \frac{2ma\lambda}{\hbar^2}$, which is where the function $\frac{2ma\lambda}{\hbar^2}\frac{1}{\kappa a} - 1$ intersects zero. On the other hand, since $\tanh(x) \leq 1$, we need $\frac{2ma\lambda}{\hbar^2}\frac{1}{\kappa a} - 1 < 1$, or $\kappa > \frac{m}{\hbar^2}\lambda$. Larger κ means larger magnitude of binding energy $E = -\frac{\hbar^2\kappa^2}{2m}$. We have $\frac{m}{\hbar^2}\lambda < \kappa < \frac{2m}{\hbar^2}\lambda$ If we compare this to the binding-energy in single δ-potential, $\kappa_1 = \frac{m}{\hbar^2}\lambda$ we see that the particle is more strongly bound in the double-well potential.

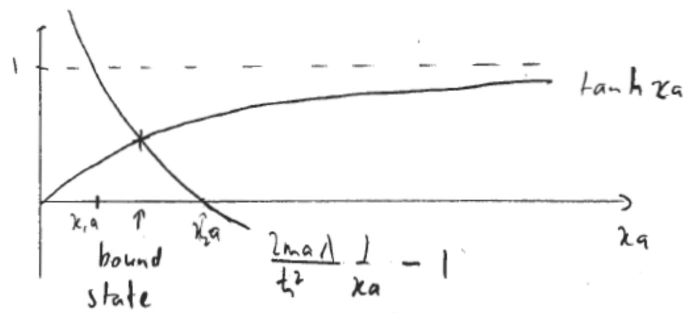


Figure XI: Graphic solution of the eigenvalue equation 16-64.

Reason. Given the discontinuity in slope due to the potential, it is possible to choose a steeper wavefunction (larger $\kappa \to$ larger binding energy) when the two δ-functions are close. Variation of binding energy with well separation a: As we decrease a, the

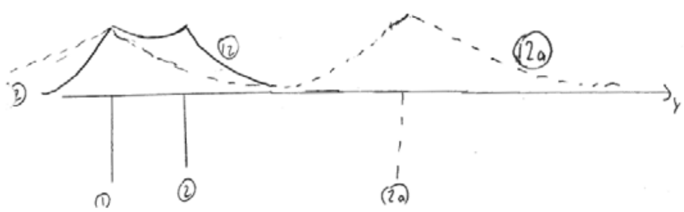


Figure XII: Comparison of the wavefunction for two different well spacings. If the wells are close, for the same wavefunction discontinuity at each δ function the wavefunction outside the two wells can decay faster (larger κ), resulting in larger binding energy $|E| = \hbar^2\kappa^2/2m$.

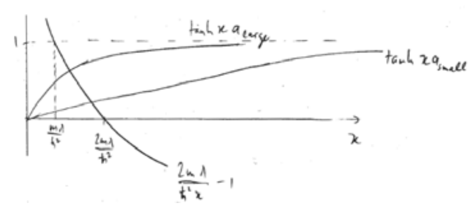


Figure XIII: Graphic comparison of the binding energies for large and small separation $2a$ between the binding sites.

binding energy increases from the value given by $\kappa = \frac{m\lambda}{\hbar^2}$ (binding energy of a single well attained at $a \to \infty$) towards the value $\kappa = \frac{2m\lambda}{\hbar^2}$, attained as $a \to 0$. Thus the binding energy quadruples. the possibility of the wavefunction in a double-well system to change so as to decrease the kinetic (and possibly potential) energy is at the origin of chemical bonds in molecules.

For the single δ-potential we have exactly one bound state (symmetric state), for the double δ-potential we always have one symmetric bound state, and we may have (depending on the potential strength) also an antisymmetric bound state. For the finite-size potential well we may have several (but always a finite number) of bound states.

Bound states in potential well

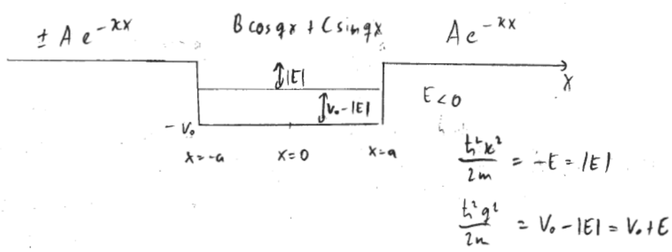


Figure I: Solutions in different regions for bound states in a potential well.

Here, instead of writing the solutions as exponentials, $\tilde{B}e^{iqx} + \tilde{C}e^{-iqx}$, we have already written them in a form that reflects the symmetry of the potential. We match $\frac{1}{u}\frac{du}{dx}$ at $x = a$:

- For even solutions: $C = 0$

$$\frac{-q\sin(qa)}{\cos(qa)} = \frac{-\kappa e^{-\kappa a}}{e^{-\kappa a}} \tag{17-1}$$

$$\kappa = q\tan(qa) \tag{17-2}$$

- For odd solutions: $D = 0$

$$\frac{q\cos(qa)}{\sin(qa)} = -\kappa \tag{17-3}$$

$$\kappa = -q\cot(qa) \tag{17-4}$$

Even solutions

Let us introduce $y = qa$, $\lambda = \frac{2m}{\hbar^2} V_0 a^2$

$$\kappa a = \sqrt{\frac{2ma^2}{\hbar^2}|E|} \tag{17-5}$$
$$= \sqrt{\frac{2ma^2}{\hbar^2}V_0 - \frac{2ma^2}{\hbar^2}(V_0 - |E|)} \tag{17-6}$$
$$= \sqrt{\lambda - q^2a^2} \tag{17-7}$$
$$= \sqrt{\lambda - y^2} \tag{17-8}$$

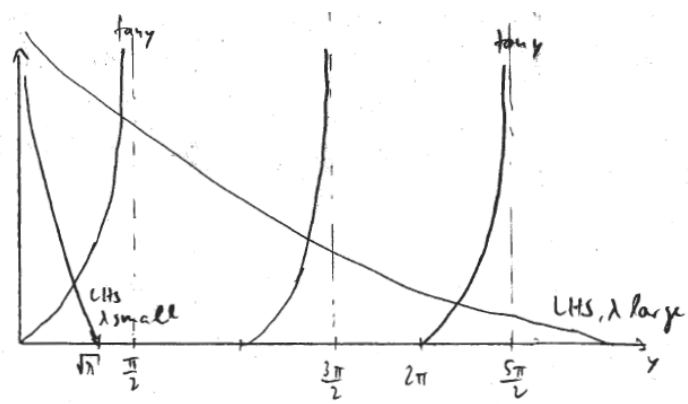


Figure II: Graphic solution of the eigenvalue equation (17-2) for symmetric bound states.

There is always at least one solution, more if $\lambda = \frac{2m}{\hbar^2} V_0 a^2$ is larger (potential deeper and/or wider). For $\lambda \gg 1$, the lowest energy solutions are approximately located at $y = qa = \left(n + \frac{1}{2}\right)\pi$, or $V_0 - |E_n| = \frac{\hbar^2 {q_n}^2}{2m} = \frac{\hbar^2\pi^2}{2ma^2}\left(n + \frac{1}{2}\right)^2$, similar to infinite well.

The existence of at least one bound state is typical of 1D problems, but not of 3D problems that behave more like odd solutions.

Odd solutions

$$\frac{\sqrt{\lambda - y}}{y} = -\cot(y) = \tan\left(\frac{\pi}{2} + y\right) \tag{17-9}$$

The looks similar to the previous plot, but with shifted RHS. For large λ, the solutions are $q_n a = n\sigma$. For small λ, a solution exists only if $\sqrt{\lambda - \left(\frac{\pi}{2}\right)^2} \geq 0$ or $\frac{2mV_0a^2}{\hbar^2} \geq \frac{\pi^2}{4}$.

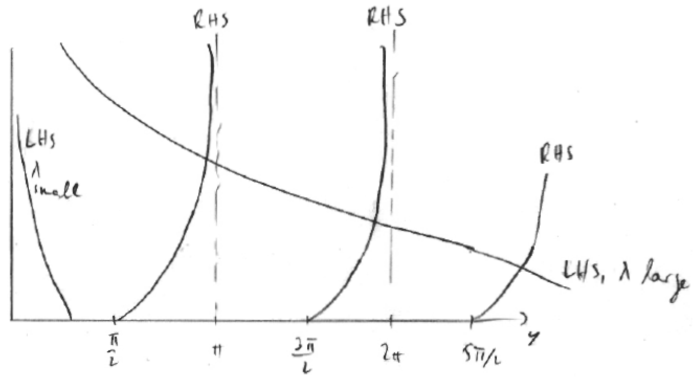


Figure III: Graphic solution of the eigenvalue equation (17-4) for antisymmetric bound states.

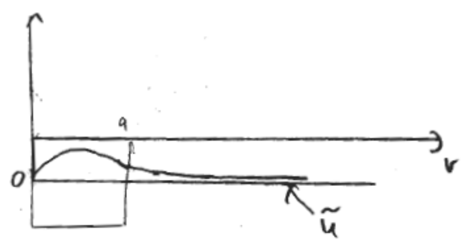


Figure IV: Graphic construction of an odd-state solution, or of a solution in 3D, where the wavefunction must vanish at the origin.

Condition for the existence of odd solutions. In 3D, we will require that a (modified) wavefunction vanishes at the origin, therefore the solutions will look like odd-parity solutions. (It is as if the wavefunction were continued at $-r$.)

Odd solutions do not always exist because the wavefunction needs to bend around sufficiently to match a decaying exponential, this requires high KE.

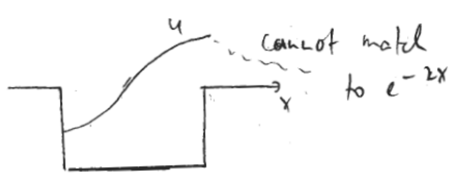


Figure V: If the well is not deep enough, the odd solution cannot bend down sufficiently to match (with continuous slope) a decaying exponential at the edge of the well.