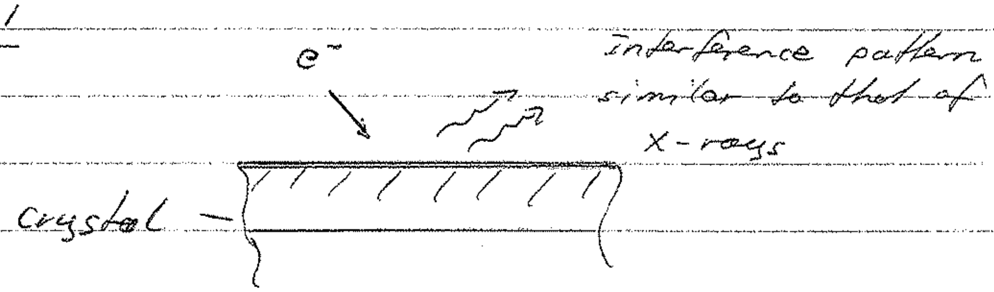
III Concepts of Quantum Mechanics

3.1 Waves and Matter

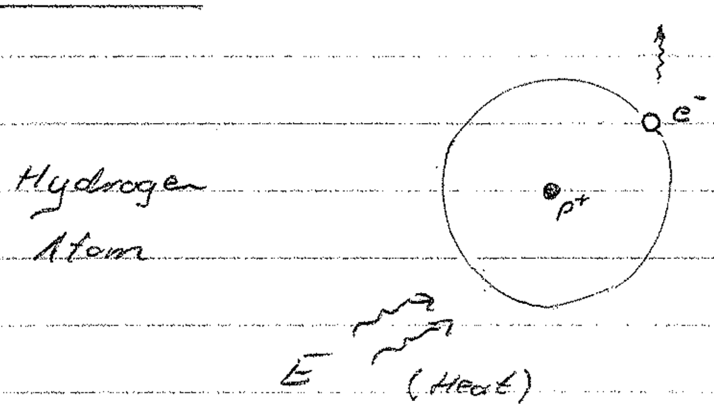
At the beginning of the 20th century, particles and waves were entities that were strictly divided. However, the outcome of some new experiments could not be explained by the methods of classical physics.

Experiment 1



Electrons can be diffracted from a crystal in a manner similar to the diffraction of X-rays. However, instruments recording the diffraction pattern confirm that each "particle" always arrives whole.

Experiment 2



When a hydrogen atom was heated to an elevated temp. and the cooled down again, the emitted light was observed at only certain discrete wavelengths; according to the classical theory, scientists expected a continuum of wavelength.

In order to explain these experiments, a new theory had to be developed. It was called

Quantum Mechanics

Note: QM does not distinguish between waves and particles, it rather combines what we call wave or particle properties to an elementary entity → "Quantum Stuff"

<u>Link between wave and particle scheme:</u>

1) de Broglie $\boxed{\lambda = \frac{h}{p}}$

λ: equivalent wavelength
p: momentum of particle
h: Plank's constant
($h = 6.63 \times 10^{-34}$ Js)

2) Plank $\boxed{E = h \cdot f = \hbar \omega}$ E: wave energy
derived from f: frequency of wave
Black Body radiation exp.

Notes: de Broglie's formula can be applied to bodies of any size, however, due to the extremely small value of Plank's constant, the resulting wave-length makes only sense if the considered bodies are extremely small.

e.g. Calculate λ for
a) a free el. travelling with the speed of $10^{3} \frac{m}{s}$
b) a 4kg bowling ball with the velocity of $10 \frac{m}{s}$

a) $\lambda = \dfrac{h}{m \cdot V} = \dfrac{6.6 \times 10^{-34} [m]}{9.1 \times 10^{-31} \times 10^{3}} \cong \underline{7.2 \times 10^{-7} m}$

b) $\lambda = \dfrac{6.6 \times 10^{-34}}{4 \times 10} [m] \cong \underline{1.6 \times 10^{-35} m}$

The resulting wavelength for the electron is within the range of physical verification. A distance as short as 10^{-35}m, however, is far beyond our means of verification (cf. size of an atom is in the range of 10^{-10}m)

Bohr's Hydrogen model (1913)

In order to explain the discrete wavelengths observed when a hydrogen atom is heated up, Bohr assumed that its angular momentum is quantized. Consequently, the single electron contained in a simple hydrogen atom exhibits discrete energy levels. They can be derived as follows:

1) Att. Coulomb force between el. and proton:

$$F_C = \frac{q^2}{4\pi\varepsilon_0 r^2} \qquad (I)$$

2) Radial force due to rotation of el. around proton.

$$F_R = m\omega^2 r \underset{\uparrow}{=} \cancel{m}\frac{(n\hbar)^2}{r^4 m^{\cancel{2}}}\, r \qquad (II)$$

$$\omega = \frac{n\hbar}{m r^2}$$

$(n\hbar)$: angular momentum (quantized)

3) Total Energy of system:

$$E_H = -E_{el} = -\frac{1}{2}m\omega^2 r^2 = -\frac{1}{2}\cancel{m}\frac{(n\hbar)^2}{m^{\cancel{2}} r^{\cancel{4}\,2}} \cancel{r^2} \qquad (III)$$

To keep the el. on current trace: $\underline{F_C = F_R}$
(Stable System)

(I) = (II) $$\frac{q^2}{4\pi\varepsilon_0 r^2} = \frac{(n\hbar)^2}{m r^3}$$

$$\underline{r_n = \frac{(n\hbar)^2 4\pi\varepsilon_0}{m \cdot q^2}} \qquad (\text{II}')$$

(II') plugged into III $\Rightarrow$ $$E_H = -\frac{1}{2}\frac{(n\hbar)^2}{m}\frac{m^2 q^4}{(n\hbar)^4 (4\pi\varepsilon_0)^2}$$

$$\Rightarrow \underline{\underline{E_H = -\frac{1}{2}\frac{m q^4}{(4\pi\varepsilon_0 n\hbar)^2}}} = -\frac{1}{2}\frac{m q^4}{(2\varepsilon_0 h)^2 n^2}$$

n: quantum number $\rightarrow$ orbit identifier

The lowest energy for the system is achieved if n=1. In this case, we obtain

$$E_H(n=1) = -\frac{1}{2}\frac{m q^4}{(4\pi\varepsilon_0 \hbar)^2} = -13.6 \text{ eV}$$

Thus, we can write:

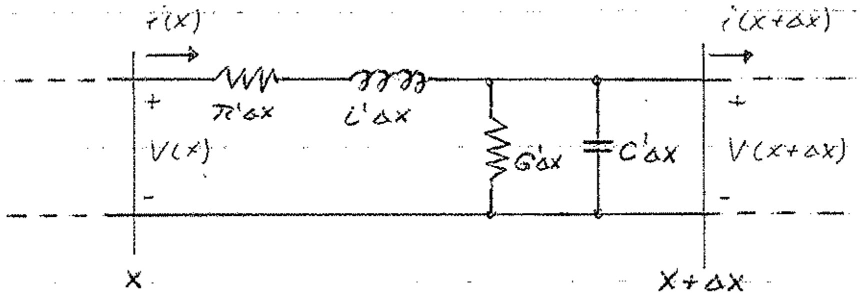
$$\underline{\underline{E_H(n) = -\frac{13.6}{n^2}\,[\text{eV}]}} \qquad n = 1, 2, \ldots$$

3.2 Properties of Waves

Example: Transmission line

How do voltage and current propagate?

Model:



line is characterized by R', L', G' and C'

Voltage drop across Δx:

1) $\Delta V(x) = V(x+\Delta x) - V(x) = -R'\Delta x\, i(x,t) - L'\Delta x \dfrac{\partial i(x,t)}{\partial t}$

Current drop across Δx:

2) $\Delta i(x) = -G'\Delta x\, V(x+\Delta x, t) - C'\Delta x \dfrac{\partial V(x+\Delta x, t)}{\partial t}$

We divide both eq. by Δx and let $\Delta x \to 0$

1') $\dfrac{\partial V(x,t)}{\partial x} = -R'\, i(x,t) - L' \dfrac{\partial i(x,t)}{\partial t}$

2') $\dfrac{\partial i(x,t)}{\partial x} = -G'\, V(x,t) - C' \dfrac{\partial V(x,t)}{\partial t}$

Telegrapher's equations

Taking the derivative $\frac{\partial}{\partial x}$ yields

1'') $\dfrac{\partial^2 V}{\partial x^2} = -R' \dfrac{\partial i}{\partial x} - L' \dfrac{\partial^2 i}{\partial x \partial t}$

2'') $\dfrac{\partial^2 i}{\partial x^2} = -G' \dfrac{\partial V}{\partial x} - C' \dfrac{\partial^2 V}{\partial x \partial t}$

Separating the Telegrapher's eq. w.r.t. voltage and current yields:

$$\frac{\partial^2 V(x,t)}{\partial x^2} = R'G'V(x,t) + [R'C' + L'G'] \frac{\partial V(x,t)}{\partial t} + L'C' \frac{\partial^2 V(x,t)}{\partial t^2}$$

$$\frac{\partial^2 i(x,t)}{\partial x^2} = R'G'i(x,t) + [R'C' + L'G'] \frac{\partial i(x,t)}{\partial t} + L'C' \frac{\partial^2 i(x,t)}{\partial t^2}$$

Special case #1 Lossless transmission line
$(R' = 0 ;\ G' = 0)$

$$\frac{\partial^2 V}{\partial x^2} = L'C' \frac{\partial^2 V}{\partial t^2}$$

$$\frac{\partial^2 i}{\partial x^2} = L'C' \frac{\partial^2 i}{\partial t^2}$$

Lossless Transmission

Compare: Classical wave equation:

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

c: propag. speed of wave (phase velocity)

Solution of classical wave eq.

We assume that $\Psi(x,t) = X(x) \cdot T(t)$

i.e. effects of time and position are independent

$$\Rightarrow \frac{\partial^2 X}{\partial x^2} T = \frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} X \quad \Big| \ \frac{1}{X \cdot T}$$

$$\frac{\partial^2 X}{\partial x^2} \frac{1}{X} = \frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} \frac{1}{T}$$

Solution for $X(x)$:

$$X(x) = C_1 e^{jkx} + C_2 e^{-jkx}$$

or

$$X(x) = A_1 \cos kx + B_1 \sin kx$$

Solution for $T(t)$:

$$T(t) = C_3 e^{j\omega t} + C_4 e^{-j\omega t}$$

or

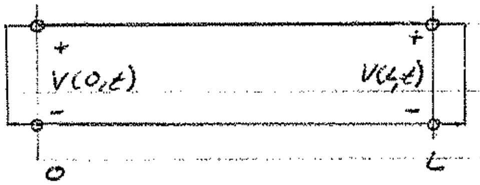
$$T(t) = A_2 \cos \omega t + B_2 \sin \omega t$$

where, ω = radian frequency of the wave
k = wave number

and $\underline{\omega = k \cdot c}$

<u>Note:</u> The coefficients C_1, C_2, C_3 and C_4 or A_1, A_2, B_1 and B_2, are determined by the <u>boundary conditions</u>. Thus, to obtain a unique solution, 4 boundary conditions must exist.

<u>Example:</u> Lossless transmission line of length L short-circuited at both ends.
Find $V(x,t)$



Boundary conditions: $V(0,t) = 0$ (I)

$V(L,t) = 0$ (II)

$V(x,0) = 0$ (initial condition) (III)

3 conditions → 1 free parameter

We have: $V(x,t) = X(x) \cdot T(t)$

$X(x) = A_1 \cos kx + B_1 \sin kx$

$T(t) = A_2 \cos \omega t + B_2 \sin \omega t$

from (I) $\Rightarrow A_1 = 0$

from (III) $\Rightarrow A_2 = 0$

from (II) $B_1 \sin kL = 0$ $\Rightarrow kL = n \cdot \pi$ $n = 1, 2, \ldots$

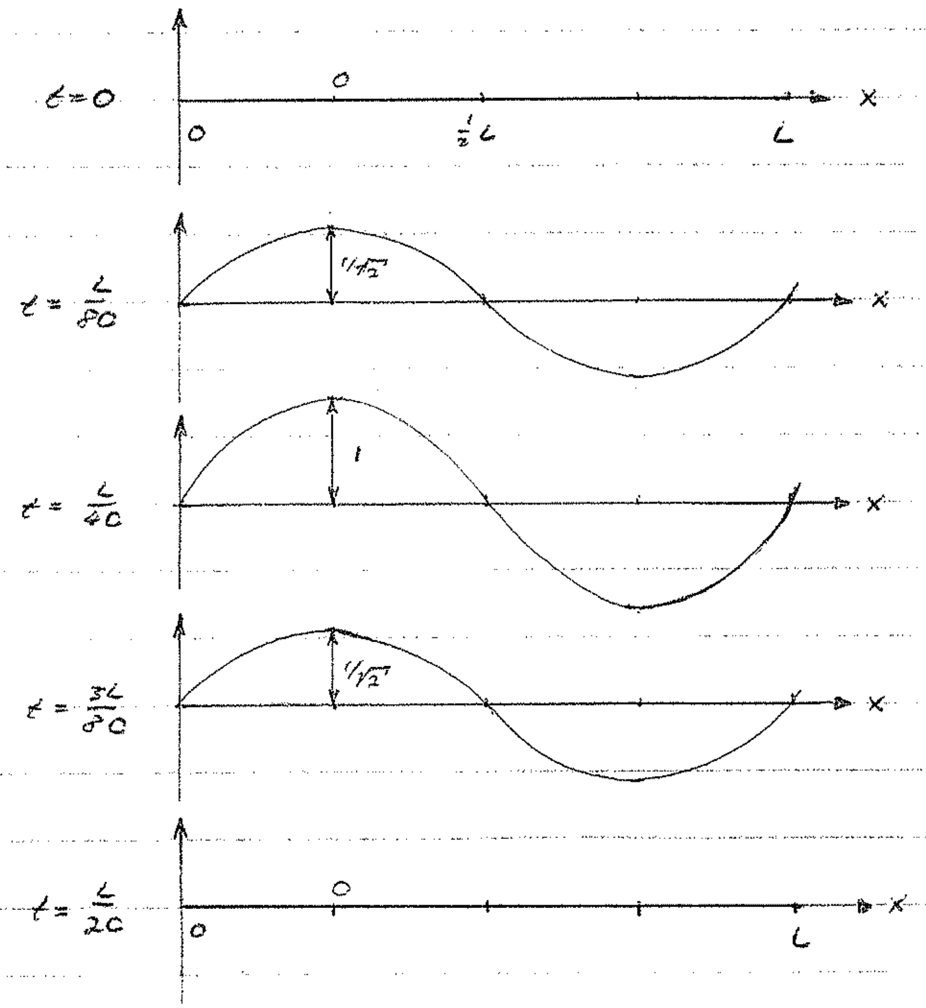
$\Rightarrow \underline{\underline{k_n = n \cdot \pi / L}}$

since $\omega = k c$ $\Rightarrow \underline{\underline{\omega_n = k_n c = n \pi \frac{c}{L}}}$

Finally: $\left\| V_n(x,t) = \overset{B_{1n} \cdot B_{2n}}{B_n} \sin\left(n\pi \frac{x}{L}\right) \sin\left(n\pi \frac{c}{L} t\right) \right\|$

Standing wave equation

e.g. $n=2$



The standing wave eq. has a periodicity in length of

$$\underline{\lambda_n = \frac{2L}{n}}$$

and in time of

$$\underline{\tau_n = \frac{2L}{nc}}$$

Note: In general, there exist several modes of standing-wave vibrations at the same time. Then

$$\left\| V(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(n\pi \frac{x}{L}\right) \sin\left(n\pi \frac{c}{L} t\right) \right\|$$

Special case # 2   Lossy $R C$ Transmission Line
($L' = 0$, $G' = 0$)

$$\left\| \begin{aligned} \frac{\partial^2 V}{\partial x^2} &= R' C' \frac{\partial V}{\partial t} \\ \frac{\partial^2 i}{\partial x^2} &= R' C' \frac{\partial i}{\partial t} \end{aligned} \right\|$$

RC Transmission Line $\rightarrow$ Diffusion eq.

Solution

$$\| V(x,t) = A \cdot \exp[j(kx - \omega t)] \|$$

where

$$| k^2 = j R' C' \omega | \qquad \omega = V_{Phase} \mathrm{Re}\{k\}$$

$$k = \sqrt{\frac{R' C' \omega}{2}} (1 + j)$$

Thus

$$\| V(x,t) = \underbrace{A \cdot \exp\left[-\sqrt{\frac{R'C'\omega}{2}}\, x\right]}_{\text{Amplitude } A(x)} \exp\underbrace{\left[j\left(\sqrt{\frac{R'C'\omega}{2}}\, x - \omega t\right)\right]}_{\text{Phase } \varphi(x,t)} \|$$

Note that

1. Wave diminishes in amplitude as it travels along the line
2. Propagation speed of points of constant phase depends on ω since

$$\text{for } \frac{\partial \varphi}{\partial t} = 0 \quad \Rightarrow \omega = \sqrt{\frac{R'C'\omega}{2}} \underbrace{\left(\frac{\partial x}{\partial t}\right)}_{V_{Phase}}$$

or

$$V_{Ph} = \sqrt{\frac{2\omega}{R'C'}} \qquad \left(\text{cf. } \quad V_{Ph} = \frac{\omega}{\mathrm{Re}\{k\}}\right)$$

$\Rightarrow$ A rectangular pulse traveling along such a line changes its shape since its different frequency components travel at different speeds.

3.3 The Schrödinger equation

In classical mechanics, the total energy of an object can be written as

$$\boxed{E = T + V}$$

E : Total Energy
T : Kinetic Energy
V : Potential Energy

where $T = \frac{1}{2} m v^2 = \frac{1}{2} \frac{p^2}{m}$

$$\Rightarrow \quad \underline{E = \frac{1}{2} \frac{p^2}{m} + V}$$

We consider now a 1-dim. wave given by

$$\boxed{\Psi(x,t) = A \cdot \exp[jkx - j\omega t]}$$

k : wave number
ω : wave frequency
$(\omega = c \cdot k)$

We try to replace k and ω in the wave eq. by the <u>momentum</u> and the <u>energy</u> of the "quantum particle".

Planck: $\left| E = h \cdot f = \hbar \omega \right|$ and $\omega = c \cdot k$

$$\Rightarrow \quad \underline{\underline{\omega = \frac{E}{\hbar}}} \quad \text{and} \quad k = \frac{E}{c \cdot \hbar}$$

Einstein: $\left| E = m \cdot c^2 \right|$

$$\Rightarrow \quad \underline{\underline{k = \frac{mc}{\hbar} = \frac{p}{\hbar}}}$$

We finally obtain:

$$\left\| \Psi(x,t) = A \cdot \exp[\,j \frac{p}{\hbar} x - j \frac{E}{\hbar} t\,] \right\|$$

To extract the energy, we take the derivative of the wave eq. w.r.t. the time t, thus

$$\frac{\partial \Psi(x,t)}{\partial t} = -j \frac{E}{\hbar} \Psi(x,t)$$

or

$$\left\| E = j\hbar \frac{1}{\Psi(x,t)} \frac{\partial \Psi(x,t)}{\partial t} \right\|$$

The kinetic energy, i.e. p^2, is obtained by taking the second derivative of Ψ w.r.t. the space coordinate x

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = -\frac{p^2}{\hbar^2} \Psi(x,t)$$

or

$$\left\| \frac{1}{2} \frac{p^2}{m} = -\frac{1}{2} \frac{\hbar^2}{m} \frac{1}{\Psi(x,t)} \frac{\partial^2 \Psi(x,t)}{\partial x^2} \right\|$$

The total energy of the "quantum particle" can now be expressed as

$$E = \frac{1}{2} \frac{p^2}{m} + V$$

$$j\hbar \frac{1}{\Psi} \frac{\partial \Psi}{\partial t} = -\frac{1}{2} \frac{\hbar^2}{m} \frac{1}{\Psi} \frac{\partial^2 \Psi}{\partial x^2} + V \quad \Big| \cdot \Psi$$

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

Schrödinger equation

Special case: potential energy V is time-independent and $\Psi(x,t) = \psi(x)\cdot\phi(t)$

$$\Rightarrow \quad \boxed{E = j\hbar \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = -\frac{1}{2}\frac{\hbar^2}{m}\frac{1}{\psi(x)}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = \text{const}}$$

i.e. The energy in the system is constant.

Solution for this special case:

A) $\phi(t) = \frac{j\hbar}{E}\frac{\partial \phi(t)}{\partial t}$

$$\| \phi(t) = A \cdot \exp[-j\frac{E}{\hbar}t] \|$$

Since $\Psi(x,t) = \psi(x)\cdot\phi(t)$ we can assume $A = 1$ without introducing any constraint on $\Psi(x,t)$

B) $\psi(x)[E - V(x)] = -\frac{1}{2}\frac{\hbar^2}{m}\frac{\partial^2 \psi(x)}{\partial x^2}$

or

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

Time-independent Schrödinger eq.

Note: The Schrödinger eq. describes the behaviour of a particle with mass m experiencing a certain potential $V(x)$.
To derive it, we have used the particle and the wave nature of the considered mass m.

Solution of the time-independent Schrödinger eq.

If the potential V is constant (or at least piecewise constant over the considered space), $\Psi(x)$ has the following solution:

$$\Psi(x) = C_1 \exp[jkx] + C_2 \exp[-jkx]$$

where

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

<u>Note</u>: If $V_0 > E$, k becomes imaginary and $\Psi(x)$ is a real exp. function in x.
If $V_0 = E$, $k = 0$ and $\Psi(x) = \text{const.}$

Physical interpretation of the wave function $\Psi(x,t)$

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

is the probability that the considered object is located in the region between x and $x + dx$

Normalization:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

It is interesting to note that this interpretation was not proposed by Schrödinger, but by another physicist (Max Born, 1926)

The Schrödinger equation

$$\boxed{j\hbar \frac{\partial \Psi(x,t)}{\partial t} \frac{1}{\Psi(x,t)} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} \frac{1}{\Psi(x,t)} + V}$$

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

<u>Physical interpretation of $\Psi(x,t)$:</u>

$|\Psi(x,t)|^2 dx$ is the probability that the particle under consideration is located in the region between x and $x + dx$.

<u>Special case:</u> Potential V is independent of time and $\Psi(x,t) = \Psi(x) \cdot \Phi(t)$

<u>Thus:</u>

$$\left| j\hbar \frac{d\Phi(t)}{dt} \frac{1}{\Phi(t)} = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} \frac{1}{\Psi(x)} + V(x) \right|$$

1) $$\boxed{E = j\hbar \frac{d\Phi(t)}{dt} \frac{1}{\Phi(t)}} \quad \Rightarrow \Phi(t) = A \cdot \exp[-j \frac{E}{\hbar} t]$$

2) $$\boxed{[E - V(x)] + \frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} \frac{1}{\Psi(x)} = 0}$$ Time-indep. Schr. eq.

<u>If $V(x) = V_0$</u>

$$\Rightarrow \left| \Psi(x) = c_1 \exp[jkx] + c_2 \exp[-jkx] \right|$$

$$k^2 = \frac{2m}{\hbar^2} [E - V_0]$$

Note: All solutions $\Psi(x)$ of the time-independent Schrödinger eq. are subject to the following conditions:

1) $\mathrm{Re}\{\Psi(x)\} < \infty$ for all x
2) $d\Psi/dx$ must be continuous $\Rightarrow$ Ψ must also be continuous (This follows from $d^2\Psi/dx^2 \sim E < \infty$)
3) $d^2\Psi/dx^2$ contains at most a finite number of finite discontinuities.

3.4 Heisenberg's uncertainty principle (1927)

Heisenberg stated that

> it is not possible to measure simultaneously the position and the momentum of a particle with arbitrary accuracy.

The uncertainty of the product of $p \cdot x$ was found to be always greater than Planck's constant h.

$$\boxed{\Delta p \cdot \Delta x \geq h}$$

Similarly, one can state that the uncertainty in the product $E \cdot t$ is also greater than or equal to h.

$$\boxed{\Delta E \cdot \Delta t \geq h}$$

$\Delta p = m \cdot \Delta V$

$\Delta x = V \cdot \Delta t$

$\Rightarrow \Delta p \cdot \Delta x = \underbrace{m \cdot V \cdot \Delta V}_{\Delta E} \cdot \Delta t$

since $E = \frac{1}{2} m V^2$

Finally, a third formulation of the uncertainty principle relates the spectral sharpness of waves with the accuracy of time

$$\boxed{\Delta f \, \Delta t \geq 1} \qquad \Delta E = h \cdot \Delta f$$
$$\Rightarrow \Delta E \, \Delta t = h \, \Delta f \, \Delta t$$

3.5. <u>Applications of Schrodinger's eq.</u>

1) <u>free particle</u>

A free particle experiences $V = 0$ everywhere. It's wave function is given by

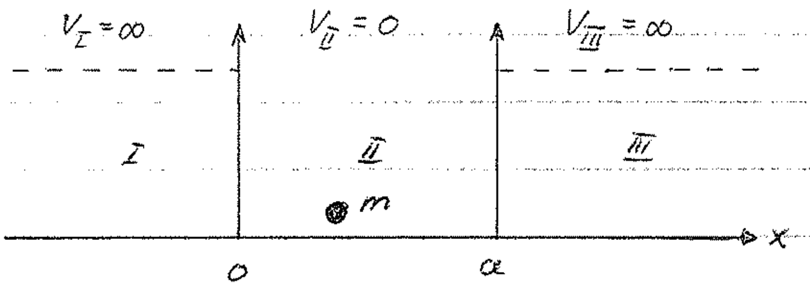
$$\boxed{\Psi(x,t) = A \cdot \exp[\,jkx - j\omega t\,]}^{**} \qquad k^2 = \frac{2m}{\hbar^2} E \qquad \omega = \frac{E}{\hbar}$$

Since $|\Psi|^2 = A^2$, i.e. independent of position x, the particle* can be found with <u>equal</u> probability <u>everywhere</u>. This agrees well with Heisenberg's uncertainty principle in that precise momentum implies undefined position.

* It is assumed that the particles energy E, and so its wave number k and angular frequency ω, is known.

** Since particle is free, its wave function is nowhere reflected and so propagates only in one direction i.e. the term $\exp[-jkx]$ does not exist.

3) Particle in infinite potential well



Particle is confined in an infinite well.

In regions I and III, where $V = \infty$, $\psi_I = \psi_{III} = 0$ is the only possible solution.

In region II, where $V=0$, we have

$$\boxed{\psi_{II}(x) = C_1 \exp[jkx] + C_2 \exp[-jkx]} \qquad k^2 = \frac{2m}{\hbar^2} E$$

Boundary conditions: 1) $\psi_I(0) = \psi_{II}(0) = 0$

2) $\psi_{II}(a) = \psi_{III}(a) = 0$

from 1) $C_1 + C_2 = 0 \Rightarrow \underline{\underline{C_2 = -C_1}}$

from 2) $C_1 e^{jka} - C_1 e^{-jka} = 0$

$C_1 \cdot 2j \sin(ka) = 0 \Rightarrow \underline{\underline{k \cdot a = n\pi}} \quad n = 1, 2, \ldots$

$$\Rightarrow \boxed{k_n = n \cdot \frac{\pi}{a} = \sqrt{\frac{2m}{\hbar^2} E_n}}$$

The second boundary condition places a restriction on the allowed energy states of the confined particle.

The allowed energy values are:

$$\underline{\underline{E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \cdot n^2 = \frac{h^2}{8ma^2} n^2}} \qquad n = 1, 2, \ldots$$

Conclusion:

| An object that is confined to a limited region in space will exhibit quantized energy states! |

Solution of time-independent Schrödinger eq.

$$\boxed{\psi_n(x) = A_n \sin(k_n x)} \qquad \text{where } A_n = 2jC_n$$

Normalization:

$$\int_0^a A_n^2 \sin^2(k_n x)\, dx = 1 \qquad \text{with } k_n = n\frac{\pi}{a}$$

$$A_n^2 \cdot \frac{1}{2} \cdot a = 1 \qquad \Rightarrow \qquad \underline{\underline{A_n = \sqrt{\frac{2}{a}}}}$$

$$\Rightarrow \left\| \psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x) \right\|$$

Complete solution:

$$\left\| \psi_n(x,t) = \sqrt{\frac{2}{a}} \sin(k_n x)\, e^{-j\omega_n t} \right\|$$

where

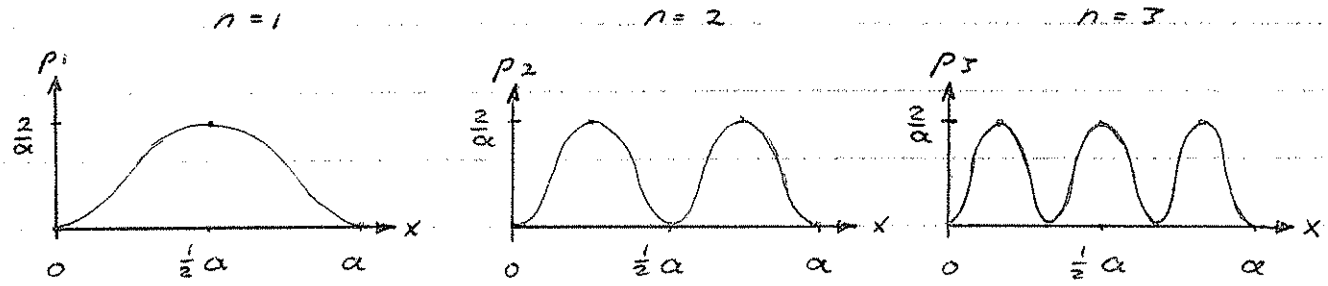
$$\left\| k_n = n\frac{\pi}{a}\ ; \quad \omega_n = \frac{E_n}{\hbar} = \frac{\pi h n^2}{4ma^2} \right\|$$

note: Complete description of particle state:

$$\left\| \psi(x,t) = \sum_{n=1}^{\infty} \psi_n(x,t) \right\|$$

The probability density function of the particle is therefore:

$$\underline{\underline{P_n(x)}} = |\Psi_n(x,t)|^2 = \Psi_n(x,t) \cdot \Psi_n^*(x,t) = \underline{\underline{\frac{2}{a}\sin^2(k_n x)}}$$



$$\boxed{p_n(x) = \frac{2}{a}\sin^2\left(n\pi\frac{x}{a}\right)}$$

The average position $\hat{x}_n$ of the particle, i.e. it's most likely position, is given by

$$\hat{x}_n = \int_{-\infty}^{\infty} |\Psi_n|^2 x \, dx = \int_0^a \frac{2}{a}\sin^2\left(n\pi\frac{x}{a}\right) x \, dx$$

$$= \int_0^a \frac{2}{a}\left[\frac{x}{2} - \frac{x}{2}\cos\left(2n\pi\frac{x}{a}\right)\right]dx$$

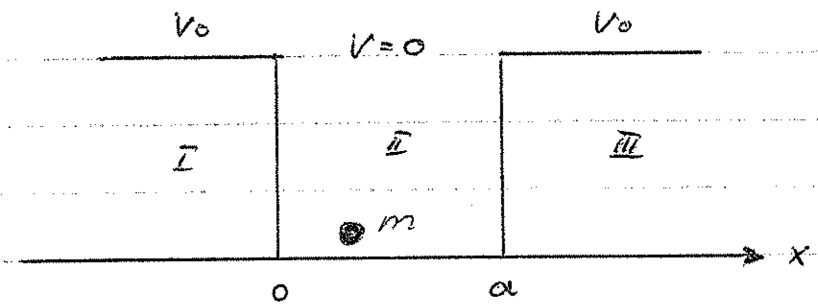
$\sin^2\alpha = \frac{1}{2}[1-\cos 2\alpha]$

$$= \int_0^a \frac{x}{a}dx - \frac{1}{a}\int_0^a x\cos\left(2n\pi\frac{x}{a}\right)dx$$

$$= \frac{a}{2} - \frac{1}{2n\pi}\left[\sin\left(2n\pi\frac{x}{a}\right)\cdot x - \int \sin\left(2n\pi\frac{x}{a}\right)dx\right]_0^a$$

$$\underline{\underline{\hat{x}_n = \frac{a}{2}}}$$

C) Particle in finite potential well



$V_0 > E$

Solution for time-indep. Schr. eq.

$$\psi(x) = c_1 e^{jkx} + c_2 e^{-jkx}$$
$$k^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$$\Rightarrow \quad k_I = k_{III} = j\sqrt{\frac{2m}{\hbar^2}(V_0 - E)} = jk_0$$
$$k_{II} = \sqrt{\frac{2m}{\hbar^2}E} = k_1$$

$$\psi_I(x) = C_{I1} e^{-k_0 x} + C_{I2} e^{k_0 x}$$
$$\psi_{II}(x) = C_{II1} e^{jk_1 x} + C_{II2} e^{-jk_1 x}$$
$$\psi_{III}(x) = C_{III1} e^{-k_0 x} + C_{III2} e^{k_0 x}$$

These solutions are subject to:

1) $Re\{\psi(x)\} < \infty$ for all x
2) $\psi(x)$ must be continuous
3) $d\psi(x)/dx$ must be continuous

From cond. 1): $\left\| \begin{array}{l} C_{I_1} = 0 \\ C_{III_2} = 0 \end{array} \right\|$

From cond. 2): $\left| \begin{array}{l} C_{I_2} = C_{II_1} + C_{II_2} \\ C_{II_1} e^{jh_1 a} + C_{II_2} e^{-jh_1 a} = C_{III_1} e^{-h_0 a} \end{array} \right|$ ① ②

From cond. 3): $\left| \begin{array}{l} C_{I_2} k_0 = jk_1 [C_{II_1} - C_{II_2}] \\ jk_1 [C_{II_1} e^{jh_1 a} - C_{II_2} e^{-jh_1 a}] = -C_{III_1} k_0 e^{-h_0 a} \end{array} \right|$ ③ ④

From eq. ① + ③ $\quad C_{II_1} + C_{II_2} = jk [C_{II_1} - C_{II_2}] \qquad k = \frac{k_1}{k_0}$

$$C_{II_1}(1 - jh) = -C_{II_2}(1 + jh)$$

$\left\| \begin{array}{l} C_{I_2} = C_{II_1} \frac{j2k}{(1+jk)} = C_{II_1} \frac{2k}{(1+k^2)} [k + j] \\ C_{II_2} = -C_{II_1} \frac{(1-jh)}{(1+jk)} = -C_{II_1} \frac{1}{(1+h^2)} [1 - h^2 - j2k] \end{array} \right\|$ ⑤ ⑥

From eq. ② + ④ $\quad C_{II_1} e^{jh_1 a} + C_{II_2} e^{-jh_1 a} = -jk [C_{II_1} e^{jh_1 a} - C_{II_2} e^{-jh_1 a}]$

$$C_{II_1} e^{jh_1 a} [1 + jh] = -C_{II_2} e^{-jh_1 a} [1 - jh]$$

$\left| \begin{array}{l} C_{II_2} = -C_{II_1} e^{j2h_1 a} \frac{(1+jk)}{(1-jh)} = -C_{II_1} e^{j2h_1 a} \frac{1}{(1+h^2)} [1 - h^2 + j2h] \\ C_{III_1} = -C_{II_1} e^{k_0 a} e^{jh_1 a} \frac{j2k}{(1-jh)} = -C_{II_1} e^{h_0 a} e^{jh_1 a} \frac{2k}{(1+k^2)} [-k + j] \end{array} \right|$ ⑦ ⑧

Since ⑥ = ⑦ $\Rightarrow \quad \frac{(1-jh)}{(1+jk)} = e^{j2h_1 a} \frac{(1+jh)}{(1-jh)}$

$$\Rightarrow \quad \left| e^{j2h_1 a} = \frac{(1-jh)^2}{(1+jh)^2} \right|$$

$$e^{jk_1 a} = \frac{(1-jh)}{(1+jh)} \quad \Rightarrow k_1 a = n\pi - 2\tan^{-1}(h)$$

$$\Rightarrow e^{jk_1 a} = (-1)^n e^{-j2\cdot\tan^{-1}(h)}$$

$$\Rightarrow K_{1_n} = \frac{1}{a}[n\pi - 2\cdot\tan^{-1}(h)] \qquad n = 1, 2, \ldots$$

Thus, we have

$$C_{I2} = C_{II1}\frac{2h}{(1+h^2)}[h+j]$$

$$C_{II2} = -C_{II1}\frac{1}{(1+h^2)}[1-h^2-j2h]$$

$$C_{III1} = -C_{II1}\, e^{\kappa_0 a}\frac{2h}{(1+h^2)}[h+j](-1)^n$$

We obtain C_{II1} from the normalization cond.

$$\int_{-\infty}^{0}|\psi_I(x)|^2dx + \int_0^a|\psi_{II}(x)|^2dx + \int_a^\infty|\psi_{III}(x)|^2dx = 1$$

$$\Rightarrow |C_{II1}|^2 = \frac{(1+h^2)}{4\frac{h^2}{\kappa_0} + 2a(1+h^2)} = \frac{(1+h^2)}{D^2}$$

$$\Rightarrow C_{II1} = \frac{(h-j)}{D}$$

We finally obtain

$$C_{II1} = \frac{h-j}{D} \qquad C_{I2} = \frac{1}{D}\,2h$$

$$C_{II2} = \frac{h+j}{D} \qquad C_{III1} = -\frac{1}{D}\,2h\,e^{\kappa_0 a}(-1)^n$$

The resulting wave function $\psi(x)$ is:

$$\psi_n(x) = \begin{cases} \frac{2}{D} k\, e^{k_0 x} & x < 0 \\ \frac{2}{D} \left[k \cos(k_1 x) + \sin(k_1 x) \right] & 0 \le x \le a \\ -\frac{2}{D} k\, e^{-k_0 (x-a)} (-1)^n & x > a \end{cases}$$

with

$$k_1 = \frac{1}{a}\left[n\pi - 2 \tan^{-1}(k) \right]\ ; \quad k_0 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$k = \frac{k_1}{k_0} = \sqrt{\frac{E}{(V_0 - E)}}$$

$$D^2 = 4\frac{k^2}{k_0} + 2a(1+k^2)$$

The particle's prob. dens. function (PDF) is:

$$|\psi_n(x)|^2 = \begin{cases} \frac{4}{D^2} k^2 e^{2k_0 x} & x < 0 \\ \frac{2}{D^2} \left[1 + k^2 + (k^2 - 1)\cos(2k_1 x) + 2k \sin(2k_1 x) \right] & 0 \le x \le a \\ \frac{4}{D^2} k^2 e^{-2k_0 (x-a)} & x > a \end{cases}$$

Note: Probability to find particle outside the well is:

$$P_0 = \int_{-\infty}^{0} \frac{4}{D^2} k^2 e^{2k_0 x} dx + \int_{a}^{\infty} \frac{4}{D^2} k^2 e^{-2k_0 (x-a)} dx$$

$$= \frac{4}{D^2} \frac{k^2}{k_0} = \frac{1}{1 + \frac{a}{2} k_0 \frac{1+k^2}{k^2}} = \frac{1}{1 + \sqrt{\frac{m a^2}{2\hbar^2}} \frac{V_0}{E} \sqrt{V_0 - E}}$$

roblem:

Sketch the PDF of an electron in a potential well with $a = 1nm$ and

a) $V_0 = 2 E_1$

b) $V_0 = 10 E_1$ (we assume $n = 1$)

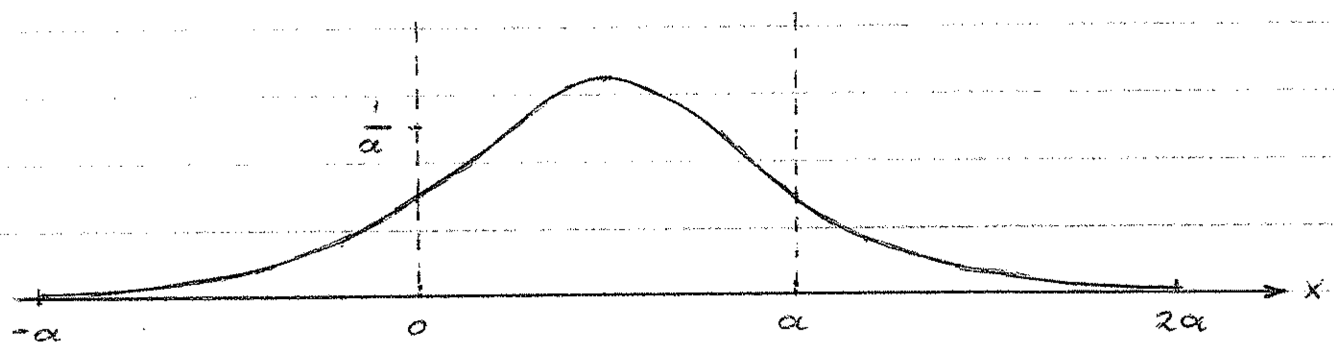
c) $V_0 = 10'000 E_1$

Solution:

a) $k_0 = k_1$ $\quad$ $k_1 = \frac{1}{a}[\pi - 2\tan^{-1}(1)] = \frac{1}{a}\frac{\pi}{2}$

$n = 1$ $\Rightarrow$ $D^2 = 2a[2 + \frac{4}{\pi}]$

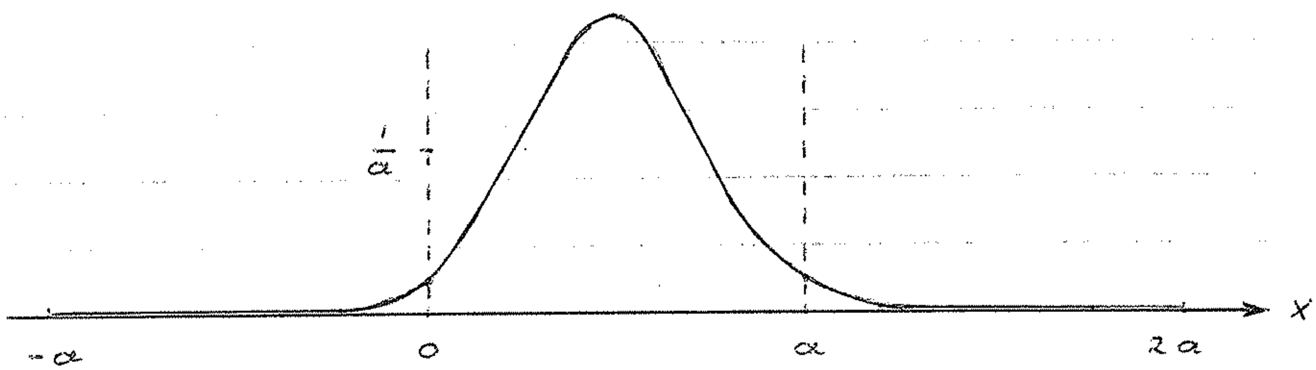
$$|\psi_1(x)|^2 = \begin{cases} \frac{1}{a[1+2/\pi]} e^{\pi\frac{x}{a}} & x < 0 \\ \frac{1}{a[1+2/\pi]} [1 + \sin(\pi\frac{x}{a})] & 0 \le x \le a \\ \frac{1}{a[1+2/\pi]} e^{-\pi[\frac{x}{a} - 1]} & x > a \end{cases}$$



b) $k_0 = 3k_1$, $k = 1/3$ $\Rightarrow$ $k_1 = \frac{1}{a}\left[\pi - 2\tan^{-1}\left(\frac{1}{3}\right)\right] \cong \frac{1}{a}\pi\frac{4}{5}$

$D^2 \cong 2a\left[1 + 1/9 + 1/12\pi\right] \approx 2a$

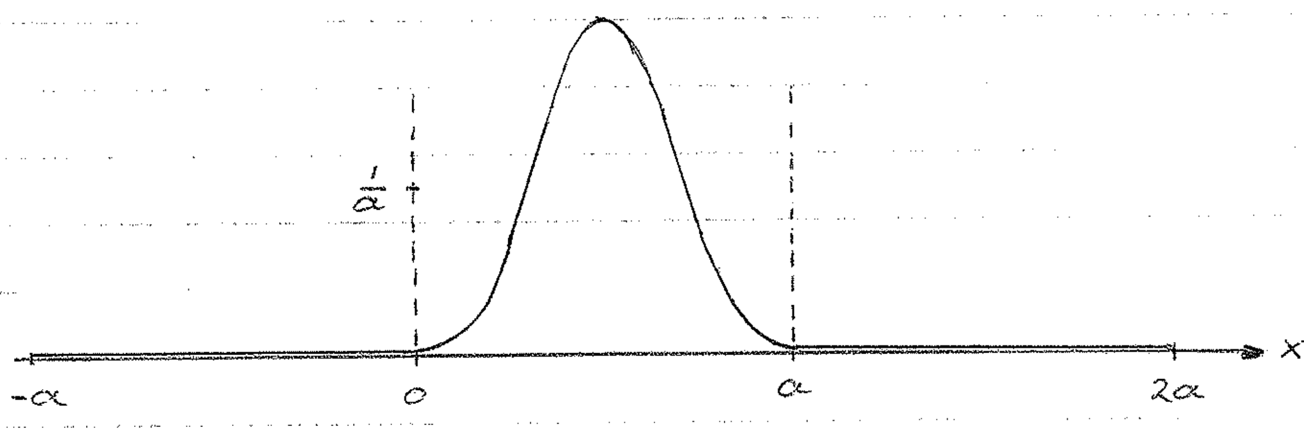
$$|\psi_1(x)|^2 \cong \begin{cases} \frac{2}{a}\frac{1}{9}\, e^{\pi\cdot 4.8\frac{x}{a}} & x<0 \\ \frac{2}{a}\frac{1}{9}\left[5 - 4\cos\left(\pi\frac{8}{5}\frac{x}{a}\right) + 3\sin\left(\pi\frac{8}{5}\frac{x}{a}\right)\right] & 0 \le x \le a \\ \frac{2}{a}\frac{1}{9}\, e^{-\pi\cdot 4.8\left(\frac{x}{a}-1\right)} & x > a \end{cases}$$



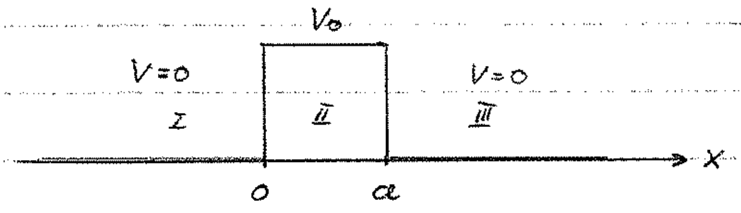
c) $k_0 = 100 k_1$, $k = \frac{1}{100}$ $\Rightarrow$ $k_1 \cong \frac{1}{a}\left[\pi - 2\tan^{-1}\left(\frac{1}{100}\right)\right] \cong \frac{1}{a}\pi$

$D^2 \cong 2a$

$$|\psi_1(x)|^2 \cong \begin{cases} 0 & x<0 \\ \frac{1}{a}\left[1 - \cos\left(2\pi\frac{x}{a}\right)\right] & 0 \le x \le a \\ 0 & x > a \end{cases}$$



Particle experiencing a potential barrier



$V_0 > E$

General form of solution:

$$\psi(x) = \begin{cases} C_1 e^{jk_1 x} + C_2 e^{-jk_1 x} & x \leq 0 \\ C_3 e^{-k_2 x} & 0 < x < a \\ C_4 e^{jk_1 x} + C_5 e^{-jk_1 x} & x \geq a \end{cases}$$

where $k_1 = \sqrt{\frac{2m}{\hbar^2} E}$ $\quad k_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

Note: The above general form of the solution contains 5 unknown coefficients, but there exist only 4 boundary conditions.

Solution of this dilemma:

Assume a particle source, e.g. at $x = -\infty$

$\Rightarrow$ Coefficient C_1 is given, i.e. we can consider it to be a free parameter.

(Recall that $\Psi(x,t) = C_1 e^{j(kx - \omega t)} + C_2 e^{-j(kx + \omega t)}$

hence, the first term in $\Psi(x,t)$ represents a wave propagating in the positive x-direction while the second term denotes a wave traveling in the negative x-direction)

The eq. resulting from the boundary cond. are:

$$\begin{array}{ll|l|} ① & & C_1 + C_2 = C_3 \\ ② & & jh_1(C_1 - C_2) = -k_2 C_3 \\ ③ & & C_3 e^{-h_2 a} = C_4 e^{jh_1 a} + C_5 e^{-jh_1 a} \\ ④ & & -h_2 C_3 e^{-h_2 a} = jh_1 (C_4 e^{jh_1 a} - C_5 e^{-jh_1 a}) \end{array}$$

Solution:

$$\left| \begin{array}{l} C_2 = C_1 \dfrac{h-j}{h+j} \\ C_3 = C_1 \dfrac{2h}{h+j} \\ C_4 = C_1 e^{-h_2 a} e^{-jh_1 a} \\ C_5 = C_1 e^{-h_2 a} e^{+jh_1 a} \dfrac{h-j}{h+j} \end{array} \right|$$

$$k = \frac{h_1}{h_2} = \sqrt{\frac{E}{V_0 - E}}$$

To get a real value for C_3, we assume $C_1 = C_0 \dfrac{h+j}{2}$

$$\left\| \begin{array}{l} C_1 = C_0 \dfrac{k+j}{2} \\ C_2 = C_0 \dfrac{k-j}{2} \\ C_3 = C_0 k \\ C_4 = C_0 e^{-k_2 a} e^{-jh_1 a} \dfrac{k+j}{2} \\ C_5 = C_0 e^{-h_2 a} e^{+jh_1 a} \dfrac{h-j}{2} \end{array} \right\|$$

C_0: free parameter

The resulting wave function is

$$\psi(x) = \begin{cases} C_0 \left[k \cos k_1 x - \operatorname{sen} k_1 x \right] & x \leq 0 \\ C_0 k e^{-k_2 x} & 0 < x < a \\ C_0 e^{-k_2 a} \left[(k \cos k_1 a + \operatorname{sen} k_1 a) \cos k_1 x \right. & x \geq a \\ \qquad \left. - (\cos k_1 a - k \operatorname{sen} k_1 a) \operatorname{sen} k_1 x \right] & \end{cases}$$

where $k_1 = \sqrt{\frac{2m}{\hbar^2} E}$ $\quad k_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$ $\quad k = \frac{k_1}{k_2} = \sqrt{\frac{E}{V_0 - E}}$

The probability to find the particle on the left hand side of the barrier is

$$P_I = C_0^2 \int_{-\infty}^{0} (k^2 \cos^2 k_1 x - \underbrace{2k \cos k_1 x \operatorname{sen} k_1 x}_{0} + \operatorname{sen}^2 k_1 x) \, dx$$

$$= C_0^2 \int_{-\infty}^{0} (k^2 \cos^2 k_1 x + \operatorname{sen}^2 k_1 x) \, dx \underset{\int \cos^2 = \int \operatorname{sen}^2}{=} C_0^2 (k^2 + 1) \int_{-\infty}^{0} \cos^2(k_1 x) \, dx$$

With $\int_{-\infty}^{0} \cos^2(k_1 x) \, dx = \frac{1}{2k_1} \pi$ where π denotes the # of periods over which we integrate ($\pi \to \infty$)

we can write:

$$P_I = C_0^2 \, \frac{k^2 + 1}{2k_1} \, \pi$$

Similarly, the probabilities to find the particle in regions II (barrier) and III (right of barrier) are:

$$P_{II} = C_0^2 \, \frac{k^2}{2k_2} \left(1 - e^{-2k_2 a}\right)$$

and $$P_{III} = C_0^2 e^{-2h_2 a} \frac{h^2+1}{2h1} \pi$$

Since $P_I + P_{II} + P_{III} = 1$ we obtain for π

$$\pi = \frac{1 - P_{II}}{C_0^2 \frac{h^2+1}{2h1}\left(1 + e^{-2h_2 a}\right)}$$

We finally obtain

$$\left| \begin{array}{l} P_I = \dfrac{(1 - P_{II})}{1 + e^{-2h_2 a}} \\[2ex] P_{III} = \dfrac{(1 - P_{II})\, e^{-2h_2 a}}{1 + e^{-2h_2 a}} \end{array} \right|$$

In the limit as $\pi \to \infty$ $\underline{\underline{P_{II} \to 0}}$. So we get the final result

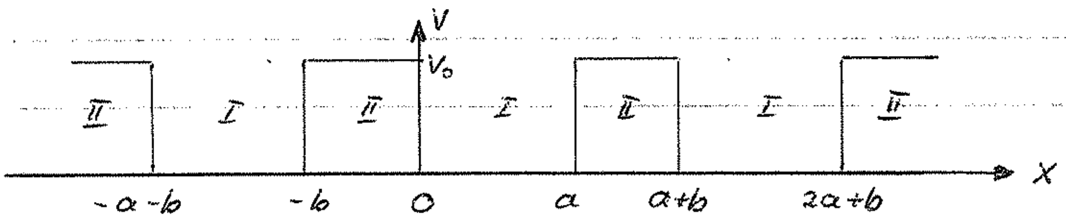
$$\left\| \begin{array}{l} P_I = \dfrac{1}{1 + e^{-2k_2 a}} \\[2ex] P_{III} = \dfrac{e^{-2h_2 a}}{1 + e^{-2h_2 a}} \end{array} \right\|$$

e.g. for $\underline{h_2 = \frac{1}{a}}$ $\qquad\qquad$ $\underline{h_2 = \frac{1}{10 \cdot a}}$

$$\left| \begin{array}{l} P_I = 0.88 \mathrel{\hat{=}} 88\% \\ P_{III} = 0.12 \mathrel{\hat{=}} 12\% \end{array} \right| \qquad \left| \begin{array}{l} P_I = 0.55 \mathrel{\hat{=}} 55\% \\ P_{III} = 0.45 \mathrel{\hat{=}} 45\% \end{array} \right|$$

3.6 The electron in a periodic potential
(Krönig - Penney Model)

We assume a one-dimensional periodic potential



Time-independent Schr. eq.

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0}$$

<u>Note:</u> There exists no exact solution for a system containing many electrons.

<u>Approximation:</u> We describe the electrons as plane waves modulated by a function with the periodicity of the lattice (Bloch Theorem*)

<u>Thus</u> $\quad \boxed{\psi(x) = u^{*}(x)\ \exp\left[jkx\right]}$

where

$$u(x) = u(x+L) = u(x+nL) \qquad L = (a+b)$$

$$\Rightarrow \frac{d\psi}{dx} = jk\,e^{jkx}\cdot u(x) + \frac{du}{dx}\,e^{jkx}$$

$$\frac{d^2\psi}{dx^2} = -k^2 e^{jkx} u + \underbrace{jk\,e^{jkx}\frac{du}{dx} + jk\,e^{jkx}\frac{du}{dx}}_{2jk\,e^{jkx}\frac{du}{dx}} + e^{jkx}\frac{d^2u}{dx^2}$$

* u is called Bloch function (Felix Bloch, 1928)

We substitute in Schrodinger's eq.

region I

$$\frac{2m}{\hbar^2} E = \alpha^2$$

region II

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

Thus, we obtain:

region I

$$-k^2 u_I \cancel{e^{jkx}} + 2jk \cancel{e^{jkx}} \frac{du_I}{dx} + \cancel{e^{jkx}} \frac{d^2u_I}{dx^2} + \alpha^2 \cancel{e^{jkx}} u_I = 0$$

$$\boxed{\frac{d^2u_I}{dx^2} + 2jk \frac{du_I}{dx} + u_I(\alpha^2 - k^2) = 0}$$

region II

$$\boxed{\frac{d^2u_{II}}{dx^2} + 2jk \frac{du_{II}}{dx} - u_{II}(\beta^2 + k^2) = 0}$$

<u>Solution:</u>

$$u_I(x) = A_1 \exp[j(\alpha - k)x] + B_1 \exp[-j(\alpha + k)x]$$

$$u_{II}(x) = A_2 \exp[(\beta - jk)x] + B_2 \exp[-(\beta + jk)x]$$

<u>Boundary</u> cond.

1) $u_I(0) = u_{II}(0)$

2) $u_I(a) = u_{II}(-b)$

3) $\left.\frac{du_I}{dx}\right|_{x=0} = \left.\frac{du_{II}}{dx}\right|_{x=0}$

4) $\left.\frac{du_I}{dx}\right|_{x=a} = \left.\frac{du_{II}}{dx}\right|_{x=-b}$

After voluminous calculations, we obtain

$$\boxed{\frac{(\beta^2 - \alpha^2)}{2\alpha\beta} \sinh(\beta b)\sin(\alpha a) + \cosh(\beta b)\cos(\alpha a) = \cos(kL)}$$

$L = a + b$

transcendental equation

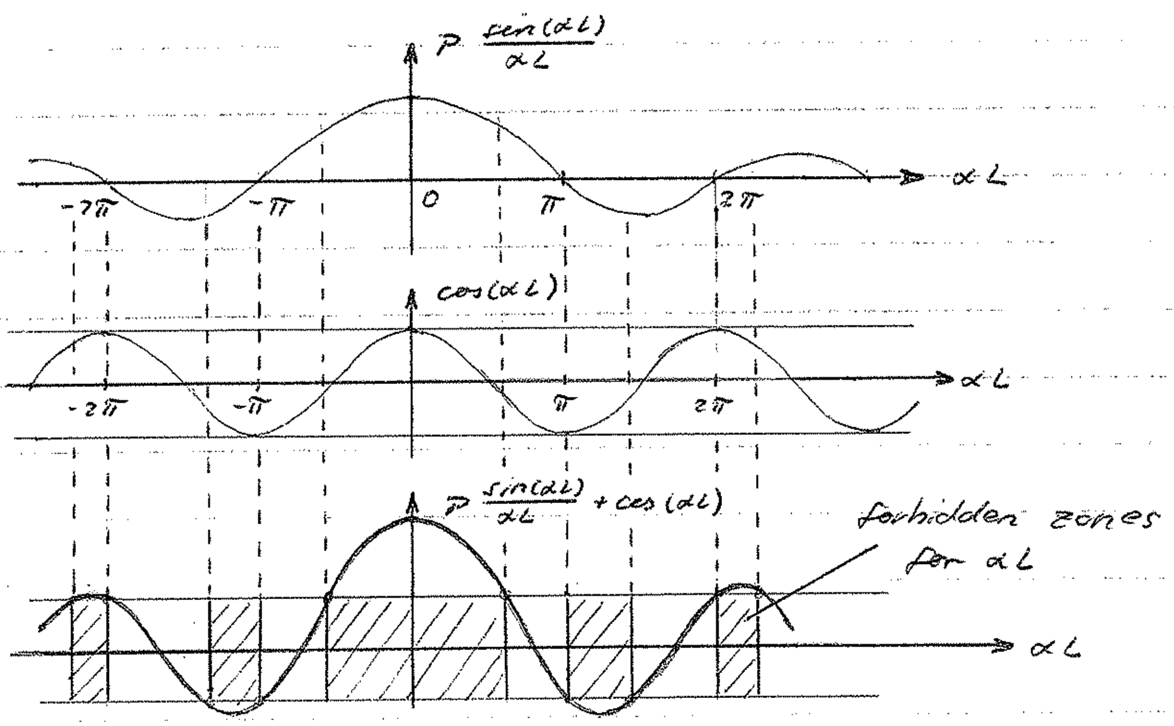
We simplify: $$\lim_{\substack{V_0 \to \infty \\ b \to 0}} \frac{\beta^2 \alpha b}{2} = P$$

$\Rightarrow \alpha \cong L \quad \beta b \cong 0$

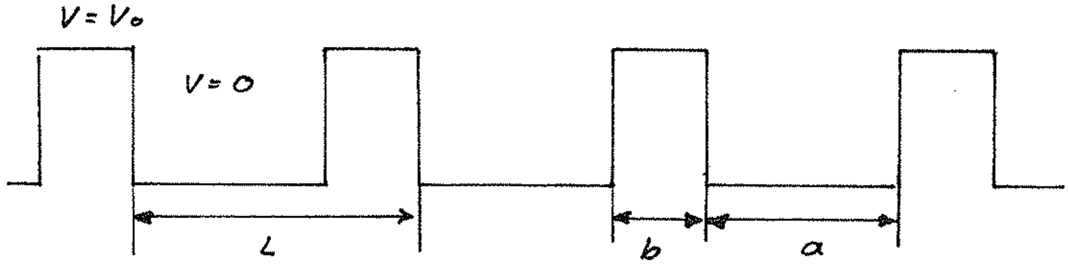
$$\Rightarrow \quad \frac{\beta}{2\alpha} \underbrace{\sinh(\beta b)}_{= \beta b} \sin(\alpha L) + \underbrace{\cosh(\beta b)}_{= 1} \cos(\alpha L) = \cos(kL)$$

$$\boxed{\frac{P}{\alpha L} \sin(\alpha L) + \cos(\alpha L) = \cos(kL)}$$

This eq. has some restrictions. The right hand side is limited to ± 1 whereas the left hand side is not. Consequently, the solutions occur for certain ranges of α only, where the left side of the above eq. is between $+1$ and -1.
(Recall: $\alpha^2 = \frac{2m}{\hbar^2} E$) $\Rightarrow$ There exist forbidden energy ranges for the electrons!



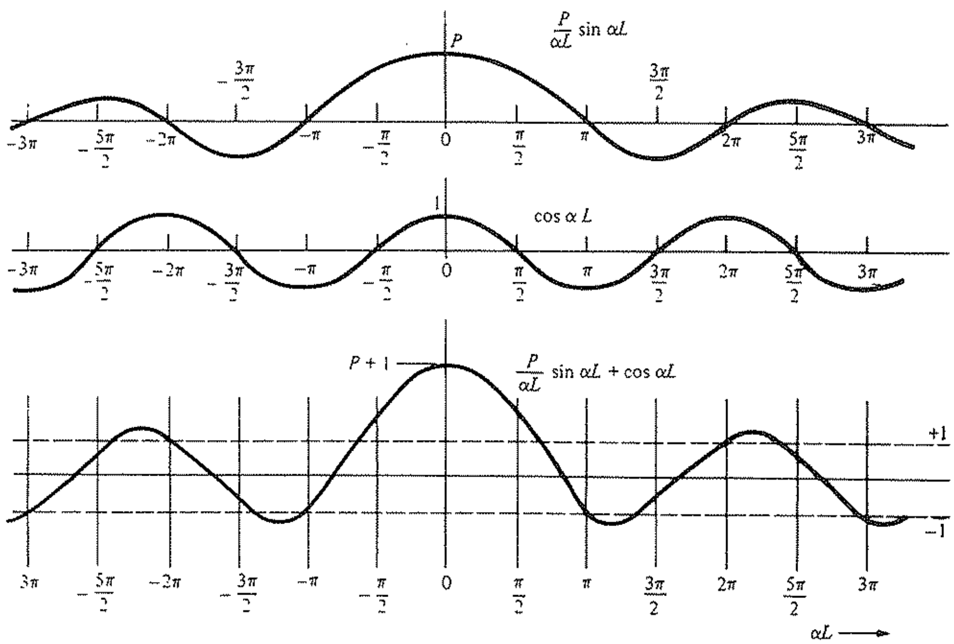
Electrons in periodic potentials



Simplified solution from Krönig - Penney Model

$$P \cdot \frac{\sin(\alpha L)}{\alpha L} + \cos(\alpha L) = \cos(kL)$$

where $P = \lim_{\substack{V_0 \to \infty \\ b \to 0}} \left(\frac{1}{2}\beta^2 ab\right)$; $\alpha^2 = \frac{2m}{\hbar^2} E$; $\beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$



Energy versus k characteristics

Recall: for a free particle we have

$$\boxed{E = \frac{1}{2}\frac{p^2}{m} = \frac{1}{2}\frac{\hbar^2 k^2}{m}}$$

In a crystal, we obtain the particles energy from the solution of the Kronig - Penney Model

$$\left\| P\,\frac{\sin(\alpha l)}{\alpha l} + \cos(\alpha l) = \cos(kl) \right\|$$

where $\alpha^2 = \frac{2m}{\hbar^2} E$

Thus $\boxed{E = \alpha^2 \frac{\hbar^2}{2m}}$

free particle

$$E = \frac{\hbar^2}{2m} k^2$$

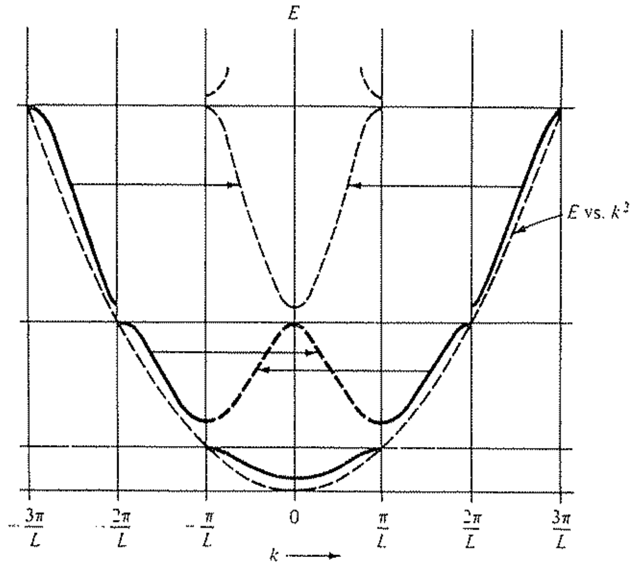
E vs. k plot results in a parabolic curve

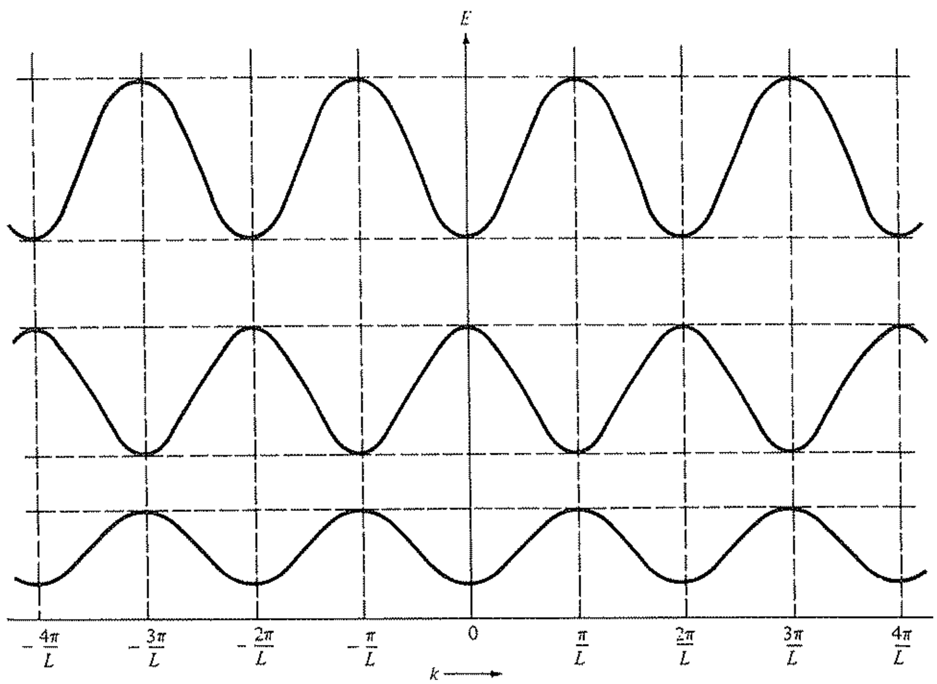
particle in crystal

$$E = \frac{\hbar^2}{2m} \alpha^2$$

Since α must satisfy the solution derived from the Kronig-Penney model, the E vs. k plot will be a discontinuous function with a curvature different from that of a parabola.

Energy versus k characteristics





3.7 The concept of the effective mass

Objective: We want a model for charge carriers in a crystal that enables us to treat the charge carrying particles as if they were free (ideal Fermi gas).

Solution: The effects of the crystal lattice are included by modifying the parameters used to describe the particle. This will be accomplished by redefining the particles mass ($m \to m^*$).

The kinetic energy of a free particle is given by:

$$\underline{\underline{E}} = \frac{p^2}{2m} = \underline{\underline{\frac{(\hbar k)^2}{2m}}}$$

The particle's velocity is given by

$$\underline{\underline{v}} = \frac{dE}{dp} = \frac{p}{m} = \frac{\hbar k}{m} = \underline{\underline{\frac{dE}{dk}\frac{1}{\hbar}}}$$

The particle's acceleration is, therefore:

$$\underline{\underline{a}} = \frac{dv}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right] = \frac{1}{\hbar}\frac{dk}{dt}\frac{d}{dk}\left[\frac{dE}{dk}\right]$$

$$\underline{\underline{= \frac{1}{\hbar}\frac{dk}{dt}\frac{d^2E}{dk^2} = \frac{dk}{dt}\frac{\hbar}{m}}}$$

Since $\frac{1}{\hbar}\frac{d^2E}{dk^2} = \frac{\hbar}{m}$ we obtain the particle's mass as

$$\underline{\underline{m = \hbar^2 \left[\frac{d^2E}{dk^2}\right]^{-1}}}$$

If we apply this formula also to particles in a crystal, where the E vs k characteristic is no longer parabolic, we obtain a value for the particle mass which is different from the mass of the free particle. We call this "pseudo mass" the "effective" mass of the particle.

Thus

$$\boxed{m^* = \frac{\hbar^2}{d^2E/dk^2}}$$

<u>Notes</u> $\frac{d^2E}{dk^2}$, i.e. the curvature in the E vs k plot, can be positive, negative and zero. Hence, the effective mass of a particle in a crystal can be positive, negative and infinite

<u>Comment</u> Mass is a quantification of the difficulty of accelerating an entity with a given force ($m = \frac{\bar{F}}{\bar{a}}$). Thus, $m^* = \infty$ implies that the particle cannot be accelerated by external forces. A neg. effective mass implies that the object reacts to an attractive force as if it would experience a repulsive force. This can happen if the external force tries to impel a particle into a region dominated by a repulsive force whose magnitude increases as the particle penetrates further into the region.

Note: The effective mass is not a simple scalar quantity; it depends on the direction under consideration ($\bar{k}$ is a vector), the carrier type and the material. Therefore, for any given material, there exist several effective masses.

Example effective masses of common semiconductors*

Material	Density-of-State masses		Conductivity masses	
	m_n^*/m_0	m_p^*/m_0	m_n^*/m_0	m_p^*/m_0
Si	1.08	0.81	0.26	0.39
Ge	0.55	0.29	0.12	0.29
GaAs	0.068	0.82	0.068	0.82
GaP	0.82	0.60	0.82	0.60

Note: The values indicated in the above table are averages!

Alternative concept to view the effective mass.

Total force that particle experiences: $\bar{F}_{tot} = \sum_i \bar{F} = m \cdot \bar{a}$

A single external force is then $\bar{F}_{ex} = m\bar{a} - \sum_i \bar{F}_{in} = m^* \bar{a}$

$$\text{where} \quad m^* = m - \sum_i \bar{F}_{in} \frac{\bar{a}}{|\bar{a}|^2}$$

* According to Muller / Kamins: Device Electronics for IC's, Tab. 1.3 pp. 54-55