Chapter 2

Wave Packets and the Uncertainty Relations

Localized waves may represent the particles 

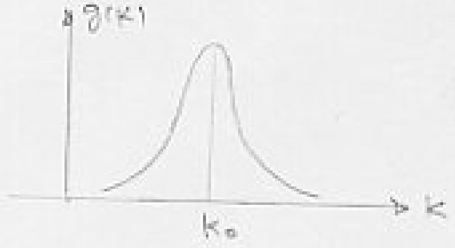
Consider; $$f(x) = \int_{-\infty}^{\infty} dk\, g(k)\, e^{ikx} \qquad (1)$$

$$\mathrm{Rel}\,(f(x)) = \int_{-\infty}^{\infty} dk\, g(k) \cos(kx) \qquad (2)$$ for $g(k)$ real

$\mathrm{Rel}\,(f(x))$: Linear superposition of waves with $\lambda = \frac{2\pi}{k}$

Because $\forall k$, $\cos(kx) = \cos\left[k\left(x + \frac{2\pi}{k}\right)\right]$

$\rightarrow$ $\mathrm{Rel}\,(f(x)) = \mathrm{Rel}\left(f\left(x + \frac{2\pi}{k}\right)\right)$



Choose; $$g(k) = e^{-a(k-k_0)^2} \qquad (3)$$

Integral evaluation:

change of variable $k' = k - k_0$

$$f(x) = \int_{-\infty}^{\infty} dk\, g(k)\, e^{i(k-k_0)x}\, e^{ik_0x} = e^{ik_0x} \int_{-\infty}^{\infty} dk'\, e^{ik'x}\, e^{-ak'^2}$$

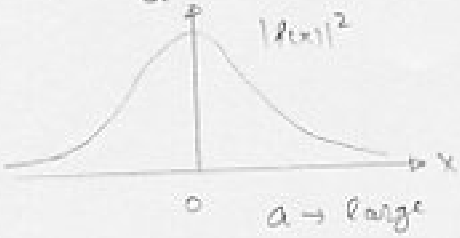
$$= e^{ik_0x} \int_{-\infty}^{\infty} dk'\, e^{-a\left[k' - \left(\frac{ix}{2a}\right)\right]^2}\, e^{-\left(\frac{x^2}{4a}\right)} \qquad (3')$$

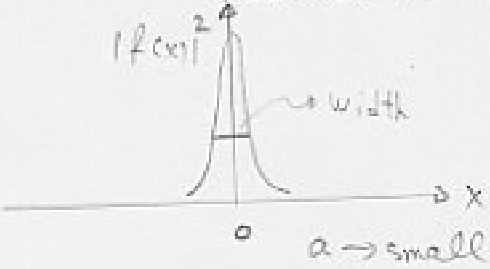
Now let $k' - \frac{ix}{2a} \equiv q$

$$f(x) = e^{ik_0x}\, e^{-\frac{x^2}{4a}} \underbrace{\int_{-\infty}^{\infty} dq\, e^{-aq^2}} = \sqrt{\frac{\pi}{a}}\, \underbrace{e^{ik_0x}}_{\text{fase factor}}\, e^{-\frac{x^2}{4a}} \qquad (4)$$

$$\rightarrow |f(x)|^2 = \frac{\pi}{a}\, e^{-\frac{x^2}{2a}} \qquad (5)$$

(because $|e^{ik_0x}|^2 = 1$)





$|f(0)|^2 = \frac{\pi}{a}$ Peak value

at $x = \pm\sqrt{2a} \rightarrow |f(\pm\sqrt{2a})|^2 = \frac{1}{e}\, |f(0)|^2$

$\rightarrow$ width of $|f(x)|^2 = 2\sqrt{2a} \equiv \Delta x$

Also $|g(k)|^2 = e^{-2a(k-k_0)^2}$ at $k = k_0 \rightarrow |g(k_0)|^2 = 1$ Peak value

and at $k = k_0 \pm \frac{1}{\sqrt{2a}}$ $\quad |g(k_0 \pm \frac{1}{\sqrt{2a}})|^2 = \frac{1}{e}\, |g(k_0)|^2$

$\rightarrow$ width of $|g(k)|^2 = \frac{2}{\sqrt{2a}} \equiv \Delta k$

$\rightarrow$ width of $|f(x)|^2$ <u>correlated</u> width of $|g(k)|^2$

$$\Delta k \cdot \Delta x \sim \frac{2}{\sqrt{2a}} \cdot 2\sqrt{2a} = 4 \qquad a\text{-indep.} \qquad (6)$$

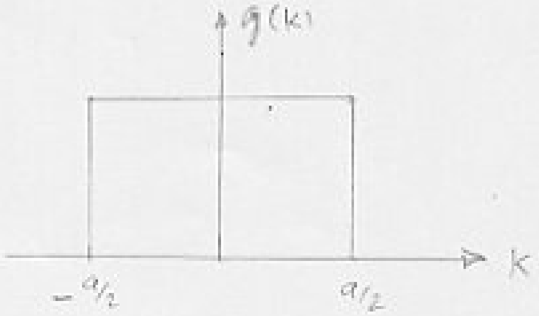
This is a general <u>property</u> of funcs, that are Fourier transforms of each other.

We represent it by $\quad \Delta x \, \Delta k \gtrsim O(1) \qquad (7)$

$O(1)$ (which is a number) may depend on $f(x)$ and $g(k)$ and it is not significantly smaller than 1.

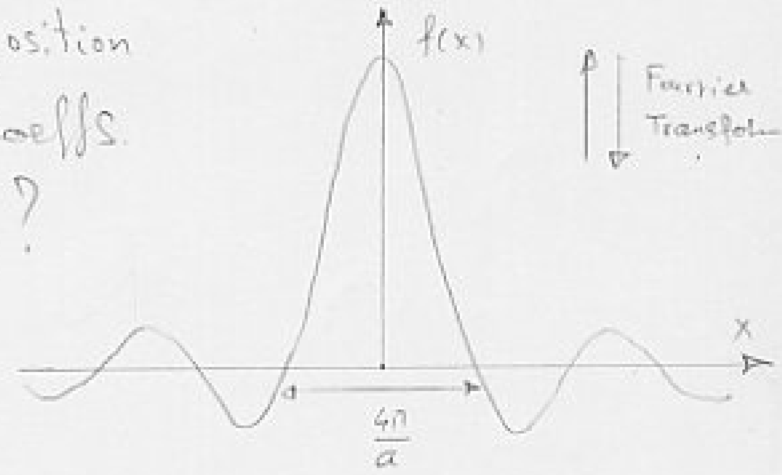
$\rightarrow$ It is impossible to make both Δx and Δk small.

This is a general feature of wave packet. But it has deep implications for Q.M.



Question:

How will a wave packet $f(x)$ (made up of a continuous superposition of simple waves e^{ikx} with the coeffs. $g(k)$) propagate in Time?



For simple wave e^{ikx} (plane wave);

$$\rightarrow e^{ikx - i\omega t}$$

where $\omega = 2\pi\nu$ and $k = \frac{2\pi}{\lambda}$

$$\rightarrow \quad e^{2\pi i \left[\frac{x}{\lambda} - \nu t\right]}$$

For propagation of light wave in vaccum there is a simple relation between ν and $\frac{1}{\lambda}$:

$$\nu = \frac{c}{\lambda}$$

$$\rightarrow e^{2\pi i(x-ct)/\lambda} = e^{ik(x-ct)}$$

$$f(x) \rightarrow f(x,t) \qquad f(x,t) = \int_{-\infty}^{\infty} dk\, g(k)\, e^{ik(x-ct)} = f(x-ct) \tag{8}$$

The wave packet localized at $x=0$ $\rightarrow$ is now localized at $x-ct=0$

(with out distortion with velocity c)

However for the waves representing the particles;

$$\omega \neq kc \qquad (\text{i.e. } \omega = 2\pi\nu \neq 2\pi\frac{c}{\lambda} = kc)$$

In general $\omega = \omega(k)$

$$\rightarrow f(x,t) = \int dk\, g(k)\, e^{ikx - i\omega(k)t} \tag{9}$$

$\omega(k) = ?$

We shall try to find it from the requirement that $f(x,t)$ resemble a freely moving classical particle.

Consider a wave packet strongly localized in k-space about k_0 (like equ(3) with $a \to$ large).

$\longrightarrow$ $f(x)$ will not sharply localized in x-space.

Now

$$\omega(k) \simeq \omega(k_0) + (k-k_0)\left(\frac{d\omega}{dk}\right)_{k_0} + \frac{1}{2}(k-k_0)^2\left(\frac{d^2\omega}{dk^2}\right)_{k_0} \qquad (10)$$

where we have assumed $\omega(k)$ is not a very rapidly varying func. of k ($\frac{d^n\omega}{dk^n} \simeq 0$ for $n \geq 2$)

For the special case Equ(3) for definiteness; using (10);

$$(9) \longrightarrow f(x,t) = e^{ik_0x}\, e^{-i\omega(k_0)t} \int dk'\, e^{-ak'^2}\, e^{-i\left(\frac{k'^2}{2}\right)\left[\frac{d^2\omega}{dk^2}\right]_{k_0} t}\, e^{ik'\left\{x - \left[\frac{d\omega}{dk}\right]_{k_0} t\right\}} \qquad (11)$$

The term $h(x) = e^{ik'\left\{x - \left(\frac{d\omega}{dk}\right)_{k_0} t\right\}}$ shows that the peak of the packet located at $x=0$ (at $t=0$) is moving with the velocity of $\left(\frac{d\omega}{dk}\right)_{k_0}$

Or mathematically the peak of the wave packet $f(x,t) = \int dk\, g(k)\, e^{i[kx - \omega(k)t]}$ tends to be where $kx - \omega t$ has a min. as a func. of k, that is

$$\frac{\partial}{\partial k}[kx - \omega t] = 0 \quad \rightarrow \quad x - \frac{d\omega}{dk} t = 0$$

→ The velocity of propagation of the packet, the <u>group</u> velocity is;

$$V_g = \left(\frac{d\omega}{dk}\right)_{k_0} \qquad (12)$$

Remark: Consider a particle of mass m moving with a velocity v;

$$E = mc^2 = \frac{m_0 c^2}{\sqrt{1-\frac{v^2}{c^2}}} = \hbar\omega \qquad (13) \qquad \rightarrow \omega = \omega(v)$$

$$p = mv = \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}} = \hbar k \qquad (14) \qquad \rightarrow k = k(v)$$

Def.: $V_p \equiv \frac{\omega}{k}$ phase velocity (the velocity of a single frequency component)

(13)(14) $\rightarrow$ $V_p = \frac{E}{p} = \frac{c^2}{v}$

Def: $V_g \equiv \frac{d\omega}{dk}$ group velocity (the velocity of wave packet propagation)

$$V_g = \frac{d\omega}{dv}\frac{dv}{dk} = \left(\frac{mv}{h\left(1-\frac{v^2}{c^2}\right)^{3/2}}\right)\left(\frac{h\left(1-\frac{v^2}{c^2}\right)^{3/2}}{m}\right) = v$$

↑ velocity of the particle

Now define; $\frac{1}{2}\left(\frac{d^2\omega}{dk^2}\right)_{k_0} = \beta$

$$\rightarrow f(x,t) = e^{i[k_0 x - \omega(k_0)t]} \int dk' \, e^{ik'(x-v_g t)} \, e^{-(a+i\beta t)k'^2} \qquad (13')$$

This is just the integral (3') led to (4) with $\begin{cases} x \rightarrow x - v_g t \\ a \rightarrow a + i\beta t \end{cases}$

$$(4) \rightarrow f(x,t) = e^{i[k_0 x - \omega(k_0)t]} \left(\frac{\pi}{a+i\beta t}\right)^{1/2} e^{-\left[\frac{(x-v_g t)^2}{4(a+i\beta t)}\right]} \qquad (14')$$

$$\rightarrow |f(x,t)|^2 = \left(\frac{\pi^2}{a^2+\beta^2 t^2}\right)^{1/2} e^{-\left[\frac{a(x-v_g t)^2}{2(a^2+\beta^2 t^2)}\right]} \qquad (15)$$

Representing a wave packet whose peak is traveling with velocity v_g, but it does not have a definite width;

i.e. the quantity $a \longrightarrow a + \frac{\beta^2 t^2}{a}$

at $t=0$ at $t=t$

The rate of spreading $\simeq$ small if $a \simeq$ large

(i.e. : The packet is spacially large to begin with)

$$\left(a + \frac{\beta^2 t^2}{a}\right)^{1/2} = \sqrt{a}\left(1 + \frac{\beta^2 t^2}{a^2}\right)^{1/2}$$

Important result:

If equ.(9) is to represent a particle with momentum p and Kinetic energy $\frac{p^2}{2m}$, then we must require that:

$$V_g = \frac{d\omega}{dk} = \frac{p}{m} \qquad (16)$$

If we further make the association that $E = \hbar\omega$ (17)

$$\text{Since } E = \frac{p^2}{2m} \rightarrow \omega = \frac{p^2}{2m\hbar} \qquad (18)$$

then the consistency demands that we make the association;

$$K = \frac{2\pi}{\lambda} = \frac{p}{\hbar} \rightarrow p = \hbar K \qquad (19)$$

$$\text{Because } \frac{d\omega}{dk} = \frac{\hbar k}{m} \rightarrow \omega = \frac{\hbar k^2}{2m} + \text{Const.} \qquad (20)$$

$$\rightarrow \hbar\omega = \frac{p^2}{2m} + \text{Const.} \qquad (21)$$

Remark:

$$\omega(k) = \frac{\hbar k^2}{2m} = \frac{\hbar k_0^2}{2m} + \frac{\hbar k_0}{m}(k-k_0) + \frac{\hbar}{2m}(k-k_0)^2 + 0$$

exact

(22)

In terms of p and E:

$$(9) \rightarrow \quad \Psi(x,t) = \underbrace{\frac{1}{\sqrt{2\pi\hbar}}}_{\text{normalized}} \int dp\, \varphi(p)\, e^{i(px - Et)/\hbar} \quad (23)$$

This wave packet is a general sol. of the partial differential equ.

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \varphi(p)\, E\, e^{i(px-Et)/\hbar}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \varphi(p)\, \frac{p^2}{2m}\, e^{i(px-Et)/\hbar} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2}$$

$$\rightarrow \quad i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} \quad \text{Schrödinger equ.} \quad (24)$$

$$(V(x) = 0)$$

Remember there is no justification on the basis of classical physics for the replacement: $\begin{cases} \omega \rightarrow \frac{E}{\hbar} \\ k \rightarrow \frac{p}{\hbar} \end{cases}$

One difficulty:

For a wave packet (for example a Gaussian packet) we finally have a noticeable spreading after a time of t.

But we know that very tiny particles, say, nuclei have no changed during a period of 3×10^9 yrs $= 10^{?}$ sec!

We shall see that this difficulty will be removed if we refer the the spreading to the growing probability that the particle is far from where it was localized at $t = 0$.

Now $\Delta K \Delta X \gtrsim 1 \quad \rightarrow \quad \Delta P \Delta X \gtrsim \hbar \qquad (25)$

The smallness of $\hbar$ guarantees that only for microscopic systems will the usual notions of classical physics fail.

Example:

a) A dust particle;

$$\begin{cases} m = 10^{-4} \, gr \\ V = 10^{4} \, cm/sec \end{cases} \rightarrow P = mV = 1 \, gr \, cm/sec$$

Assume $\Delta P = 10^{-6}$

$$\Delta P \Delta X \approx \hbar \qquad 10^{-6} \Delta X \approx 1.0545 \times 10^{-27} \text{ erg sec}$$

$$\Delta X \approx 10^{-21} \text{ cm} < 10^{-7} r_{Proton}$$

b) Electron in Bohr atom;

$$V = \frac{Z\alpha c}{n} \rightarrow P = \frac{mZ\alpha c}{n} \qquad \text{for } Z=1 \quad P = \frac{m\alpha c}{n}$$

and $\Delta P \sim P$

Also $r = \frac{n^2}{Z\alpha} \frac{\hbar}{mc}$ for $Z=1$ $r = \frac{n^2 \hbar}{m\alpha c}$

$\Delta X \sim r$

In what follows, we will discuss a number of Gedankenexperiments in which we will show in detail how the <u>wave-particle</u> duality acts to conspire to prohibit a violation of the relation $\Delta p \Delta x \gtrsim \hbar$.

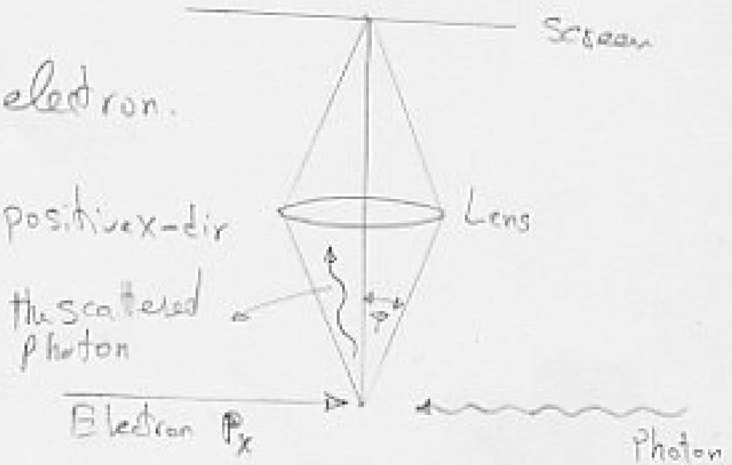
a) Measurement of position of an electron;

Aim: Measuring the position of an electron.

Suppose; P_x : well defined in positive x-dir

Measuring device; Microscope

(Lens + Scream)



The resolution of microscope (Known from optics);

$$\Delta x \sim \frac{\lambda}{S\varphi}$$

One may make $\Delta x \to$ small by $\begin{cases} \lambda \to \text{small} \\ S\varphi \to \text{large} \end{cases}$

We will show this can be done at the expense of losing the information about P_x.

The direction of the scattered Photon is undetermined within the angle subtended by the aperture.

$$\to \Delta P_x \sim 2\frac{E}{c} S\varphi = 2\frac{h\nu}{c} S\varphi \qquad \text{for the electron}$$

$$\Delta P_x \Delta X \sim 2\frac{h\nu}{c} S\varphi \frac{\lambda}{S\varphi} \sim 4\pi\hbar$$

Can we get around this difficulty?

The dir. of the photon correlated with its momentum

If we could somehow measure the recoil of screen

$\xrightarrow{\text{then}}$ photon momentum can be specified $\longrightarrow$ and hence the electron mom.

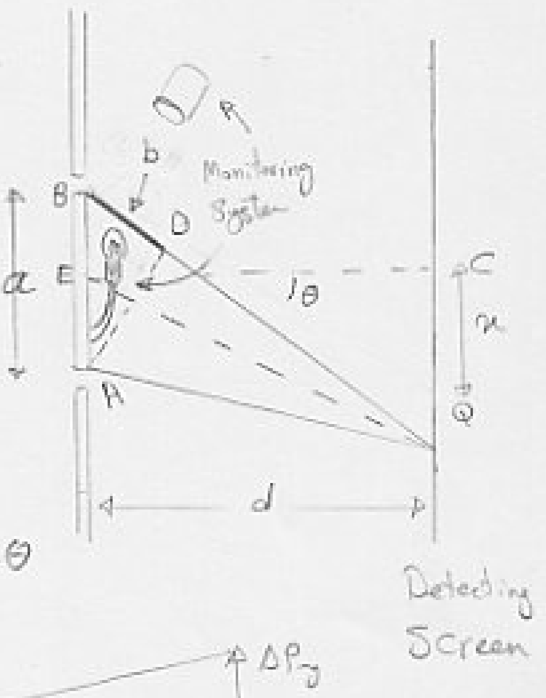
True, but: once we include the microscope as part of the observed system, we must worry about the about its location, since its momentum is to be specified.
But the microscope too, must obey the uncertainty relation and if its momentum is to be specified, its position will be less determined.

b) The two-slit experiment

$b = a \sin\theta = n\lambda$ constructive interference

$\Delta\, ABD \sim \Delta\, QEC$

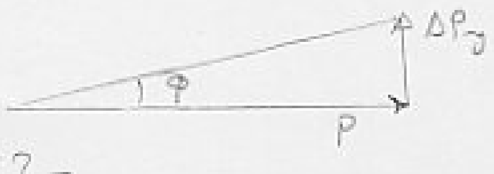
Source of electron



$$\frac{b}{x} = \frac{a}{EQ}$$

But $EQ \simeq d$

$$\Rightarrow \frac{b}{x} = \frac{a}{d} \qquad x = \frac{bd}{a} = \frac{a \sin\theta\, d}{a} = d \sin\theta$$



The distance between two maxima l is given by:

$$l = d\,\delta\theta_{n+1} - d\,\delta\theta_n = d\left((n+1)\frac{\lambda}{a} - n\frac{\lambda}{a}\right) = \frac{d\lambda}{a}$$

The monitor determines the position of an electron to an accuracy $\Delta y < \frac{a}{2} \xrightarrow{i.e.}$ it tells us which slit the electron went through.

$$\Delta Y \Delta P_y > h \quad \rightarrow \Delta P_y > \frac{2h}{a}$$

$$\rightarrow \frac{\Delta P_y}{P} > \frac{2}{a}\frac{h}{P} = \frac{2\lambda}{a} \quad \text{but } \delta\varphi = \frac{\Delta P_y}{P} \rightarrow \delta\varphi > \frac{2\lambda}{a}$$

$$l' = d\,\delta\varphi \underset{\min}{=} \frac{2d\lambda}{a} > l$$ $\rightarrow$ The presence of the monitor will wipe out the interference pattern.

c) The <u>reality</u> of orbits in the Bohr atom;

$$R_n = \frac{\hbar n^2}{\alpha mc} \qquad \text{acc. to Bohr atomic model}$$

The accuracy for a position measurement for a given orbit must be such that

$$\Delta x \ll R_n - R_{n-1} \simeq \frac{2\hbar n}{\alpha mc}$$

$$\Delta x \Delta P_x \gtrsim \hbar \quad \rightarrow \Delta P_x \gg \frac{mc\alpha}{2n}$$ uncontrolable mom. transfer to the electron

$$E \simeq \frac{P^2}{2m} \rightarrow \Delta E \simeq \frac{P\Delta P}{m} = \frac{P}{m}\Delta P = V\Delta P = \underset{\substack{\uparrow \\ z=1 \\ (P16)}}{\frac{c\alpha}{n}} \cdot \frac{mc\alpha}{2n} = \frac{1}{2}\frac{mc^2\alpha^2}{n^2}$$

uncertainty in the energy of electron

→ $\Delta E >$ binding energy of the electron

→ such a measurement, as likely as not, will kick the electron out of the orbit!

d) The energy-time uncertainty relation;

$$\Delta p \, \Delta x \geq \hbar \rightarrow \underbrace{\frac{p \Delta p}{m}}_{\Delta E} \underbrace{\frac{\Delta x \, m}{p}}_{\Delta t} \geq \hbar \qquad \left(p = m \frac{\Delta x}{\Delta t} \right)$$

Such a relation might also be deduced from the form of the wave packet (23) since E and t appear in the same reciprocal relation as p and x

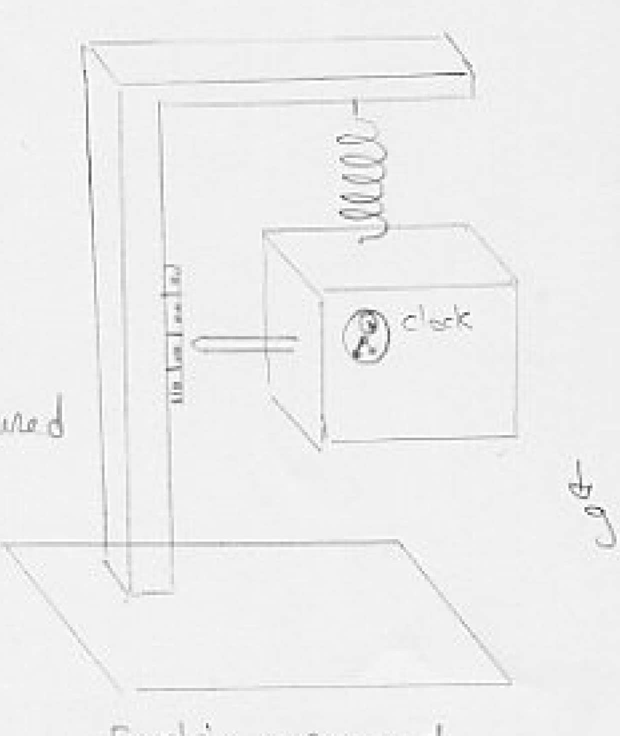
Einstein experiment: (Gedankenexperiment);

(to show violation of $\Delta E \Delta t \geq \hbar$)

A clock controls a shutter to open a hole for a short time Δt.

The radiation inside the box scapes

The scaped radiation can be measured very accurately by weighing the box before and after opening the box.



Einstein experiment

Bohr's rebuttal of argument:

1- A weighing implies the reading of a scale pointer with an accuracy Δx.

$\longrightarrow \Delta p \geq \frac{\hbar}{\Delta x}$ uncertainty in the mom. of box

2 - Δm: detected mass

T: weighing time

$\int F\,dt = g\Delta m T$ $\qquad$ $g\Delta m T \gg \underset{\text{mom. of box}}{\Delta p}$ (must be)

$g T \Delta m \gg \frac{\hbar}{\Delta x}$

3 - Acc. to equivalence principle;

$\frac{\Delta T}{T} = \frac{g\,\Delta x}{c^2}$ $\qquad$ Δx causes a change in the rate of clock.

$\frac{\Delta T}{T} \gg \frac{g}{c^2}\frac{\hbar}{g T \Delta m}$ $\rightarrow \Delta m c^2\, \Delta T \gg \hbar$

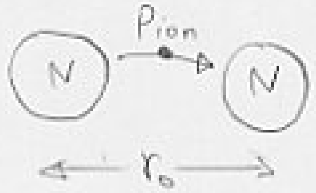
$\rightarrow \Delta E\, \Delta T \gg \hbar$.

$\rightarrow |V| \sim 3\times10^{-5}$ ergs ~ 20 Mev

(the order is correct in) nucleus
in the atoms it is of order of ev

Example c) Yukawa meson theory of nuclear forces

$\Delta E \sim m_\pi c^2$ energy imbalance in pion emission



This can take place for a time;

$\Delta T \sim \frac{\hbar}{m_\pi c^2}$ $\qquad$ $\underbrace{c\Delta T}_{r_0} \sim \frac{\hbar}{m_\pi c}$ the range of the particle traveling

If $r_0 = 1.4\times10^{-13}$ cm

$$r_0 \simeq \frac{\hbar}{m_\pi c} \rightarrow m_\pi c^2 \simeq \frac{\hbar c}{r_0} = \frac{10^{-27}\times3\times10^{10}}{1.4\times10^{-13}} \text{ ergs} \simeq 130 \text{ Mev}$$

We know that $m_\pi c^2 \simeq 140$ Mev

Example a) Hydrogen atom;

$$\Delta p \Delta x \simeq \hbar \rightarrow pr \sim \hbar$$

$$E = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r} \quad , \quad \frac{\partial E}{\partial r} = -\frac{\hbar^2}{mr^3} + \frac{e^2}{r^2} = 0$$

$$\rightarrow r = \frac{\hbar^2}{me^2} = \frac{\hbar}{mc\alpha} \quad \rightarrow E = -\frac{1}{2} mc^2 \alpha^2 \quad \text{exact.}$$

The fact that we obtained the exact value of the energy is, of course, a swindle, since we could equally well have written $pr \sim h$ and we would then have obtained a different result. But the order is <u>correct</u>.

Main point;

In contrast to cl. theory, the energy is <u>bounded</u> from <u>below</u>, because of the uncertainty relation;

$$V = -\frac{e^2}{r} \quad , \quad r \rightarrow \text{small} \Rightarrow |V| \rightarrow \text{large} \quad (\Delta x : \text{small})$$

$$\rightarrow K = \frac{\hbar^2}{2mr^2} \underset{\text{(Kinetic energy)}}{\rightarrow \text{large}} \quad (\Delta p : \text{large})$$

Example b) Nuclear forces;

$$\text{The range} \sim 10^{-13}\ \text{cm} \quad \rightarrow p \sim \frac{\hbar}{r} \sim 10^{-14}\ \text{gr cm/sec}$$

$$\rightarrow \frac{p^2}{2M} \sim \frac{10^{-28}}{3.2 \times 10^{-24}} \sim 3 \times 10^{-5}\ \text{ergs}$$

M : Proton mass

For a bound system $|V| > |K|$