Lecture 1

Barrier and Wells

One dimensional problem

1. General Discussion

$S(x,t)$ probabity of finding a particle passing through x at time t ; The Potential Step

T = transmitted coefficient

R = reflected coefficient

$E > V_0$ oscillating e^{ikx}, e^{-ikx}

$E < V_0$ exponential $e^{\kappa x}$, $e^{-\kappa x}$

Lecture 1

General Discussion   Barriers and Wells

Time dependent Schrodinger in one dimension

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

$\psi \longrightarrow \psi(x,t)$

ψ is complex

$\psi^* \psi \, dx$ = probability of finding the particle between x and $x + dx$ at time

$\downarrow$

$|\psi|^2$

$\equiv P(x,t)\, dx$

$\downarrow$

probability density   current $\longleftrightarrow$ probability flux

Theorem: If $V(x,t)$ is real, i.e.,

$$V^*(x,t) = V(x,t)$$

then $\frac{\partial}{\partial t} P(x,t) + \frac{\partial}{\partial x} S(x,t) = 0 \qquad (II)$

with $S(x,t) = \frac{\hbar}{2im}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right]$

$\downarrow$

probability current density (flux)

- The definition of $P(x,t)$ and $S(x,t)$ and existence is the basis of our physical interpretation

- (II) expresses conservation of probability

When $V(x,t) = V(x)$
$\downarrow$
time - independent

Seperation of variable method can be used.

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

with

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

$\downarrow$
time - independent Schrodinger equation

is a solution of the time dependent Schrodinger equation

Requirements for acceptable solutions $\psi(x)$

(i) $\psi(x)$ is square integrable *

(ii)(a) $\psi(x)$ must be finite

(b) $\psi(x)$ must be continuous

(c) $\frac{d\psi}{dx}$ must be finite

(d) $\frac{d\psi}{dx}$ must be continuous **

* For unbounded motion, we shall leave the normalization constant open

** If $V(x) = V_0\,\delta(x-a)$, then (d) is modified into

$$\left.\frac{d\psi}{dx}\right|_{a+\epsilon} - \left.\frac{d\psi}{dx}\right|_{a-\epsilon} = \frac{2m}{\hbar^2} V_0\,\psi(a)$$

$E < V_0$

Region I

as before

Region II

$$\psi_{II}(x) = \underbrace{C}_{0} e^{k_2 x} + D e^{-k_2 x}$$

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

Pentrating depth

uncertainty relation

Transmission coefficient.

Reflection coefficient

Example

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.

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

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

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

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

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

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

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

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

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

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

$\Rightarrow$ $S(x,t) \longrightarrow$ 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
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_E(x) + V(x)\psi_E(x) = E\psi_E(x)$$
$\llcorner$ time independent Schrodinger equation.

$$\psi_E(x) \equiv \psi(x)$$

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) $\longleftrightarrow$ 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 $\epsilon \to 0$
if V is finite

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

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

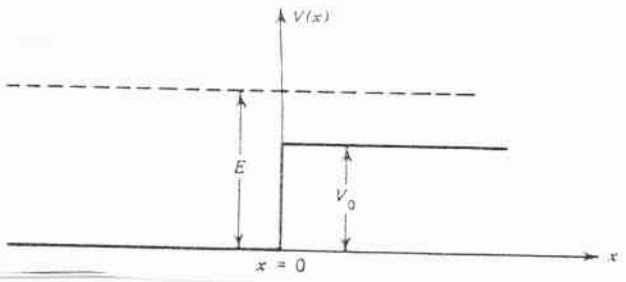
$$\Rightarrow \left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon} \frac{2m}{\hbar^2}\left[V_0\,\delta(x-a) - E\right]\psi(x)\,dx$$

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

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

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

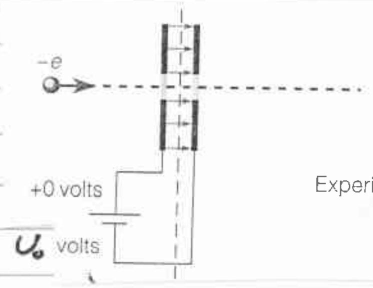
$$\Rightarrow \frac{d^2}{dx^2}\psi_1 = -\frac{2mE}{\hbar^2}\psi_1 = -k_1^2\psi_1$$

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

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

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

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



Experimental setup

$V_0 = eU_0$

Experimental setup

The Schrodinger equation

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

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

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

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

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

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

Continuity equation at $x=0$

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

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

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

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

$$\Rightarrow \psi(x) = \begin{cases} A e^{ik_1 x} + A \dfrac{k_1-k_2}{k_1+k_2} e^{-ik_1 x} & x<0 \\ A \dfrac{2k_1}{k_1+k_2} e^{ik_2 x} & x \geq 0 \end{cases}$$

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

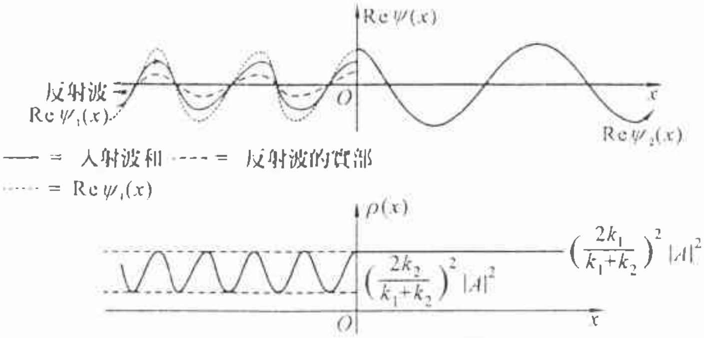
$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

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

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

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

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



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

$\psi(x)$= 能量本徵函數， $\rho(x)$=概率密度

Reflection Coefficient and Transmission Coefficient

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

$\downarrow$
reflection coefficient

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

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

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

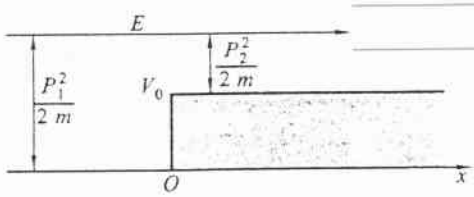
$$= \frac{\left(\frac{2k_1}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{-ik_2x}\frac{d}{dx}e^{ik_2x} - e^{ik_2x}\frac{d}{dx}e^{-ik_2x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

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

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

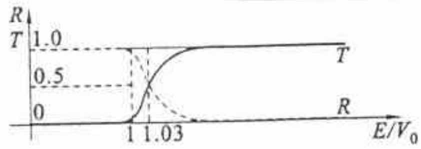
- $\rho(x,t)$ is independent of time
  Probability conservation

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

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

Furthermore, $R + T = 0$

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



$E < V_0$

In region (I)

$$\psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

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

In region (II)

Schrodinger equation

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

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

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

$$\Rightarrow \psi_2(x) = Ce^{k_2 x} + De^{-k_2 x}$$

cannot increase exponentially as $x \to \infty$

$\Rightarrow C = 0$

$$\Rightarrow \psi_2(x) = De^{-k_2 x}$$

Continuity equation at $x = 0$

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

$$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \quad \Rightarrow \quad ik_1(A-B) = -k_2 D$$

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

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

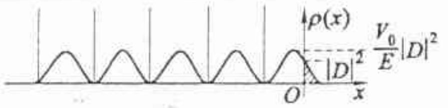
$$\Rightarrow \psi(x,t) = \psi(x)e^{-i\omega t}$$

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

$$\rho(x,t) = \begin{cases} |D|^2\left(\cos k_1 x - \frac{k_2}{k}\sin k_1 x\right)^2 & x<0 \\ |D|^2 e^{-2k_2 x} & x>0 \end{cases}$$

$\rho(x,t)$ 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

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

$$\text{Transmitted probability flux} = \frac{\hbar}{2im}|D|^2\left(e^{-k_2 x}\frac{d}{dx}e^{-k_2 x} - e^{-k_2 x}\frac{d}{dx}e^{-k_2 x}\right)$$
$$= 0$$

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

Furthermore $S = 0$ for all x

22. The conduction electrons in metals are held inside the metal by an average potential called the inner potential of the metal. Calculate, for the one-dimensional model given by $V(x) = -V_0$ if $x < 0$ and $V(x) = 0$ if $x > 0$ (Fig. II.10), the probability of reflection and of transmission of a conduction electron approaching the surface of the metal with total energy E, (i) if $E > 0$, and (ii) if $-V_0 < E < 0$.

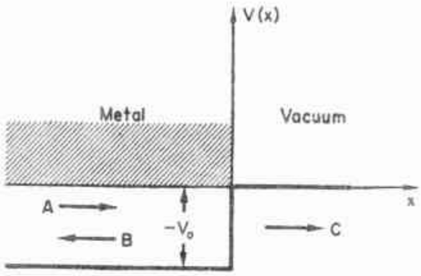


FIG. II.10.

23. **A beam of mono-energetic electrons strikes the surface of a metal at normal incidence. Calculate the reflection probability of these electrons if $E = 0{\cdot}1$ eV and $V_0 = 8$ eV.**

22. By making the substitution

$$\psi(x, t) = \psi(x)\, e^{-\frac{i}{\hbar}Et} \tag{22.1}$$

in the Schrödinger equation

$$i\hbar\frac{\partial\psi(x, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x, t),$$

we obtain, for $x < 0$,

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E+V_0)\,\psi_1 = 0,$$

and, for $x > 0$,

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}E\psi_2 = 0.$$

The general solutions of these equations are

$$\psi_1 = Ae^{\frac{i}{\hbar}qx} + Be^{-\frac{i}{\hbar}qx}, \quad q = [2m(E+V_0)]^{1/2}, \qquad x < 0,$$

$$\psi_2 = Ce^{\frac{i}{\hbar}px} + De^{-\frac{i}{\hbar}px}, \quad p = \sqrt{2mE}, \qquad x > 0.$$

According to classical mechanics, if $E > 0$, the electron has sufficient energy to overcome the potential barrier at the surface of separation and hence it will leave the metal. In the quantum-mechanical treatment the answer is not so simple.

The electron wavefunction is

$$\psi(x, t) = \begin{cases} Ae^{\frac{i}{\hbar}(qx-Et)} + Be^{-\frac{i}{\hbar}(qx+Et)}, & \text{if} \quad x < 0 \\ Ce^{\frac{i}{\hbar}(px-Et)} + De^{-\frac{i}{\hbar}(px+Et)}, & \text{if} \quad x > 0. \end{cases}$$

The term with the coefficient A represents a plane wave which arrives at the surface from the left (incident particle), the term with B represents the reflected wave, the term with C represents the transmitted wave and that with D represents a wave arriving at the surface from the right. Since such a wave does not exist under the conditions of this problem we put $D = 0$. The continuity conditions at $x = 0$ then yield the equations

$$A+B = C, \quad q(A-B) = pC, \tag{22.2}$$

whence

$$B = \frac{q-p}{q+p}A, \quad C = \frac{2q}{q+p}A.$$

It can be seen that the certainty of transmission (which would correspond to a total lack of reflection, i.e. to $B = 0$) prescribed by classical mechanics, occurs only in the trivial case $q = p$, i.e. $V_0 = 0$. Since

$$|\mathbf{j}_A| = |A|^2\frac{q}{m}, \quad |\mathbf{j}_B| = |B|^2\frac{q}{m}, \quad |\mathbf{j}_C| = |C|^2\frac{p}{m},$$

we obtain in fact

$$T = \frac{|\mathbf{j}_C|}{|\mathbf{j}_A|} = \left|\frac{C}{A}\right|^2\frac{p}{q} = \frac{4qp}{(q+p)^2} = \frac{4\sqrt{E(E+V_0)}}{(\sqrt{E+V_0}+\sqrt{E})^2}, \tag{22.3}$$

$$R = \frac{|\mathbf{j}_B|}{|\mathbf{j}_A|} = \left|\frac{B}{A}\right|^2 = \left(\frac{q-p}{q+p}\right)^2 = \frac{V_0^2}{(\sqrt{E+V_0}+\sqrt{E})^4}, \tag{22.4}$$

$$T+R = 1.$$

Note that, according to quantum mechanics, reflection occurs with a probability different from zero even if $E > 0$. However, if $E \gg V_0$ the reflection probability decreases rapidly with increasing energy:

$$R \approx \frac{V_0^2}{16E^2}. \tag{22.5}$$

On the other hand, if $0 < E \ll V_0$, we have the approximate formula

$$R \approx 1 - 4\sqrt{\frac{E}{V_0}}. \tag{22.6}$$

For the commonest metals, $V_0 \sim 10$ eV, and the reflection probability for an electron with $E = 0{\cdot}1$ eV is approximatively 60%.

If $-V_0 < E < 0$ the total energy of the electron is not sufficient for it to leave the metal, according to classical mechanics, so that we should have $T = 0$ and $R = 1$.

In fact, in this case, $q = [2m(V_0-|E|)]^{1/2}$, $p = i(2m|E|)^{1/2}$, and the solution bounded in the region $x > 0$ is

$$\psi_2 = Ce^{-(x/2d)} \quad \text{where} \quad d = \hbar(8m|E|)^{-1/2}.$$

The continuity conditions at $x = 0$ give

$$A+B = C, \quad \frac{i}{\hbar}q(A-B) = -\frac{1}{2d}C,$$

whence

$$\frac{B}{A} = -\frac{1+\frac{2i}{\hbar}qd}{1-\frac{2i}{\hbar}qd}, \quad \frac{C}{A} = -2\frac{\frac{2i}{\hbar}qd}{1-\frac{2i}{\hbar}qd}.$$

It follows from the expression for ψ_2 that $\mathbf{j}_C = 0$, and hence $T = 0$ and $R = |B/A|^2 = 1$. Thus, as in classical theory, an electron having a total energy smaller than the potential barrier height will be reflected with certainty. A new result, however, is that the probability of finding the electron outside the metal ($x > 0$) is different from zero, since

$$|\psi_2(x)|^2 = 4|A|^2\left(1+\frac{\hbar^2}{4q^2d^2}\right)^{-1} e^{-x/d} = 4|A|^2\frac{V_0-|E|}{V_0}e^{-x/d}.$$

This phenomenon is similar to that of the "total internal reflection" which occurs when the passage of light from a denser medium to a less dense one is impossible because the angle of incidence exceeds a certain critical angle. The theory of wave optics shows that, in the less dense medium, there is then a wave whose amplitude decreases exponentially, in analogy with the exponentially decreasing electron wave considered above.

23. Since the electrons, with momentum $p = \sqrt{2mE}$, encounter a potential drop $-V_0$ at the metal surface, they will all enter the metal, according to classical mechanics, and, because of the law of conservation of energy, they will acquire a final momentum $q = [2m(E+V_0)]^{1/2}$ after doing so.

According to quantum mechanics, on the other hand, some of the electrons may be reflected by the metal surface. Using the notation of the preceding problem, $D\exp(-i/\hbar px)$ now represents the incident wave, $C\exp(i/\hbar px)$ the reflected wave, and $B\exp(-i/\hbar qx)$ the transmitted wave inside the metal. In this case, $A = 0$. The continuity conditions at the point $x = 0$ give $C+D = B$, $p(C-D) = -qB$, whence

$$R = \frac{|\mathbf{j}_C|}{|\mathbf{j}_D|} = \left|\frac{C}{D}\right|^2 = \left(\frac{p-q}{p+q}\right)^2$$

and

$$T = \frac{|\mathbf{j}_B|}{|\mathbf{j}_D|} = \left|\frac{B}{D}\right|^2\frac{q}{p} = \frac{4pq}{(p+q)^2}.$$

Thus, if $E = 0{\cdot}1$ eV and $V_0 = 8$ eV, the reflection probability is

$$R = \left(\frac{\sqrt{E}-\sqrt{E+V_0}}{\sqrt{E}+\sqrt{E+V_0}}\right)^2 = \left|\frac{1-\sqrt{1+\frac{V_0}{E}}}{1+\sqrt{1+\frac{V_0}{E}}}\right|^2 = \left(\frac{8}{10}\right)^2 = 0{\cdot}64,$$

which is greater than the probability (0·36) of entering the metal. The higher the energy of the incident electrons, however, the less probable is their reflection. For example, the probability of reflection of an electron bombarding an anticathode in the usual Röntgen X-ray tube ($V_0 \approx 10$ eV, $E = 10^5$ eV) is approximately $6{\cdot}2\times10^{-10}$.

For greater familiarity with the phenomena of electron reflection at, and penetration into, metals, we suggest that the reader make a plot of the quantities R and T as functions of E.

The Potential Barrier

Divide the region into three part.

Solution in different regions

Matching the boundary condition ⇒ the wave function

$\rho(x)$, $S(x)$

T = transmisson
R = reflection   coefficient

discussion on the physical meaning

T , R

resonance

exponential decrease.

Examples , Application
Extension , and Approximation

Field Emission

Scanning Tunneling Microscope

Radioactivity

The Potential Step

Specify the potential

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

$E > V_0$

Region I_1

$$\psi_I(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

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

Region II

$$\psi_{II}(x) = C e^{ik_2 x} + D e^{-ik_2 x}$$

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

Physical interpretation

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

$$= \underbrace{A e^{ik_1 x - i\omega t}}_{\text{incident wave}} + \underbrace{B e^{-ik_1 x - i\omega t}}_{\text{reflected wave}}$$

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

$$= C e^{ik_2 x - i\omega t} + \underbrace{D}_{0} e^{-ik_2 x - i\omega t}$$

nothing to reflected the wave.

$$\psi(x) = A e^{ik_1 x} + B e^{-ik_1 x} \qquad x<0$$

$$\psi(x) = C e^{ik_2 x} \qquad x>0$$

Continuity equation at $x=0$

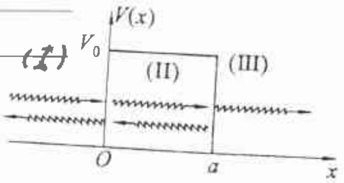
$$\Rightarrow \quad A + B = C \qquad \Rightarrow \qquad B = \frac{k_1 - k_2}{k_1 + k_2} A$$

$$k_1(A-B) = k_2 C \qquad\qquad C = \frac{2k_1}{k_1+k_2} A$$

R = reflection coefficient

T = transmission coefficient

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
↓
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
↓
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 $x=a$.

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

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

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

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

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)

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

$$\psi_2(x,t) = \psi_2(x)e^{-i\omega t}$$

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

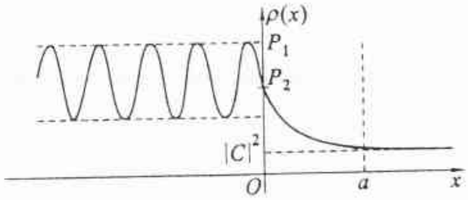
$$\psi_3(x,t) = \psi_3(x)e^{-i\omega t} = Ce^{i(k_1 x-\omega t)}$$

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

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

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

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

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

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

$$= \left[1 + \frac{\sinh^2 k_2 a}{4\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} = \left[1 + \frac{(e^{k_2 a} - e^{-k_2 a})^2}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1}$$

$$= \left[1 + \frac{e^{2k_2 a}(1 - 2e^{-2k_2 a} + e^{-4k_2 a})}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1}$$

T is a function of E, V_0 and a.

This is the fundamental equation for discussing the tunneling problem.

If $k_2 a \gg 1$, then

$$T \sim \left[\frac{e^{2k_2 a}}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2k_2 a}$$

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

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

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

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

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 林清凉 "近代物理" I 第十章]

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

⇒ we want to obtain an approximate expression 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 juxtaposition of square potential barrier (See the following figure

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

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

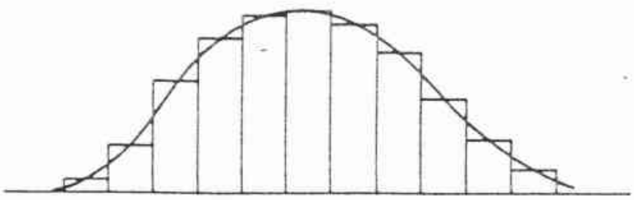
$$\simeq -2\int dx\sqrt{\frac{2m}{\hbar^2}[V(x)-E]}$$

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

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

⇒ (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.

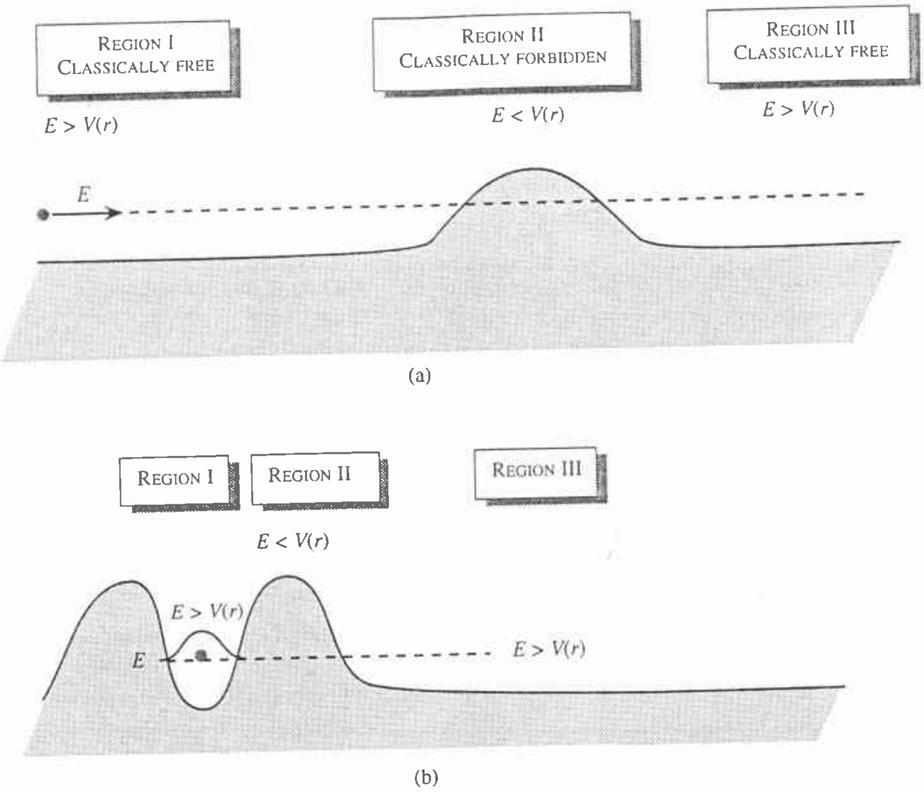
TUNNELING OF PARTICLES

- The general problem of quantum mechanical tunneling
- Tunneling as a stationary state problem: Tunneling through a barrier
- Important technological applications of tunneling
- Tunneling through multiple barriers: Resonant tunneling

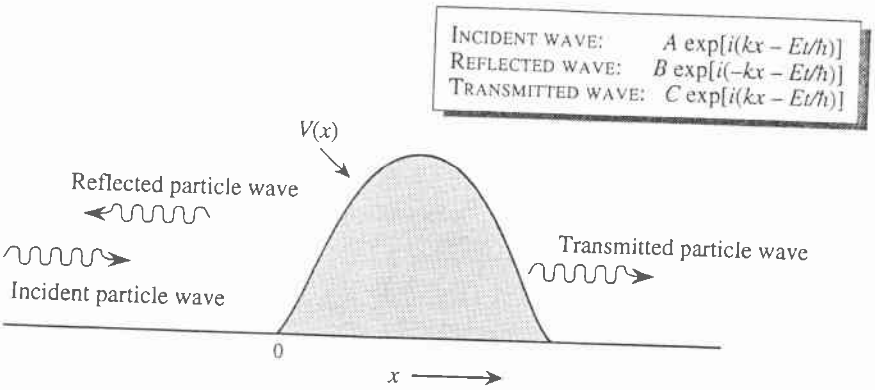
TOPICS STUDIED	KEY OBSERVATIONS
Tunneling of particles	In quantum mechanics, when particles are treated as waves, they can traverse through regions where their energy is less than the potential energy. Their trajectories are completely different from what one expects from classical physics.
Tunneling as a stationary state problem	The time-independent problem can be used to calculate the tunneling behavior of particles. Physically, the time-independent problem corresponds to a constant flux of particles in space. A number of analytical and numerical approaches have been developed to solve such problems.
Applications of tunneling	Tunneling of particles has many important applications in technology. These include: • Scanning tunneling microscopes for studying precise positions of atoms on a surface. • Producing low-resistance ohmic contacts for semiconductor devices. • Tunnel diodes for microwave applications. • Field emission devices. • Radioacitve materials for medical and anthropological uses.
Tunneling through multiple barriers	When particles tunnel through multiple barriers, the tunneling probability has strong resonances as a function of particle energy. This concept is exploited in a number of devices.

Applications.

General Tunneling Problem.



A schematic view of two categories of tunneling problems. (a) A particle starts from the unbound state on the left in region I where it is free to move classically (i.e., $E \geq V(r)$) and tunnels through a classically "forbidden" region (II) into a classically allowed region (III). In (b) the particle is initially in "bound region" and tunnels through a "forbidden" region (II) into a classically allowed region (III).



A generic description of the tunneling problem. Particles are incident from the left with an energy E. A certain fraction of the particle current is reflected and the rest is transmitted.

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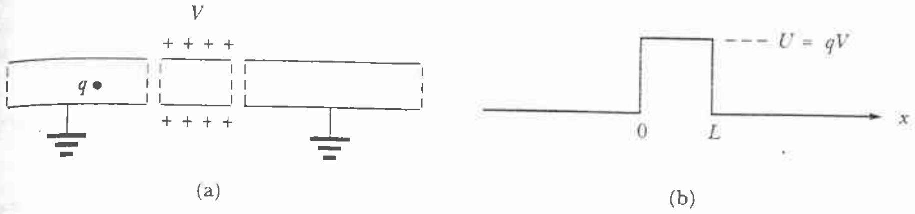
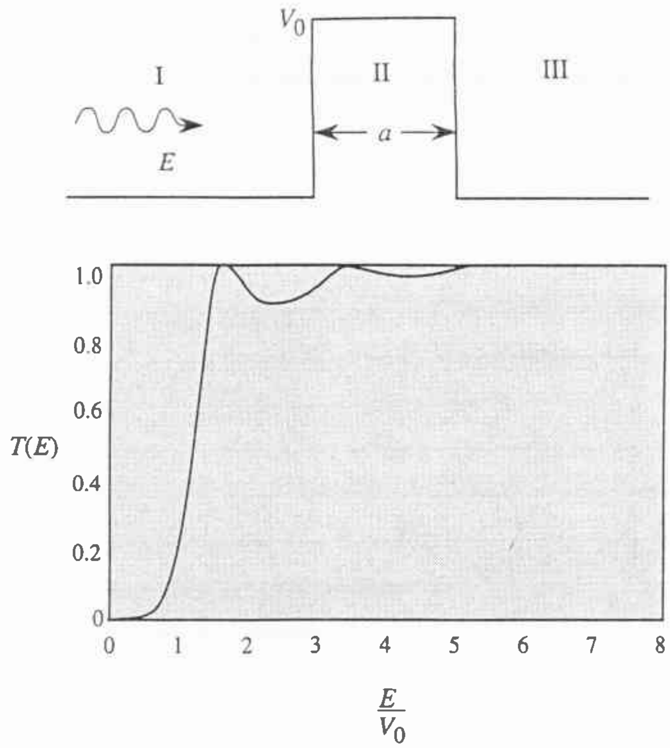
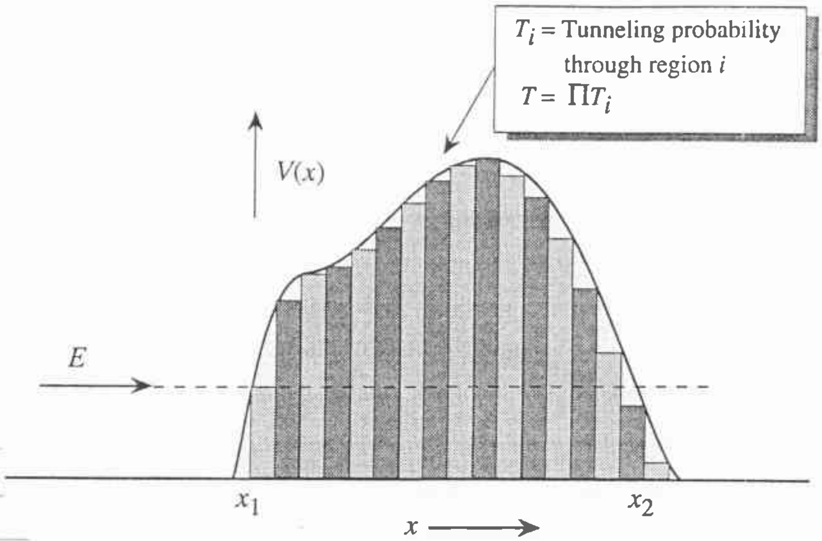


(a) Aligned metallic cylinders serve as a potential barrier to charged particles. The central cylinder is held at some positive electric potential V, and the outer cylinders are grounded. A charge q whose total energy is less than qV is unable to penetrate the central cylinder classically, but can do so quantum mechanically by a process called *tunneling*. (b) The potential energy seen by this charge in the limit where the gaps between the cylinders have shrunk to zero size. The result is the square barrier potential of height U.

Simplest way to realize a potential barrier



(a) Tunneling of a particle through a potential barrier. (b) The transmission coefficients for an electron as a function of energy for $V_0 = 1.0$ eV, $a = 7.77$ Å. The results are typical of transmittance through a barrier. Notice that even for $E > V_0$, the probability goes through values less than unity; i.e., some reflection occurs.



: An approximation scheme used to calculate particle tunneling with energy E through a smoothly varying potential.

FIELD	APPLICATIONS
Solid-state electronics	• Ohmic contact technology • Tunnel diodes and mircrowave devices • Tunneling-based microaccelerometers and other sensors • Resonant tunneling switches
Medicine	• Radioactivity in diagnostics • Radiation therapy
Biological sciences	Radioactive dyes injected in insects to track their activities
Material science	✓Surface characterization by scanning tunneling microscope
Anthropology	Carbon-dating to determine age of objects
Manufacturing sciences	Radioactive tracers to keep track of wear-and-tear of machine parts

Important applications of particle tunneling in various fields.

✓

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Basic Formula

We have developed an analytical expression for the tunneling probability for simple square barriers

In the "wide" barrier approximation ($d \ll a$)

$$T \sim \frac{16\, E(V_0 - E)}{V_0^2}\, e^{-2\gamma a} \qquad \gamma = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \equiv \frac{1}{2d}$$

[The tunneling expression is dominated by the exponential term]

As a further approximation, we take the prefactor to be unity

$$T \sim e^{-2\gamma a}$$

Now we will develope a simple approximation which is quite accurate and yet can be applied analytically to many problem of interest.

Divide the potential into hatched region

$$T \sim \prod_i T_i = e^{-\frac{1}{\hbar}\sum_i [8mV(x_i)-E]^{\frac{1}{2}} \Delta x_i}$$

[This is valid only if the potential is smoothly varying compared to the de Broglie wavelength)

Now increasing the number of subdivisions while ensuring $d_i \ll \Delta x_i$

[Note, when $E > V(x_i)$, $T_i \sim 1$]

$$\Rightarrow \quad T = e^{-\frac{1}{\hbar}\int_{x_1}^{x_2} [8mV(x)-E]^{\frac{1}{2}} dx}$$

where x_1 and x_2 are points where $E = V(x)$

turning points

This is the starting point for the application of tunneling.

Example. Trianglar Barrier and Trapzoidal Barrier

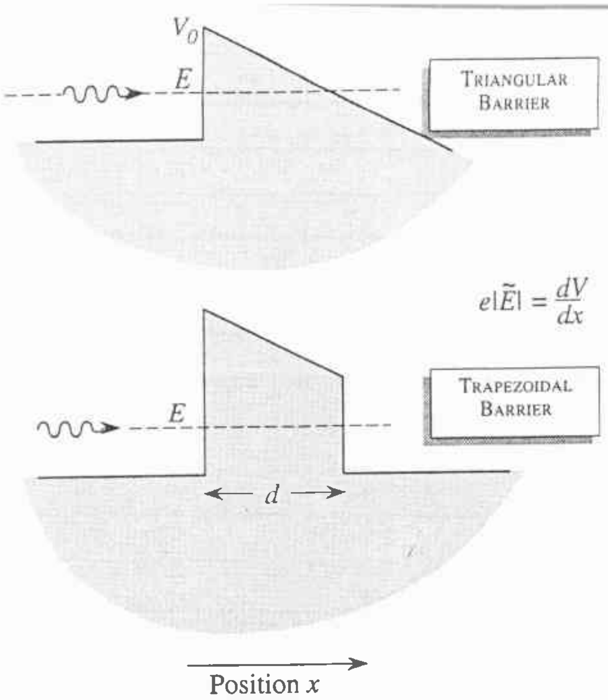

Figure 6.6: (a) Triangular and (b) trapezoidal barriers through which an electron with energy E can tunnel. Such barriers are encountered in many electronic device structures. The potential shape is described by an electric field $\tilde{E}$.

Triangle $\quad T = e^{\frac{-4(2m)^{\frac{1}{2}}}{3e|E|\hbar}(V_0 - E)^{3/2}}$

Fowler - Nordheim formula

Trapezoidal, $\quad T = e^{\frac{-4(2m)^{\frac{1}{2}}}{3\hbar e|E|}\left[(V_0 - E)^{3/2} - (V_0 - E - e|\tilde{E}|d)^{3/2}\right]}$

Task, find the good model for $V(x)$

in application.

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6.2 GENERAL TUNNELING PROBLEM

The general problem of particle tunneling can be loosely classified into two categories, both of which involve the propagation of a particle with energy E through a region of potential energy $V(r)$, where in some regions, the particle energy is smaller than the potential energy. This region is classically forbidden to the particle, but, as discussed in the Introduction, when the particle is described through a wave description, tunneling can occur. In the first category of problems we have a situation, as shown in Fig. 6.2a, where there is a region of space where the particle can be represented by a "free" state. The particle can be represented by a momentum in this free space region where the electron energy E is greater than the background potential energy, which may be considered to be uniform. In this example, the tunneling problem involves the particle coming from the left and striking the potential barrier, with the particle having a finite probability of tunneling through and a finite probability of being reflected back.

In the second category of tunneling problems, the particle is initially confined to a "quantum well" region in a "quasi-bound" state, as shown in Fig. 6.2b. In the quasi-bound state, the particle is primarily confined to the quantum well, but has a finite probability of tunneling out of the well and escaping. The key difference between the two cases is that in the first problem the wavefunction corresponding to the initial state is essentially unbound, whereas in the second case it is primarily confined to the quantum well region.

Tunneling Through Wide Barriers

In many applications, the transmission probability for tunneling is very small. Inside a barrier, the wave function is essentially proportional to $e^{-\alpha x}$, or $e^{-x/\delta}$, where $\delta \equiv 1/\alpha$ is the penetration depth.[2] If $L \gg \delta$, very little of the wave will "survive" to $x = L$. The condition for a "wide" barrier is thus

$$\frac{1}{\delta}L = \alpha L = \frac{\sqrt{2m(U_0 - E)}}{\hbar}L \gg 1 \qquad \textbf{(5-11)}$$

It is wide if L is large, or E is much less than U_0, or both.

It is left as an exercise to show that if (5-11) holds, the transmission probability of (5-10) is given by the approximation

$$T \cong 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)e^{-2[\sqrt{2m(U_0-E)}/\hbar]L} \qquad \textbf{(5-12)}$$

Example 5.2

An electron encounters a barrier of height 0.100 eV and width 15 nm. What is the transmission probability if its energy is (a) 0.040 eV? (b) 0.060 eV?

[2] The solution within the barrier is not strictly a decaying exponential, but contains an exponentially *increasing* part $e^{+\alpha x}$. In most cases, this part is inconsequentially small.

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Solution

First we see if condition (5-11) holds.

For 0.040 eV:

$$\frac{L}{\delta} = \frac{\sqrt{2(9.11 \times 10^{-31}\ \text{kg})(0.100 - 0.040) \times 1.6 \times 10^{-19}\ \text{J}}}{1.055 \times 10^{-34}\ \text{J·s}} 15 \times 10^{-9}\ \text{m}$$

$$= 18.8$$

For 0.060 eV:

$$\frac{L}{\delta} = \frac{\sqrt{2(9.11 \times 10^{-31}\ \text{kg})(0.100 - 0.060) \times 1.6 \times 10^{-19}\ \text{J}}}{1.055 \times 10^{-34}\ \text{J·s}} 15 \times 10^{-9}\ \text{m}$$

$$= 15.4$$

In both cases, the barrier is wide, many times the penetration depth. Now, noting that we have just calculated the arguments of the exponential in (5-12),

$$T_{0.040\ \text{eV}} = 16\frac{0.04}{0.1}\left(1 - \frac{0.04}{0.1}\right)e^{-2\times 18.8} = 1.8 \times 10^{-16}$$

$$T_{0.060\ \text{eV}} = 16\frac{0.06}{0.1}\left(1 - \frac{0.06}{0.1}\right)e^{-2\times 15.4} = 1.8 \times 10^{-13}$$

As expected, for both barriers the transmission probability *for a single event* is very small. But in many real situations, barriers are constantly bombarded by particles. If electrons at either of these energies were to strike the barrier 10^{20} times each second, there would be a significant flux of escaping particles. Such high frequency is not at all unrealistic; alpha-particles *almost* trapped in an atomic nucleus typically get 10^{20} chances to tunnel out every second. Alpha decay is discussed in the next section.

The example illustrates another important point: When transmission probabilities are very small, they vary sharply with energy. Both probabilities are small, but a modest 50% increase in particle energy results in a transmission probability about a thousand times larger. This sensitivity is due to the exponential dependence in (5-12), and the smaller the probability, the more pronounced is the variation.[3]

Electrons with energies of 1.0 eV and 2.0 eV are incident on a barrier 10.0 eV high and 0.50 nm wide. (*a*) Find their respective transmission probabilities. (*b*) How are these affected if the barrier is doubled in width?

Solution

(*a*) For the 1.0-eV electrons

$$k_2 = \frac{\sqrt{2m(U - E)}}{\hbar} = \frac{\sqrt{(2)(9.1 \times 10^{-31}\ \text{kg})[(10.0 - 1.0)\ \text{eV}](1.6 \times 10^{-19}\ \text{J/eV})}}{1.054 \times 10^{-34}\ \text{J} \cdot \text{s}} = 1.6 \times 10^{10}\ \text{m}^{-1}$$

Since $L = 0.50$ nm $= 5.0 \times 10^{-10}$ m, $2k_2L = (2)(1.6 \times 10^{10}\ \text{m}^{-1})(5.0 \times 10^{-10}\ \text{m}) = 16$, and the approximate transmission probability is

$$T_1 = e^{-2k_2L} = e^{-16} = 1.1 \times 10^{-7}$$

One 1.0-eV electron out of 8.9 million can tunnel through the 10-eV barrier on the average. For the 2.0-eV electrons a similar calculation gives $T_2 = 2.4 \times 10^{-7}$. These electrons are over twice as likely to tunnel through the barrier.

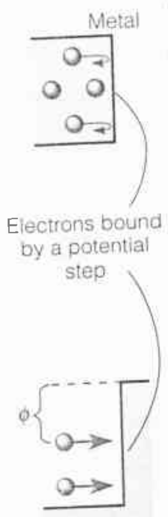
(*b*) If the barrier is doubled in width to 1.0 nm, the transmission probabilities become

$$T_1' \doteq 1.3 \times 10^{-14} \qquad T_2' = 5.1 \times 10^{-14}$$

Evidently T is more sensitive to the width of the barrier than to the particle energy here.

Field Emission.

To remove an electron from a given kind of metal requires a certain minimum amount of energy
⇒ the work function Φ
↓
in effect, the metal's electrons reside in a potential well, the result of their attraction to the positive ions

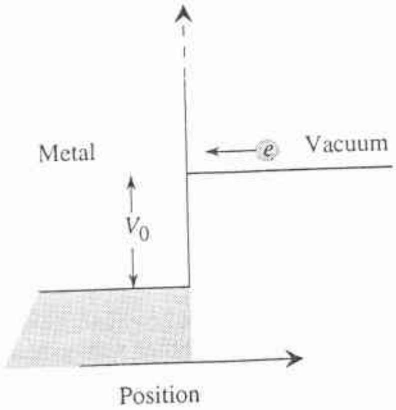


Due to the random thermal distribution of speeds, at a given temperature a small fraction of the electrons have sufficient kinetic energy to escape the metal.

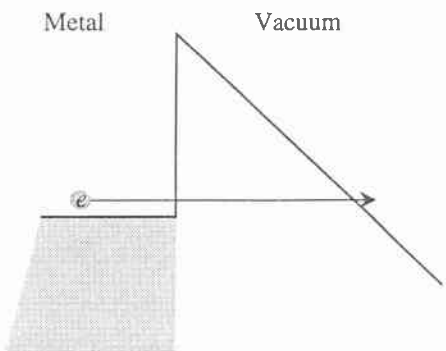
Heating a metal filament to enhance this effect
⇒ thermionic emission
↓
used a source of electron beams
↓
such as those in the conventional (elongated) cathode ray tubes used in TV and computer monitors.

Postive electrode modifies the potential energy function "seen" by the electrons
⇒ tunneling ⇒ field emission (cold)

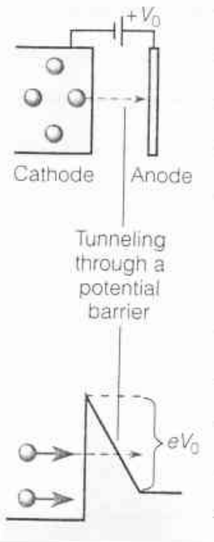
Field Emission Devices

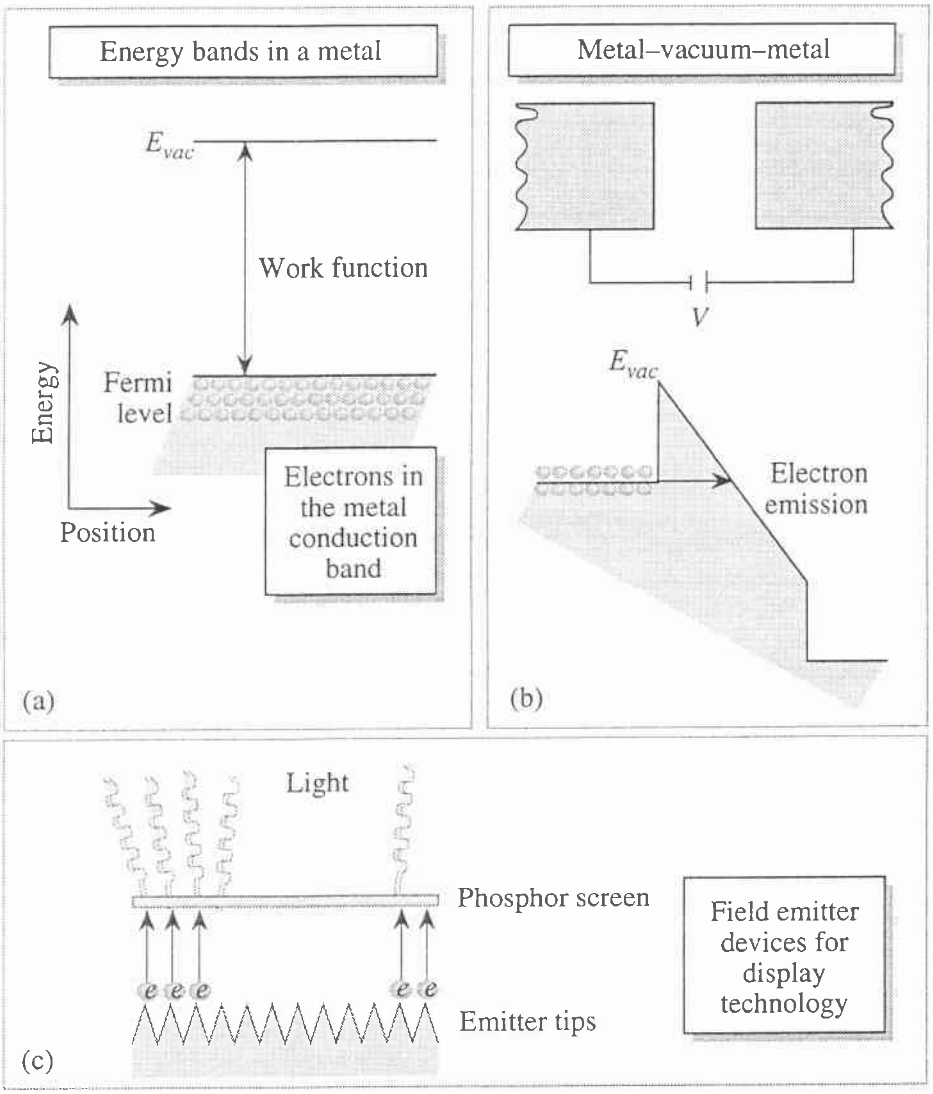


Potential profile of a metal–vacuum interface region.



Potential profile of a metal–vacuum interface with a field across the junction.





(a) Schematic of the electronic energies in a solid-state material. (b) Metal–vacuum–metal junction under applied field. (c) Schematic of a display device based on field emission tips.

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Flat panel display

The metal (or semiconductor) emitters are formed into sharp tips to enhance the field produced by the applied potential

The voltage across tips is controlled by a driver circuitry.

The phosphor screen is seperated from the tips by a very small gap (submicron) ⇒ entire system is "paper-thin."

Each pixel (picture element) is "illuminated" by its own set of tips ⇒ thin, low-power-consuming display system.

(a) (b)

Figure 5.12 Electrons in a metal (a) behave as though in a finite well. An electric field (b) alters the "wall," so that tunneling may occur.

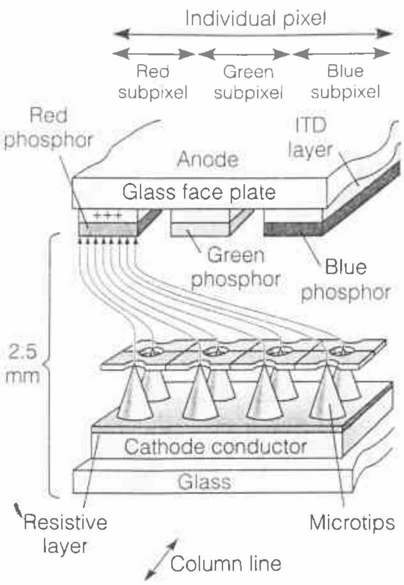
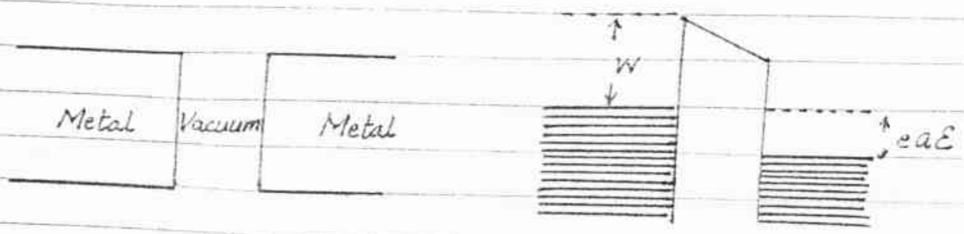


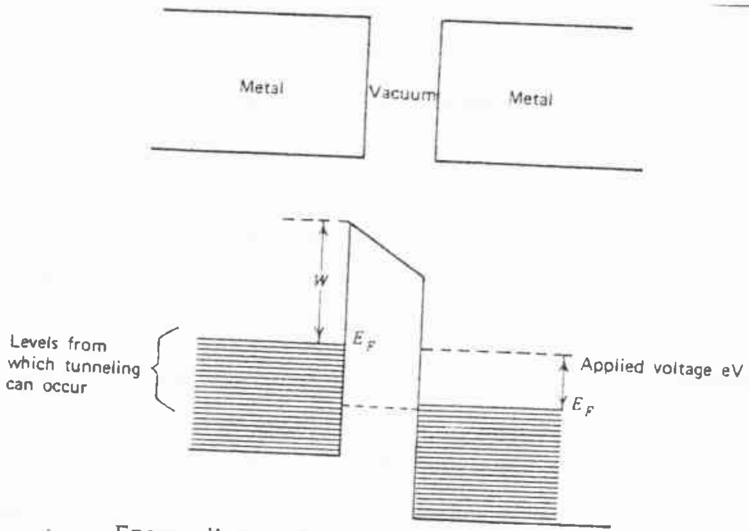
Figure 5.13 One pixel of a field emission display. Applying a positive bias turns on any of the three different colors of subpixel.

Field emission is now being tried as the source of illumination in a new kind of flat-screen display, the aptly named Field Emission Display (FED) shown in Figure 5.13. Its potential advantages over the liquid crystal displays commonly used in laptop computers include wider viewing angle and quicker response.

Tunneling between two metals seperated by vacuum



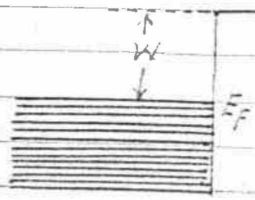
Ni - Nio - Pb with gap of 50Å



Energy diagram for tunneling between two metals separated by vacuum. Tunneling between metals is possible only when there are empty states on the right. Such empty states are created when eV is applied to lower the Fermi level on the right.

$$|T|^2 \sim e^{-2\sqrt{\frac{2mW}{\hbar^2}}\,a}$$

Field Emission



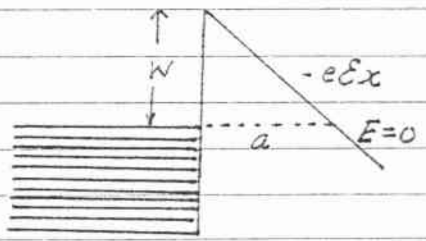
Electrons in a metal
↓
held in a metal by a potential
↓
first approximation, described by a box of finite depth

Pauli's exclusion principle
↓
no two electrons can occupy than a given state
↓
stack up to an energy E_F
↓
Fermi energy

Workfunction : difference between the Fermi energy and top of the well
photoelectric effect

Electrons can be removed by transferring energy to them
↓
for example , use photons

Cold emission → applying an external electric field $\mathcal{E}$



$$W \rightarrow W - e\mathcal{E}x$$

$$|T|^2 \sim e^{-2\int_0^a dx \sqrt{\frac{2m(W-e\mathcal{E}x)}{\hbar^2}}}$$

for electron at the top of the "sea"

a is determined by $W = e\mathcal{E}a$

$$\Rightarrow a = \frac{W}{e\mathcal{E}}$$

$$\int dx\,(A+Bx)^{\frac{1}{2}} = \frac{(A+Bx)^{3/2}}{3B/2}$$

$$\Rightarrow |T|^2 = e^{-\frac{4\sqrt{2}}{3}\sqrt{mW}/\hbar^2 (W/e\mathcal{E})}$$

↓

Fowler - Nordheim formula
↓
only describe cold emission qualitatively since we have neglected many effects

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編號： 8-41C
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Metal - superconductor tunneling

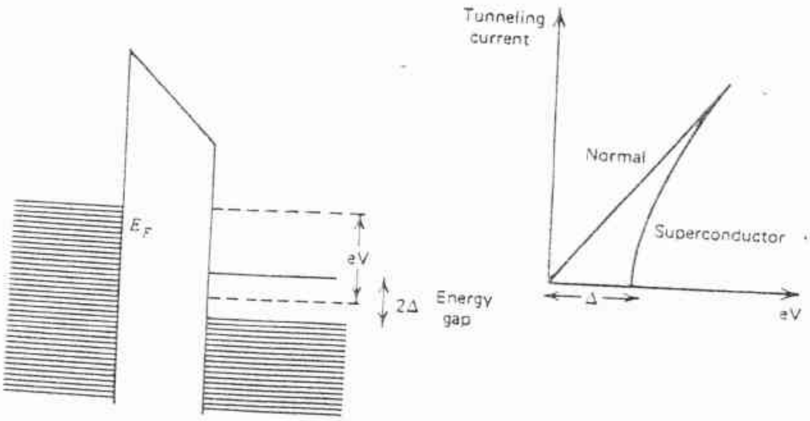
Gap in energy level

$E_F - \Delta$ and $E_F + \Delta$

$\Delta \sim 10^{-3}\ eV$ $\quad E_F \sim 10\ eV$

Level density just below and just above the gap is very large
$ea\mathcal{E} < \Delta$ there will be no tunneling

Superconductor - oxide - superconductor
"Photon-assisted" tunneling → photon energy cause breakup of the electron pairs



Energy diagram for tunneling from metal to superconductor. In contrast to the metal–metal tunneling shown in Figure 5-6, no tunneling is allowed into the energy gap. This affects the current-voltage characteristic as shown.

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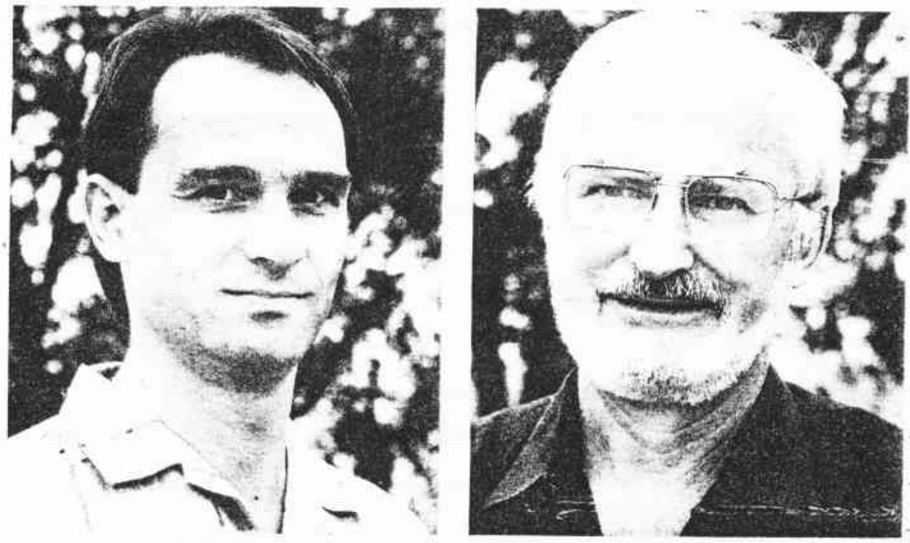
Scanning Tunneling Microscope
(STM)



BINNIG ROHRER

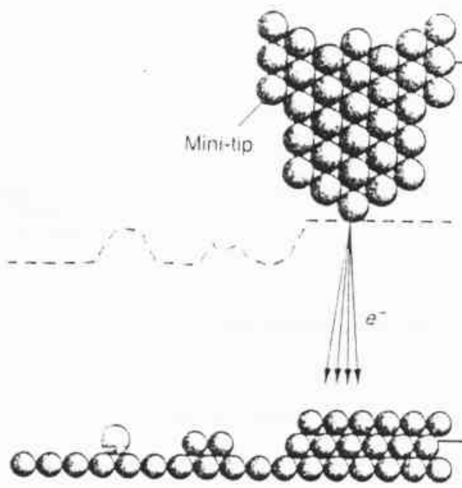
Study surfaces on an atomic scale of size.

STM was invented in 1981 by Gert Binning and Heinrich Rohrer, who shared the 1986 Nobel Prize in physics with Ernst Ruska, the inventor of the electron microcopy.

The extreme sensitivity of tunneling probability to width in a wide barrier is the root of the ulility of the STM

A narrow gap between a conducting speciman and the tip of a tin probe acts a potential barrier to electrons bound in the speciman.

A small bias voltage applied between the probe and the speciman causes the electrons to tunnel through the barrier sepering the two surfaces if the space are close enough together.



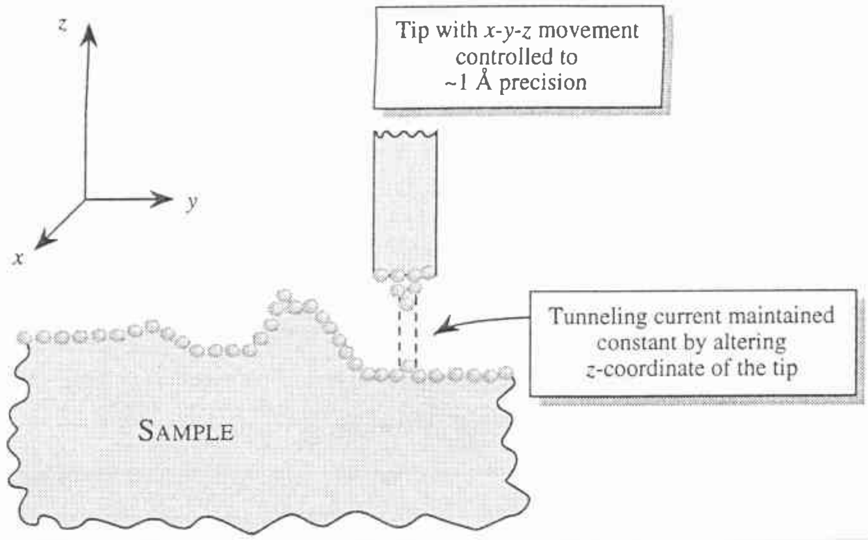
The tunneling current is extremely sensitive to the size of the gap.. ie., the width of the barrier, between the probe and speciman

A change of only 0.5 nm (about the diameter of one atom) in the width of the barrier can cause the tunneling current change by as much as a factor of 10^4.

As the probe scans the specimen, a constant tunneling current is maintained by a piezoelectric feedback system that keeps the gap constant.

⇒ the surface of the speciman can be mapped out by the vertical motion of the probe.

✓


Tip with x-y-z movement
controlled to
~1 Å precision
z
y
x
Tunneling current maintained
constant by altering
z-coordinate of the tip
SAMPLE

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Key :

Tip with x-y-z movement controlled to ~ 1Å precision.

Early work of Binnig and Rohrer.

- a vacuum enviornment
- a very elaborate system for the suppression of vibration.

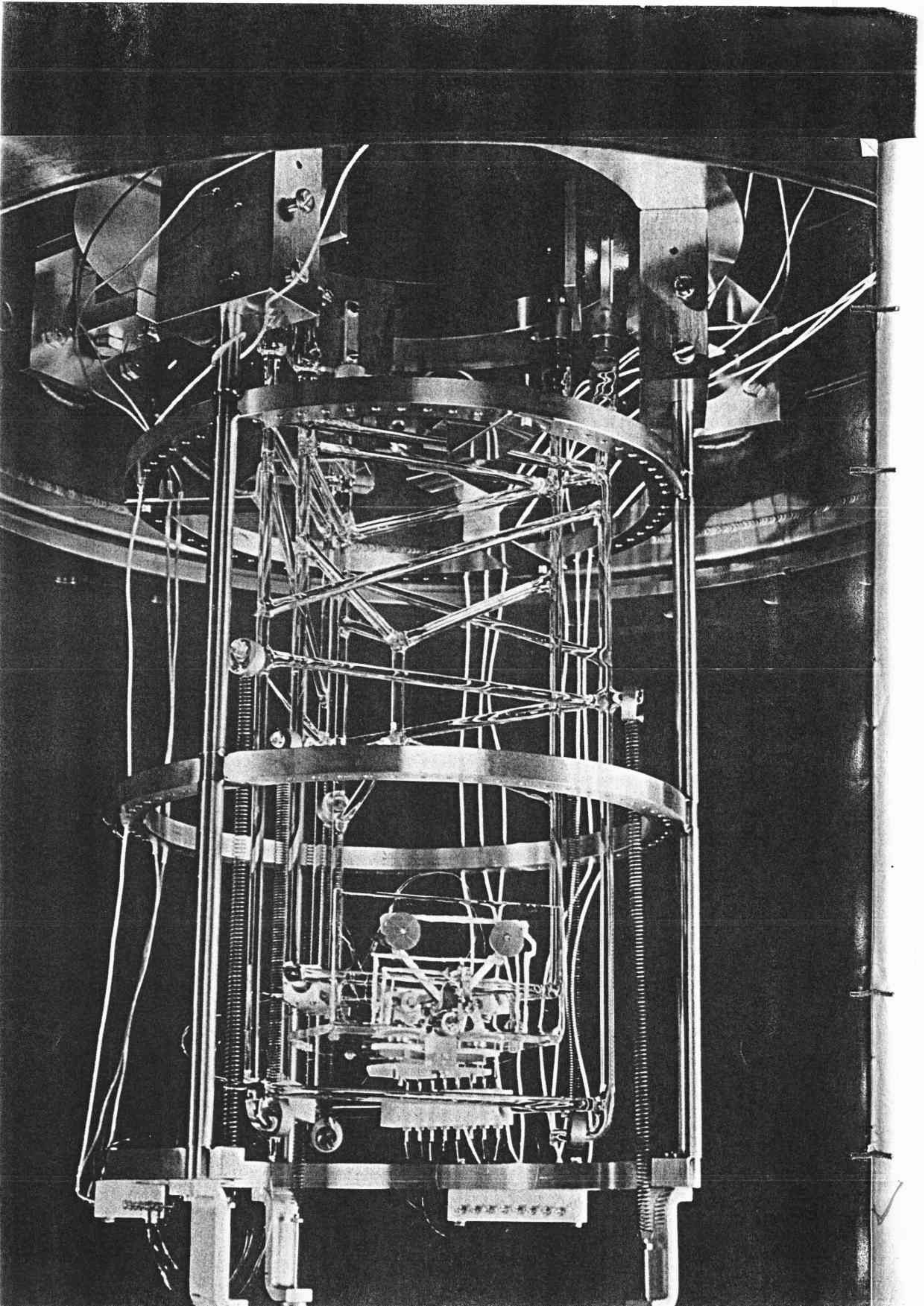
relative position of
probe and specimen
remain fixed.

SCANNING TUNNELING MICROSCOPE has two stages, suspended from springs, that nestle within a cylindrical stainless-steel frame. The innermost stage contains the microscope mechanism. To achieve high-resolution images of surface structures the microscope must be shielded from even such small vibrations as those caused by footsteps and sound. The copper plates (attached to the bottom of the stainless-steel frame) and the magnets (attached to the bottom of the inner and outer stages) damp vibrations. Any disturbance causes the copper plates to move up and down in the field generated by the magnets. The movement induces eddy currents in the plates. The interaction of the eddy currents with the magnetic field retards the motion of the plates and hence the motion of the stages. For work required in a vacuum a steel cover is placed over the outer frame of the microscope.

The original apparatus was magnetically levitated on a superconducting lead bowl resting on a heavy stone slab atop a bed of inflated rubber tires

Two stages, or sections, suspended from springs, nestle within the stainless-steel cylindrical frame of the microscope and protect the tunneling gap from vibration. Both stages, triangular in cross section, are made of glass rods. The second stage slips into the first stage, from which it is suspended by three springs. The first stage in turn is suspended from the outer frame, also by three springs. The second stage carries the heart of the microscope: it contains both the sample and the scanning needle.

When the entire microscope sits in a vacuum, air resistance is minimal and the first and second stages could, if they were disturbed, bounce up and down almost indefinitely. To stop this motion we rely on the phenomenon of eddy-current damping. We let copper plates attached to the bottom of the first and second stages slide between magnets attached to the outer frame. As each plate slides up and down, the magnetic field causes the conducting electrons of the copper to move around, inducing a so-called eddy current. The reaction between the eddy current and the magnetic field retards the motion of the plate and thereby protects the microscope from even the smallest vibrations.



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· Piezoelectric drive

The thickness of certain ceramics changes when a voltage is applied across them

↓

piezoelectricity

Once the gross vibrations have been stopped the sample can be positioned. This is done with a specially developed drive that carries the sample across a horizontal metal plate on the second stage. The body of the drive consists of a slab of piezoelectric material that expands or contracts when voltage is applied. The drive has three metallic feet, arranged in triangular fashion, that are coated with a thin layer of insulating material. They can be clamped to the metal plate by establishing a voltage between them and the metal plate.

We move the drive in the following manner. Suppose, for instance, we clamp only one foot and apply a voltage to the piezoelectric body so that it contracts. The other two feet will move slightly. We then clamp those two feet, release the third foot and remove the applied voltage so that the body expands back to its original size. The drive has just moved one step. The step width can be varied between 100 and 1,000 angstroms. Since the drive can rotate about each of its feet, it can walk along the plate in any desired direction.

When the drive has carried the sample to the wanted tunneling position, we begin scanning the surface of the sample. We use a rigid tripod made of three piezoelectric sticks to move the tip of the scanning needle. When we apply a voltage to expand or contract one of the sticks, the other two bend slightly. Consequently the tip moves in a straight line over distances as great as 10,000 angstroms. Furthermore, this motion is quite sensitive to the magnitude of the applied voltage: a voltage on the order of .1 volt results in a motion of 1.0 angstrom. The precision of the tripod's drive is so good that at present only vibration limits the vertical resolution of the sample's surface. This resolution at present is in the range of approximately a few hundredths of an angstrom.

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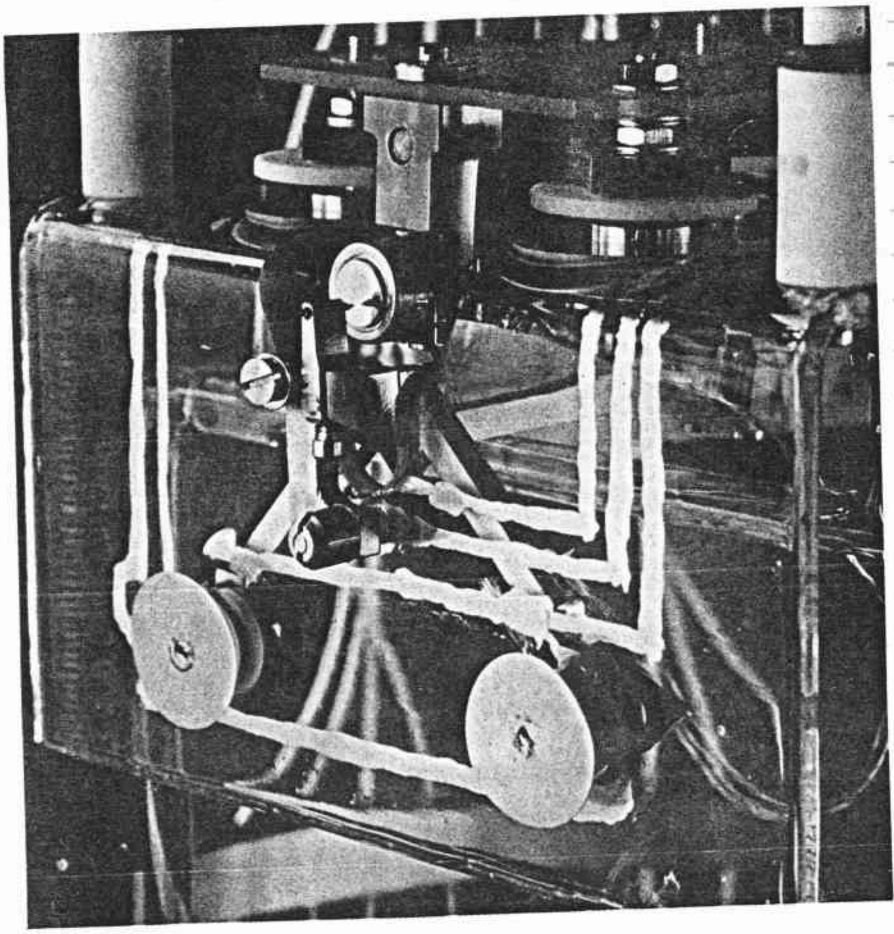
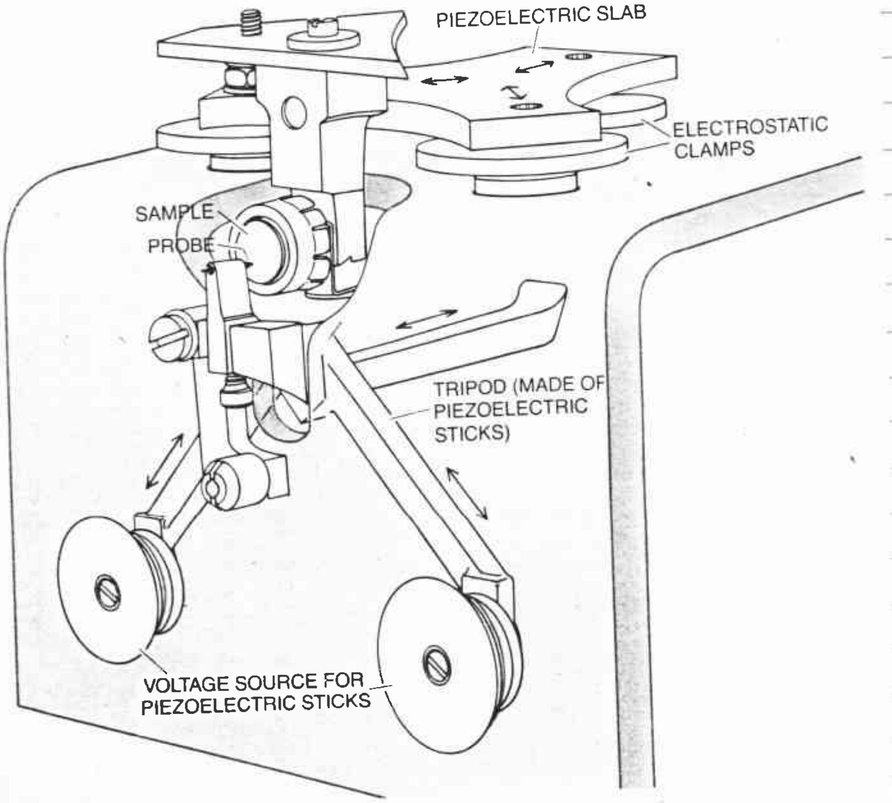
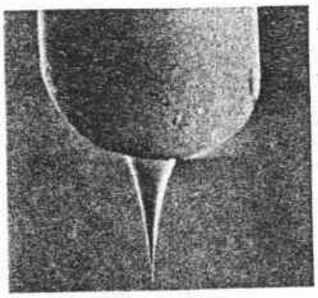




MICROSCOPE DEVICE contains a sample and a scanning needle. Piezoelectric materials, which expand or contract when voltage is applied to them, enable the device to resolve features that are only about a hundredth the size of an atom. A piezoelectric drive positions the sample on a horizontal metal plate. A piezoelectric tripod then sweeps the scanning needle over the surface of the sample, simultaneously achieving high stability and precision.

· Sharpness of the tip of the probe.



The tungsten probe of a scanning tunneling microscope.

The lateral resolution of the surface is limited by the sharpness of the tip. In this instance nature has been kind to the vacuum tunneler. It is relatively easy to make a sharp tip that yields a lateral resolution of about six to 12 angstroms: one simply grinds the end of a needle, which is usually made of tungsten.

To achieve a lateral resolution of two angstroms, however, the needle must have a single atom sitting securely on top of its tip. Such an atom usually comes from the sample itself. It is dislodged by high electric fields that are caused by applying a voltage difference of from two to 10 volts between the sample and the tip. Since luck plays a large role in the final stage, we are trying to sharpen the tip by bombarding it with a high-energy beam of ions. This causes the atoms on the surface to sputter away in a highly controlled manner.

The probe turned out to be even more local than their fondest hopes. Employing stylus tips with curvature radii on the order of a thousand angstroms, Binnig and Rohrer had expected a horizontal resolution of about 50 Å—not nearly good enough to resolve individual atoms. But when they started scanning, they certainly did see atoms. "We had thought this kind of resolution would require a big effort," Binnig told us. "But we got atomic scale resolution more or less as a gift."

The gift comes from the fact that these 1000-Å tips are inevitably rough on a smaller scale, with accidental protuberances serving as tips only a few atoms wide. With these protuberances doing the probing, the scanning instruments achieved a horizontal resolution of about 4 Å very early on. Now it's down to 1 Å. In recent months the IBM Zurich group has been replacing these fortuitous probing tips with monatomic tips carefully created by field-ion microscopy techniques devised by Hans-Werner Fink. The end of the tip is the world's smallest manmade pyramid: three layers consisting respectively of seven, three and finally one single atom. Putting the last single atom in place is "a miracle," says Rohrer.

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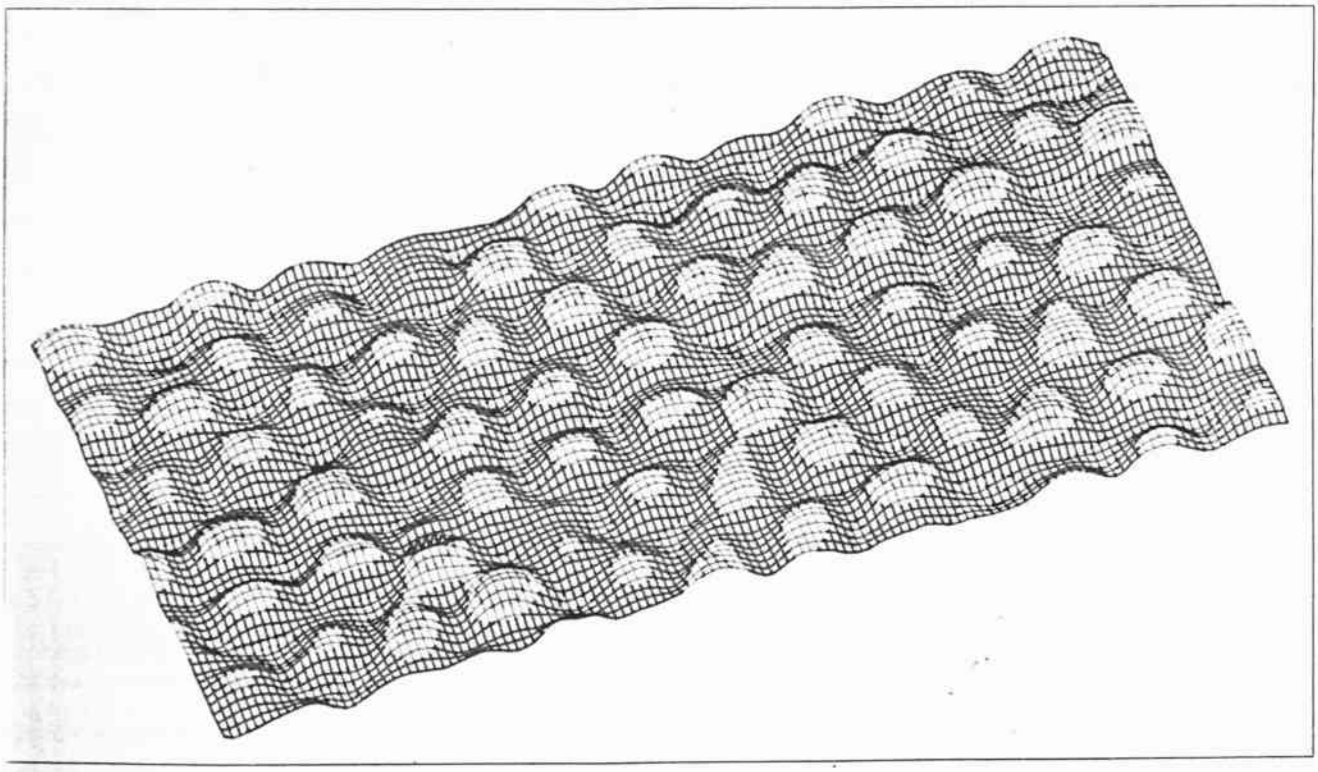

SURFACE OF SILICON as disclosed by the scanning tunneling microscope consists of a pattern of diamond-shaped unit cells. Each cell measures 27 angstrom units (one angstrom unit is one ten-billionth of a meter) on a side. The cell is called the 7-by-7 because each side measures seven atomic units. Each 7-by-7 contains 12 bumps that are arranged in two groups of six. The bumps, which have never before been resolved, apparently correspond to the surfaces of individual atoms. They stand as much as 1.3 angstroms above the rest of the surface. The image was formed by applying a voltage so that electrons flowed from the needle tip to the surface.

The STM must be ranked as one of the most indispensable tools in modern technology. Its uses are already legion—studying geometry and composition of a seeming endless list of surfaces; locating important biological molecular groups, such as the fundamental building blocks of DNA; mapping microscopic "vortices" in certain kinds of superconductors; nudging atoms from one point on a surface to another—and they continue to expand.

Actually, the result of an STM scan is not a true topographical map of surface height but a contour map of constant electron density on the surface. This means that atoms of different elements appear differently, which greatly increases the value of the STM as a research tool.

Although many biological materials conduct electricity, they do so by the flow of ions rather than of electrons and so cannot be studied with STMs. A more recent development, the **atomic force microscope** (AFM) can be used on any surface, although with somewhat less resolution than an STM. In an AFM, the sharp tip of a fractured diamond presses gently against the atoms on a surface. A spring keeps the pressure of the tip constant, and a record is made of the deflections of the tip as it moves across the surface. The result is a map showing contours of constant repulsive force between the electrons of the probe and the electrons of the surface atoms. Even relatively soft biological materials can be examined with an AFM and changes in them monitored. For example, the linking together of molecules of the blood protein fibrin, which occurs when blood clots, has been watched with an AFM.

Articles by Roger A. Freedman and Paul K. Hansma
Binnig and Rohrer are given in Appendix E

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α Decay
(Alpha)

Certain heavy nuclei are observed to decay by emission of an α particle (made of two protons and two neutrons) with a kinetic energy of a few MeV

In an α decay, the daughter nucleus has two fewer protons and two fewer neutrons than the parent nucleus

The kinetic energy of the α-particles are measured to be in a relatively small range from 4 to 9 MeV

The lifetime of the α-decay process vary dramatically from 10^{-7} sec to 10^{10} years.
(The half-life is defined as the time required for one half the nuclei in a sample to decay)

For example

$$^{238}U \longrightarrow {}^{234}Th + \alpha$$

E_k of α particle $= 4.18$ MeV

$$t_{1/2} = 4.5 \times 10^{9} \text{ years}$$

$$^{212}Po \longrightarrow {}^{208}Pb + \alpha$$

$$E_k = 8.78 \text{ MeV}$$

$$t_{1/2} = 0.3\ \mu\text{sec.}$$

" Why do similar decays yield α-particle energies of the same order of magnitude while the lifetimes differ by more than 23 order of magnitude ? "

The answer is to be found in quantum tunneling.

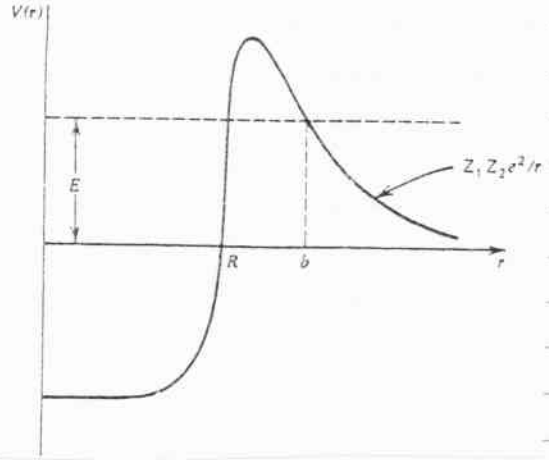
$\downarrow$

first proposed by
Gamow
in 1928

8-52

George Gamow, 1904–1968, whose work in 1928 showed that alpha particles can behave as waves. In so doing, he solved the long-standing puzzle about the half-life of alpha decay. This demonstrated for the first time that quantum mechanics applies to nuclei. (AIP Emilio Segrè Visual Archives.)

$V(r)$ between the daughter nucleus and the α particle.



We approximate $V(r)$ as an attractive "square well" (short - range) due to the strong interaction plus a repulsive Coulomb component outside the nuclues.

$|T|^2 \sim e^{-G}$

with $$G \cong 2\int_R^b \left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \left(\frac{Z_1 Z_2 e^2}{r} - E\right)^{\frac{1}{2}} dr$$

(m = mass of the α particle)

b is determined by $E = \frac{Z_1 Z_2 e^2}{b} \sim \frac{1}{2} m v^2$

$$G \sim 2\int_R^b \left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} Z_1 Z_2 e^2 \left(\frac{1}{r} - \frac{1}{b}\right) dr$$

Z_1 = charge of the daughter nucleus

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

For $b \gg R$ (valid for low energy α)

$$\Rightarrow \quad G \sim \frac{2\pi Z_1 Z_2 e^2}{\hbar v} \sim \frac{Z_1}{\sqrt{E}}$$

$$t_{1/2} \sim \frac{2R}{v'} e^{G} \quad *$$

$$\ln t_{1/2} \sim C_2 + C_1 \frac{Z_1}{\sqrt{E}}$$

very rough result

Comparison with experimental result are shown in the next graph.

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number of decays / time $= \dfrac{\text{number of times } \alpha \text{ strikes}}{\text{time}}$

$\times$ transmission probability

$$= \frac{\text{one strike}}{\text{time to cross diameter}} \times \text{transmission probability}$$

$$= \frac{1}{\text{diameter of nucleus/speed}} \times \text{transmission probability}$$

$$= \frac{v}{2R_{nucl.}} \times \text{transmission} = \lambda$$

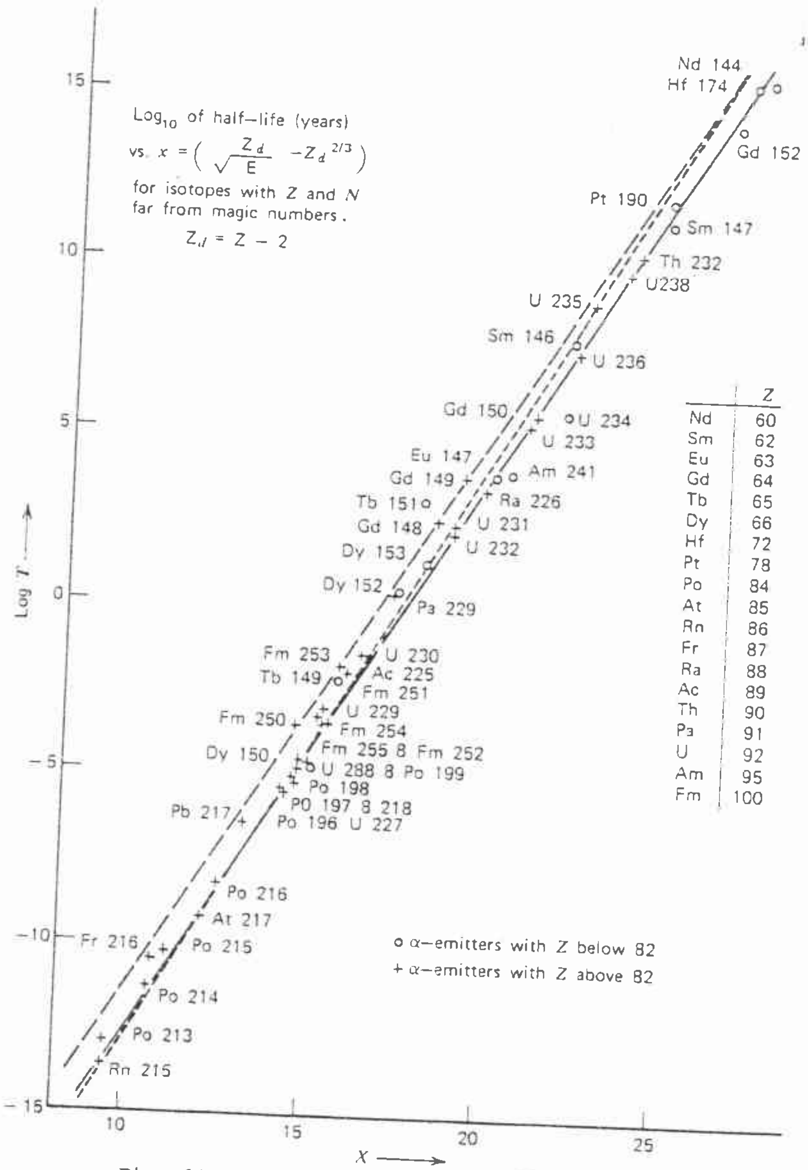
$$\frac{dN}{dt} = -\lambda$$

$$N = N_0 e^{-\lambda t}$$

$$\frac{1}{2} = e^{-\lambda t_{1/2}}$$

$$\ln 2 = \lambda t_{\frac{1}{2}}$$

$$t_{\frac{1}{2}} = \frac{\ln 2}{\lambda}$$



Plot of $\log_{10} 1/\tau$ versus $C_2 - C_1 Z_1/\sqrt{E}$ with $C_1 = 1.61$ and a slowly varying $C_2 = 28.9 + 1.6Z_1^{2/3}$. (From E. K. Hyde, I. Perlman, and G. T. Seaborg, *The Nuclear Properties of the Heavy Elements*, Vol. 1, Prentice-Hall, Englewood Cliffs, N.J. (1964), reprinted by permission.)

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Remarks.

- Even with such crude model, the agreement is impressive.

- For higher α energies, G depends on R.

- The idea was proposed in 1928
  ↓
  first application of quantum mechanics to nuclear physics.

For a more detailed discussion, see Appendix F

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

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{1/2}\int_R^b dr\sqrt{\frac{Z_1Z_2e^2}{4\pi\varepsilon_0 r} - E} \tag{4B-2}$$

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 $b = Z_1Z_2e^2/4\pi\varepsilon_0 E$. 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.

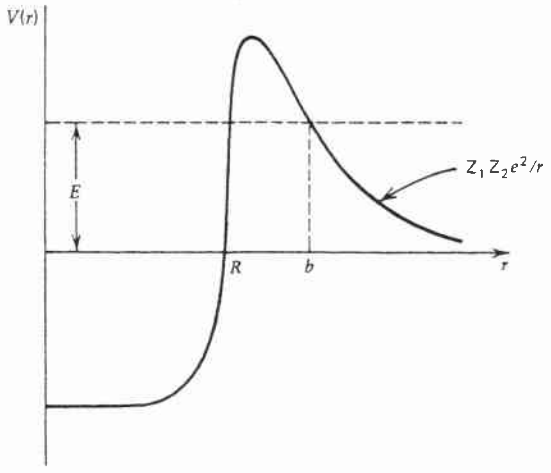


Figure 4B-1 Potential barrier for α decay.

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.

(Finite) Potential Well

Even, Odd Solution

General discussion of the solution

Single and Double
δ - function

Periodic Potential.

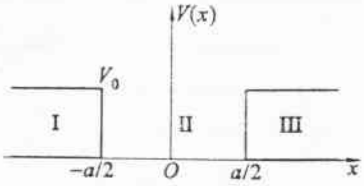
Summary

Three Lectures of M.I.T. 8.04
Quantum Physics

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

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

are also eigenfunctions of the Schrodinger equation with eigenvalue E

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

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

$\Rightarrow$ 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 $x = -\frac{a}{2}$

$$\psi_1(x = -\tfrac{a}{2}) = \psi_2(x = -\tfrac{a}{2})$$

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

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

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

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

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.,

$$q \tan qa = \kappa \qquad (A)$$

· 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.

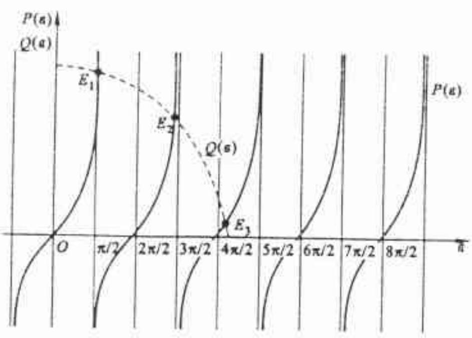
Analytic solutions are difficult to find, we usually solved it using graphic method, i.e., plot LHS, RHS as function of E. The intersection $\Rightarrow$ eigenvalues of E

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

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

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

(a circle when Q is plotted against ϵ.



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

Odd solution.

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

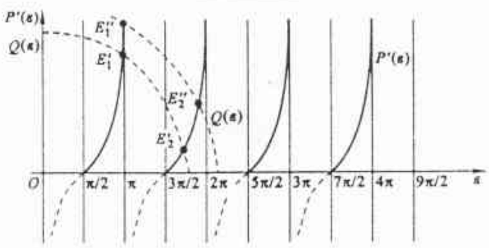
$\psi_2(x) = A \sin k_2 x$ $\quad -\frac{a}{2} < x < \frac{a}{2}$

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

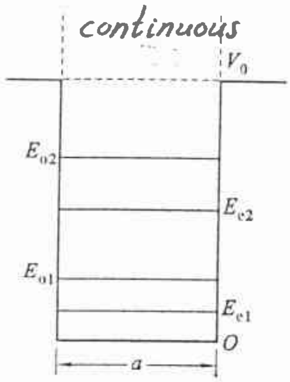
$k_2 \cot \frac{k_2 a}{2} = -k_1$ (from matching the boundary conditions)

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

Again, graphic method can be used to find $E_{o1}, E_{o2}, \cdots$



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.

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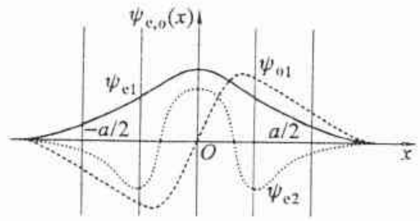
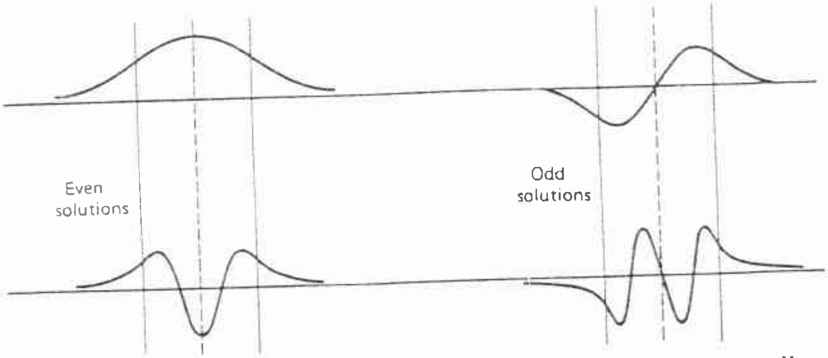
總號:

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.

$V_0 \to \infty \Rightarrow$ infinite well.