History of Physics

- Christian Huygens on wave nature of light (~1678)
- Newton's *Principia* for mechanics (~1687)
- Maxwell's *A Dynamic Theory of the Electromagnetic Fields* (~1864)
- Electron was discovered in 1897 (J.J. Thomson)
- A few strange phenomena had to be resolved, but that would be a matter of time

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Key points of this chapter

- Where and why did classical mechanics fail?
- Photoelectric effect: photons behave as particles
- Duality principle of de Broglie
- Davisson-Germer experiment
- Uncertainty relation of Heisenberg
- Schrodinger's Wave equation
- Pauli's exclusion principle

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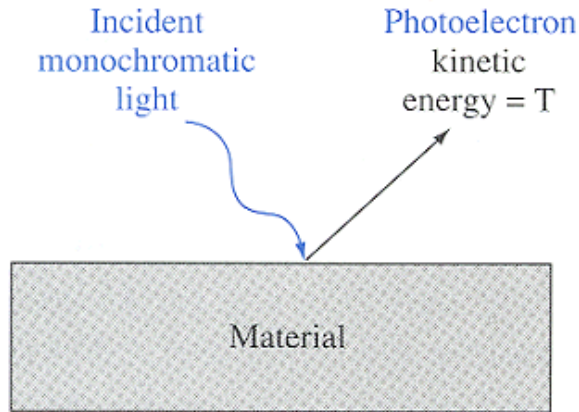Max Planck (1858–1947).

h= Planck's constant

$6{,}625*10^{-34}$ Js

Proposed that electromagnetic energy is emitted only in quantized form and is always a multiple of smallest unit $E = h\square$, where $\square$ is the frequency of emitted radiation.
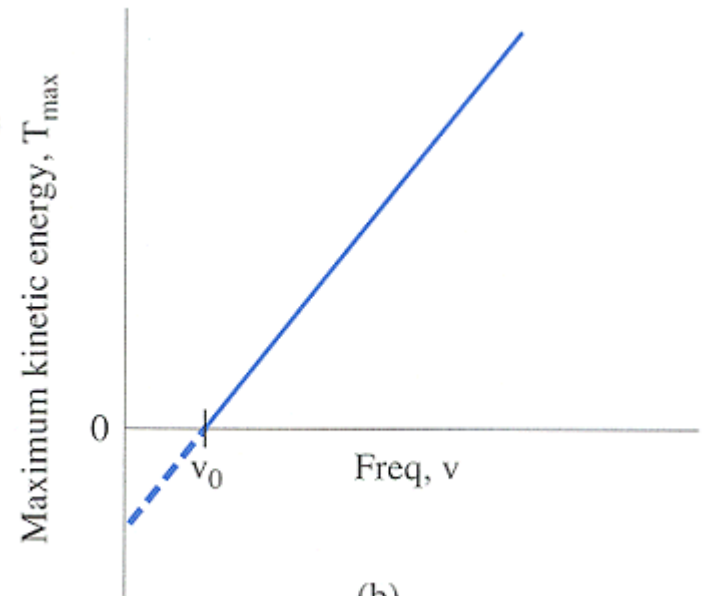
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In 1900:
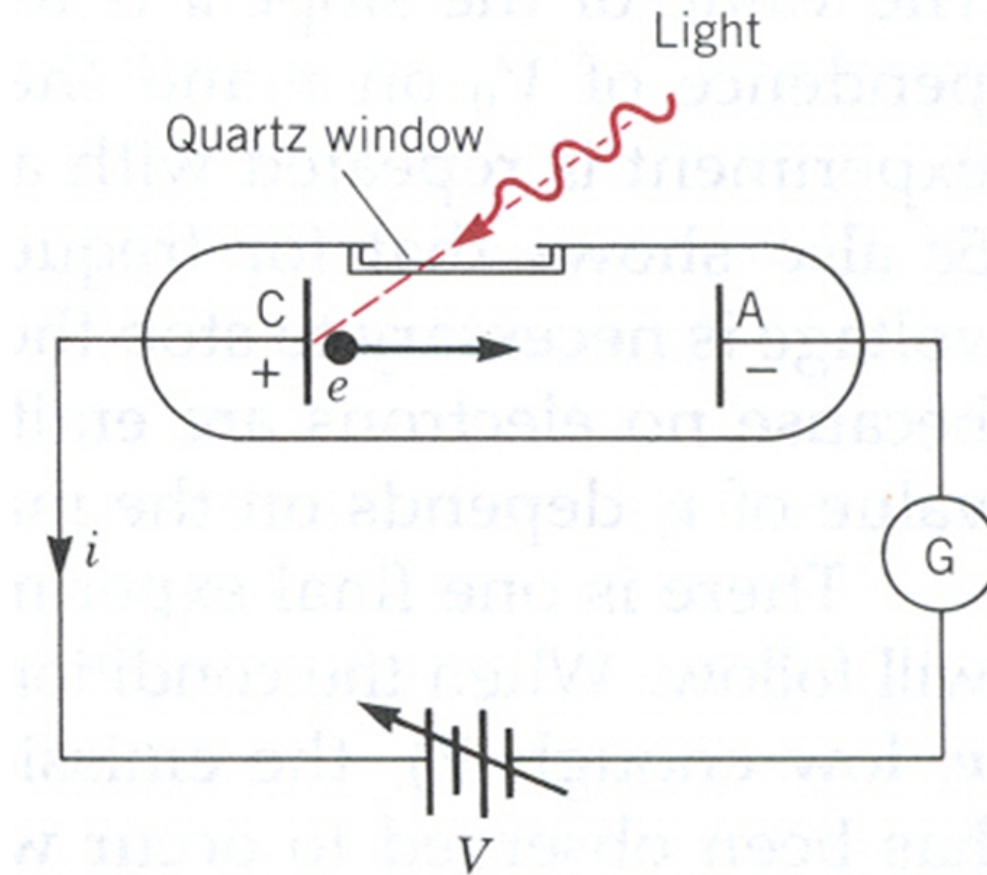
Experimental setup for the study of photoelectric effect

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Observations of photoelectric effect

(a)

Photoelectric effect

(b)

The maximum kinetic energy of photoelectrons as a function of incident frequency.

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Observations :

- When monochromatic light is incident on a clean surface of a material photoelectrons are emitted from the surface.

- According to classical physics, if light intensity is high enough to overcome work function, photoelectron should be emitted. But this is not always observed.

- Max kinetic energy (T_{max}) of electron   ∝   Frequency of incident light $\big|$ $\square > \square_0$

- Rate of photoelectron emission   ∝   intensity of incident light

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Einstein's explation

- Light behaves as a particles that transfers its energy to an electron
- The energy of a light particle (photon) is E=hν
- The energy in excess of workfunction (2-5 eV) is converted into kinetic energy of the photoelectrons.

$$T_{\max} = \frac{1}{2}mv^2 = h\nu - h\nu_0 \ (\nu \geq \nu_0)$$

where h$\square_0$ is the work function of the material

But if a photon can behave as a particle, is it also possible that a particle can behave as a wave?

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Someone was thinking about it...

Can we express momentum in terms of wavelength?

Who & where?

de Broglie was a telecom engineer who spent most of his time on top of the Eiffel tower thinking about waves !

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Louis Victor Pierre Raymond duc de Broglie

Born: 15 Aug 1892 in Dieppe, France

Died: 19 March 1987 in Paris, France

Louis de Broglie (1892 – 1987)

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Wave-particle duality principle

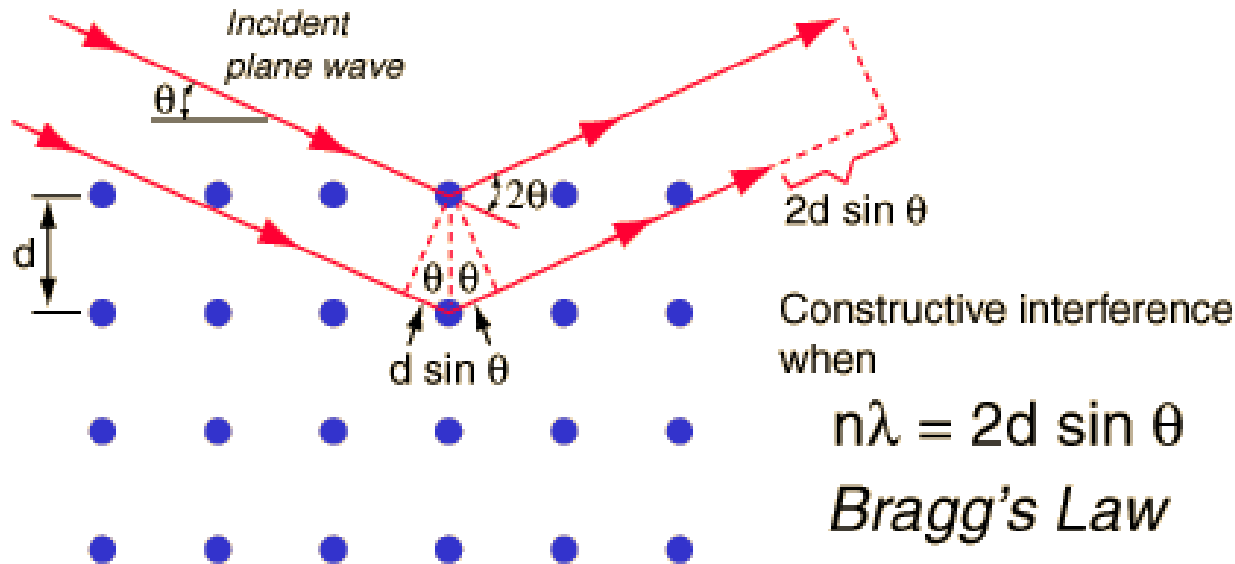From Einstein's special theory of relativity, momentum of a photon is given by -

$$p = h/\lambda$$

de Broglie Hypothesized that wavelength of all particles can also be expressed as –

$$\lambda = h/p$$

This is the duality principle of de Broglie

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Let us look at Bragg's Law first: light interfering with a single crystal
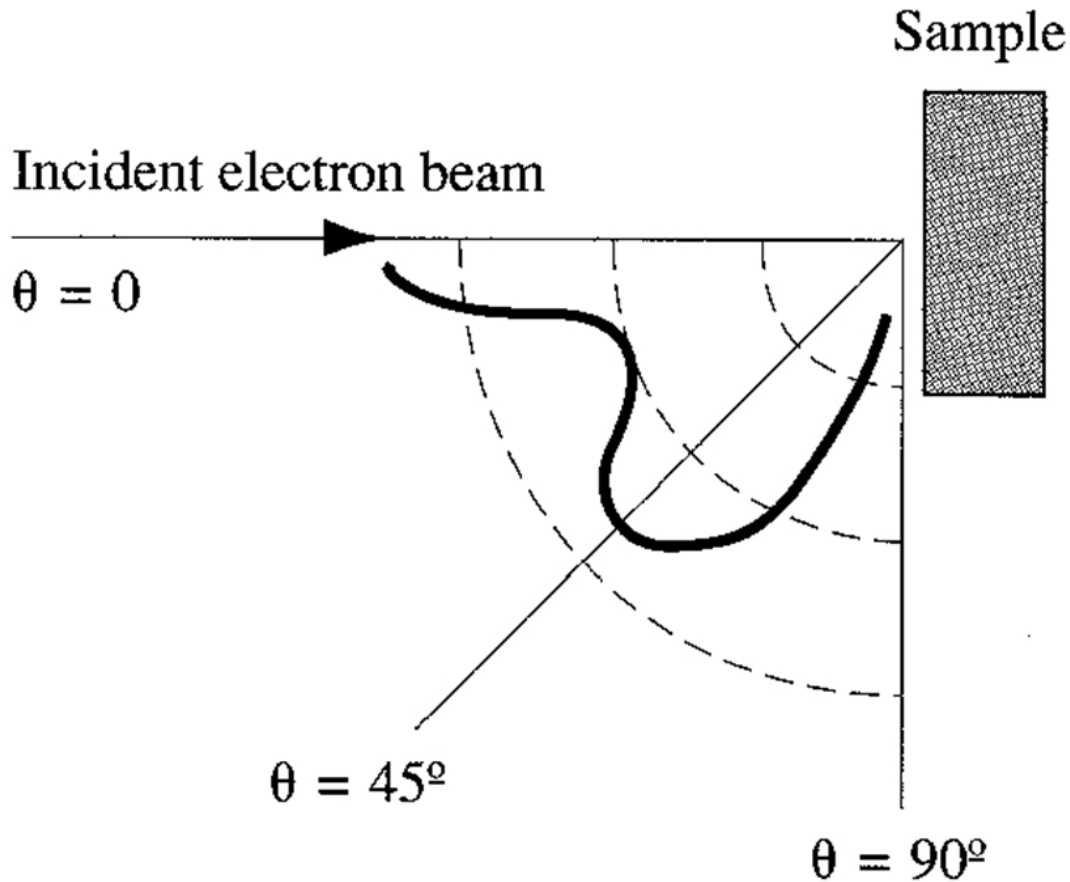

Based on the angle of incidence of light, there is either constructive interference or destructive interference.

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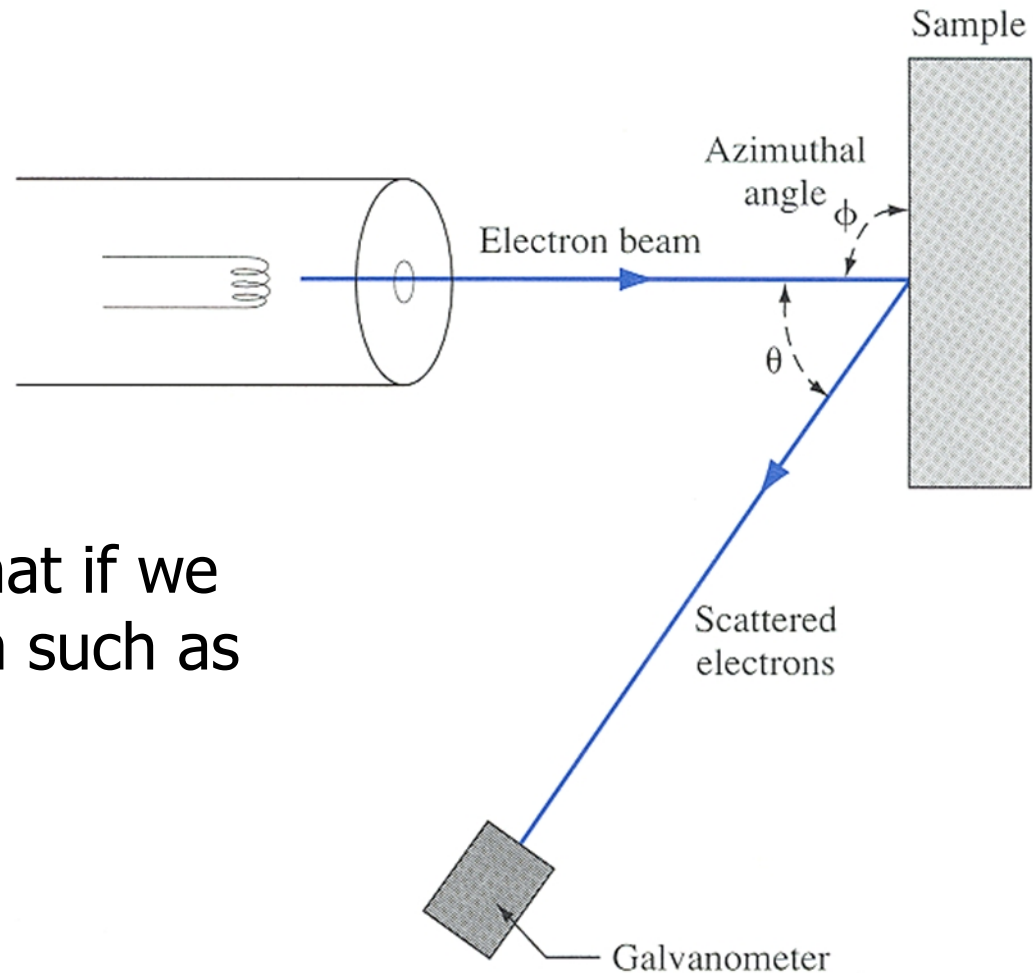
Instead of light, what if we use a particle beam such as electrons?

Experimental arrangement of Davisson-Germer experiment (1927)

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Davisson Germer Experiment

Sample

Incident electron beam

$\theta = 0$

$\theta = 45^\circ$

$\theta = 90^\circ$

Result similar to Bragg reflection (interference)

Scattered electron flux as a function of scattering

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Werner Heisenberg 1901-1976

Friend of Bohr, who was important for nuclear program of allies

Head of German nuclear war program.

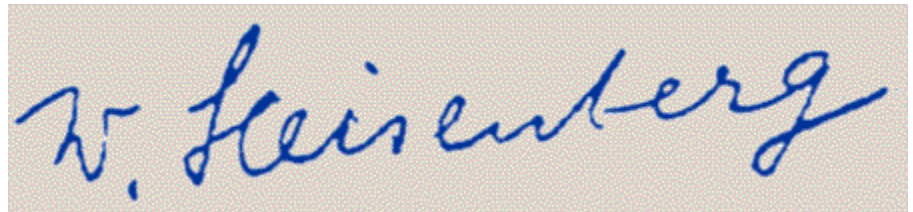Did he do intentionally miscalculations?

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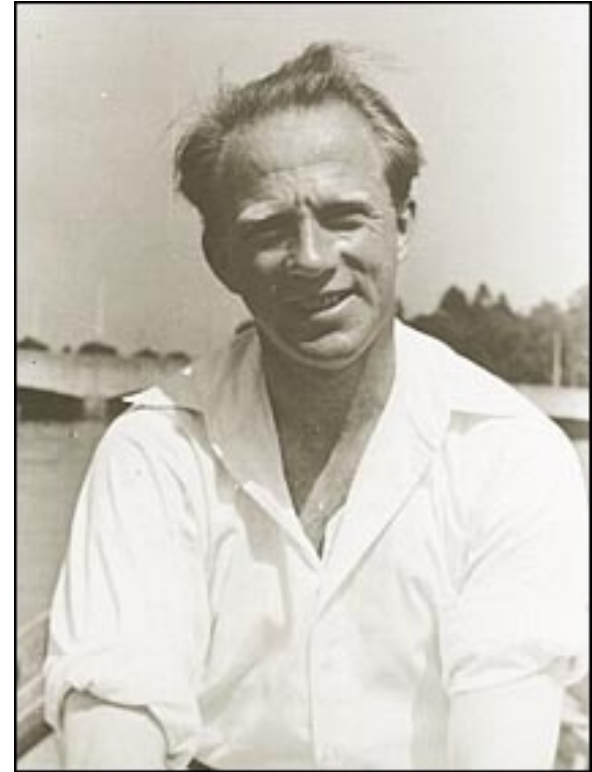
Heisenberg's uncertainty principle (1927):

the **Heisenberg uncertainty principle** states that locating a particle in a small region of space makes the momentum of the particle uncertain; and conversely, that measuring the momentum of a particle precisely makes the position uncertain.

In formula:
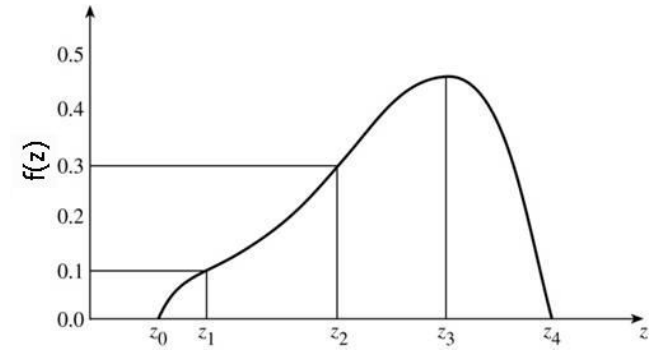$$\Delta p \Delta x \geq \hbar$$
$$\Delta E \Delta t \geq \hbar$$

So we can only express things in terms of probabilities!!!

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Probability

Probability is the likelihood that an event will occur. In our present discussion, probability refers to the likelihood of finding an electron at a certain position

Probability density function (pdf) is a function which gives the probability distribution for all possible locations.

Example : Imagining a one dimensional confinement of electron, if $[z_0, z_4]$ is the set of all possible locations, then f(z) as shown in figure can be the pdf of the electron location.

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Probability

When the set of all possible locations is a continuous range as in this example, the probability of finding the electron at one particular location is zero.
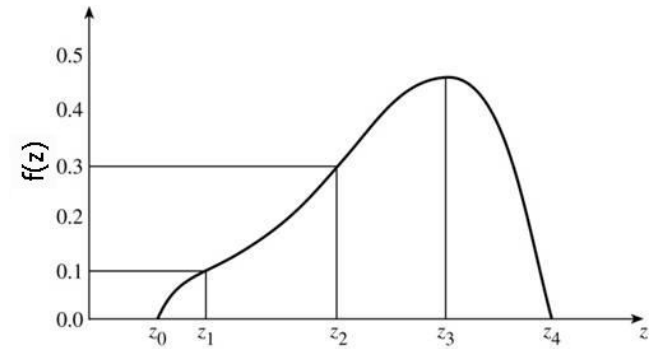
But the probability of finding the electron in a small range say between z_1 and z_1+dz is finite and is given by $f(z_1)dz$

Since the electron is confined between z_0 and z_4,

$$\int_{z_0}^{z_4} f(z)dz = 1$$

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Erwin Schrödinger (1887-1961).

Schrodinger introduced the wave function for any particle, which was later interpreted as the square-root of probability density function of finding the particle at a particular position.

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SCHRODINGER'S WAVE EQUATION

One-dimensional Schrodinger's wave equation-

$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = j\hbar\frac{\partial \Psi(x,t)}{\partial t}$$

Where Ψ(x,t) is the wave function, V(x) is the potential function experienced by the particle, m is the mass of the particle and ħ=h/2Π

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Potential function

Potential here refers to the potential of the electron (electronic potential).

Example : electronic potential of an atom on an electron
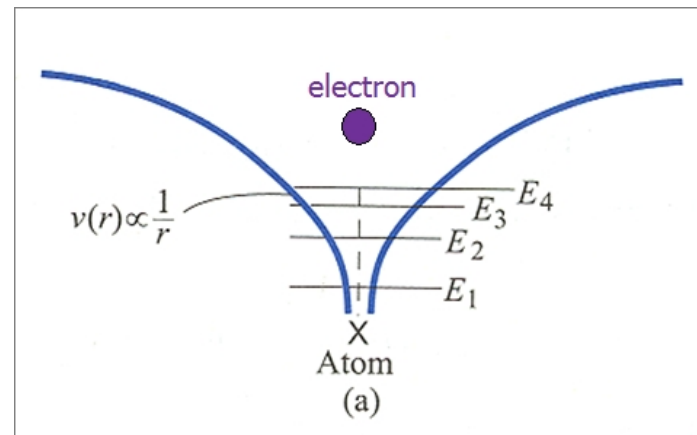
Potential function of an isolated atom

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How to solve the wave equation?

Separation of variables: $\Psi(x, t) = \psi(x)\phi(t)$

Substituting this form into the Schrodinger's equation :

$$\frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = j\hbar \cdot \frac{1}{\phi(t)} \cdot \frac{\partial \phi(t)}{\partial t}$$

$= \text{CONSTANT} = \eta$

Hence we have two differential equations each having one variable only

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$$\eta = j\hbar \cdot \frac{1}{\phi(t)} \cdot \frac{\partial \phi(t)}{\partial t}$$

$$\Phi(t) = e^{-j\left(\frac{\eta}{\hbar}\right)t} \longrightarrow$$ Time dependent portion of wave function

This is an oscillation with radian frequency $\eta/\hbar \Rightarrow \omega = \eta/\hbar$

$\hbar\omega = \eta$, Comparing with equation E=hν, η is the ***TOTAL*** energy **E** of the particle

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From previous slide, η = E

Therefore
$$\frac{-\hbar^2}{2m} \cdot \frac{1}{\psi(x)} \cdot \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

The time-independent Schrödinger wave equation (TISE)

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Physical meaning of the wave function

The time dependent wave function is -

$$\Psi(x, t) = \psi(x)\phi(t) = \psi(x)e^{-j(E/\hbar)t}$$

Hypothesis of Born (1926):

$|\Psi(x,t)|^2 dx$ is the *probability* that the particle can be found in the *interval [x , x + dx]*

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$$|\Psi(x, t)|^2 = \Psi(x, t) \cdot \Psi^*(x, t)$$

$$\Psi(x, t)\psi^*(x, t) = [\psi(x)e^{-j(E/\hbar)t}][\psi(x)e^{+j(E/\hbar)t}]$$

$$= \psi(x)\psi^*(x)$$

$$|\Psi(x, t)|^2 = \psi(x)\psi^*(x) = |\psi(x)|^2$$

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Important potential functions

We first apply Schrodinger's equation to some simple situations, the results of which will be used to analyze more complicated cases later.

●

(a)   (b)   (c)   (d)
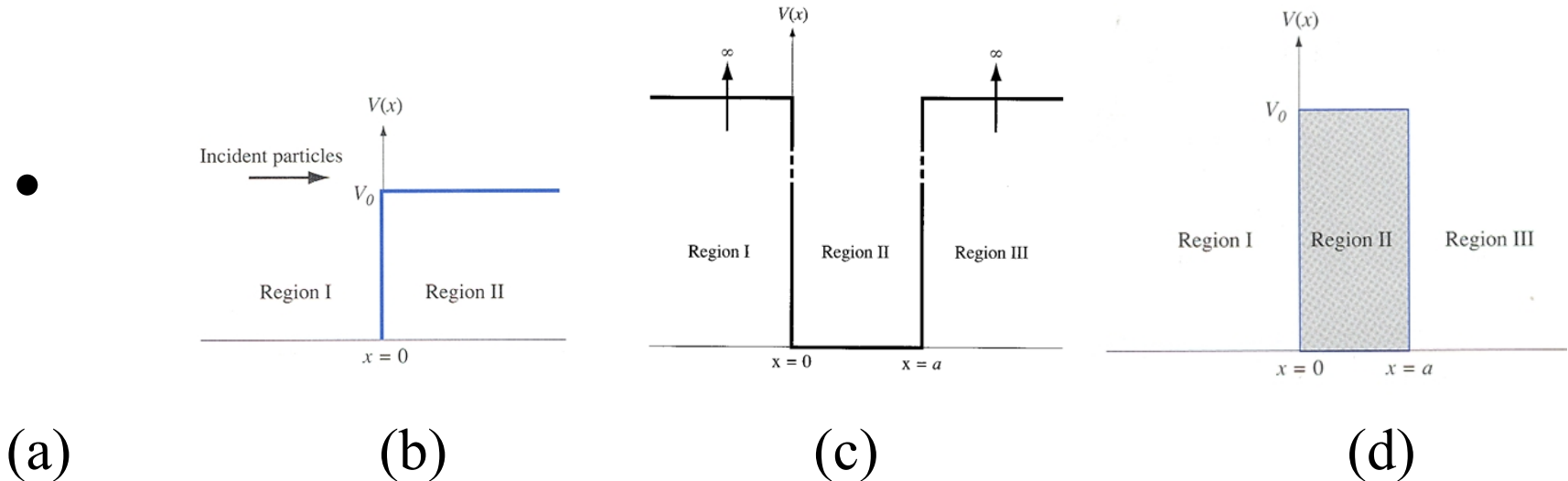
a) Electron in free space, b) The step potential function, c) The infinite potential well and d) The barrier potential function

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Boundary Conditions

Condition 1. $\psi(x)$ must be finite, single-valued, and continuous.

Condition 2. $\partial\psi(x)/\partial x$ must be finite, single-valued, and continuous.

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Examples of functions that are not well-behaved. (a) A function that becomes infinite at $x = x_o$. (b) A function that is not single-valued everywhere. (c) A function with a discontinuity at $x = x_o$.
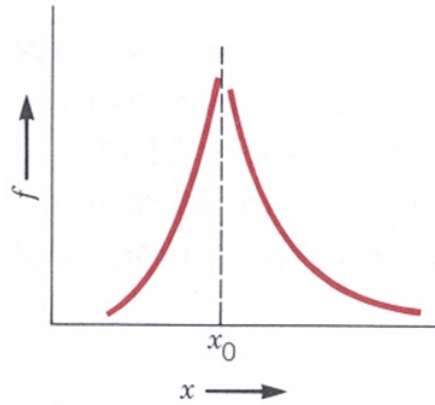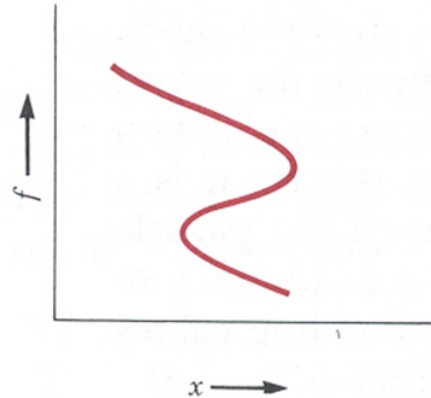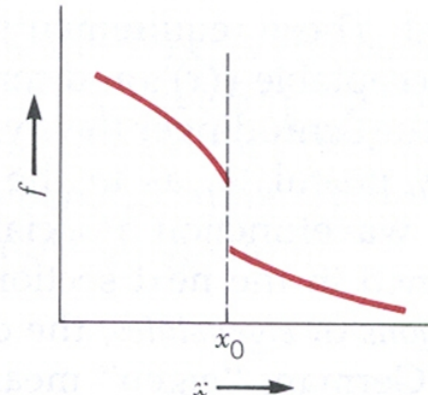
(a)   (b)   (c)

"Probability integral" is infinity

Different probability at the same position

Different probability for left to right and for right to left.

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Before solving the Schrodinger's wave equation it is helpful to consider general solutions for-

$$\frac{\partial^2 \psi(x)}{\partial x^2} - c^2 \psi(x) = 0$$

When $-c^2 > 0$

$$\psi(x) = Ae^{j|c|x} + Be^{-j|c|x}$$

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

When $-c^2 < 0$

$$\psi(x) = Ae^{cx} + Be^{-cx}$$

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Applications of Schrodinger's wave equation

Electron in free space $\Rightarrow$ Potential energy V = 0

•

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

Referring to previous

slide, $|c| = \dfrac{\sqrt{2mE}}{\hbar}$

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$$\psi(x) = A \exp\left[\frac{jx\sqrt{2mE}}{\hbar}\right] + B \exp\left[\frac{-jx\sqrt{2mE}}{\hbar}\right]$$

$$\phi(t) = e^{-j\left(E/\hbar\right)t}$$

Time dependent wave function is then -

$$\Psi(x,t) = A \exp\left[\frac{j}{\hbar}(x\sqrt{2mE} - Et)\right] + B \exp\left[\frac{-j}{\hbar}(x\sqrt{2mE} + Et)\right]$$

This is the equation for a travelling wave.

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General expression for a travelling wave is -

$$\Psi(x, t) = A \exp[j(kx - \omega t)] \qquad k = \frac{2\pi}{\lambda}$$

From previous solution, $k = \dfrac{\sqrt{2mE}}{\hbar}$

$$\lambda = \frac{h}{\sqrt{2mE}} \qquad \lambda = \frac{h}{p}$$

Hence a particle with a well defined energy also has a well defined wavelength and momentum

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The Infinite Potential Well
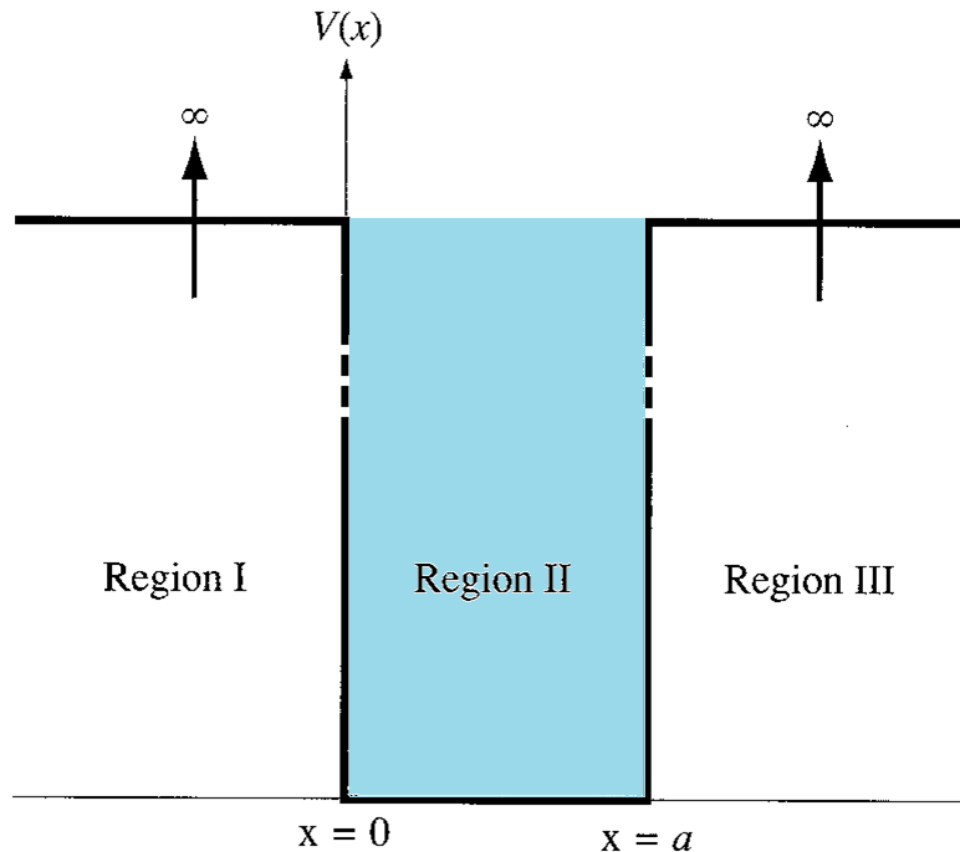
Potential function of the infinite potential well

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TISE $\Rightarrow$ $\quad \dfrac{\partial^2 \psi(x)}{\partial x^2} + \dfrac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$

V(x)$\rightarrow\infty$ and E $\rightarrow$finite,   so Ψ(x)=0 in regions I and III

In region II, where V(x)=0, TISE reduces to -

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

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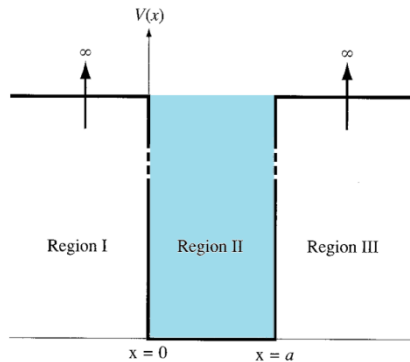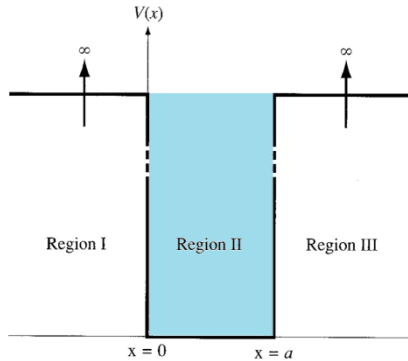
$$\psi(x) = A_1 \cos Kx + A_2 \sin Kx$$

$$K = \sqrt{\frac{2mE}{\hbar^2}}$$

To satisfy boundary condition that Ψ(x) is continuous

$$\psi(x = 0) = \psi(x = a) = 0$$

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$$\psi(x) = A_1 \cos Kx + A_2 \sin Kx$$

boundary condition at

$$\psi(x = 0) = 0 \Rightarrow \mathbf{A_1 = 0}$$

$$\psi(x = a) = 0 \Rightarrow \mathbf{A_2 \sin \textit{Ka} = 0}$$

This results in $Ka = n \, \pi,$

or $K = n \, (\pi/a)$

with n = 1, 2,.......

K = 2 $\pi / \lambda = n \, (\pi/a)$
½λ = a/n
with n = 1, 2,.......

$$\Rightarrow \psi(x) = A_2 \, sin\{ n \frac{\pi}{a} x\}$$

½λ

½λ

½λ

½λ

ψ_n

$x = 0$ $x = a$

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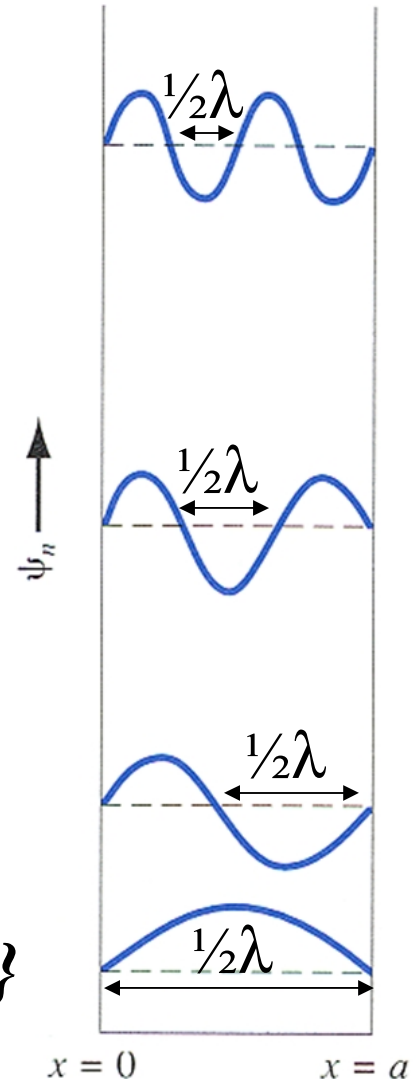
$$K = \frac{n\pi}{a} \quad \text{and} \quad K = \sqrt{\frac{2mE}{\hbar^2}}$$
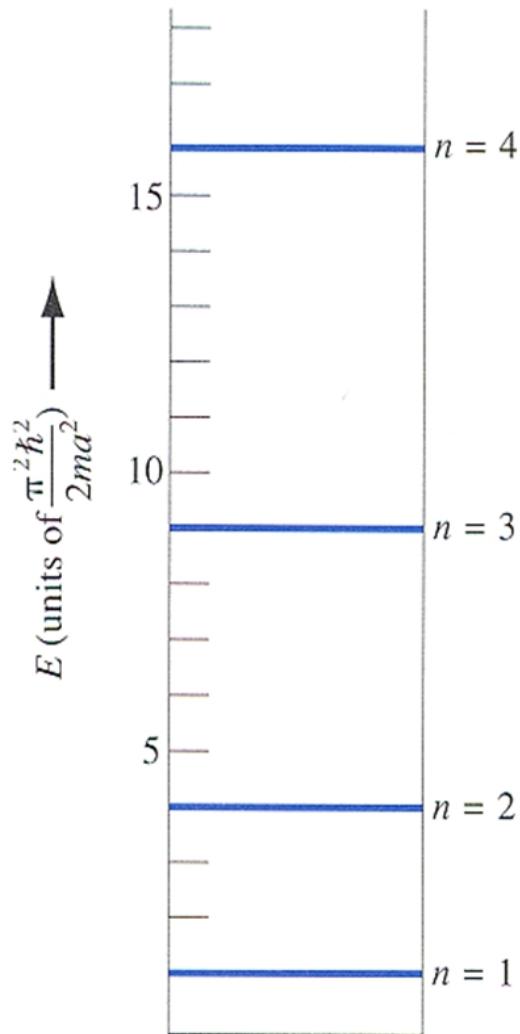
$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

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

$$n = 1, 2, 3, \ldots$$

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Since particle can only exist between x=0 and x=a,

$$\int_0^a \Psi(x)\Psi^*(x)dx = 1$$

V(x)

∞   ∞

Region I   Region II   Region III

x = 0   x = a

$$\psi(x) = A_2 \sin Kx \rightarrow real\ function$$

$$\psi(x) = \psi^*(x)$$

$$\int_0^a A_2^2 \sin^2 Kx\,dx = 1$$

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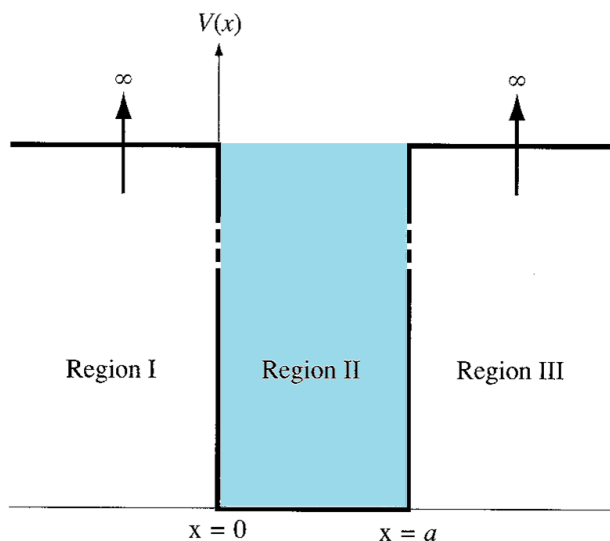
$$\Rightarrow \quad A_2 = \pm\sqrt{\frac{2}{a}}, \pm j\sqrt{\frac{2}{a}}$$

Any of these values → same conclusions

For simplicity we take $A_2 = +\sqrt{\frac{2}{a}}$

$$\psi(x) = \sqrt{\frac{2}{a}}\sin Kx$$

$$\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \quad n = 1, 2, 3, \ldots$$

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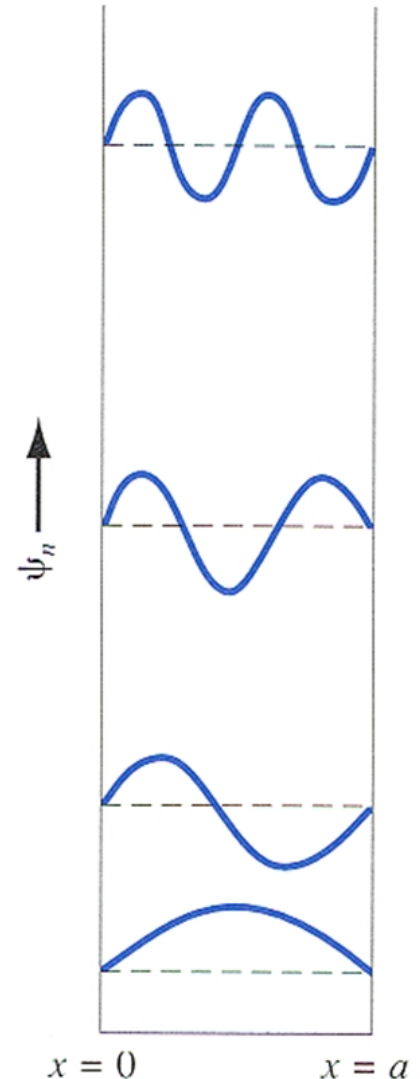
Particle in an infinite potential well
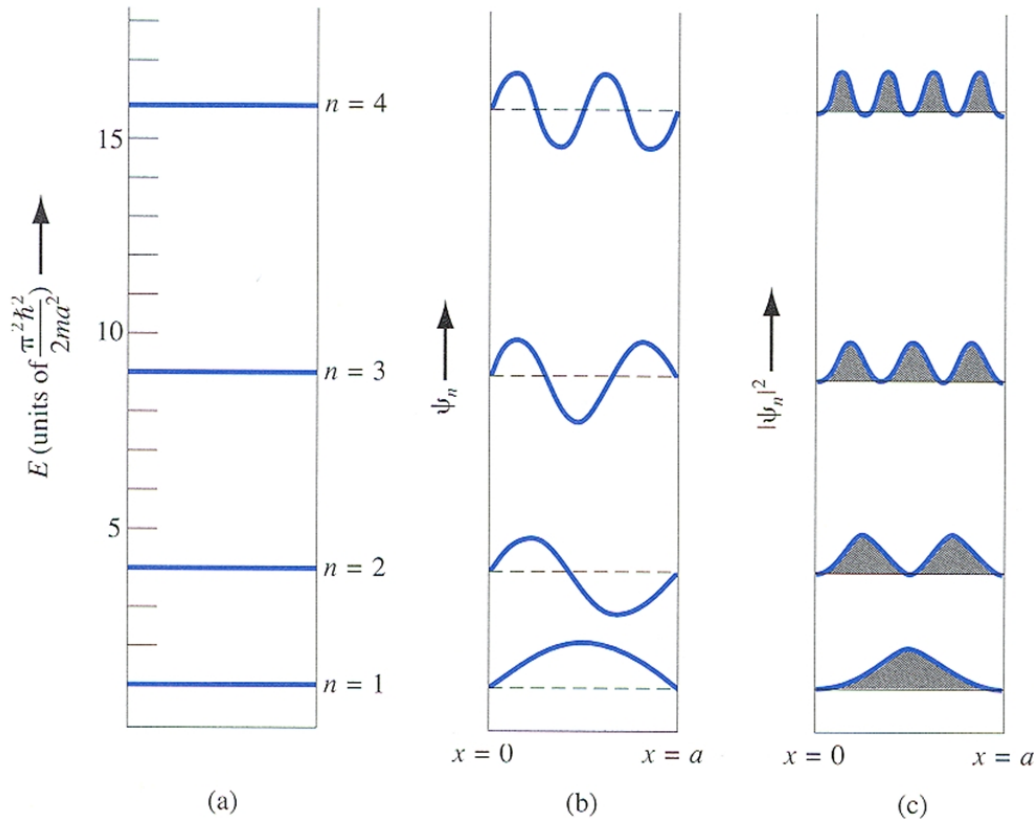
a) Four lowest discrete energy levels, b) corresponding wave functions and c) corresponding probability functions

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The Step Potential Function

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

Energy of incident particle $E < V_0$

Incident particles →

$V(x)$

V_0

in region I, in which $V = 0$ In region II, the potential is $V = V_0$.

Region I   Region II

$x = 0$

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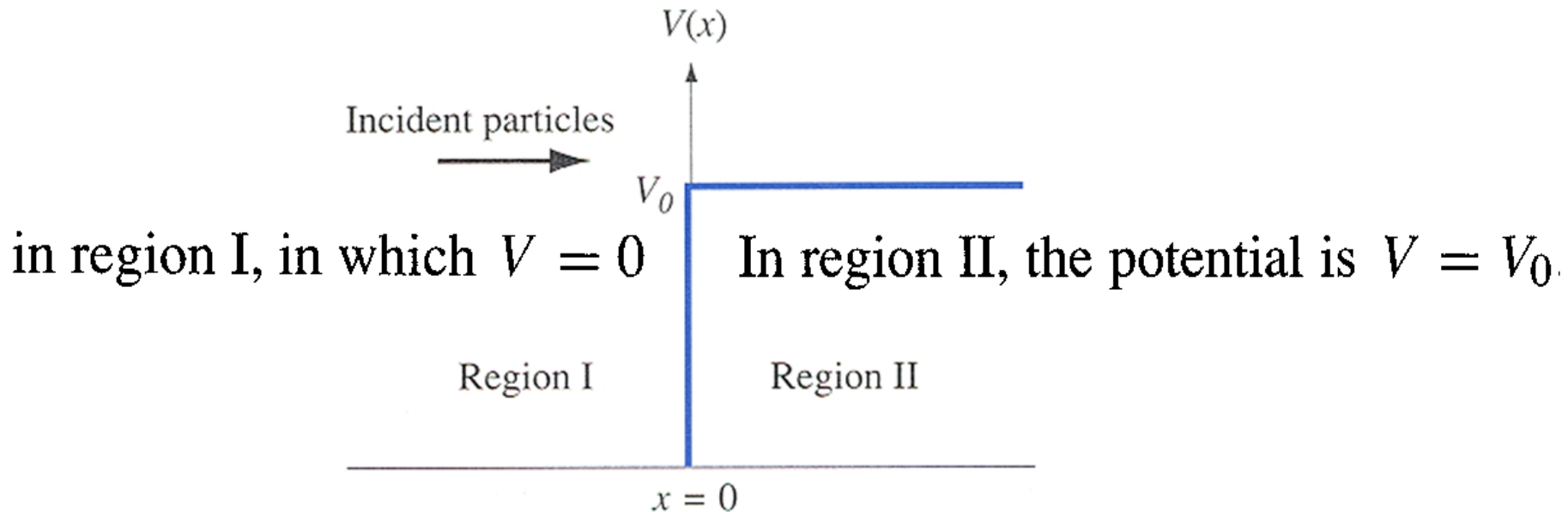
TISE → $$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

In region I, V=0 → $$\frac{\partial^2 \psi_1(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi_1(x) = 0$$

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} (x \leq 0) \qquad K_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

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$$A_1 e^{jK_1 x} \longrightarrow$$

$$B_1 e^{-jK_1 x} \longleftarrow$$

Incident particles $\longrightarrow$

$V(x)$

V_0

Region I   Region II

$x = 0$
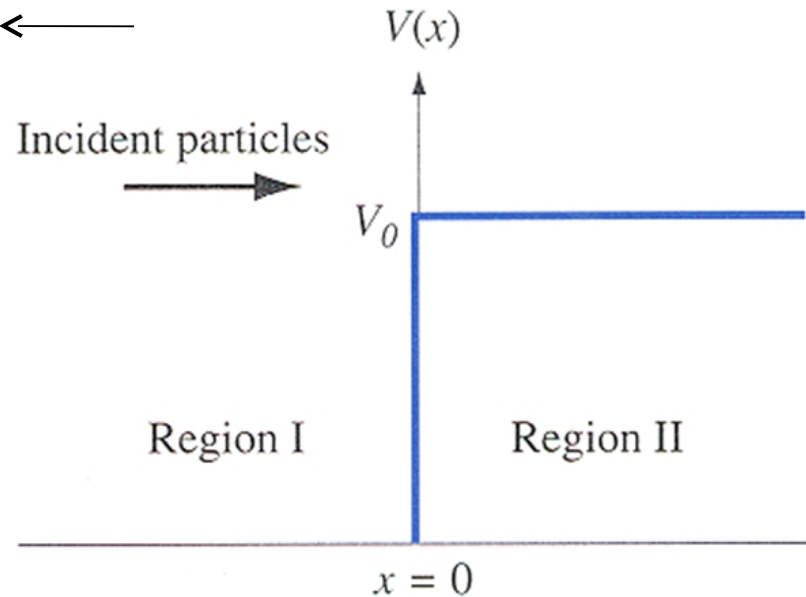
In $A_1 e^{j(k_1 x - \frac{\eta}{\Box} t)} \longrightarrow$ A given phase moves towards +x as time progresses → wave travelling in +x direction

Similarly $B_1 e^{-j(k_1 x + \frac{\eta}{\Box} t)} \longrightarrow$ wave travelling in -x direction

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In region II, $V=V_0$ and we assume $E<V_0$

$$\frac{\partial^2 \psi_2(x)}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2(x) = 0$$

$$\psi_2(x) = A_2 e^{-K_2 x} + B_2 e^{+K_2 x} \; (x \geq 0)$$

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

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in region I, in which $V = 0$

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \quad (x \leq 0) \qquad K_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

In region II, the potential is $V = V_0$. $\quad E < V_0$

$$\psi_2(x) = A_2 e^{-K_2 x} + B_2 e^{+K_2 x} \quad (x \geq 0)$$

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$V(x)$

Incident particles

V_0

Region I

Region II

$x = 0$

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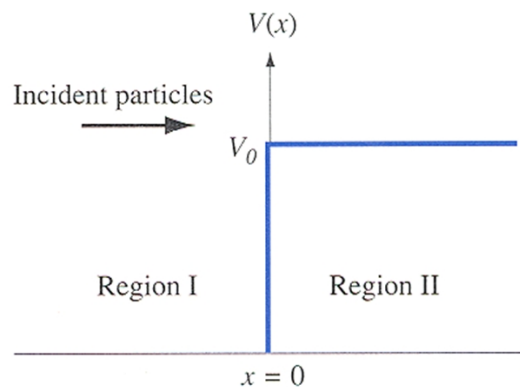
$$\psi_2(x) = A_2 e^{-K_2 x} + B_2 e^{+K_2 x} \ (x \geq 0)$$

$\Psi_2(x)$ must remain finite even as x $\rightarrow \infty$ $\rightarrow$ $B_2 = 0$

$$\psi_2(x) = A_2 e^{-K_2 x} \ (x \geq 0)$$

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$$\text{Reg I} \Rightarrow \psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \, (x \leq 0)$$

$$\text{Reg II} \Rightarrow \psi_2(x) = A_2 e^{-K_2 x} \, (x \geq 0)$$

The wave function at $x = 0$ must be continuous

$$\psi_1(0) = \psi_2(0) \quad \rightarrow \quad A_1 + B_1 = A_2$$

$V(x)$

Incident particles →

V_0

Region I

Region II

$x = 0$

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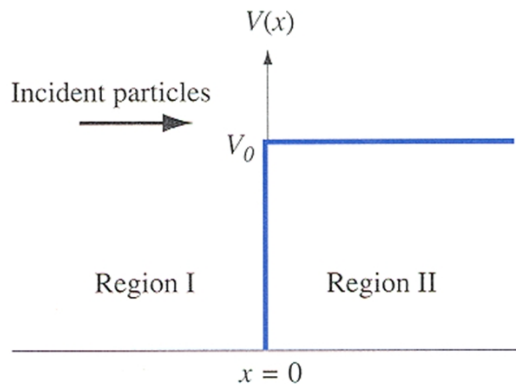
$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \ (x \leq 0)$$

$$\psi_2(x) = A_2 e^{-K_2 x} \ (x \geq 0)$$

V(x)

Incident particles

V_0

Region I

Region II

$x = 0$
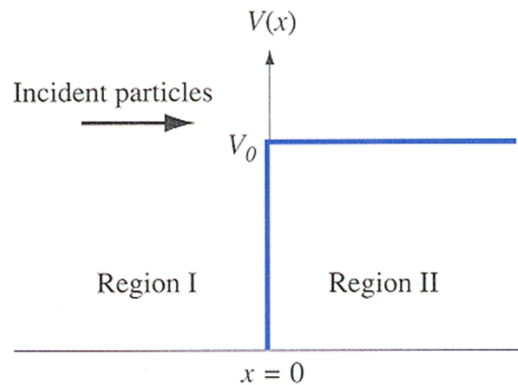
The first derivatives of the wave functions must also be continuous at x=0

$$\left.\frac{\partial \psi_1}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_2}{\partial x}\right|_{x=0}$$

$$jK_1 A_1 - jK_1 B_1 = -K_2 A_2$$

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$$\psi_1(0) = \psi_2(0) \quad \Rightarrow \quad A_1 + B_1 = A_2$$

$$\left.\frac{\partial \psi_1}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_2}{\partial x}\right|_{x=0} \quad \Rightarrow \quad jK_1A_1 - jK_1B_1 = -K_2A_2$$

Two equations and three unknowns ! So we cannot solve for all three but we can express two co-efficients in terms of the remaining one.

$$B_1 = \frac{-(K_2^2 + 2jK_1K_2 - K_1^2)A_1}{(K_2^2 + K_1^2)} \qquad A_2 = \frac{2K_1(K_1 - jK_2)A_1}{(K_2^2 + K_1^2)}$$

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What is the form of ψ_1 and ψ_2?
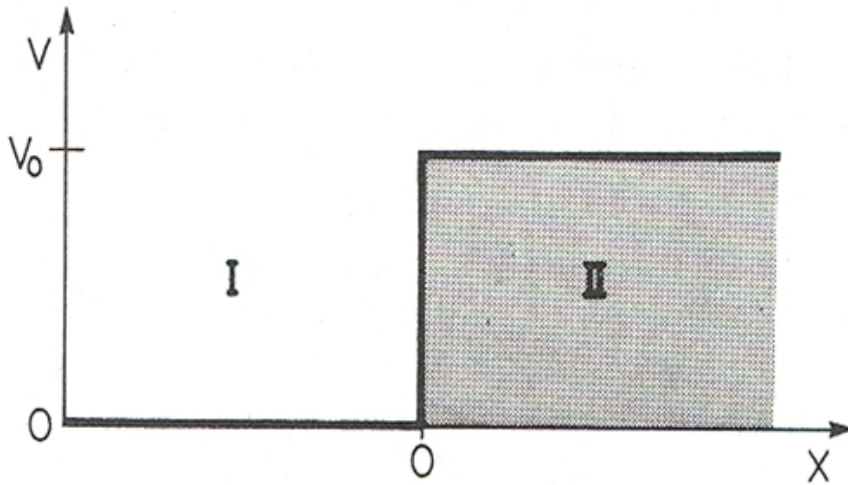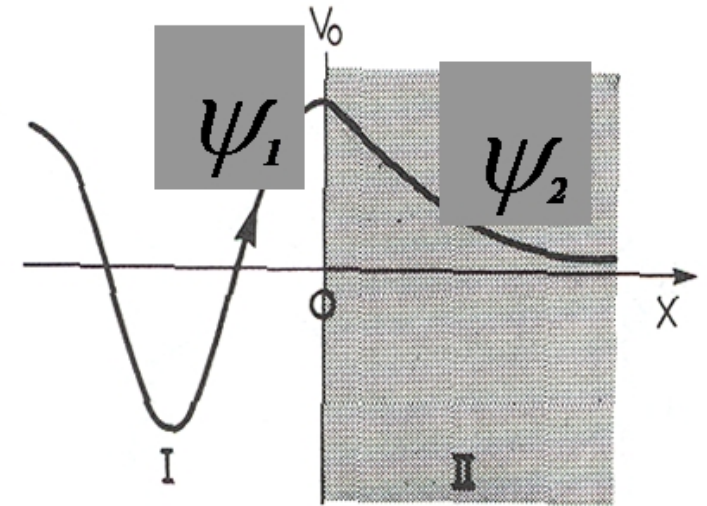
Potential barrier

Wave function at potential barrier

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$$B_1 = \frac{-(K_2^2 + 2jK_1K_2 - K_1^2)A_1}{(K_2^2 + K_1^2)}$$
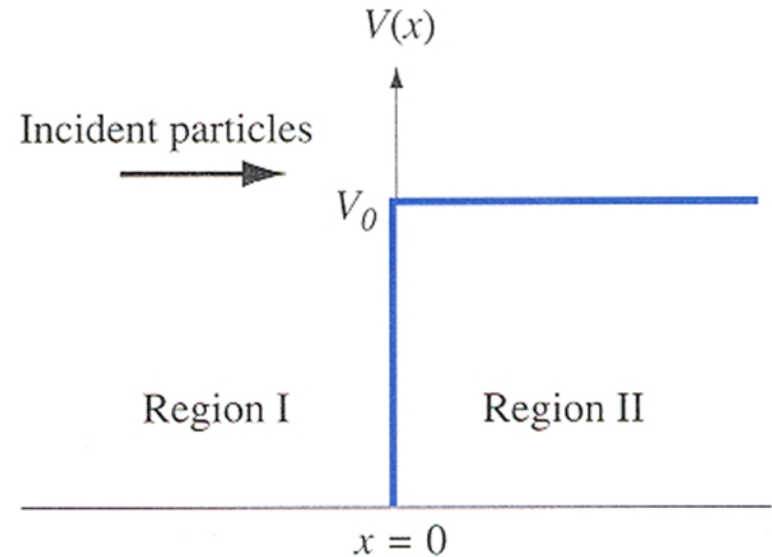
The probability density function of the reflected wave is -

$$B_1 \cdot B_1^* = \frac{(K_2^2 - K_1^2 + 2jK_1K_2)(K_2^2 - K_1^2 - 2jK_1K_2)A_1 \cdot A_1^*}{(K_2^2 + K_1^2)^2}$$

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Reflection coefficient = R = $\dfrac{reflected \text{ flux}}{incident \text{ flux}}$

$$R = \frac{v_r . B_1 . B_1^{*}}{v_i . A_1 . A_1^{*}}$$

Where v_i and v_r are the velocities of incident and reflected waves.

Now, $K_1 = \sqrt{\dfrac{2mE}{\hbar^2}}$ and $E = 1/2 mv^2$ when $V=0$

Since K_1 applies to both incident and reflected waves in $x \leq 0$,

$$v_r = v_i$$

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$$R = \frac{v_r \cdot B_1 \cdot B_1^*}{v_i \cdot A_1 \cdot A_1^*} = \frac{B_1 \cdot B_1^*}{A_1 \cdot A_1^*}$$

$$R = \frac{B_1 \cdot B_1^*}{A_1 \cdot A_1^*} = \frac{(K_2^2 - K_1^2)^2 + 4K_1^2 K_2^2}{(K_2^2 + K_1^2)^2} = 1.0$$

Total reflection at an arbitrary step function V$_0$, if E<V$_0$

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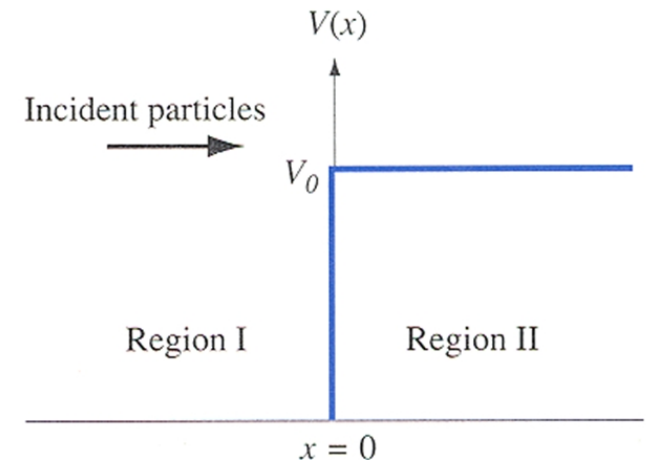
Transmitted wave co-efficient $A_2=A_1+B_1$, hence A_2 is not equal to 0

➔pdf $|\Psi_2(x)|^2$ of finding the particle in region II is not zero

There is finite probability that incident particle will penetrate the potential barrier and exist in region II.

But since reflection coefficient is 1, all particles in region II will eventually turn around and move back into region I.

Quantum mechanical snooker!!!

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The potential barrier

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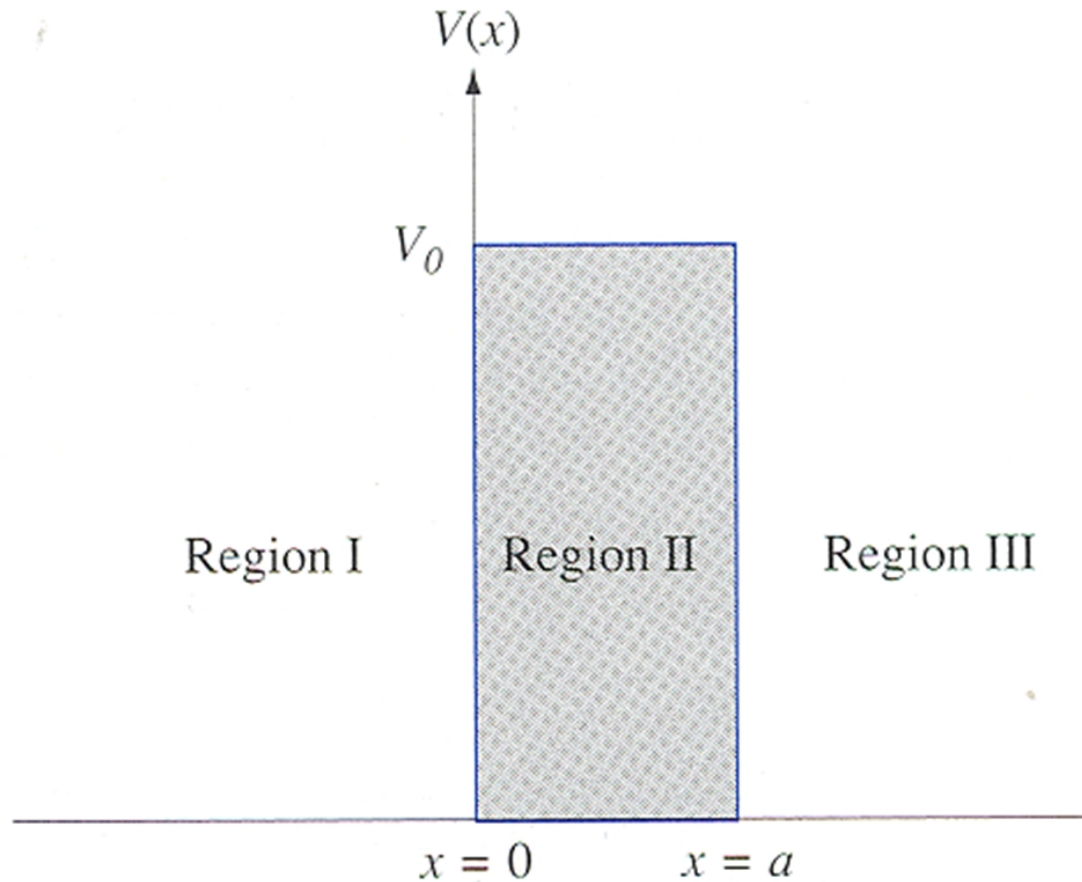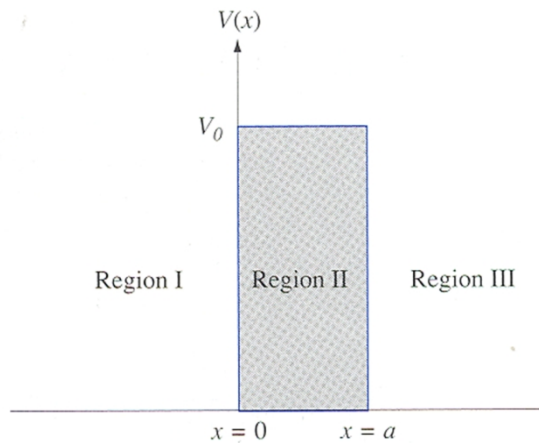
Reg.I: $\quad \psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \quad K_1 = \sqrt{\dfrac{2mE}{\hbar^2}}$

Reg.II: $\quad \psi_2(x) = A_2 e^{K_2 x} + B_2 e^{-K_2 x} \quad K_2 = \sqrt{\dfrac{2m}{\hbar^2}(V_0 - E)}$

Reg.III: $\quad \psi_3(x) = A_3 e^{jK_1 x} + B_3 e^{-jK_1 x}$

(since regions I and III are $K_3 = K_1$)

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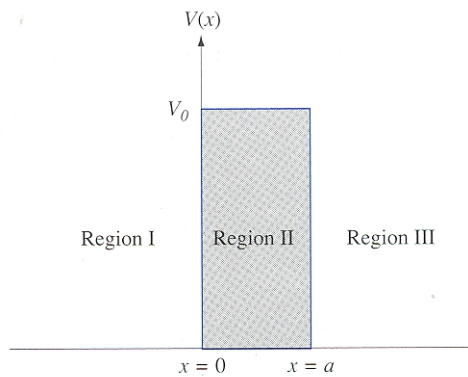
Figure 2.7 The potential barrier function

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x}$$

$$\psi_2(x) = A_2 e^{K_2 x} + B_2 e^{-K_2 x}$$

$$\psi_3(x) = A_3 e^{jK_1 x} + B_3 e^{-jK_1 x}$$

Boundary conditions:

ψ_3 can have component only in +x direction

hence $B_3 = 0$;

At x = 0:

$$\psi_1(0) = \psi_2(0); \quad \frac{\partial}{\partial x}\psi_1(0) = \frac{\partial}{\partial x}\psi_2(0)$$

At x = a:

$$\psi_2(a) = \psi_3(a); \quad \frac{\partial}{\partial x}\psi_2(a) = \frac{\partial}{\partial x}\psi_3(a)$$

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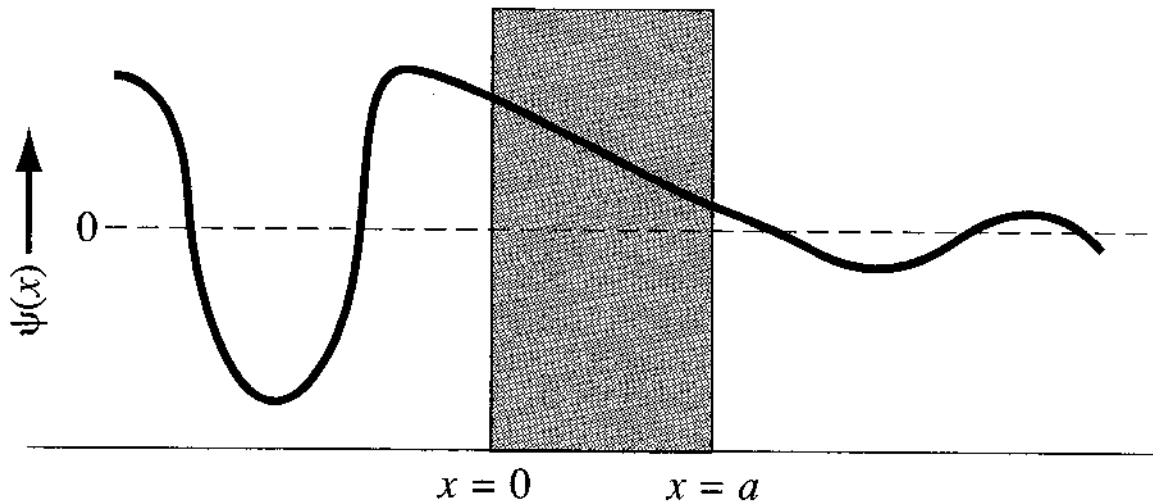
Figure 2.8 The wave functions through the potential barrier

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transmission coefficient $\quad T = \dfrac{v_t \cdot A_3 \cdot A_3^*}{v_i \cdot A_1 \cdot A_i^*} = \dfrac{A_3 \cdot A_3^*}{A_1 \cdot A_1^*}$

$$T \cong 16\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right)\exp(-2K_2 a)$$

$E \ll V_0$

$K_2 = \sqrt{\dfrac{2m}{\hbar^2}(V_0 - E)}$

- We can see that T is not zero, a result which cannot be explained from classical physics

- T is exponentially dependent on a. Thinner the barrier, higher is the transmission co-efficient.

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Extension of wave theory to atoms.

• For simplicity potential function of one electron atom or hydrogen atom is considered.

•Schrodinger's wave equation to be solved in three dimensions.

•Potential function is spherically symmetric → so use spherical co-ordinates.

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The spherical co-ordinate system

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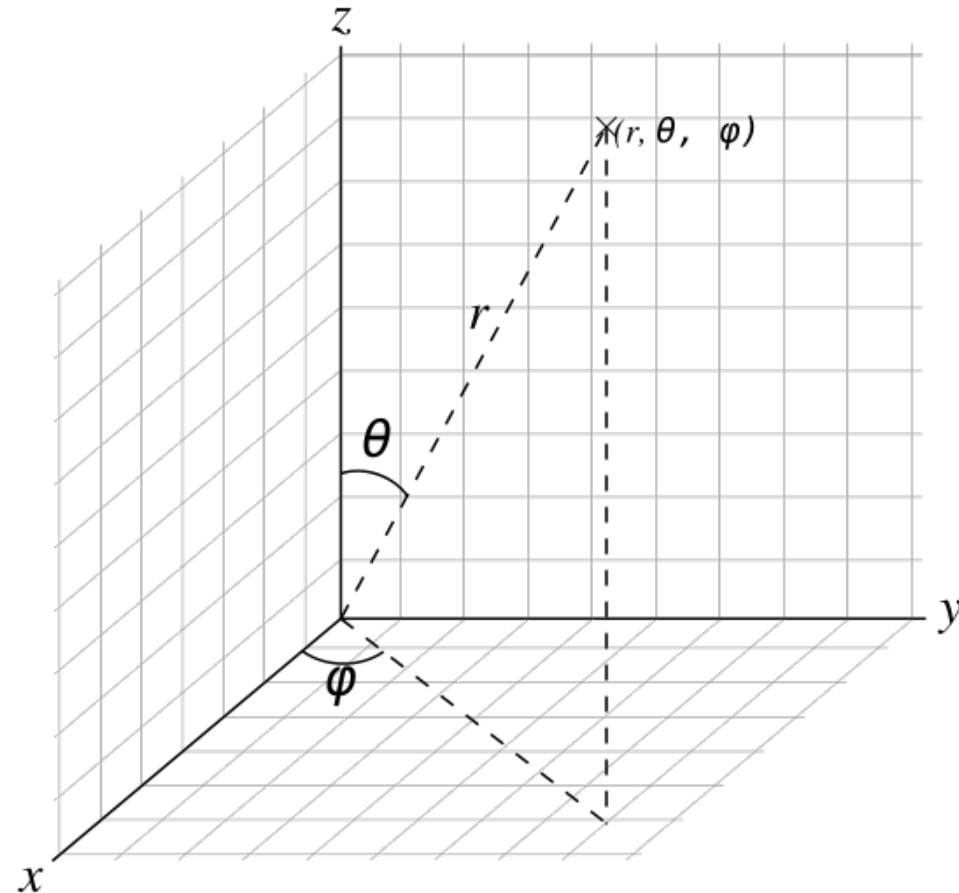
1D:
$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = j\hbar\frac{\partial \Psi(x,t)}{\partial t} \quad \text{[2.4]}$$

CARTESIAN COORDINATES

3D:
$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(x,y,z,t)\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

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TISE in spherical co-ordinates $\longrightarrow$ $\dfrac{\hbar^2}{2m_0}\nabla^2\psi\,(r,\theta,\varphi)+\{E-V(r)\}\psi\,(r,\theta,\varphi)=0$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)$$

Expanding the laplacian operator the TISE in spherical co-ordinates is -

$$\frac{1}{r^2}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)+\frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\Psi}{\partial\varphi^2}+\frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial\Psi}{\partial\theta}\right)+\frac{2m_0}{\hbar^2}\left(E-V(r)\right)\Psi=0$$

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Separation of variables $\longrightarrow$ $\Psi\left(r,\theta,\varphi\right) = R(r)\Theta\left(\theta\right)\Phi\left(\varphi\right)$

Substituting this form of solution, the TISE is -

$$\frac{\sin^2\theta}{R}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\varphi^2} + \frac{\sin\theta}{\Theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial\Theta}{\partial\theta}\right) + r^2\sin^2\theta\,\frac{2m_0}{\hbar^2}\left(E-V\right) = 0$$

Each term is a function of only one of r, θ and φ. Grouping terms of the same variable and equating to a constant we can get three equations.

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The equation for φ can be written as -

$$\frac{1}{\Phi} \cdot \frac{\partial^2 \Phi}{\partial \phi^2} = -m^2 \quad \Rightarrow \quad \Phi = e^{jm\varphi}$$

Wave function should be single valued → m=0,±1, ±2, ±3

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Similarly the equations in r and θ can be solved in terms of constants n and l. The separation of variables constants n, l and m are known as principal, azimuthal (orbital) and magnetic quantum numbers and related by –

n=1,2,3…   l=n-1,n-2,n-3,…0 |m|=l,l-1,…,0

Each set of quantum numbers → a quantum state which an electron can occupy

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Electron energy can be written as –

$$E_n = \frac{- m_0 e^4}{\left(4\pi \, \varepsilon_0^{\,2}\right) 2\hbar^2 n^2}$$

where m_0 is the electron mass and n is the principal quantum number.

• Energy is negative → electron is bound to nucleus

• n is integer → Energy can have only discrete values.

• electron being bound in a finite region of space → quantized energy

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For the lowest energy state, n=1, l=m=0 and the wave function is given by -

$$\psi_{100} = \frac{1}{\sqrt{\pi}} \cdot \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

(a)
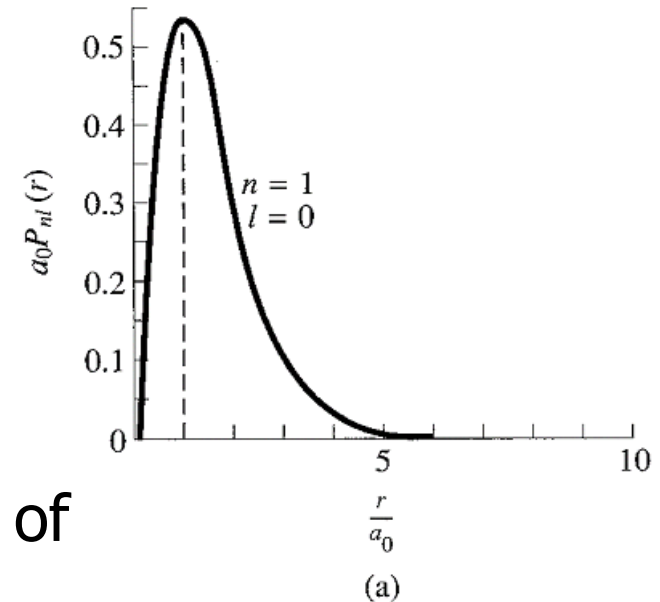
The value of r for which the probability of finding the electron is maximum is -

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_0 e^2} = 0.529 \text{ Å} \quad \longrightarrow \quad \text{Bohr radius}$$

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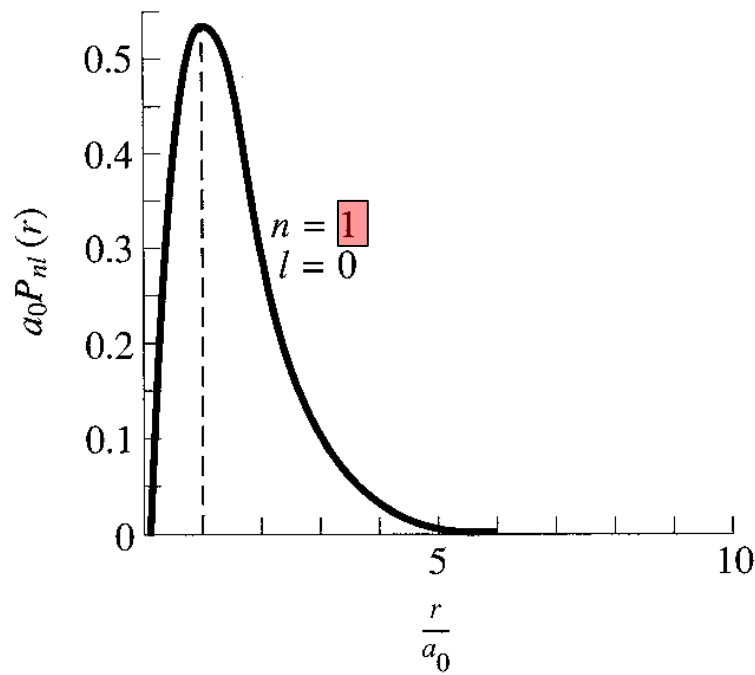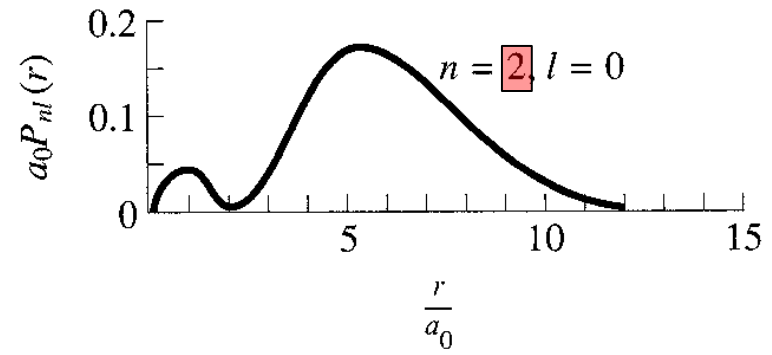
Radial probability density function for the one-electron atom for a) n=1, l=m=0 and b) n=2, l=m=0.

• Radius of second energy shell > radius of first energy shell
• finite (but small) probability that this electron can be at smaller radius.

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One more quantum number !

Every electron has an intrinsic angular momentum or spin. This spin is quantized, designated by spin quantum number **s** and take values **+1/2** or **-1/2**

E_1 E_2

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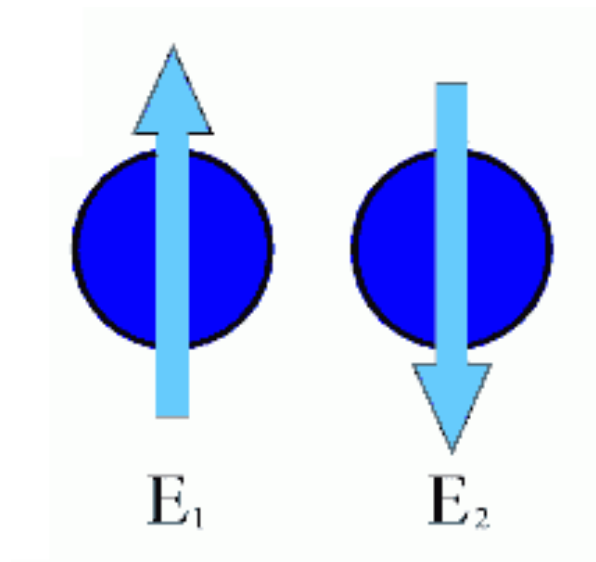
Pauli Exclusion Principle

"no two electrons in any given system (atom, molecule or crystal) can have the same set of quantum numbers"

• This principle not only determines the distribution of electrons in an atom but also among the energy states in a crystal as will be seen later.

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Periodic Table

• In 1869 Mendeleev demonstrated that a periodic relationship existed between the properties of an element and its atomic weight.

•But it was only quantum mechanics which provided a satisfactory explanation for the periodic table of elements.

•Each row in the periodic table corresponds to filling up of one quantum shell of electrons.

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Initial portion of the periodic table

From the concept of quantum numbers and Pauli exclusion principle we can explain the periodic table.

Element	Notation	n	l	m	s
Hydrogen	$1s^1$	1	0	0	$+\frac{1}{2}$ or $-\frac{1}{2}$
Helium	$1s^2$	1	0	0	$+\frac{1}{2}$ and $-\frac{1}{2}$
Lithium	$1s^2 2s^1$	2	0	0	$+\frac{1}{2}$ or $-\frac{1}{2}$
Beryllium	$1s^2 2s^2$	2	0	0	$+\frac{1}{2}$ and $-\frac{1}{2}$
Boron	$1s^2 2s^2 2p^1$	2	1		
Carbon	$1s^2 2s^2 2p^2$	2	1		
Nitrogen	$1s^2 2s^2 2p^3$	2	1	$m = 0, -1, +1$	
Oxygen	$1s^2 2s^2 2p^4$	2	1	$s = +\frac{1}{2}, -\frac{1}{2}$	
Fluorine	$1s^2 2s^2 2p^5$	2	1		
Neon	$1s^2 2s^2 2p^6$	2	1		

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• Hydrogen → single electron in lowest energy state (n=1,l=m=0). However spin can be +1/2 or -1/2

•Helium → two electrons in lowest energy state and this shell is full. Valence energy shell (which mainly determines the chemical activity) is full and hence helium is an inert element.

•Lithium → three electrons. 3rd electron must go into second energy shell (n=2)

•When n=2, l=0 or 1 and when l=1, m=0,±1. In each case s=±½. So this shell can accommodate 8 electrons.

•Neon has 10 electrons and hence the n=2 shell is also full making neon also an inert element.

•Thus the period table can be built. At higher atomic numbers, the electrons begin to interact and periodic table deviates a little from the simple explanation.

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PERIODIC TABLE OF THE ELEMENTS

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