Quantum Theory

Thornton and Rex, Ch. 6

Matter can behave like waves.

1) What is the wave equation?

2) How do we interpret the wave function $\psi(x,t)$?

Light Waves

Plane wave: $\psi(x,t) = A\cos(kx-\omega t)$

wave (ω,k) $\Leftrightarrow$ particle (E,p):

1) Planck: $E = h\nu = \hbar\omega$
2) De Broglie: $p = h/\lambda = \hbar k$

A particle relation:

3) Einstein: $E = pc$

A wave relation:

4) $\omega = ck$ (follows from (1),(2), and (3))

The wave equation:

$$\boxed{\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = \frac{\partial^2\psi}{\partial x^2}}$$

Matter Waves

Equations (1) and (2) must hold.
(wave (ω,k) $\Leftrightarrow$ particle (E,p))

Particle relation (non-relativistic, no forces):

3') $E = 1/2\ m\ v^2 = p^2/2m$

The wave relation:

4') $\hbar\omega = (\hbar k)^2/2m$
(follows from (1),(2), and (3'))

$\Rightarrow$ Require a wave equation that is consistent with (4') for plane waves.

The Schrödinger Equation

1925, Erwin Schrodinger wrote down the equation:

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

The Schrödinger Equation

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

(Assume V is constant here.)

A general solution is

$$\begin{aligned}\psi(x,t) &= A\, e^{i(kx-\omega t)} \\ &= A\,(\cos(kx-\omega t) + i\sin(kx-\omega t))\end{aligned}$$

$$\Rightarrow\ \hbar\omega = \frac{\hbar^2 k^2}{2m} + V$$

$$\Rightarrow\ E = \frac{p^2}{2m} + V$$

What is $\psi(x,t)$?

Double-slit experiment for light:

$$I(x) \approx |E(x)|^2 + |B(x)|^2$$

Probability of photon at x is $\propto I(x)$.

Max Born suggested:

$|\psi(x,t)|^2$ is the probability of finding a matter particle (electron) at a place x and time t.

Probability and Normalization

The probability of a particle being between x and x + dx is:

$$P(x)\,dx = |\psi(x,t)|^2\,dx$$

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

The probability of being between x_1 and x_2 is:

$$P = \int_{x_1}^{x_2} \psi^*\psi\,dx$$

The wavefunction must be normalized:

$$P = \int_{-\infty}^{\infty} \psi^*\psi\,dx \quad = \; 1$$

Properties of valid wave functions

1. ψ must be finite everywhere.

2. ψ must be single valued.

3. ψ and $d\psi/dx$ must be continuous for finite potentials (so that $d^2\psi/dx^2$ remains single valued).

4. $\psi \rightarrow 0$ as $x \rightarrow \pm \infty$.

These properties (boundary conditions) are required for physically reasonable solutions.

Heisenberg's Uncertainty Principle

Independently, Werner Heisenberg, developed a different approach to quantum theory. It involved abstract quantum states, and it was based on general properties of matrices.

Heisenberg showed that certain pairs of physical quantities ("conjugate variables") could not be simultaneously determined to any desired accuracy.

We have already seen:

- $\Delta x \, \Delta p \geq \hbar/2$

It is impossible to specify <u>simultaneously</u> both the position and momentum of a particle.

Other conjugate variables are (E,t) (L,θ):

- $\Delta t \, \Delta E \geq \hbar/2$
- $\Delta \theta \, \Delta L \geq \hbar/2$

Expectation Values

Consider the measurement of a quantity (example, position x). The average value of many measurements is:

$$\overline{x} = \frac{\sum N_i \, x_i}{\sum_i N_i}$$

For continuous variables:

$$\overline{x} = \frac{\int_{-\infty}^{\infty} P(x)\, x \, dx}{\int_{-\infty}^{\infty} P(x)\, dx}$$

where $P(x)$ is the probability density for observing the particle at x.

Expectation Values (cont'd)

In QM we can calculate the "expected" average:

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \psi \; x \; dx}{\int_{-\infty}^{\infty} \psi^* \psi \; dx} = \int \psi^* \psi \; x \; dx$$

The expectation value.

Expectation value of any function $g(x)$ is:

$$\langle g(x) \rangle = \int_{-\infty}^{\infty} \psi^* \; g(x) \; \psi \; dx$$

What are the expectation values of p or E?

First, represent them in terms of x and t:

$$\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial x}\left(Ae^{i(kx-\omega t)}\right) = ik\,\psi = \frac{ip}{\hbar}\psi$$

$$\Rightarrow \; p\,\psi = -i\hbar \frac{\partial \psi}{\partial x}$$

Define the <u>momentum operator:</u>

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

Then:

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p}\, \psi \, dx = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} \, dx$$

Similarly,

$$\frac{\partial \psi}{\partial t} = -i\omega\,\psi = \frac{-iE}{\hbar}\,\psi$$

$$\Rightarrow E\,\psi = i\hbar\,\frac{\partial \psi}{\partial t}$$

so the Energy operator is:

$$\hat{E} = i\hbar\,\frac{\partial}{\partial t}$$

and

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^* \hat{E}\,\psi\,dx = i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial t}\,dx$$

A self-consistency check:

The classical system obeys:

$$E = K + V = \frac{p^2}{2m} + V$$

Replace E and p by their respective operators and multiplying by ψ:

$$\hat{E}\,\psi = \left(\frac{\hat{p}^2}{2m} + V\right)\psi$$

The Schrodinger Equation!

Time-independent Schrodinger Equation

In many (most) cases the potential V will not depend on time.
Then we can write:

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

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar\,(-i\omega)\,\psi = \hbar\omega\,\psi = E\,\psi$$

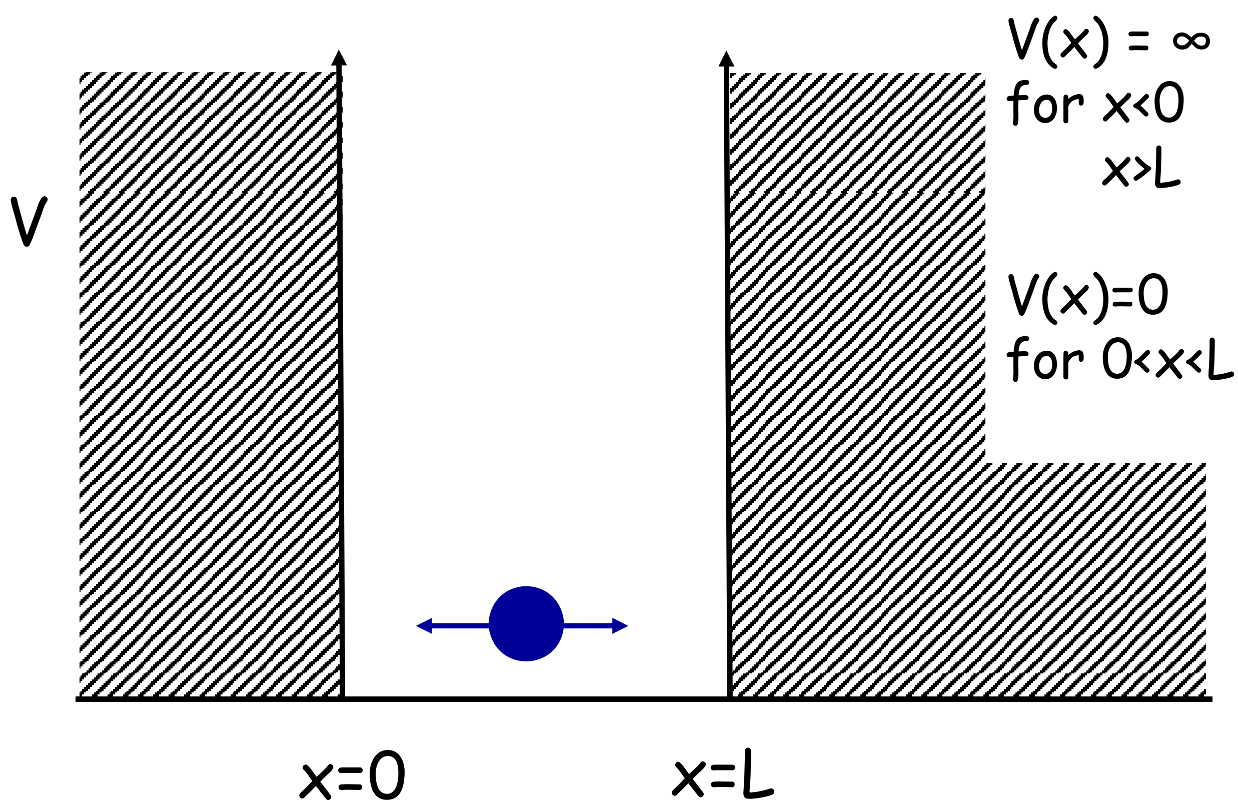
This gives the time-independent S. Eqn:

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

The probability density and distributions are constant in time:

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

The infinite square well potential



The particle is constrained to $0 < x < L$.

Outside the "well" $V = \infty$,

$$\Rightarrow \psi = 0$$

for $x<0$ or $x>L$.

Inside the well, the t-independent S Eqn:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{d\,x^2} = E\,\psi$$

$$\Rightarrow \frac{d^2\psi}{d\,x^2} = \frac{-2mE}{\hbar^2}\psi = -\,k^2\,\psi$$

(with $k = \sqrt{2mE/\hbar^2}$)

A general solution is:

$$\psi(x) = A \sin kx + B \cos kx$$

Continuity at $x=0$ and $x=L$ give

$\psi(x=0) = 0$

$\Rightarrow$ $B=0$

and $\psi(x=L) = 0$

$$\boxed{\Rightarrow \psi(x) = A \sin kx \quad \text{with } kL=n\pi \quad n=1,2,3,\ldots}$$

Normalization condition gives

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

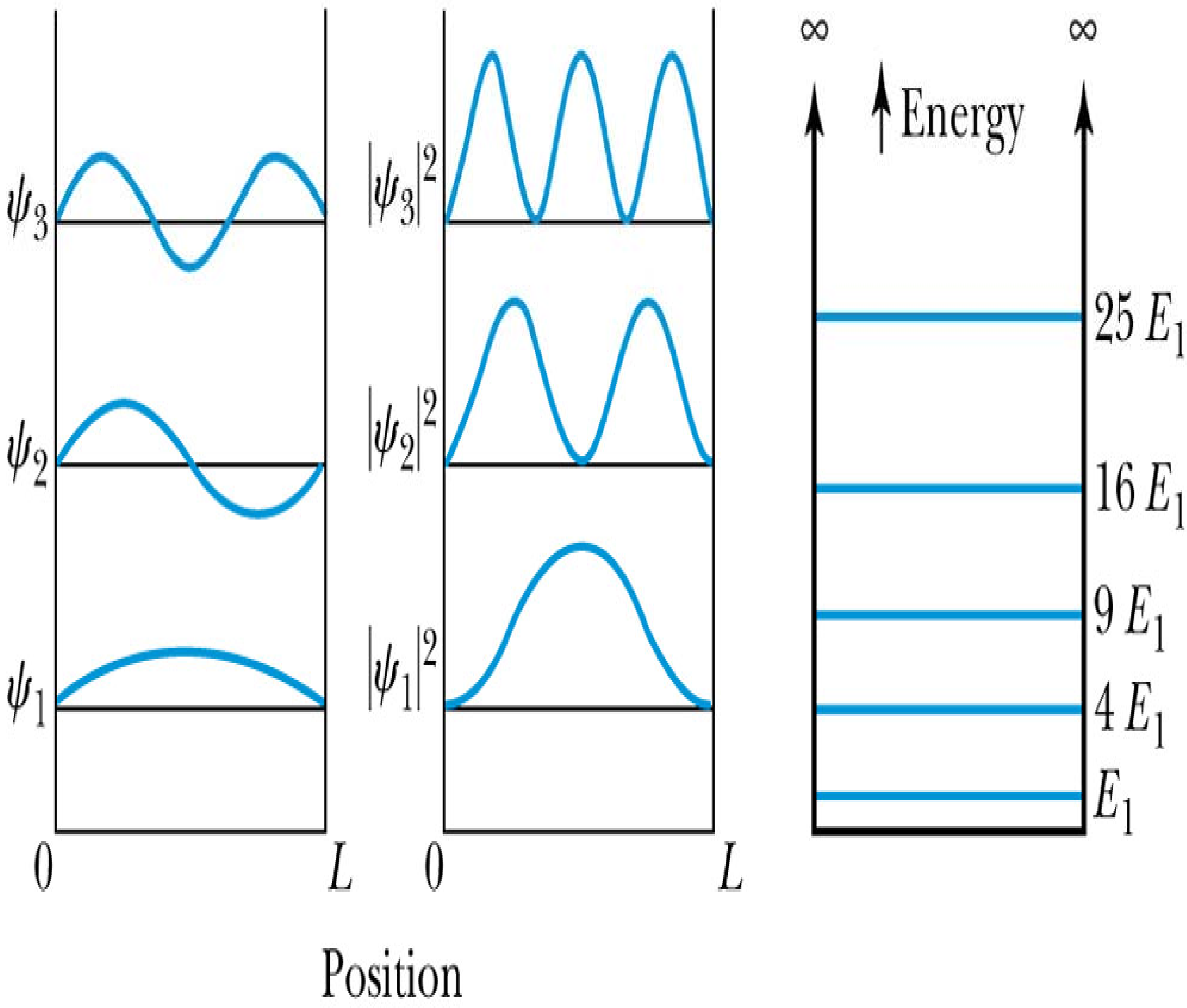
so the normalized wave functions are:

$$\psi_n(x) = \sqrt{2/L}\;\sin(k_n x) \qquad n=1,2,3,\,.\,.\,.$$

with $k_n = n\pi/L = \sqrt{2mE_n/\hbar^2}$

$$\boxed{\Rightarrow \; E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$$

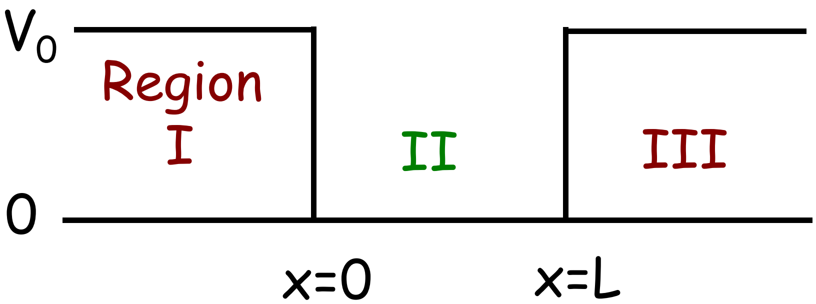
The possible energies (<u>Energy levels</u>) are quantized with n the <u>quantum number.</u>



ψ_3
ψ_2
ψ_1
$|\psi_3|^2$
$|\psi_2|^2$
$|\psi_1|^2$
0
L
0
L
Position
∞
∞
Energy
$25\,E_1$
$16\,E_1$
$9\,E_1$
$4\,E_1$
E_1

Fig 6.3, pg 213

Finite square well potential



$V(x) = V_0$
for $x<0$
$x>L$

$V(x)=0$
for $0<x<L$

Consider a particle of energy $E < V_0$.
Classically, it will be bound inside the well

Quantum Mechanically, there is a finite probability of it being outside of the well (in regions I or III).

Regions I and III:

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

$$\Rightarrow\ d^2\psi/dx^2 = \alpha^2\,\psi \quad \text{with } \alpha^2 = \underbrace{2m(V_0-E)/\hbar^2}_{>0}$$

The solutions are exponential decays:

$\psi_I(x) = A\,e^{\alpha x}$ Region I ($x<0$)

$\psi_{III}(x) = B\,e^{-\alpha x}$ Region III ($x>L$)

In region II (in the well) the solution is

$\psi_{II}(x) = C\cos(kx) + D\sin(kx)$

with $k^2 = 2mE/\hbar^2$ as before.

Coefficients determined by matching wavefunctions and derivatives at boundaries.

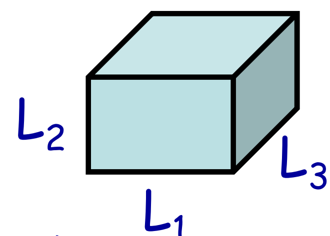
The 3-dimensional infinite square well

S. time-independent eqn in 3-dim:

$$\underbrace{\frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)}+V\psi = E\psi$$

$$\Rightarrow \qquad \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

The solution:



$\psi = A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z)$

with $k_1 = n_1\pi/L_1$, $k_2 = n_2\pi/L_2$, $k_3 = n_3\pi/L_3$.

Allowed energies:

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2}+\frac{n_2^2}{L_2^2}+\frac{n_3^2}{L_3^2}\right)$$

If $L_1 = L_2 = L_3 = L$ (a cubical box)
the energies are:

$$E = \frac{\pi^2 \hbar^2}{2m L^2} \left(n_1^2 + n_2^2 + n_3^2 \right)$$

The ground state $(n_1 = n_2 = n_3 = 1)$ energy is:

$$E_0 = \frac{3 \pi^2 \hbar^2}{2m L^2}$$

The first excited state can have
$(n_1, n_2, n_3) = (2,1,1)$ or $(1,2,1)$ or $(1,1,2)$

There are 3 different wave functions
with the same energy:

$$E_1 = \frac{6 \pi^2 \hbar^2}{2m L^2}$$

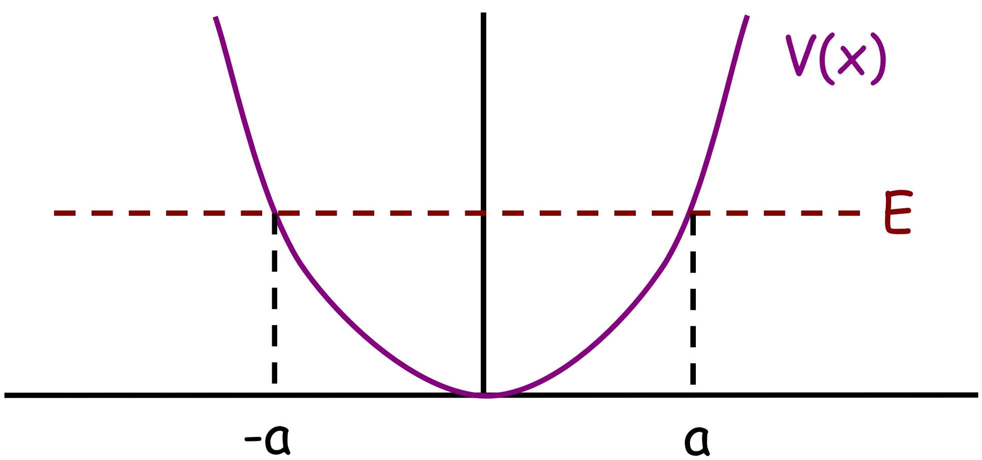
The 3 states are degenerate.

Simple Harmonic Oscillator

Spring force: $F = -\kappa x$

$$\Rightarrow V(x) = \frac{1}{2}\kappa x^2$$

A particle of energy E in this potential:



$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{d x^2} + \frac{1}{2}\kappa x^2 \psi = E\psi$$

$$\frac{d^2\psi}{d\,x^2} = (\alpha^2 x^2 - \beta)\,\psi$$

with

$$\beta = \frac{2m\,E}{\hbar} \qquad \text{and} \qquad \alpha^2 = \frac{m\,\kappa}{\hbar^2}$$

The solutions are:

$$\psi_n(x) = H_n(x)\; e^{-\alpha x^2/2}$$

Hermite Polynomial
(oscillates at small x)

Gaussian
(exponential
decay at large x)

The energy levels are

$$E_n = (n + 1/2) \hbar \omega$$

where $\omega^2 = \kappa/m$ is the classical angular frequency.

The minimum energy ($n=0$) is

$$E_0 = \hbar \omega /2$$

This is the <u>ground state</u> (lowest) energy, sometimes called zero-point energy.

In this system, ground state labeled by $n=0$, while in box, labeled by $n=1$.

The lowest energy state saturates the Heisenberg uncertainty bound:

$$\Delta x \, \Delta p = \hbar/2$$

We can use this to calculate E_0.

In the SHM, $\langle PE \rangle = \langle K \rangle = E/2$.

$$\Rightarrow \quad \kappa \langle x^2 \rangle /2 = \langle p^2 \rangle /(2m) = E/2$$

$$\Rightarrow \quad \kappa \, \Delta x^2 \qquad = \Delta p^2/m \qquad = E$$

$$\Rightarrow \quad \Delta x = \Delta p \,/ \sqrt{m \, \kappa}$$

From uncertainty principle: $\Delta x = \hbar/(2\Delta p)$

So $E = \kappa \, \Delta x \, \Delta x = \kappa \, (\Delta p \,/ \sqrt{m \, \kappa})(\hbar/(2\Delta p))$

$$= (\hbar/2) \sqrt{\kappa \,/\, m} \qquad = \hbar \, \omega \,/2$$

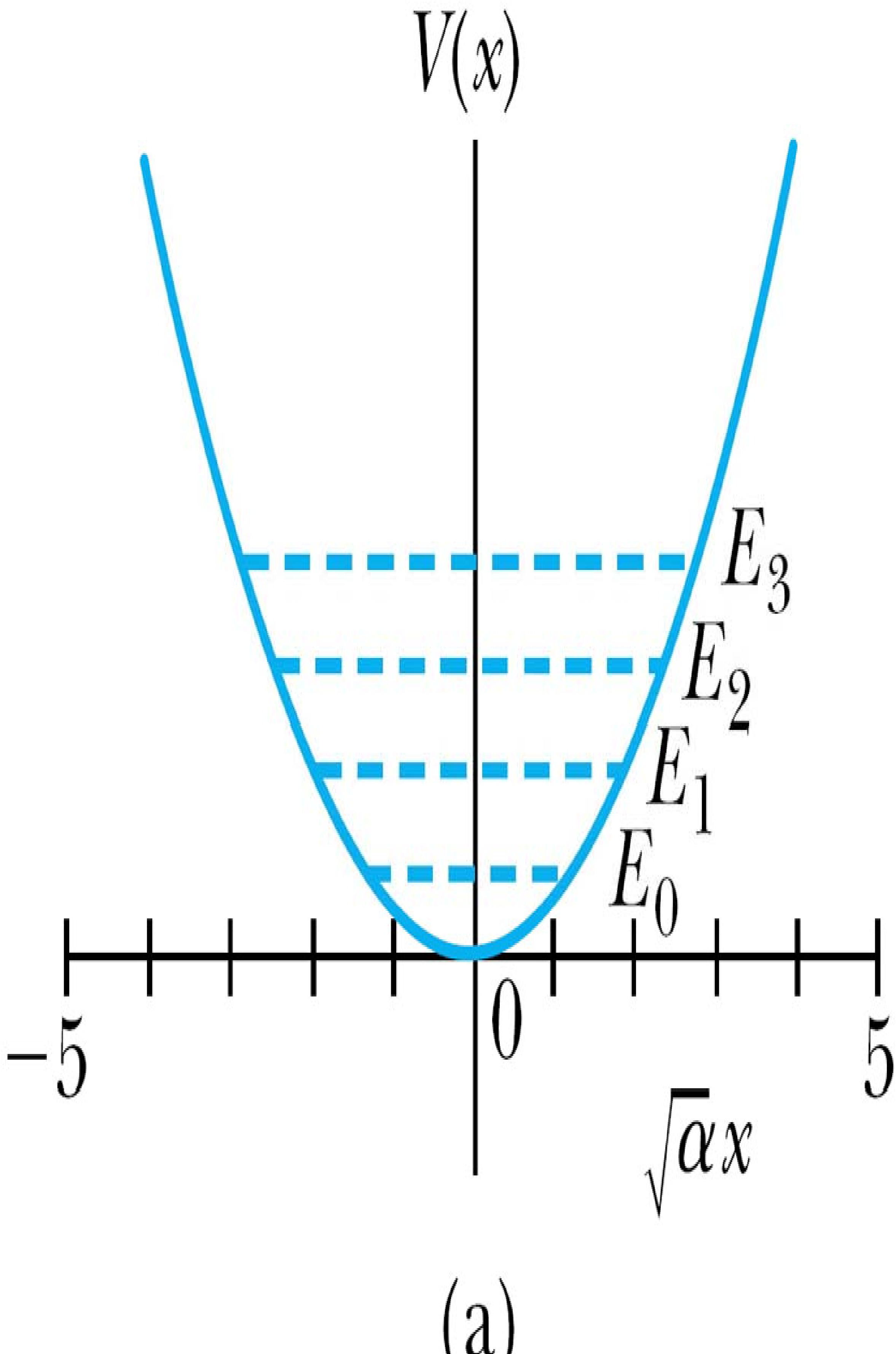


Fig 6.10a, pg 223

Polynomials wiggle more as n increases

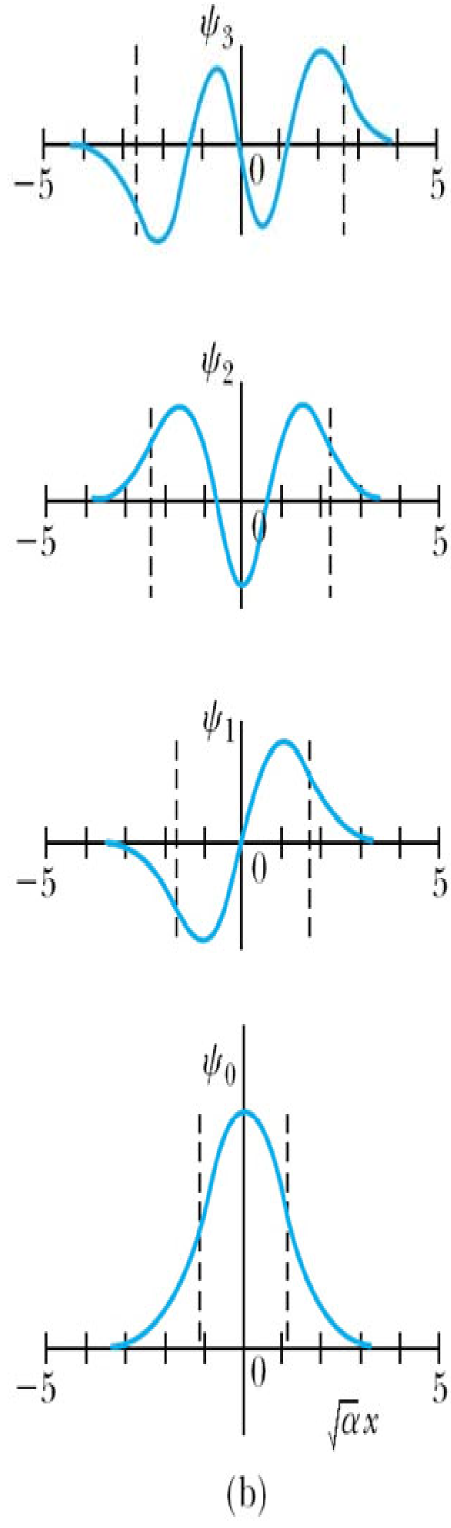


Fig 6.10b, pg 223

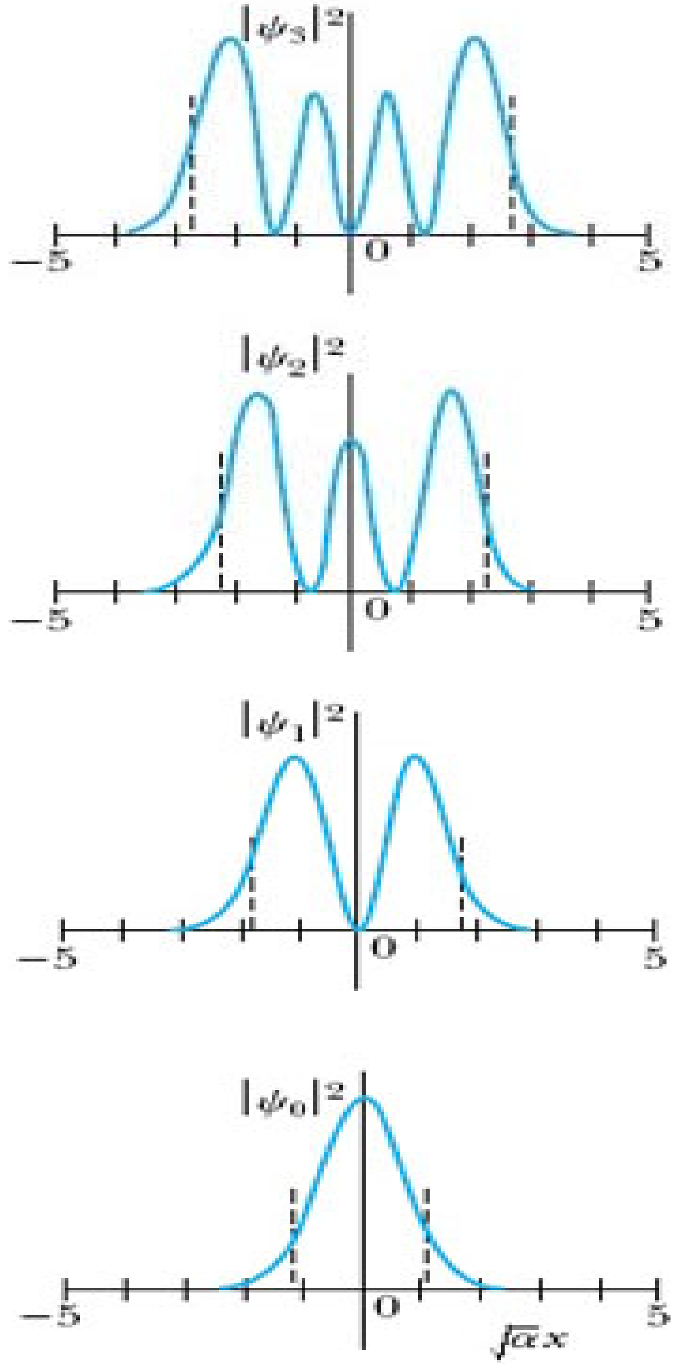
Wave functions

$$\psi_3(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} \left(\sqrt{\alpha}\, x\right)\left(2\alpha x^2 - 3\right) e^{-\alpha x^2/2}$$

$$\psi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} \left(2\alpha x^2 - 1\right) e^{-\alpha x^2/2}$$

$$\psi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\; x e^{-\alpha x^2/2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$



(c)

Fig 6.10c, pg 223

Eventually, wiggles too narrow to resolve:
As n increases, transition to classical

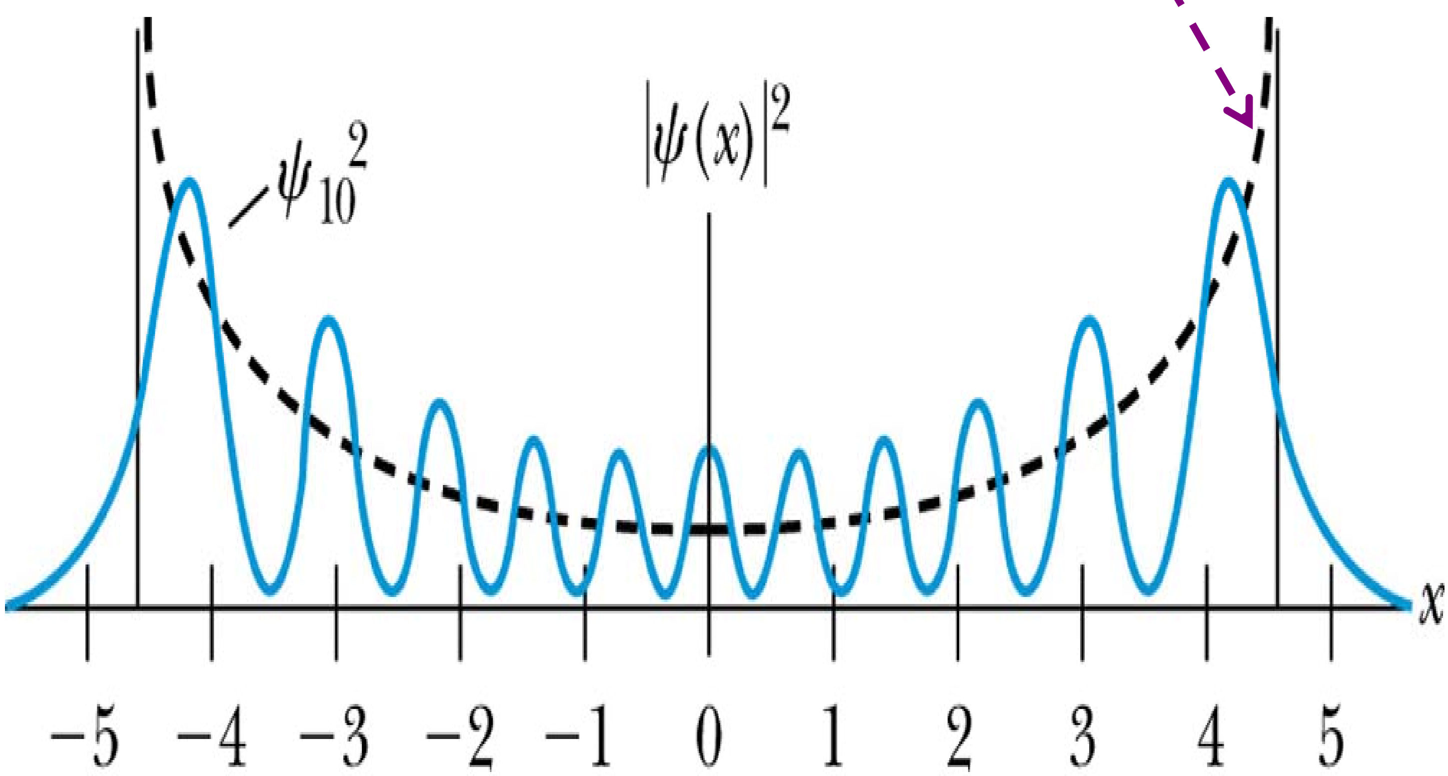
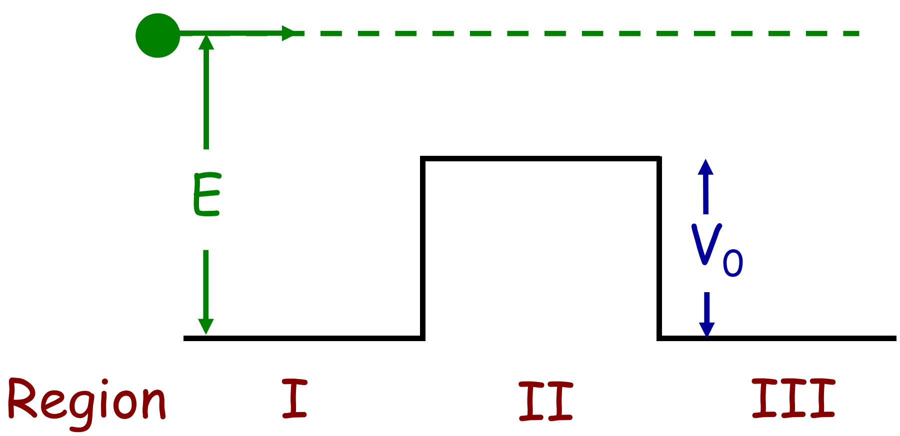


Fig 6.11, pg 223

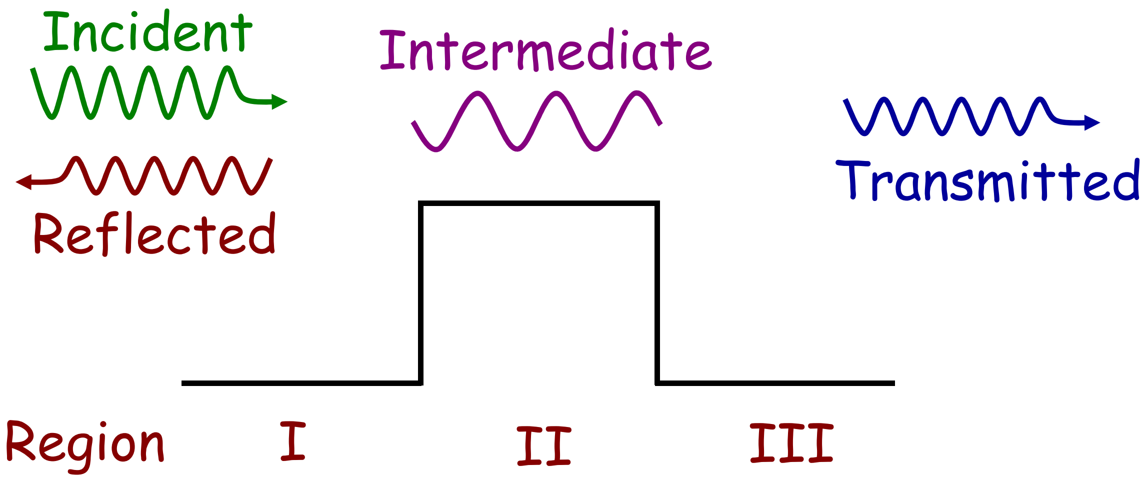
Barriers and Tunneling

A particle of total energy E approaches a change in potential V_0. Assume $E>V_0$:



Classically, the particle slows down over the barrier, but it always makes it past into region III.

Quantum Mechanically, there are finite probabilities of the particle being reflected as well as transmitted.



Solutions:

Incident Reflected

I $\quad \psi_I = A\,e^{ikx} + B\,e^{-ikx}$

II $\quad \psi_{II} = C\,e^{ik'x} + D\,e^{-ik'x}$ Intermediate

III $\quad \psi_{III} = F\,e^{ikx}$

Transmitted

with

$$k = \sqrt{2mE/\hbar^2} \qquad\qquad k' = \sqrt{2m(E-V_0)/\hbar^2}$$

Coefficients determined by continuity of ψ and derivative at boundaries.

The probability of reflection is

$R = |B|^2 / |A|^2$

The probability of transmission is

$T = |F|^2 / |A|^2$

In general there will be some reflection and some transmission.

The result for transmission probability is

$$\frac{1}{T} = 1 + \frac{V_0^2 \sin^2(k'L)}{4E(E - V_0)}$$

(Note T=1 for $k'L = n\pi$, $n = 1, 2, 3, \ldots$)

If $E<V_0$ ⟶ no transmission classically.

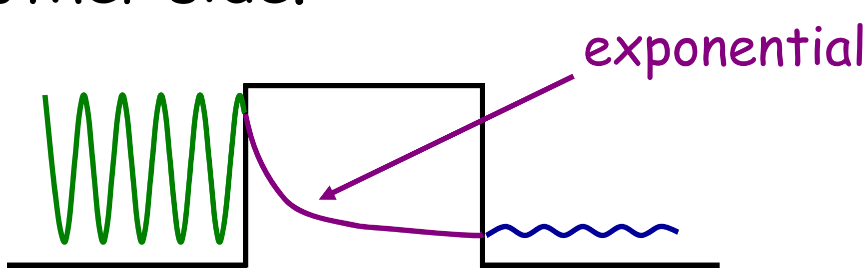
But in QM, probability of transmission is nonzero.

For $E<V_0$ intermediate wavefunctions are:

$$\psi_{II} = C\, e^{\alpha x} + D\, e^{-\alpha x}$$

where $\alpha^2 = 2m(V_0-E)/\hbar^2$

The intermediate solution decays exponentially, but there is a finite probability for the particle to emerge on the other side.



This process is called tunneling.

The probability for transmission is

$$\frac{1}{T} = \left[1 + \frac{V_0^2 \sinh^2(\alpha L)}{4E(V_0 - E)} \right]$$

for $\alpha L >> 1$

$$T \approx 16\,(E/V_0)\,(1-E/V_0)\,e^{-2\alpha L}$$

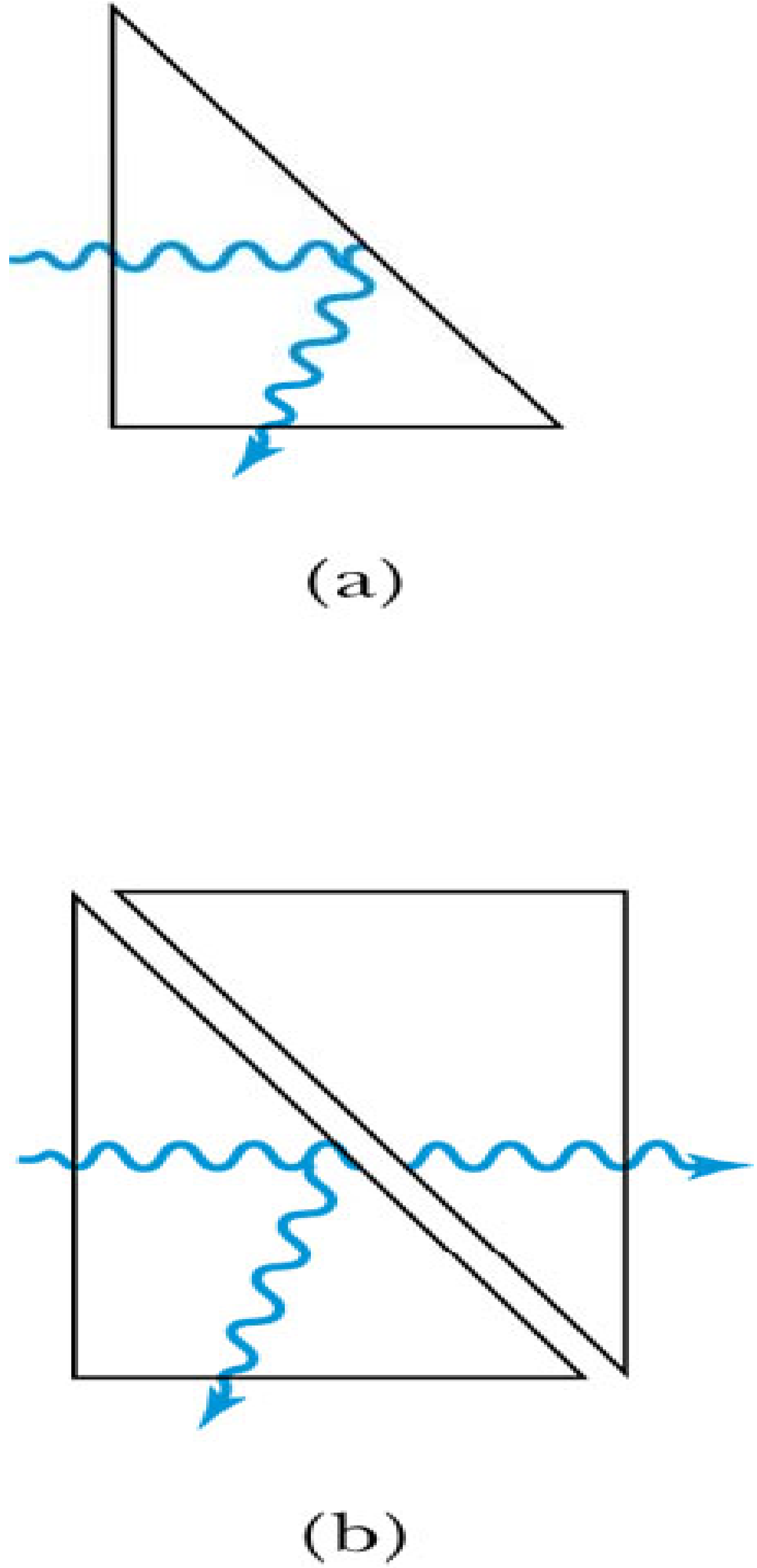
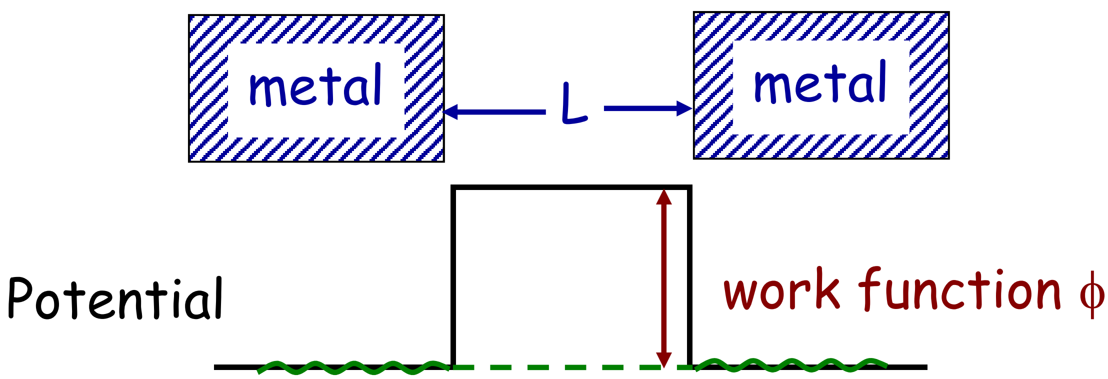


Fig 6.16, pg 229

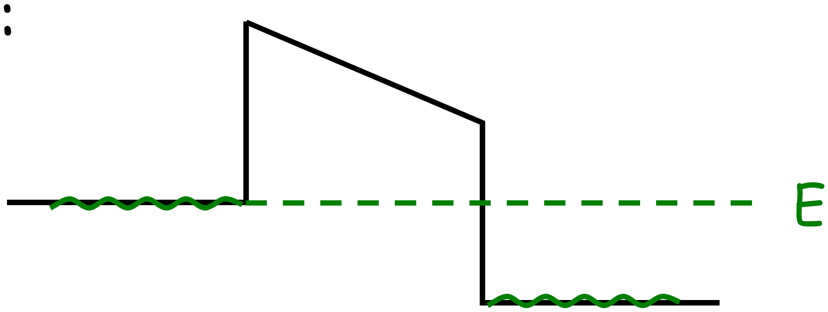
Applications of tunneling:

1) Scanning Tunneling Microscope

Consider two metals separated by vacuum:



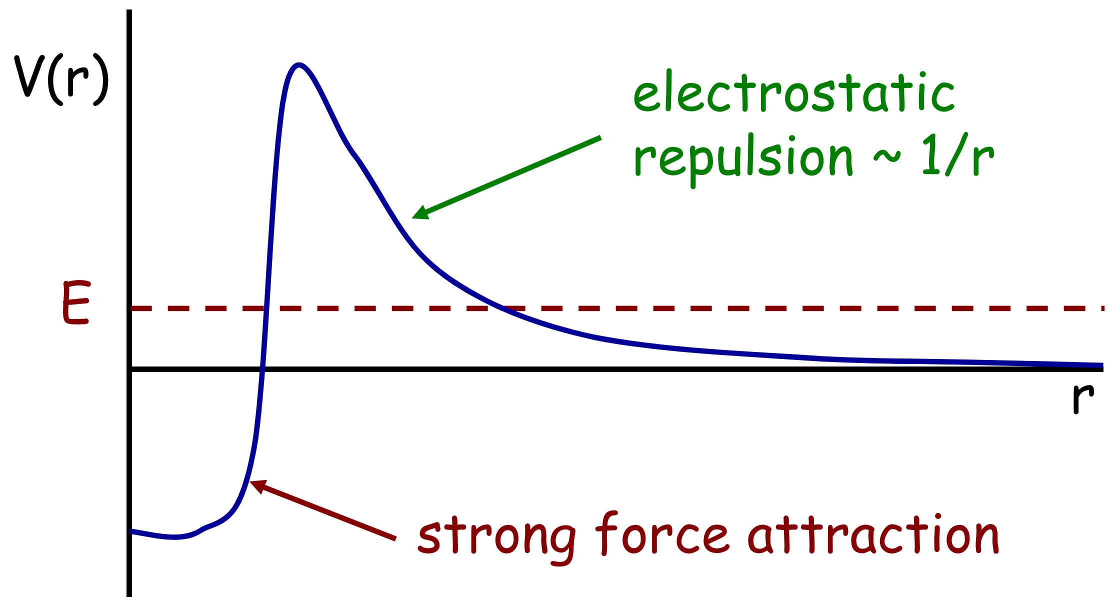
Apply a voltage difference between the metals:



- The current ~ Tunneling Probability
  ~ $e^{-\alpha L}$
- Very sensitive to distance L
- With thin metal probe can map the surface contours of the other metal at the atomic level.

2) Nuclear α-Decay

The potential seen by the α-particle looks like:



Because the decay is limited by the probability of tunneling, small changes in the potential or energy of the α particle lead to large changes in the nuclear lifetime.

^{232}Th $\tau \approx 2 \times 10^{8}$ yr
^{212}Po $\tau \approx 4 \times 10^{-7}$ s

$\Rightarrow$ 22 orders of magnitude!