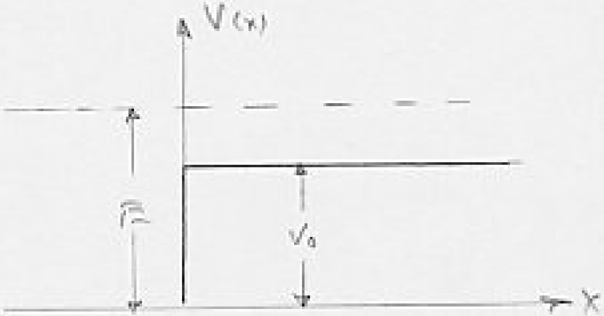
Chapter 5

One-Dimensional Potentials:



A- The Potential Step

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases} \qquad (1)$$

The Schrödinger equ.;

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

$$\rightarrow \quad \frac{d^2 u(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right] u(x) = 0 \qquad (3)$$

We introduce;
$$\frac{2mE}{\hbar^2} = k^2 \quad , \quad \frac{2m(E-V_0)}{\hbar^2} = q^2 \qquad (4)$$

For region $x<0$ $\quad V(x)=0 \quad \rightarrow u(x) = e^{ikx} + R e^{-ikx}$ $\qquad (5)$

$$j(x) = \frac{\hbar}{2im}\left[\psi^*(x)\frac{d\psi(x)}{dx} - \frac{d\psi^*(x)}{dx}\psi(x)\right] \qquad (6)$$

$$j(x) = \frac{\hbar}{2im}\left[(e^{-ikx} + R^* e^{ikx})(ik e^{ikx} - ikR e^{-ikx}) - \text{Complex conjugate}\right]$$

$$= \frac{\hbar k}{m}\left(1 - |R|^2\right) \qquad (7)$$

e^{ikx} : Incoming wave with flux $\frac{\hbar k}{m}$

Re^{-ikx} : Reflected wave (by $V(x)$) with flux $\frac{\hbar k |R|^2}{m}$

For $x>0$, $V(x) = V_0 \quad \rightarrow u(x) = T e^{iqx}$ $\qquad (8)$

$$j(x) = \frac{\hbar q}{m}|T|^2 \qquad (9)$$

Since $\frac{\partial P(x,t)}{\partial t} = 0$ $\left(V \neq V(t) \rightarrow \frac{\partial}{\partial t} P(x,t) = \frac{\partial}{\partial t} \left| e^{iHt/\hbar} \psi(x) \right|^2 = 0 \right)$

$$\rightarrow \frac{\partial P(x,t)}{\partial t} + \frac{\partial j(x)}{\partial x} = 0 \quad \rightarrow \frac{\partial j(x)}{\partial x} = 0 \qquad j(x) = \text{const.} \quad (10)$$

$$\rightarrow j(x)_{left} = j(x)_{right} \quad \rightarrow \frac{\hbar k}{m}\left(1 - |R|^2\right) = \frac{\hbar q}{m} |T|^2 \quad (11)$$

From the continuity of the wave func.;

$$\left(e^{ikx} + R e^{-ikx} \right)\Big|_{x=0} = \left(T e^{iqx} \right)\Big|_{x=0} \quad \rightarrow 1 + R = T \quad (12)$$

Remark: In spite of the fact that the potential is discontinuous, the <u>slope</u> of the wave func. is continuous.

$$(3) \rightarrow \int_{-\epsilon}^{\epsilon} \frac{d^2 u(x)}{dx^2} dx = \int_{-\epsilon}^{\epsilon} dx \frac{2m}{\hbar^2} \left[V(x) - E \right] u(x) \quad (13)$$

$$\left(\frac{du}{dx}\right)_{\epsilon} - \left(\frac{du}{dx}\right)_{-\epsilon} = \int_{-\epsilon}^{0} dx \frac{2m}{\hbar^2} \left[0 - E \right] \left(e^{ikx} + R e^{-ikx} \right) \quad (14)$$

$$+ \int_{0}^{\epsilon} dx \frac{2m}{\hbar^2} \left[V_0 - E \right] \left(T e^{iqx} \right) \quad (15)$$

$$\left(\frac{du}{dx}\right)_{\epsilon} - \left(\frac{du}{dx}\right)_{-\epsilon} = \frac{-2mE}{\hbar^2} \left[\frac{1}{ik} e^{ikx} - \frac{R}{ik} e^{-ikx} \right]_{-\epsilon}^{0} + \frac{2m}{\hbar^2}(V_0 - E) \left[\frac{T}{iq} e^{iqx} \right]_0^{\epsilon}$$

$$= -\frac{2mE}{\hbar^2} \left[\frac{1}{ik}\left(1 - e^{-ik\epsilon}\right) - \frac{R}{ik}\left(1 - e^{ik\epsilon}\right) \right] + \frac{2m}{\hbar^2}(V_0 - E) \frac{T}{iq}\left(e^{iq\epsilon} - 1 \right)$$

$$\left(\frac{du}{dx}\right)_{\epsilon} - \left(\frac{du}{dx}\right)_{-\epsilon} = 0 \quad (16) \qquad \text{slope} = \left(\frac{du}{dx}\right)\Big|_{x=x_0}$$

$\epsilon \rightarrow 0$

Remark: If the pot. contains a term like $V_0\,\delta(x-a)$, then

$$\left(\frac{du}{dx}\right)_{a+\epsilon}-\left(\frac{du}{dx}\right)_{a-\epsilon}=\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon}dx\,V_0\,\delta(x-a)\,u(x)+0 \qquad (17)$$

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

The continuity of the derivative of the wave func. implies that;

$$ik\left(e^{ikx}-Re^{-ikx}\right)_{x=0}=iqT\left(e^{iqx}\right)_{x=0} \qquad (18)$$

$$\rightarrow\ ik(1-R)=iqT \qquad (19)$$

$$(12)\,(19)\rightarrow\ R=\frac{k-q}{k+q} \qquad T=\frac{2k}{k+q} \qquad (20)$$

$$\rightarrow\ \frac{\hbar k}{m}|R|^2=\frac{\hbar k}{m}\left(\frac{k-q}{k+q}\right)^2 \quad \text{Reflected flux} \qquad (21)$$

$$\frac{\hbar q}{m}|T|^2=\frac{\hbar k}{m}\,\frac{4kq}{(k+q)^2} \quad \text{Transmitted "}$$

Some points:

1) In contrast to cl. M., acc. to which a particle going over a pot. step would slow down (to conserve energy) but would never be reflected, here we do have a certain fraction of the incident particles reflected.
This is the consequence of the wave properties of the particle.

2) By the help of (21) we can check that the conservation law (11) is satisfied.

3) For $E >> V_0$, i.e. $q \to k$ (from below)

$$\frac{\text{Reflected flux}}{\text{Incident flux}} = \frac{|R|^2}{1} \longrightarrow 0 \qquad (22)$$

This agrees with intuition, which tells us that at very high energies, the presence of the step is but a small perturbation on the propagation of the wave.

4) If $E < V_0 \to q = \text{imaginary}$

For $x > 0 \to u(x) = T e^{-|q|x}$ (23)

$$|R|^2 = \left(\frac{k - i|q|}{k + i|q|}\right)\left(\frac{k - i|q|}{k + i|q|}\right)^* = 1 \qquad (24)$$

Thus, as in classical mechanics, there is now total reflection.

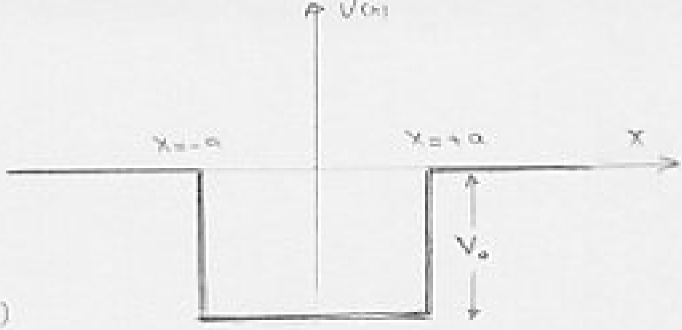
However, $T = \frac{2k}{k + i|q|}$ (25)

does not vanish, and a part of the wave penetrates into the forbidden region (tunneling).

Note that $j_{\text{right}}(x) = \frac{\hbar}{2mi}|T|^2\left(e^{-|q|x}(-|q|e^{-|q|x}) - (-|q|e^{-|q|x})e^{-|q|x}\right) = 0$

(26)

B. The potential Well



$$V(x) = \begin{cases} 0 & x<-a \\ -V_0 & -a<x<a \\ 0 & x>a \end{cases} \qquad (27)$$

The shrodinger equ.:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) - V_0 u(x) = E u(x) \qquad -a<x<a$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) = E u(x) \qquad x<-a\ ,\ x>a \qquad (28)$$

$$K^2 = \frac{2mE}{\hbar^2} \qquad q^2 = \frac{2m(E+V_0)}{\hbar^2} \qquad (\text{For } E>0) \quad (29)$$

The sol.:

$$u(x) = e^{ikx} + R e^{-ikx} \qquad x<-a$$

$$u(x) = A e^{iqx} + B e^{-iqx} \qquad -a<x<a \qquad (30)$$

$$u(x) = T e^{ikx} \qquad x>a$$

Incoming flux $= \frac{\hbar k}{m}$

Reflected " $= \frac{\hbar k |R|^2}{m}$ (31)

Transmitted " $= \frac{\hbar k |T|^2}{m}$

Flux conservation: $J_L = J_M = J_R$

$$\frac{\hbar k}{m}(1-|R|^2) = \frac{\hbar q}{m}(|A|^2-|B|^2) = \frac{\hbar k}{m}|T|^2 \qquad (32)$$

$$\begin{cases} u_L(x)\big|_{x=-a} = u_M(x)\big|_{x=-a} \rightarrow e^{-ika} + R e^{ika} = A e^{-iqa} + B e^{iqa} \\ \dfrac{du_L(x)}{dx}\Big|_{x=-a} = \dfrac{du_M(x)}{dx}\Big|_{x=-a} \rightarrow ik(e^{-ika} - R e^{ika}) = iq(A e^{-iqa} - B e^{iqa}) \end{cases} \quad (33)$$

$$\begin{cases} u_M(x)\big|_{x=a} = u_R(x)\big|_{x=a} \longrightarrow A e^{iqa} + B e^{-iqa} = T e^{ika} \\ \dfrac{du_M(x)}{dx}\Big|_{x=a} = \dfrac{du_M(x)}{dx}\Big|_{x=a} \longrightarrow iq(A e^{iqa} - B e^{-iqa}) = ikT e^{ika} \end{cases} \quad (34)$$

$$\rightarrow \quad R = i\, e^{-2ika} \frac{(q^2-k^2)\,\mathrm{Sin}(2qa)}{2kq\,\mathrm{Cos}(2qa) - i(q^2+k^2)\,\mathrm{Sin}(2qa)}$$

$$T = e^{-2ika} \frac{2kq}{2kq\,\mathrm{Cos}(2qa) - i(q^2+k^2)\,\mathrm{Sin}(2qa)} \quad (35)$$

If $E >> V_0 \quad \Longrightarrow q \simeq k \quad \Rightarrow R \rightarrow 0$

If $E \rightarrow 0 \quad \Rightarrow k \rightarrow 0 \quad \Rightarrow T \rightarrow 0 \quad (36)$

A special Case:

$\mathrm{Sin}\, 2qa = 0 \quad \rightarrow 2qa = n\pi \rightarrow 4q^2a^2 = n^2\pi^2 \quad (37)$

$\rightarrow E = -V_0 + \dfrac{\pi^2 n^2 \hbar^2}{8ma^2} \quad n = 1, 2, 3 \ldots \quad (38)$

In this case; $R = 0$

This is actually a model of what happens in the scattering of low energy electrons (0.1 eV) by noble gas atoms (neon, argon - -).

In this case, $T \to$ large (anomalously)

This effect, first observed by Ramsauer and Townsend, is described as a transmission resonance.

More accurate discussion must involve 3-dim. considerations.

In wave language, the effect is due to a destructive interference between the wave reflected at $x = -a$ and the wave reflected once, twice, thrice - - -, at the edge $x = a$.

The resonance cond. : $2qa = n\pi$

$$\to \quad \lambda = \frac{2\pi}{q} = \frac{4a}{n} \qquad (39)$$

For $E < 0$, when the pot. is negative (i.e. $V_0 > 0$),

$$\frac{2mE}{\hbar^2} = -k^2 \qquad (40)$$

$$u(x) = C_1 e^{kx} \qquad x < -a$$

$$u(x) = C_2 e^{-kx} \qquad x > a$$

(to be bounded at $x \to \pm\infty$)

(41)

Since (41) are real funcs., it is more convenient to write the sol. inside the well in the form:

$$u(x) = A\cos(qx) + B\sin(qx) \qquad -a < x < a \qquad (42)$$

$$q^2 = \frac{2m}{\hbar^2}(V_0 - |E|) > 0 \qquad (43)$$

Matching the sols. and derivatives at the edges $x = \pm a$:

$$\begin{cases} u_L(x)\big|_{x=-a} = u_M(x)\big|_{x=-a} \longrightarrow C_1 e^{-ka} = A\cos(qa) - B\sin(qa) \\ \dfrac{du_L(x)}{dx}\Big|_{x=-a} = \dfrac{du_M(x)}{dx}\Big|_{x=-a} \longrightarrow kC_1 e^{-ka} = q\left(A\sin(qa) + B\cos(qa)\right) \end{cases} \qquad (44)$$

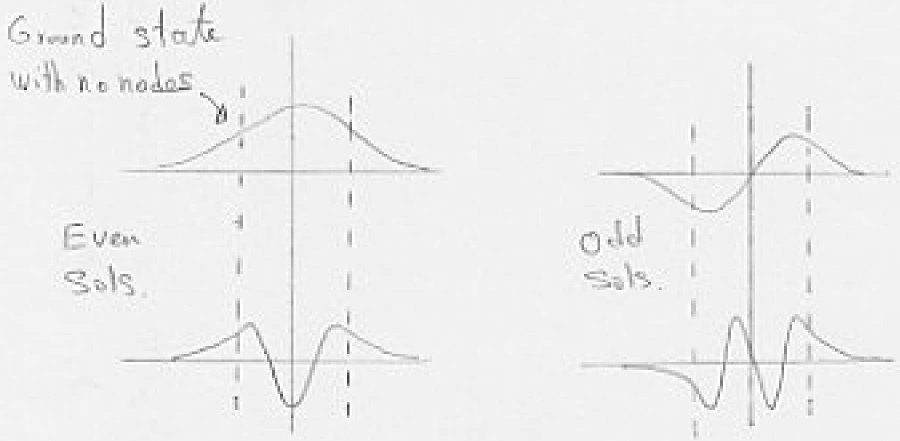
$$\begin{cases} u_R(x)\big|_{x=a} = u_M(x)\big|_{x=a} \longrightarrow C_2 e^{-ka} = A\cos(qa) + B\sin(qa) \\ \dfrac{du_R(x)}{dx}\Big|_{x=a} = \dfrac{du_R(x)}{dx}\Big|_{x=a} \longrightarrow -kC_2 e^{-ka} = -q\left(A\sin(qa) - B\cos(qa)\right) \end{cases} \qquad (45)$$

$$\rightarrow k = q\,\frac{A\sin(qa) - B\cos(qa)}{A\cos(qa) + B\sin(qa)} = q\,\frac{A\sin(qa) + B\cos(qa)}{A\cos(qa) - B\sin(qa)} \qquad (46)$$

Also $AB = 0 \longrightarrow A = 0,\ B \neq 0$ or $B = 0,\ A \neq 0$ (47)

$\longrightarrow$ The sols. are either even in x $(B = 0)$

or odd " " $(A = 0)$



$$(46)(47) \rightarrow \begin{cases} k = q \tan qa & \text{even sols.} \\ k = -q \cot g\, qa & \text{odd "} \end{cases} \qquad (48) \quad \text{conds. for energy}$$

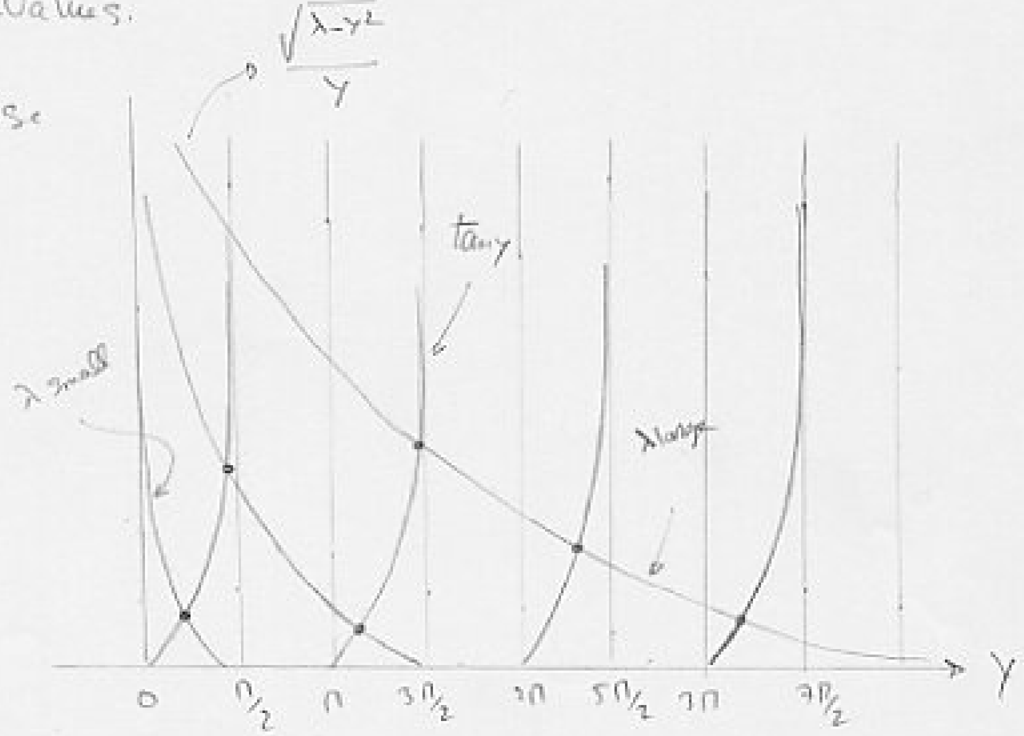
a) For even sols.;

with the notation $\lambda \equiv \frac{2mV_0 a^2}{\hbar^2}$ $\qquad y \equiv qa$

$$(48) \rightarrow \frac{\sqrt{\lambda - y^2}}{y} = \tan y \qquad (49) \quad (\text{for the first eqn.})$$

The points of intersection determine the eigenvalues.

Remark: we choose $\tan y > 0$ curves because of $\sqrt{\ }$.



The larger λ is, the further the curves for $\frac{\sqrt{\lambda - y^2}}{y}$ go;

i.e. when the pot. is deeper ($V_0 \to$ large)

and or " " " " broader ($a \to$ large)

$\longrightarrow$ There are more bound states.

The Fig. shows that no matter how small λ is, there will always be at least one bound state.

This is characteristic of one-dim. attractive pots., and not true for 3-dim. pots, which behave much more like the odd-sol. problem.

As $\lambda \longrightarrow$ large, the eigenvalues tend to become equally spaced in y, with the intersection points given by,

$$y \simeq (n+\tfrac{1}{2})\frac{\pi}{2} \quad n = 0,1,2,\ldots \quad (50) \quad (\text{see the Fig.})$$

This is just the eigenvalue cond. for the even sols. of the infinite box, and this is as might be expected, since for the deep-lying states in the potential, the fact that it is not really infinitely deep, does not matter very much.

b) The odd sols.;

$$(48) \longrightarrow \frac{\sqrt{\lambda - y^2}}{y} = -\cot y \qquad (51)$$

Since $-\cot y = \tan(\frac{\pi}{2}+y)$, the plot is the same as before with the tangent curves shifted by $\pi/2$.

For $\lambda \to$ large $\qquad y \simeq n\pi \quad n=1,2,3 \qquad (52)$

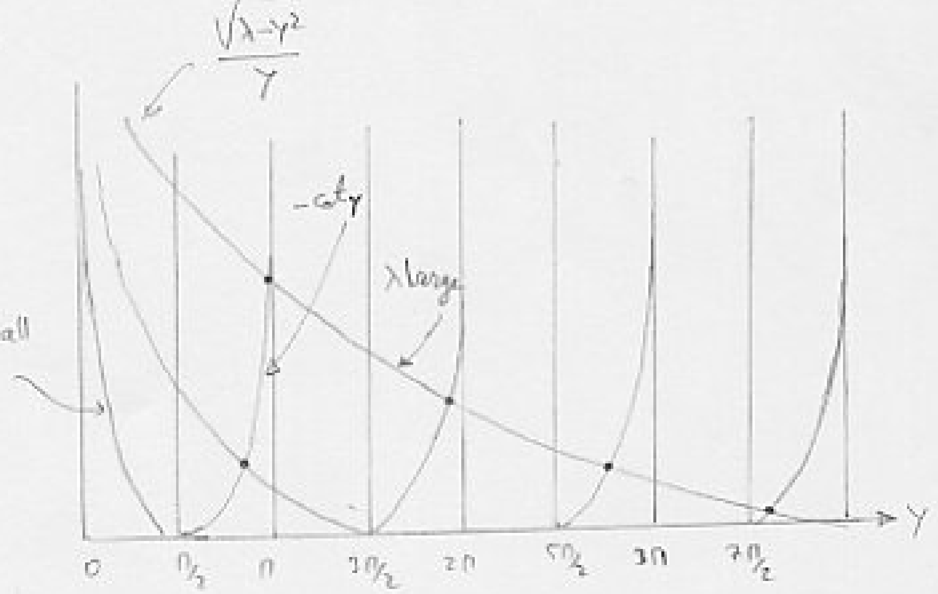
Note that:

There will only be an intersection if:

$\sqrt{\lambda - (\frac{\pi}{2})^2} > 0$

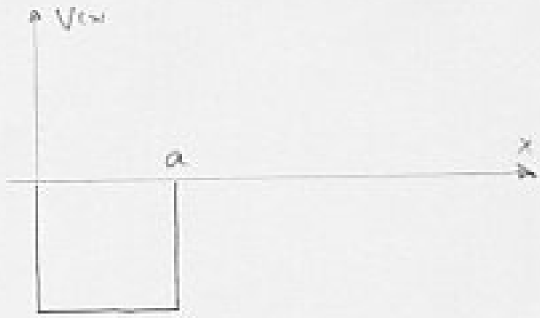
That is

$$\frac{2mV_0a^2}{\hbar^2} \geq \frac{\pi^2}{4} \qquad (53)$$



All, $u_{odd}(x=0) = 0$

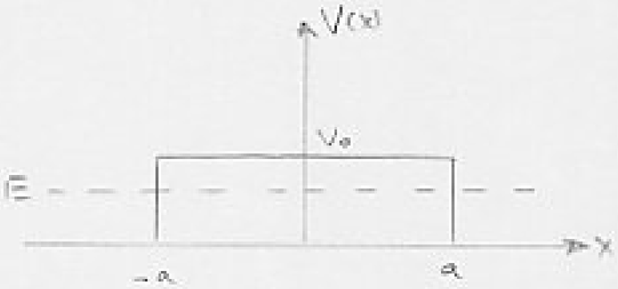
Hence the bound state problem for odd sols. will be the <u>same</u> as for the pot. well shown below, since in the later, the cond $u(0)=0$ would be imposed.



C. The Potential Barrier

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

We limit our discussion to energies such that $E < V_0$, that is, no peneteration of the barrier would occur in cl. phys.



$$\frac{d^2 u(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\, u(x) = 0 \qquad (54)$$

inside the barrier

or $$\frac{d^2 u(x)}{dx^2} - \kappa^2 u(x) = 0 \qquad \kappa^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

The general sol.,

$$u(x) = A e^{\kappa x} + B e^{-\kappa x} \qquad -a < x < a \qquad (55)$$

$$u(x) = e^{ikx} + R e^{-ikx} \qquad x < -a$$

$$u(x) = T e^{ikx} \qquad x > a$$

where $k^2 = \dfrac{2mE}{\hbar^2}$

We need not go through the trouble of solving this, since the results can be read off from (35) with the substitution

$$q \to ik = i\sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \qquad (56)$$

Thus for example: $$T = e^{-2ik} \frac{2kK}{2kK \cosh(2ka) - i(K^2 - k^2)\sinh(2ka)} \qquad (57)$$

Note that: $$\cos(x+iy) = \cos x \cosh y - i \sin x \sinh y$$
$$\sin(x+iy) = \sin x \cosh y + i \cos x \sinh y \qquad (58)$$

$$(57) \to \quad |T|^2 = \frac{(2kK)^2}{(K^2+k^2)^2 \sinh^2(2ka) + (2kK)^2} \qquad (59)$$

Note that $|T|^2 \neq 0$ even $E < V_0$

This is a wave phenomenon, and in Q.M. it is also exhibited by particles (tunneling).

For $ka \to$ large

$$|T|^2 \simeq \left(\frac{4kK}{K^2+k^2}\right)^2 e^{-4ka} \qquad (60)$$

Remark:
$\sinh x \sim \frac{1}{2} e^{x}$
for $x \gg 1$

Remark:

$$\cosh x = \frac{1}{2}(e^{x} + e^{-x})$$
$$\sinh x = \frac{1}{2}(e^{x} - e^{-x})$$

Since $\kappa a = \left[\frac{2ma^2}{\hbar^2}(V_0 - E)\right]^{1/2}$ (61)

$\rightarrow |T|^2$ becomes sensitive func. of $\begin{cases} a \\ (V_0 - E) \end{cases}$

For other kind of barriers (arbitrary shape of Pot.), WKB approx. is used.

Another approx. method for arbitriary barrier;

$$(60) \rightarrow \ln |T|^2 \simeq -2\underbrace{\kappa(2a)}_{\text{Dominant term}} + 2\ln \frac{4(ka)(\kappa a)}{(ka)^2 + (\kappa a)^2} \qquad (62)$$

under most circumstances (for any reasonable size of κa).

Since transmission coeffs. are multiplicative when they are small, i.e. $|T|^2 = |T_1|^2 |T_2|^2 \cdots |T_n|^2$ (63)

(independent events)

Then we may write approximately;

$$\ln |T|^2 \simeq \sum_{\text{Partial barriers}} \ln |T_{\text{partial barriers}}|^2 \simeq -2 \sum \Delta x \langle \kappa \rangle$$

$$\simeq -2 \int_{\text{barrier}} dx \sqrt{\frac{2m}{\hbar^2}(V(x) - E)} \qquad (64)$$

$\langle \kappa \rangle$: ave. of κ for each barrier

The approx. is least accurate near the turning points; where $E \simeq V(x)$, because in this case (60) is not a good, approx. to (59)

V(x) must also be slowly varying func. of x, since otherwise the approx. of a curved barrier by a stack of square ones is only possible if the later are narrow, and then again (60) is poor approx..

i.e. $a \xrightarrow{\text{must be}} \text{small} \Rightarrow ka \rightarrow \text{small}$

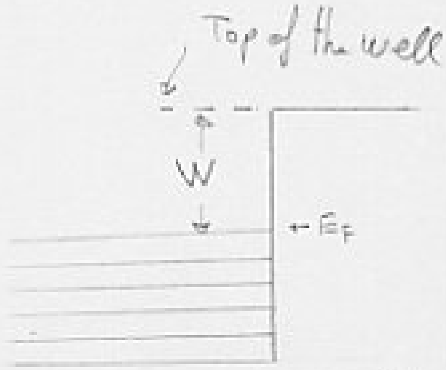
For most purposes, it is still a fair approx. to write:

$$|T|^2 \simeq e^{-2\int dx \sqrt{\frac{2m}{\hbar^2}(V(x)-E)}} \qquad (65)$$

with integration over the region in which the square root is real.

D. Tunneling Phenomena

a) Consider electrons in metal.



Electrons in metal held by a pot., which to first approx., may be described by a box of finite depth

The levels are filled taking into account the Pauli exclusion principle.

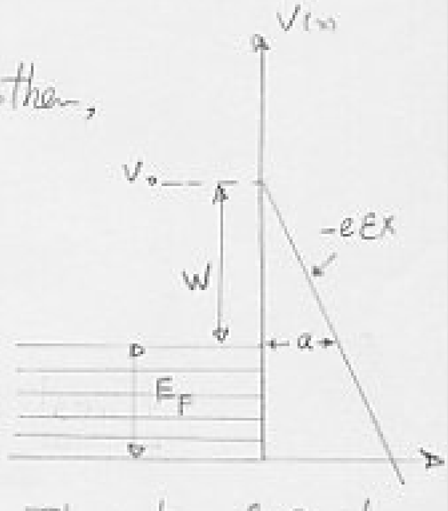
W: work fnc.

When $T > 0°K$, a few electrons are thermally excited to higher levels.

(but the number is small even at room temperature)

The electrons can be removed by transferring energy to them,

{ either by photons
{ or by heating them



They can also be removed by the application of an external electric field $\mathcal{E}$ (Cold emission).

The external $\mathcal{E}$ change the shape of the pot. from $W \xrightarrow{\text{to}} (W - e\mathcal{E}x)$ (seen by the electrons at the top of Fermi sea)

The pot.: $W \xrightarrow{-e\mathcal{E}x} W - e\mathcal{E}x$ (seen by the electron at the Fermi sea level)

$$|T|^2 \simeq e^{-2\int_0^a dx \left[\frac{2m}{\hbar^2}(W - e\mathcal{E}x)\right]^{1/2}} \quad (66)$$

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

$$\rightarrow \quad |T|^2 = e^{-(4\sqrt{\frac{2}{3}})\sqrt{mW}/\hbar^2 \,(W/e\mathcal{E})} \quad (67)$$

← Fowler–Nordheim Formula

Recall:
$V(x) - E = [\underbrace{E_F + W}_{V_0} - e\mathcal{E}x] - E_F$
and $E = E_F = V_0 - W$

where $V_0 - e\mathcal{E}a = V_0 - W$

$\rightarrow a = \dfrac{W}{e\mathcal{E}}$ barrier thickness at the top of Fermi sea.

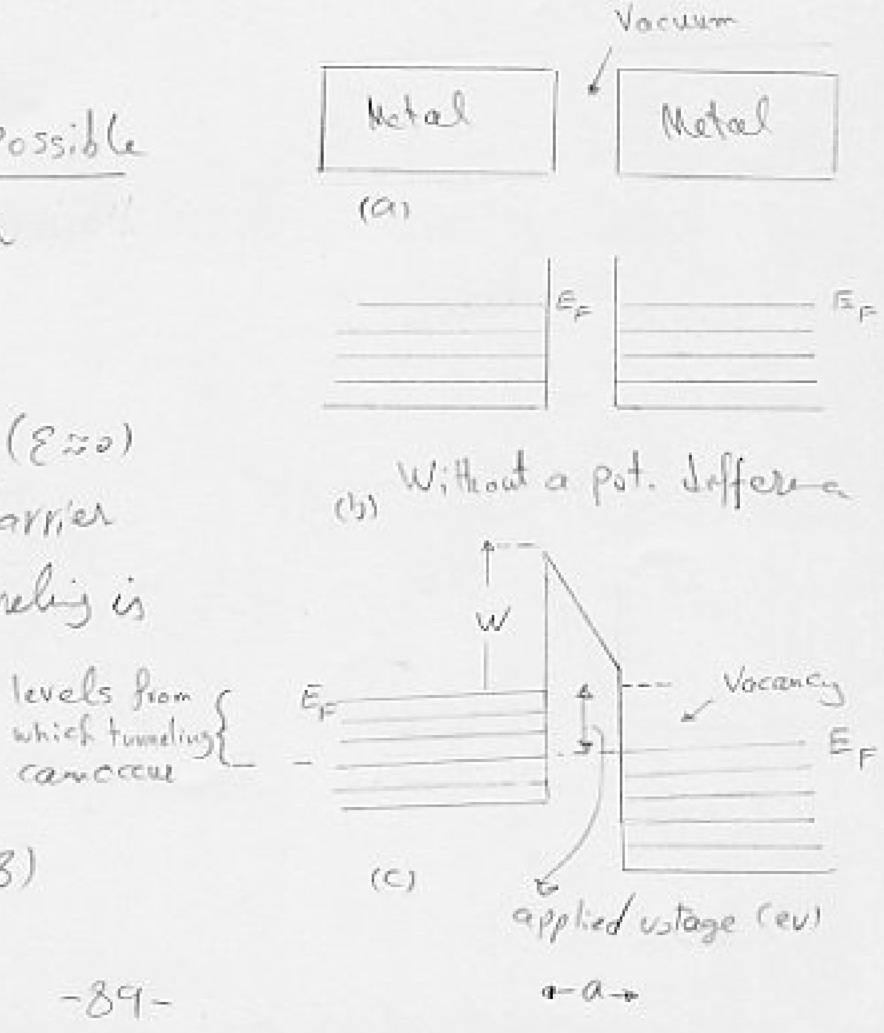
There is another effets, to be considered;

i) That is the attraction of the electron back to the plate, caused by the image charge.

ii) There are surface imperfections in metal surface, which change the electric field locally, and since $\mathcal{E}$ appear in the exponent, this can make a large difference

Two metal plates:

The same effect appears if we bring two metal plates close together.



In Fig. b tunneling is impossible because the levels on both sides are filled.

Eeven a weak electric field ($\mathcal{E} \simeq 0$) can change the shape of the barrier as shown in Fig. c. Tunneling is possibe in this case

With $\mathcal{E} \simeq 0$;

$$|T|^2 \simeq e^{-2\sqrt{\frac{2mW}{\hbar^2}}\,a} \qquad (68)$$

Such a factor acts as a <u>resistance</u>.

This expression is very sensitive to a, and since

$$W \sim O(\text{eV}) \longrightarrow a \sim O(\text{angstroms})$$

It has not proved possible to make metal plates sufficiently flat and parallel.

The formula has been applied to the interpretation of currents flowing between two plates with an <u>oxide</u> between them (Ni-NiO-Pb), where the gap can be made as small as 50 Å and it is qualitatively correct.

b) α - Decay

Parent $\longrightarrow {}^4_2He$ + Daughter

This phenomena can be explained by the tunneling effect.

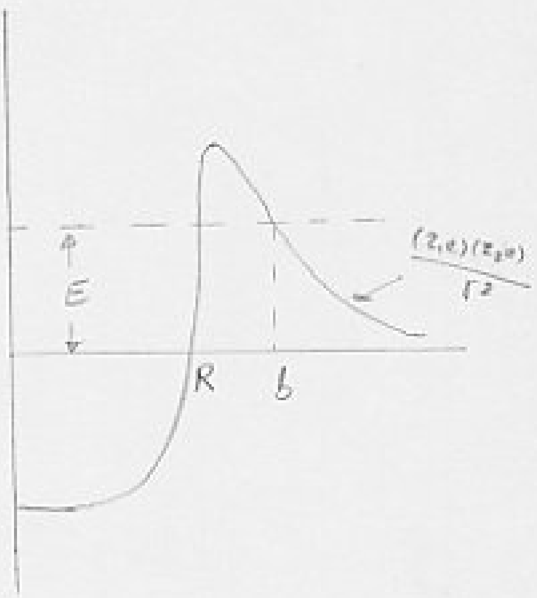
The barrier is caused by the Coulomb pot. between the daughter and the α-particle.

Remark: 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 decay is only inhibited by the existance of the barrier.

$V(r) = K \frac{Z_1 Z_2 e^2}{r}$
here K is absorbed in e^2

$$|T|^2 = e^{-G}$$

where $G = 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_R^b dr \left(\frac{Z_1 Z_2 e^2}{r} - E\right)^{\frac{1}{2}} \qquad (69)$$



Z_1: for the daughter nucleus

$Z_2 = 2$: for α-particle

$$\frac{Z_1 Z_2 e^2}{b} - E = 0 \Rightarrow E = \frac{Z_1 Z_2 e^2}{b} \qquad (70)$$

R: nuclear radius

b: Turning point (determined by the vanishing of integrand)

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{1/2} (Z_1 Z_2 e^2)^{1/2} \int_R^b dr \left(\frac{1}{r} - \frac{1}{b}\right) \qquad (71)$$

$$\int_R^b dr \left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} = \sqrt{b} \left[\cos^{-1}\left(\frac{R}{b}\right)^{1/2} - \left(\frac{R}{b} - \frac{R^2}{b^2}\right)^{1/2} \right] \qquad (72)$$

At low energies (relative to the height of the Coulomb barrier at $r = R$)

we have $b \gg R$ (see the Fig.)

$\rightarrow$ the second term negligible.

and, $\cos^{-1} x \simeq \frac{\pi}{2} - x$ for $|x| \ll 1$ (73)

$$\rightarrow \quad G \simeq 2\left(\frac{2m Z_1 Z_2 e^2 b}{\hbar^2}\right)^{1/2} \left[\frac{\pi}{2} - \underbrace{\left(\frac{R}{b}\right)^{1/2}}_{\simeq 0}\right] \qquad (74)$$

with $b = \frac{Z_1 Z_2 e^2}{E}$ (75)

Setting $E = \frac{mv^2}{2}$ (v: out of the nucleus) (76)

$$G \simeq \frac{2\pi Z_1 Z_2 e^2}{\hbar v} = 2\pi \alpha Z_1 Z_2 \left(\frac{c}{v}\right) \qquad (77)$$

The time taken for an α-particle to get out the nucleus may be <u>estimated</u> as follows:

$P = e^{-G}$ the probability of getting through the barrier on a single encounter. (78)

1 (number of encounters)	e^{-G}	
$n \simeq ?$	1	

$n \simeq e^{+G}$ number of encounters to get through. (79)

$$t = \frac{2R}{V} \qquad \text{the time between encounters} \qquad (80)$$

V: the α velocity inside the nucleus (rather a fuzzy concept)

$$\rightarrow \quad \tau \simeq \frac{2R}{V} e^{G} \qquad \text{lifetime} \qquad (81)$$

$V_{in} \simeq V_{out}$ (approx.), For $E = 1$ Mev α-particles

$$\rightarrow V = \sqrt{\frac{2E}{m}} = c\sqrt{\frac{2E}{mc^2}} = 3\times10^{10}\sqrt{\frac{2(1)}{4(940)}} \simeq \frac{3}{43}\times10^{10}\ \text{cm/sec} \qquad (82)$$

where $m_\alpha c^2 = 4\times940$ Mev

Also, for R we take

$$R \simeq 1.5\times10^{-13} A^{\frac{1}{3}}\ \text{cm}$$

and for $A = 126$ $\qquad \frac{2R}{V} = 2.6\times10^{-21} \qquad (83)$

Also, G can be written in the form;

$$(74) \rightarrow \quad G \simeq 2\left(\frac{2m(z_1 z_2 e^2)^2}{\hbar^2 E}\right)^{1/2}\frac{\pi}{2} = 2\left(\frac{2m Z_1^2\, 2^2\, e^4}{\hbar^2 E}\right)^{\frac{1}{2}}\frac{\pi}{2} \qquad (84)$$

$$= 4\,\frac{Z_1}{\sqrt{E}}\left(\frac{2me^4}{\hbar^2}\right)^{\frac{1}{2}}\frac{\pi}{2} = 4\,\frac{Z_1}{\sqrt{E(\text{Mev})}}$$

$$\frac{\pi}{2}\left(\frac{2me^4}{\hbar^2}\right)^{\frac{1}{2}} = \frac{\pi}{2}\left(2mc^2\frac{e^4}{\hbar^2c^2}\right)^{\frac{1}{2}} = \frac{\pi}{2}\left(2mc^2\alpha^2\right)^{\frac{1}{2}} = \frac{\pi}{2}\alpha\sqrt{2mc^2} = \frac{1}{137}\sqrt{2\times4\times940}\,\frac{\pi}{2}$$

$$= 1$$

Remark:

$z = x+iy \quad , w = \ln z \quad \rightarrow e^{w} = z \qquad (z \neq 0)$ (1)

$$\begin{cases} w = u+iv \\ z = |z|e^{i\theta} = re^{i\theta} \end{cases} \quad (2)$$

(2) in (1) $\rightarrow \quad e^{u+iv} = re^{i\theta} \quad (3)$

$|e^{u+iv}| = |re^{i\theta}| \quad \rightarrow \quad e^{u} = r = |z| \quad (4)$

$\rightarrow \quad u = \ln|z|$

Also, $v = \theta = \arg z$

$$\ln z = \ln|z| + i \arg z = \ln\sqrt{x^2+y^2} + i \arg(x+iy)$$

Due to the last term, the complex natural logarithm is infinitely many-valued.

The value of $\ln z$ corresponding to the principal value of $\arg z$, that is $-\pi < \arg z \leqslant \pi$ is called principal value of $\ln z$ ($\operatorname{Ln} z$).

$$\ln z = \operatorname{Ln} z \pm 2n\pi i \qquad (n = 1, 2, \ldots)$$

a) For z: real, positive $\begin{cases} \text{the principal value of } \arg z = 0 \\ \text{and } \operatorname{Ln} z = \underbrace{\ln z}_{\text{real}} \end{cases}$

b) For z: real, negative $\begin{cases} \text{the principal value of } \arg z = \pi \\ \text{and } \operatorname{Ln} z = \ln|z| + i\pi \end{cases}$

Ex.

i) $\ln(-1) = \pm\pi i, \pm 3\pi i, \pm 5\pi i, \ldots$ $\quad$ $\operatorname{Ln}(-1) = \pi i$

ii) $\ln i = \frac{\pi}{2} i, -\frac{3\pi}{2} i, \frac{5\pi}{2} i, -\frac{7\pi}{2} i, \frac{9\pi}{2} i, \ldots$ $\quad$ $\operatorname{Ln} i = \frac{\pi}{2} i$

iii) $\operatorname{Ln}(-i) = -\frac{\pi}{2} i$

iv) $\operatorname{Ln}(-2-2i) = \ln\sqrt{8} - \frac{3}{4}\pi i$

Also we have th relations;

a) $\ln(z_1 z_2) = \ln z_1 + \ln z_2$, b) $\ln\left(\frac{z_1}{z_2}\right) = \ln z_1 - \ln z_2$

Ex.

$z_1 = z_2 = e^{\pi i} = -1$

If we take $\ln z_1 = \ln z_2 = \pi i$, then (a) holds provided we write

$\ln(z_1 z_2) = \ln 1 = 2\pi i$

It is not true for th principal value $\operatorname{Ln}(z_1 z_2) = \ln 1 = 0$.

Also we have; $\frac{d}{dz} \ln z = \frac{1}{z}$

and $z^c = e^{c \ln z}$

$z^c = e^{c \operatorname{Ln} z}$ $\quad$ principal value of z^c

Since $\log_A x = \frac{\ln x}{\ln A}$

$$\log_{10}\frac{1}{\tau} = \log_{10}\left(\frac{v}{2R}e^{-G}\right) = \log_{10}\left(\frac{v}{2R}\right) + \log_{10} e^{-G}$$

$$= \text{Const.} + \log_{10} e^{-G} = \text{const.} + \frac{\ln e^{-G}}{\ln 10} = \text{const.} + \frac{-G}{2.30}$$

$$= \text{const.} - 1.73\frac{Z_1}{\sqrt{E(\text{Mev})}} \qquad (85) \quad \text{for low energy } \alpha\text{-particles}$$

A good fit to the lifetime data of a large number of α emitters is obtained with the formula;

$$\log_{10}\frac{1}{\tau} = C_2 - C_1\frac{Z_1}{\sqrt{E}} \qquad (86)$$

where $C_1 = 1.61$ and $C_2 = 28.9 + 1.6\, Z_1^{2/3}$

Thus the very simple considerations give a rather remarkable fit to the data.

The fact that the probability of a reaction (e.g. capture) between nuclei is attenuated by the factor

$$e^{-2\left(\frac{Z_1 Z_2}{\sqrt{E}}\right)}$$

implies that at $\begin{cases} E \to \text{low} \\ Z \to \text{high} \end{cases}$, such reactions are <u>rare</u>.

That is why all attempts to make thermonuclear reactors concentrate on the burning of hydrogen (Z; low) (actually heavy hydrogen - deuterium).

$$ {}_1H^2 + {}_1H^2 \longrightarrow {}_2He^3 + n \quad (3.27\ \mathrm{Mev}) $$

$$ {}_1H^2 + {}_1H^2 \longrightarrow {}_1H^3 + p \quad (4.03\ \mathrm{Mev}) $$

$$ {}_1H^2 + {}_1H^3 \longrightarrow {}_2He^4 + n \quad (17.6\ \mathrm{Mev}) $$

Since reations involving higher Z elements would require much higher energies (higher temperatures), with correspondingly greater confinement problems.

For the same reason, neutrons are used in nuclear reactors to fission the heavy elements.

Protons, at low energies available, would not be able to get near enough to the nuclei to react with them.

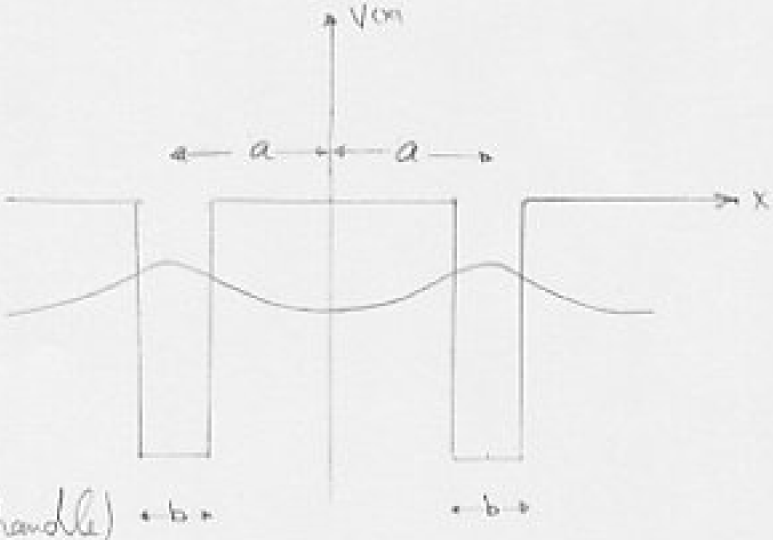
E. One-Dimensional Model of Molecule

Some aspects of what gives rise to molecules are exhibited by the example of a particle in a double potential well.

For algebraic simplification;

We assume;

$$\begin{cases} \text{depth } (V_0) \to \text{great} \\ \text{width } (a) \to \text{zero} \\ V_0\, a = \text{const.} \end{cases}$$



$\to$ δ-fnc. well (easy to handle)

Now consider a single attractive pot. well;

$$\frac{2m}{\hbar^2} V(x) = -\frac{\lambda}{a}\,\delta(x) \qquad (87)$$

For $E<0$

$$\frac{d^2u(x)}{dx^2} - k^2 u(x) = -\frac{\lambda}{a}\,\delta(x)\,u(x) \qquad (88)$$

where $\quad k^2 = \dfrac{2m|E|}{\hbar^2}$

The sol. everywhere, except at $x=0$, must satisfy the equ.,

$$\frac{d^2u(x)}{dx^2} - k^2 u(x) = 0 \qquad (89)$$

$$\to \quad u(x) = \begin{cases} A e^{-kx} & x>0 \\ B e^{kx} & x<0 \end{cases} \qquad (90)$$

$u_L(0) = u_R(0) \quad \rightarrow \quad A = B \qquad (91)$

we choose $A = B = 1$ (we can normalize afterwards)

But the derivative of the wave func. is no longer continuous.

$$\left(\frac{du}{dx}\right)_{x=0_+} - \left(\frac{du}{dx}\right)_{x=0_-} = -\frac{\lambda}{a} u(0) \qquad (92)$$

$$\rightarrow \quad -k - k = -\frac{\lambda}{a} \qquad \text{(eigenvalue cond.)}$$

$$\rightarrow \quad k = \frac{\lambda}{2a} \qquad (93)$$

For double square well;

$$\frac{2m}{\hbar^2} V(x) = -\frac{\lambda}{a}\left[\delta(x-a) + \delta(x+a)\right] \qquad (94)$$

Since $V(x) = V(-x)$ → The sols. have definite parity

i) For the even sol.,

$$u(x) = \begin{cases} e^{-kx} & x > a \\ A \cosh kx & -a < x < a \\ e^{kx} & x < -a \end{cases} \qquad (95)$$

Remark: $\cosh kx = \frac{1}{2}(e^{kx} + e^{-kx})$ (a combination of the two sols.)

Also because of the symmetry the coeffs. for e^{-kx} and e^{kx} are the same.

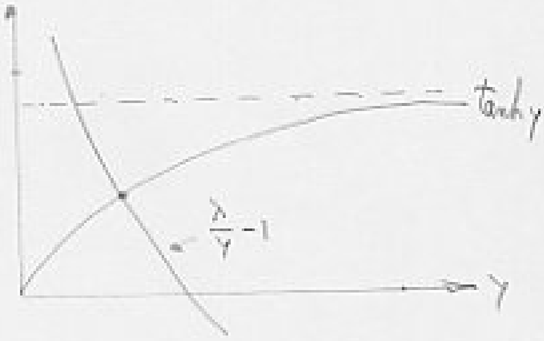
$$u_R(x)\Big|_{x=a} = u_{in}(x)\Big|_{x=a} \rightarrow e^{-\kappa a} = A\cosh \kappa a \quad (96)$$

Because of the symmetry, it is sufficient to apply the discontinuity cond. for the derivative at $x=a$. Nothing new will come of the application at $x=-a$.

$$-\kappa e^{-\kappa a} - \kappa A \sinh \kappa a = -\frac{\lambda}{a} e^{-\kappa a} \quad (97)$$

$$(96)(97) \rightarrow \tanh \kappa a = \frac{\lambda}{\kappa a} - 1 \quad (98) \quad \text{eigenvalue cond.}$$

There is only <u>one</u> intersection point.



When $y = \lambda$,

$$\underbrace{\tanh y}_{>0} = \underbrace{\frac{\lambda}{y} - 1}_{0} \quad (99)$$

$\rightarrow$ The intersection point occurs for $y < \lambda$

On the other hand since $\tanh y < 1$;

$$\frac{\lambda}{y} < 2 \quad \text{(must be) at the intersection point}$$

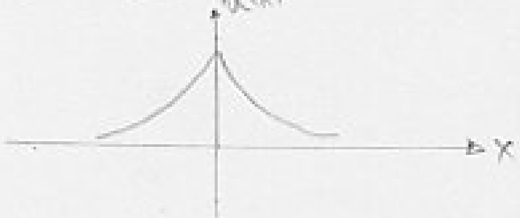
$$\rightarrow \quad \kappa > \frac{\lambda}{2a} \quad (100)$$

Comparing (93) and (100) $\rightarrow$ the energy for double well is a <u>larger</u> negative number

$\rightarrow$ The energy is <u>lower</u> (larger <u>binding</u> energy).

Note that this is not because somehow, the strength of a pair of potentials is larger than a single potential, as might be the case if one compared an electron bound to two protons with an electron bound to one proton.

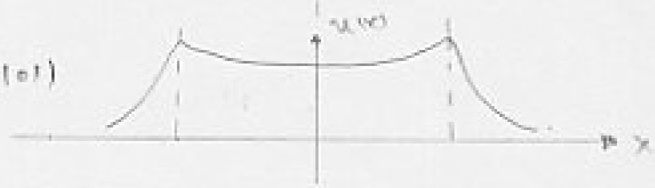
The larger binding is there because as fig. indicates, it is easier to accommodate a sharply dropping exponential to a symmetric func (here $\cosh \kappa x$) with discontinuity in slope as given, than it is to accommodate it to an equally sharply dropping exponential on the other side of the potential.



ii) The odd sol. will have the form,

$$u(x) = \begin{cases} e^{-\kappa x} & x > a \\ A \sinh \kappa x & -a < x < a \\ -e^{\kappa x} & x < -a \end{cases} \qquad (101)$$

because of antisymmetry



Again because of antisymmetry, it is sufficient to apply the conds. at $x = a$

Continuity of the wave func.;

$$u_R(x)\Big|_{x=a} = u_M(x)\Big|_{x=a}$$

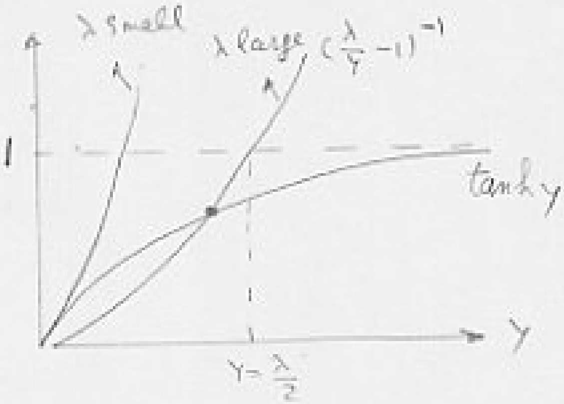
$$e^{-\kappa a} = A \sinh \kappa a \qquad (102)$$

and the discontinuity equation reads;

$$-k e^{-ka} - kA \cosh ka = -\frac{\lambda}{a} e^{-ka} \qquad (103)$$

$$(102)(103) \longrightarrow \cosh ka = \frac{\lambda}{ka} - 1 \qquad (104) \text{ eigenvalue cond.}$$

$$\rightarrow \tanh ka = \left(\frac{\lambda}{ka} - 1\right)^{-1} \qquad (105)$$



There will only be an intersection if the slope of $\tanh y$ at the origin is larger than that of $\left(\frac{\lambda}{y}-1\right)^{-1}$,

That is;

$$\left[\frac{d}{dy} \tanh y\right]_{y=0} > \left[\frac{d}{dy}\left(\frac{\lambda}{y}-1\right)^{-1}\right]$$

$$\left[1-\tanh^2 y\right]_{y=0} > \left[\frac{1}{\lambda-y} + \frac{y}{(\lambda-y)^2}\right]_{y=0}$$

$$1 > \left[\frac{1}{\lambda} + 0\right] \quad \rightarrow \lambda > 1 \qquad (106)$$

At $y = \frac{\lambda}{2} \rightarrow \left(\frac{\lambda}{y} - 1\right)^{-1} = 1$

and since $\tanh \infty = 1$

then the intersection has to occur for $y < \frac{\lambda}{2}$

$$\rightarrow ka < \frac{\lambda}{2} \rightarrow k < \frac{\lambda}{2a} \qquad (107)$$

Thus the odd sol., if there is a bound state, is less strongly bound than even sol.

The wave func., which has to go through zero, is forced to be steep between the walls, and thus can only accommodate to a less rapidly falling exponential (less strongly bound).

Depending on the size of λ, there may or may not exist an excited state.

Let us consider a superposition of the ground state $u_e(x)$, with energy E_e and the excited state $u_o(x)$, with energy E_o,

$$\psi(x) = u_e(x) + \alpha u_o(x) \quad (108)$$

we choose α so that,

$$\int_{-\infty}^{0} dx \, |\psi(x)|^2 \longrightarrow \text{small} \quad (109)$$

$\longrightarrow$ The particle localized, as far as possible, on the right side.

After time t: $\psi(x,t) = u_e(x) e^{-iE_e t/\hbar} + \alpha u_o(x) e^{-iE_o t/\hbar}$

$$= e^{-iE_e t/\hbar} \left[u_e(x) + \alpha e^{-i(E_o - E_e)t/\hbar} u_o(x) \right] \quad (110)$$

After a time such that:

$$e^{-i(E_o-E_e)t/\hbar} = -1 \qquad (111)$$

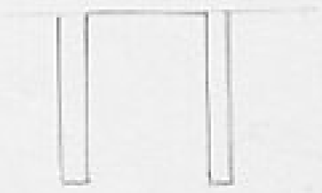
the particle will localized on the left side

Thus there is an oscillatory behavior, the particle going back and forth between the two potentials, with frequency:

$$\omega = 2\omega_{oe} = 2\,\frac{E_o-E_e}{\hbar} \qquad (112)$$

One may investigate that for $\lambda \to$ large

$$T = \frac{2\pi}{\omega_{oe}} \simeq \text{tunneling time across the barrier}$$



This is a model for the ammonia molecule.

Such a frequency can be measured with high precision, and thus we have at our disposal a very accurate clock.

F. The Kronig-Penny Model

Metals generally have a crystalline structure, that is, the ions are arranged in a way that exhibits a spacial periodicity. This periodicity has an effect on the motion of free electron in the metal, and this effect is exhibited in the simple model that we will now discuss. For this periodicity we require that:

$$V(x+a) = V(x) \qquad (113)$$

$$\text{Since } -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \xrightarrow{x \to x+a} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \quad \text{(unaltered)} \qquad (114)$$

$\to$ H : invariant by $x \to x+a$

For $V(x) = 0 \longrightarrow \psi(x) = e^{ikx}$ (115)

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

The displacement yields, $\psi(x+a) = e^{ik(x+a)} = e^{ika}\,\psi(x)$ (116)

$$|\psi(x+a)|^2 = |\psi(x)|^2 \qquad (117)$$

$\to$ The observables will therefore be the same at x and x+a, (we can not tell whether we are at x or x+a).

We have a similar argument with $V(x) \neq 0$, but $V(x) = V(x+a)$

In our example we shall insist that $\psi(x)$ and $\psi(x+a)$ differ only by a phase factor not necessarily of the form e^{ika} (due to $V(x)\neq 0$, $V(x)=V(x+a)$)

To simplify the algebra, we will take a series of repulsive δ-func potentials,

$$V(x) = \frac{+\hbar^2}{2m}\frac{\lambda}{a}\sum_{n=-\infty}^{\infty}\delta(x-na) \quad (118)$$

Away the points $x = na$, the sol. will be that of the free particle equ.,

$$\psi(x) \sim A\sin kx + B\cos kx \quad (119)$$

Let us assume that in the region $R_n = \{(n-1)a \leq x \leq na\}$, we have

$$\psi(x) = A_n \sin k(x-na) + B_n \cos k(x-na) \quad (120)$$

and for $R_{n+1} = \{na \leq x \leq (n+1)a\}$

$$\psi(x) = A_{n+1}\sin k(x-(n+1)a) + B_{n+1}\cos k(x-(n+1)a) \quad (121)$$

Continuity of $\psi(x)$ at $x = na$

$$-A_{n+1}\sin ka + B_{n+1}\cos ka = B_n \quad (122)$$

and the discontinuity cond. here reads;

$$kA_{n+1}\cos ka + kB_{n+1}\sin ka - kA_n = \frac{\lambda}{a}B_n \quad (123)$$

(P)

(122)(123) $\rightarrow$ $\begin{cases} A_{n+1} = A_n \cos ka + (g \cos ka - \sin ka) B_n \\ B_{n+1} = (g \sin ka + \cos ka) B_n + A_n \sin ka \end{cases}$ (124)

where $g = \dfrac{\lambda}{ka}$

The requirement that the wave funcs (120) and (121) be related by

$$\psi(R_{n+1}) = e^{i\varphi}\psi(R_n) \qquad (125)$$

(because the probabilities must be the same due to the periodic pot.)

is satisfied if; $\begin{cases} A_{n+1} = e^{i\varphi} A_n \\ B_{n+1} = e^{i\varphi} B_n \end{cases}$ (126)

(126) $\xrightarrow{in}$ (124) $\rightarrow$

$$(e^{i\varphi} - \cos ka)(e^{i\varphi} - g \sin ka - \cos ka) = \sin ka\,(g \cos ka - \sin ka) \qquad (127)$$

consistency cond.

$$\rightarrow e^{2i\varphi} - e^{i\varphi}(2\cos ka + g \sin ka) + 1 = 0$$

$$\rightarrow e^{i\varphi} - (2\cos ka + g \sin ka) + e^{-i\varphi} = 0$$

$$\rightarrow \cos\varphi = \cos ka + \frac{1}{2} g \sin ka \qquad (128)$$

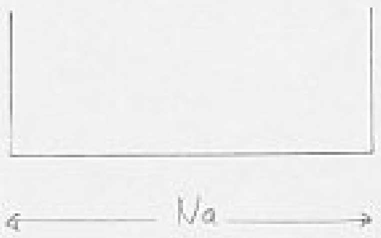
If we take periodic boundary conds for our crystal so that;

$$\psi(R_{n+N}) = \psi(R_n) \qquad (129)$$

then from (125) $\longrightarrow$ $e^{iN\varphi} = 1$ (130)

$\rightarrow \quad \varphi = \frac{2\pi}{N} m \qquad m = 0, \pm 1, \pm 2 \qquad (131)$

We denote φ by qa, where



q: the wave number of an electron in a box of length Na

with periodic boundary conds. and without any pot., that is, without any ions present (equ 129).

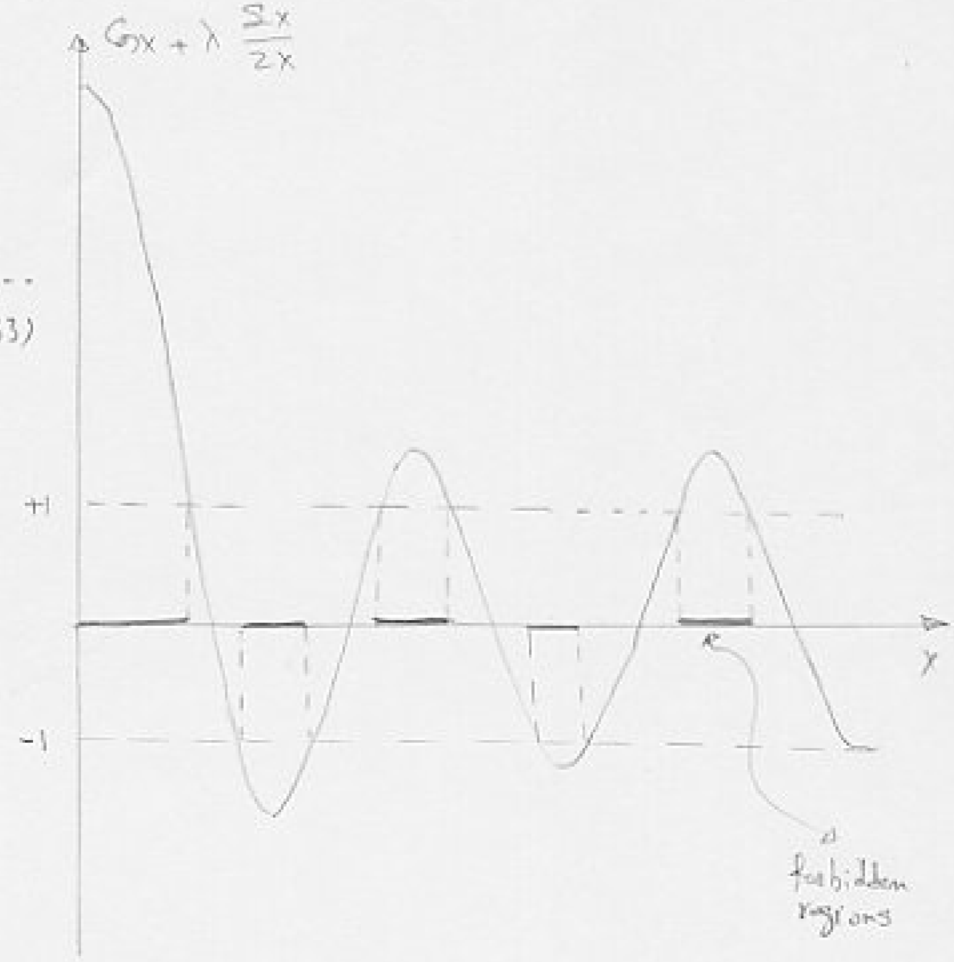
$$(128) \longrightarrow \quad \cos qa = \cos ka + \frac{1}{2}\lambda \frac{\sin ka}{ka} \qquad (132)$$

$|\cos qa| \leq 1 \longrightarrow$ There is a restriction on the values for the right side (consequently on the possible ranges of the energy $E = \frac{\hbar^2 k^2}{2m}$)

Note that the onset of a forbidden band corresponds to the cond.:

$$ka = n\pi \quad , \quad n = \pm 1, \pm 2, \dots \qquad (133)$$

$$\left(\cos n\pi + \frac{1}{2}\lambda \frac{\sin n\pi}{n\pi} = \pm 1 \right)$$

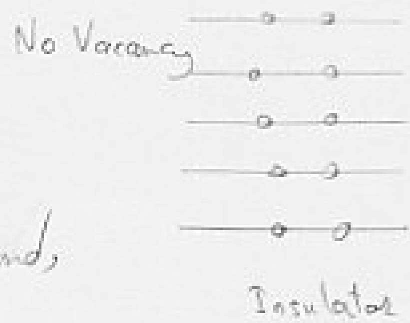


The Kronig-Penny model has some relevance to the theory of metals, insulators and semiconductors if we take into account the exclusive Pauli principle.

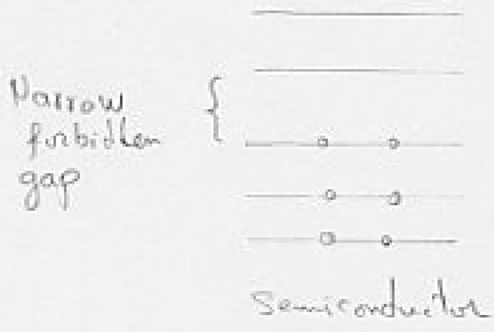
If an external electric field is applied:

i) The electrons will occupy the vacant states in metals.

ii) Insulators have completely filled bands, Only if the electric field is strong enough, the electrons jump across a forbidden energy gap and go into an empty allowed energy band, (breakdown).



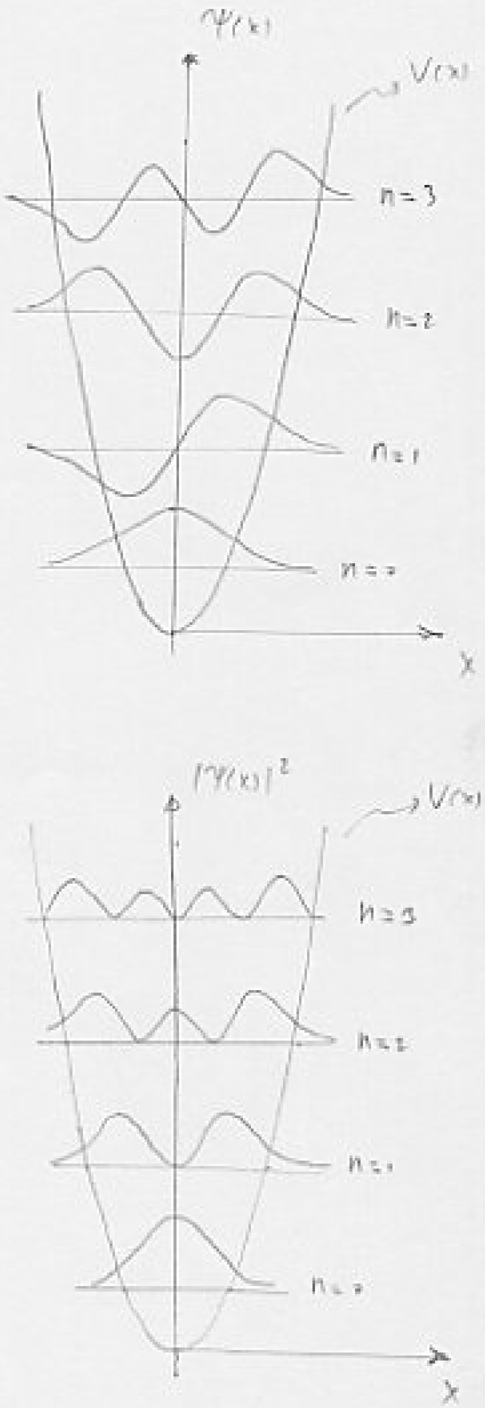
iii) The semiconductor is an insulator with a very narrow forbidden gap. There, small changes of conds. for example, a rise in temperature, can produce the jump and the insulator becomes a conductor.



G. The Harmonic Osc.

The classical Hamiltonian;

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \qquad (134)$$



The eigenvalue equ.;

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + \frac{1}{2}kx^2u(x) = Eu(x) \qquad (135)$$

we introduce, $\omega = \sqrt{\frac{k}{m}}$

write $\qquad \epsilon = \frac{2E}{\hbar\omega}$

and the change of variable $\quad y = \sqrt{\frac{m\omega}{\hbar}}\,x$

$$\rightarrow \frac{d^2u}{dy^2} + (\epsilon - y^2)u = 0 \qquad (136)$$

$\forall\, \epsilon$ (eigenvalue);

as $y^2 \rightarrow \infty \qquad ; \; (\epsilon - y^2) \simeq -y^2$

$$\rightarrow \frac{d^2u_0(y)}{dy^2} - y^2u_0(y) = 0 \qquad (137)$$

u_0 : Asymptotic sol.

We multiply by $2\frac{du_0}{dy}$

$$2\frac{du_0}{dy}\left(\frac{d^2u_0(y)}{dy^2}\right) - y^2 u_0(y)\left(2\frac{du_0(y)}{dy}\right) = 0$$

$$\rightarrow \frac{d}{dy}\left(\frac{du_0}{dy}\right)^2 - y^2\frac{d}{dy}(u_0^2) = 0 \qquad (139)$$

$$\rightarrow \frac{d}{dy}\left[\left(\frac{du_0}{dy}\right)^2 - y^2 u_0\right] = -2y u_0^2 \qquad (140)$$

If we <u>neglect</u> the right side (we later will check that this assumption is correct) then;

$$\frac{d}{dy}\left[\left(\frac{du_0}{dy}\right)^2 - y^2 u_0\right] = 0 \qquad (141)$$

$$\rightarrow \left(\frac{du_0}{dy}\right)^2 - y^2 u_0 = C \quad \rightarrow \quad \frac{du_0}{dy} = \sqrt{C + y^2 u_0^2} \qquad (142)$$

Since $\begin{cases} u_0(y=\infty) = 0 \\ \frac{du_0}{dy}(y=\infty) = 0 \end{cases} \rightarrow C = 0$

$$\rightarrow \frac{du_0}{dy} = \pm y u_0$$

$$\rightarrow u_0(y) = e^{-y^2/2} \qquad (143)$$ acceptable sol. at infinity

We can now check that

$$2y u_0^2 = 2y e^{-y^2}$$

is indeed negligible compared with

$$\frac{d}{dy}(y^2 u_0^2) = \frac{d}{dy}(y^2 e^{-y^2}) = 2y e^{-y^2} - 4y^3 e^{-y^2}$$

$$\simeq -4y^3 e^{-y^2} \qquad (144) \text{ (for large } y)$$

Now, we introduce a new func. $h(y)$, such that;

$$u(y) = h(y)\, e^{-y^2/2} \qquad (145)$$

$h(y)$: will represent the short range behavior, $(y \approx 0)$

$$(136) \rightarrow \quad \frac{d^2 h(y)}{dy^2} - 2y \frac{dh(y)}{dy} + (\epsilon - 1)\, h(y) = 0 \qquad (146)$$

Let us attempt a power series expansion;

$$h(y) = \sum_{m=0}^{\infty} a_m y^m \qquad (147)$$

$(147) \xrightarrow{\text{in}} (146)$ and equating the coefficients of y^m;

$$(m+1)(m+2)\, a_{m+2} = (2m - \epsilon + 1)\, a_m \qquad (148)$$

Thus, given a_0 and a_1, the even and odd series can be generated seperately. That they donot mix is a consequence of the invariance of the H under reflections.

For arbitrary ϵ, and for large m (say $m > N$)

$$a_{m+2} \simeq \frac{2}{m} a_m \qquad (149)$$

$h(y) =$ (a polynomial in y of deg. $< N$) +

$$a_N \left[y^N + \frac{2}{N} y^{N+2} + \frac{2^2}{N(N+2)} y^{N+4} + \frac{2^3}{N(N+2)(N+4)} y^{N+6} + \cdots \right]$$

(150)

The series may be written in the form

$$a_N y^2 \left(\frac{N}{2}-1\right)! \left[\frac{(y^2)^{N/2-1}}{(N/2-1)!} + \frac{(y^2)^{N/2}}{(N/2)!} + \frac{(y^2)^{N/2+1}}{(N/2+1)!} + \cdots \right]$$

(150')

We add some terms to (150') to make it $\sim y^2 e^{y^2}$ and subtract the similar term from the first term in (150).

$$\to h(y) \sim (\text{a polynomial}) + c y^2 e^{y^2} \quad (151)$$

(151) $\xrightarrow{\text{in}}$ (145)

$$u(y) \sim e^{-y^2/2} (\text{a polynomial}) + c y^2 e^{y^2/2} \qquad (152)$$

$$\to u(y \to \infty) \longrightarrow \infty$$

An acceptable sol. can be found if the recursion relation terminates, that is, if;

$$(148) \to a_{m+2} = \frac{2m - \epsilon + 1}{(m+1)(m+2)} a_m \qquad (153)$$

$\rightarrow \quad 2m - \epsilon + 1 = 0 \quad$ for $\quad m = N \quad$ a certain number

$$\rightarrow \quad \epsilon = 2N + 1 \qquad (154)$$

(154) → (148) :

$$a_{2k} = (-2)^k \frac{N(N-2)\cdots(N-2k+4)(N-2k+2)}{(2k)!} a_0$$

$$a_{2k+1} = (-2)^k \frac{(N-1)(N-3)\cdots(N-2k+3)(N-2k+1)}{(2k+1)!} a_1 \qquad (155)$$

Results:

1) (154) → $E = \hbar\omega(n+\frac{1}{2})$ (156)

This is a form that looks familiar, since the relation between E and ω is the same as that discovered by Planck for the radiation field modes.

This is no accident, since a decomposition of the electromag. field into normal modes is essentially a decomposition into Harmonic oscillators that are decoupled.

2) $h(y) = C H_n(y)$ $\qquad$ $H_n(y)$: Hermite Polynomials

Harmonic osc. prob. is important in Q.M. as in Cl.M., because any small perturbation of a system from its equilibrium state will give rise to small oscillations, which are ultimately decomposable into normal modes. That is, indep. oscillators.

3) (156) $\rightarrow$ $E_0 = \frac{1}{2}\hbar\omega \neq 0$

This is purely quantum mechanical effect and can be interpreted in terms of the uncertainty principle.

It is the zero-point energy that is responsible for the fact that helium does not freeze at extremely low temperatures but remains liquid down to temperatures of the order of 10^{-3} °K, at normal pressures.

ω is larger for lighter atoms, which is why the effect is not seen for nitrogen, say. It also depends on detailed features of the interatomic forces, which is why liquid hydrogen does freeze.