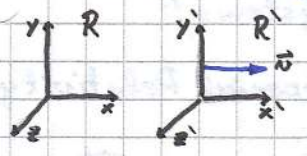
2015: INTRODUCTION TO QUANTUM MECHANICS

Inertial reference system - system in which 1ST Newton law holds! Any sytem that is moving with constant velocity w.r.t. original system is also inertial...



$$\left.\begin{aligned} x' &= x - vt \\ y' &= y \\ z' &= z \\ t' &= t \end{aligned}\right\}$$ GALILEO'S TRANSFORMATION

PRINCIPLE OF CLASSICAL RELATIVITY

PS. Good Physical law should be the same in all inertial systems!

Look if 3RD Newton is same in R and R`!

$\vec{F} = m\vec{a}$ in R ... in R`: $\vec{F}' = \vec{F}$; $m' = m$ ... $\vec{r}' = \vec{r} - \vec{v}t \Rightarrow \vec{a}' = \ddot{\vec{r}}' = \ldots = \vec{a} \Rightarrow \vec{F}' = m'\vec{a}'$ ✓ OK!

After discovering Maxwell equations it was soon clear that something is wrong... Maxwell equations or Galileo's tran. is wrong. This led to...

Let's first see how Galileo tran. change Maxwell equations:

$$\left.\begin{aligned} \vec{F} &= q(\vec{E} + \vec{v}\times\vec{B}) \quad \ldots \text{ in } R \\ \vec{F}' &= q\left(\vec{E}' + (\vec{v} - \vec{u})\times\vec{B}'\right) \ldots \text{ in } R' \end{aligned}\right\}$$ Principle of Sp.Rel. $\vec{F} = \vec{F}' \Rightarrow \vec{E} + \vec{v}\times\vec{B} = \vec{E}' + (\vec{v} - \vec{u})\times\vec{B}'$

We get... $\vec{E} - (\vec{E}' - \vec{u}\times\vec{B}') + \vec{v}\times(\vec{B} - \vec{B}') = 0 \rightarrow$ must be true for any velocity!

This is true if: $\vec{E} = \vec{E}' - \vec{v}\times\vec{B}$ and $\vec{B} = \vec{B}'$ → Now put this into Maxwell equations!

First we demonstrate that "del" operator remains same in R and R`: $\nabla = \nabla'$

And the time derivative changes to: $\frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - \vec{v}\cdot\nabla'$

$$\vec{\nabla}\cdot\vec{E} = \rho/\varepsilon_0 \qquad \vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\vec{\nabla}\cdot\vec{B} = 0 \qquad \vec{\nabla}\times\vec{B} = \mu_0\vec{J} + \mu_0\varepsilon_0\frac{\partial\vec{E}}{\partial t}$$

Now look... $\vec{\nabla}\times\vec{E} = \vec{\nabla}'\times\left[\vec{E}' - \vec{v}\times\vec{B}'\right] = \vec{\nabla}'\times\vec{E}' - \vec{\nabla}'\times(\vec{v}\times\vec{B}') = \vec{\nabla}'\times\vec{E}' + (\vec{v}\cdot\vec{\nabla}')\vec{B}'$

$\frac{\partial\vec{B}}{\partial t} = \frac{\partial}{\partial t'}\vec{B}' - (\vec{v}\cdot\vec{\nabla})\vec{B}'$ ... OK ✓ No problem here!

But... $\vec{\nabla}\cdot\vec{E} = \vec{\nabla}'\cdot\vec{E}' - \underbrace{\vec{\nabla}\cdot(\vec{v}\times\vec{B}')}_{\neq 0} = \rho/\varepsilon_0$ ... $\rho = \rho'$

0 ... In general not zero! ⇒ Here is the problem!

Also the 4TH Maxwell equation doesn't transform "well" under Galileo transform!

P.S. The two Maxwell equations that contain sources ... ρ and $\vec{J}$ ... do not transform in the "nice" way under Galileo's transformations!

Now we will try to find transformation that does not make problems...

What are general Space-Time properties? upr. Space-Time are HOMOGENOUS...

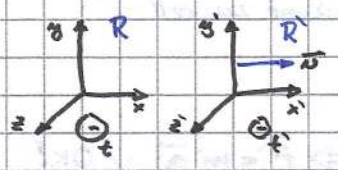
(same if we measure here and now as if in Japan 10 years ago)

① Space and Time properties: a) Space and Time are HOMOGENOUS!

b) Space is IZOTROPIC!

② Principle of Special Relativity ... all laws are same in inertial systems!

① and ② is all we need to find transformations used in Einstein's Special Relativity!



... we are looking for transf. $\underbrace{x' = F(x,t,a);\ t' = G(x,t,a)}$ (some functions; some parameter (not accelerat.))

PS. y and z are same (because $\vec{v}$ in x (or x') direction)

$$\left[\begin{array}{l} dx' = \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial t}dt \\ dt' = \frac{\partial G}{\partial x}dx + \frac{\partial G}{\partial t}dt \end{array}\right\}$$ Just Math. → But Space and Time are homogenous → can not depend on particular x and t.

Homogenous ⇒ derivatives are constants ⇒ F and G are LINEAR fun. of x and t!

$$\Rightarrow \left[\begin{array}{l} x' = \alpha(a)x + \beta(a)t \\ t' = \delta(a)x + \varepsilon(a)t \end{array}\right.$$

PS. remember... a is just some parameter... we will see that is some limiting speed (speed of light)

For the ORIGIN $O'(x'=0)$ ... $0 = \alpha(a)x + \beta(a)t \Rightarrow x = -\frac{\beta(a)}{\alpha(a)}t$

But we can see ("from picture") that ... $x(t) = vt$

$$\Rightarrow v = -\frac{\beta(a)}{\alpha(a)}$$

So instead of parameter a we can use v as a parameter!

$$\left\{\begin{array}{l} \gamma(v) \equiv \alpha(a) \\ \gamma(v)A(v) \equiv \delta(a) \\ -\gamma(v)B(v) \equiv \varepsilon(a) \end{array}\right.$$

So we can write: (I) $\left[\begin{array}{l} x' = \gamma(v)[x - vt] \\ t' = \gamma(v)[A(v)t - B(v)x] \end{array}\right.$

Now we will also use the fact that space is izotropic (until now we used homogenous).

Space is izotropic: $R \to R'$ must be same $-R \to -R'$ (p.s. $v \to -v$) ... LIKE IF WE ARE LOOKING IN MIRROR.

So... (II) $\left[\begin{array}{l} -x' = \gamma(-v)[-x + vt] \to x' = \gamma(-v)[x - vt] \\ t' = \gamma(-v)[A(-v)t + B(-v)x] \end{array}\right.$

Now compare (I) and (II) ... we can see that must ... $\left\{\begin{array}{l} \gamma(v) = \gamma(-v) \\ A(v) = A(-v);\ B(v) = -B(v) \end{array}\right.$

Now we use ② ... Principle of Special Relativity ... $R \to R'$ must be same as $R' \to R$ ... (p.s. $v \to -v$) THERE IS NO PREFRENTIAL REFERENCE SYSTEM

So... (III) $\left[\begin{array}{l} x = \gamma(v)[x' + vt'] \\ t = \gamma(v)[A(v)t' + B(v)x'] \end{array}\right\}$ we already used relations ...

Now we put (II) and (III) together ... $x = \gamma(v)\{\gamma(v)[x - vt] + v\gamma(v)[A(v)t - B(v)x]\}$

First we get ... $x = \gamma^2(v)[1 - vB(v)]x + \gamma^2(v)v[A(v) - 1]t$ ... must be three for arbitary x and t!

$$x, t \text{ arbitary} \Rightarrow \left[\begin{array}{l} \gamma^2(v)[1 - vB(v)] = 1 \\ A(v) = 1 \end{array}\right.$$

Now we look at 3 inertial systems $R \xrightarrow{v} R' \xrightarrow{u} R''$, $R \xrightarrow{w} R''$ ... v, u, w relative velocities...

Transformations must hold for all 3 systems...

$$R' \to R'' \Rightarrow \begin{aligned} x'' &= \gamma(u)[x' - ut'] \\ t'' &= \gamma(u)[t' - B(u)x'] \end{aligned}$$

we already used previously derived fact that $A(u) = 1$!

We put all together...

$$\begin{aligned} x'' &= \gamma(u)\gamma(v)[1 + uB(v)]\left(x - \frac{u+v}{1+uB(v)}t\right) \\ t'' &= \gamma(u)\gamma(v)[1 + vB(u)]\left(t - \frac{B(v)+B(u)}{1+vB(u)}x\right) \end{aligned}$$

we did $R \to R'$ and $R' \to R''$ ... $R \to R''$

But we can also do direct transform $R \to R''$...

$$x'' = \gamma(w)[x - wt]$$
$$t'' = \gamma(w)[t - B(w)x]$$

Both must be same ($R \to R' \to R'' = R \to R''$)...

After... we get... $1 + uB(v) = 1 + vB(u) \Rightarrow \frac{B(v)}{v} = \frac{B(u)}{u} = b = \text{const.} \Rightarrow \boxed{B(v) = bv}$

because arbitary v and u

Now we use fact $B(v) = bv$ in equation from before $\gamma^2[1 - uB] = 1$...

We get... $\gamma^2(v)[1 - vB(v)] = 1 = \gamma^2(v)[1 - bv^2] \Rightarrow \boxed{\gamma(v) = \frac{1}{\sqrt{1 - bv^2}}}$

We can see that all this would go $\to$ Galileo ($A = 1; B = 0; \gamma = 1$) if $b = 0$!

Now we must determine b in some way... if $b = 0$ we find just Galileo's transf...

We know Galileo's are wrong $\Rightarrow b \neq 0$... now can be $b > 0$ or $b < 0$...

If we compare equations for $R \to R''$ and $R \to R' \to R''$ we find... $w = (v + u)/(1 + bvu)$

We need this relation to discuss the possible values for b...

1.) $b = 0 \to$ Galileo ... we know it's wrong

$w = \frac{u+v}{1+buv}$; $u, v > 0$

2.) $b < 0$ (assume there is no limit speed in universe) $v, u > 0 \Rightarrow w < 0$ (can be)

(there is some limit speed V_L) CAN NOT BE $w > V_L \Rightarrow$ ... take $u = v = \frac{V_L}{2} \Rightarrow w > V_L$ $\to$ PARADOX!

3.) $b > 0$ ... we can see from $\gamma = 1/\sqrt{1 - bv^2}$ that units $[b] = [s^2/m^2]$ $(1/(\text{velocity})^2)$

Set... $b = 1/x^2$ ... experimentaly we show $x = c$ ... speed of light!

Finally...

$$\boxed{\begin{aligned} x' &= \gamma(v)[x - vt] \\ t' &= \gamma(v)\left[t - \frac{v}{c^2}x\right] \\ \gamma(v) &= 1/\sqrt{1 - v^2/c^2} \end{aligned}}$$

LORENTZ TRANSFORM

P.S. $y' = y$; $z' = z$ in our case!

PS. For velocity...

$$w = \frac{v + u}{1 + \frac{vu}{c^2}}$$

... if $u = v = c \Rightarrow w = c$ (by Galileo $w = 2c$!)

What are consequences of this?

Events ... (x_1, y_1, z_1, t_1); (x_2, y_2, z_2, t_2) ... asume that are simultaneus in R ...

Simultaneus in R $\Rightarrow \Delta t = t_2 - t_1 = 0 \longrightarrow$ R`... $\Delta t` = -\gamma(v)\frac{v}{c^2}\Delta x$ ... NOT SIMULTANEUS!

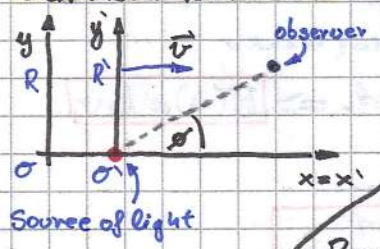
[In general ... $\Delta t = \gamma(v)\left[\Delta t` + \frac{v}{c^2}\Delta x`\right]$ ... if the two events occure at the same position in R` ($\Rightarrow \Delta x` = 0$) $\Rightarrow \boxed{\Delta t = \gamma(v)\Delta t`}$

$\Delta t`$ = proper duration (in system where two events occure in same possition)!

This equation was probably 1st tested with decay of Muons! (cosmic rays)

P.S. Proper time duration is always smalar than the one measured in moving system...

DOPPLER EFFECT



proper frequency?

$\nu` = \nu_R$ ; $\nu = \frac{\nu_R}{1 - \frac{v}{c}\cos\phi} = \frac{\nu`}{1 - \frac{v}{c}\cos\phi}$ ... in CLASSICAL MECHANICS

What about if we take into acount relativity effects?

Then the two frequencies will not be the same anymore!

$\beta = \frac{v}{c} \longrightarrow \nu = \frac{\nu_R}{1 - \beta\cos\phi} \longrightarrow \boxed{\nu = \frac{\nu`\sqrt{1-\beta^2}}{1 - \beta\cos\phi}}$ RELATIVISTIC DOPPLER EFFECT

$\Delta t = \gamma\Delta t` \Rightarrow \nu` = \nu_R\gamma$ → the frequency is not the same if we use the relativity effects!

① $\phi = 0$ (the source is dirrectly aprocking observer)

$\nu` - \nu$ sistemu R`

$$\nu = \nu`\frac{\sqrt{1-\beta^2}}{1-\beta} = \nu`\sqrt{\frac{1+\beta}{1-\beta}} \Rightarrow \nu > \nu` \text{ (VIOLET SHIFT)}$$

$\nu_R - \nu$ sistem R

② $\phi = \pi$ (the source is getting directly away from observer)

ν - for source

$$\nu = \nu`\frac{\sqrt{1-\beta^2}}{1+\beta} = \nu`\sqrt{\frac{1-\beta}{1+\beta}} \Rightarrow \nu < \nu` \text{ (RED SHIFT)}$$

What about space "deformation"? Suppose we have a rule at rest in system R!

$L_p = x_2 - x_1$ = proper length!

$$\left.\begin{aligned} x_1 &= \gamma\left[x_1` + v\underbrace{t_0}\right] \\ x_2 &= \gamma\left[x_2` + v\underbrace{t_0}\right] \end{aligned}\right\} \Rightarrow \boxed{L_p = x_2 - x_1 = \gamma\left[x_2` - x_1`\right] = \gamma L`}$$

measured length of moving stick is smaller than proper!

Note: COORDINATES MUST BE TRANSFORMED AT THE SAME MOMENT t_0!

PS. There can be some paradoxs in "in ind" experiments if the measurement is not done at the same moment in time! Time is not absolute anymore!

Until now the only invariant in relativity is the speed of light c!

We will introduce now another one...

Imagine... $\underset{\text{EMISSION of LIGHT}}{(x_1, y_1, z_1, t_1)} \longrightarrow \underset{\text{ARRIVAL of LIGHT}}{(x_2, y_2, z_2, t_2)}$ ... what is the distance?...

$$l_{12} = c(t_2 - t_1) = \sqrt{(x_2-x_1)^2 + (y_2-y_1)^2 + (z_2-z_1)^2}$$

So we have: $c^2(t_2-t_1)^2 - (x_2-x_1)^2 - (y_2-y_1)^2 - (z_2-z_1)^2 = 0 \rightarrow$ in system R

But also in R': $c^2(t_2'-t_1')^2 - (x_2'-x_1')^2 - (y_2'-y_1')^2 - (z_2'-z_1')^2 = 0 \rightarrow$ in system R'

So we have that... $\boxed{s_{12}^2 = c^2(t_2-t_1)^2 - (x_2-x_1)^2 - (y_2-y_1)^2 - (z_2-z_1)^2}$ is INVARIANT...

But note that $=0$ only if moving with speed of light!

Note... $ds^2 = c^2dt^2 - dx^2 - dy^2 - dz^2$ in system $R \rightarrow$ now we move to a proper system R' (here $dx = dy = dz = 0$) $\Rightarrow ds^2 = c^2 d\tau^2$; $d\tau$ - proper time

That means that $d\tau = ds/c$ is INVARIANT! (PROPER TIME IS INVARIANT)

1) $s_{12} = 0$ LIGHT-LIKE 2) $s_{12} > 0$ TIME-LIKE 3) $s_{12} < 0$ SPACE-LIKE

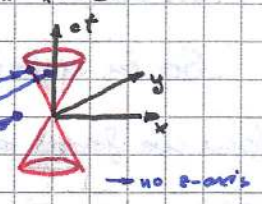
First we focus on TIME-LIKE events ($s_{12} > 0$) $\Rightarrow$ we can always find such a system R' in which $l_{12}' = 0$ ... $s_{12}'^2 = c^2(t_2'-t_1')^2 > 0$

Now for SPACE-LIKE event ($s_{12} < 0$) $\Rightarrow$ we can find R' such that $t_2' = t_1' \rightarrow s_{12}' = -l_{12}' < 0$

What about LIGHT-LIKE events... $(0,0,0,0)$ = emission of wave from O at $t=0$

Then: $\boxed{c^2t^2 = x^2 + y^2 + z^2}$ HYPER CONE (CONE IN 4-DIMENSIONS)

This is called LIGHT CONE... $\boxed{\begin{array}{l}\text{on cone = LIGHT-LIKE}\\ \text{inside cone = TIME-LIKE}\\ \text{outside cone = SPACE-LIKE}\end{array}}$



Imagine an event inside a cone $\Rightarrow s > 0$ ... you can not go outside or cross through origin to other part of cone (because origin is LIGHT-LIKE $s=0$).

That means that you are stuck in the ABSOLUTE FUTURE (or past!). We can not violate the principle of causality!

4-DIMENSIONAL SPACE-TIME $\Rightarrow$ 4-vector $\boxed{\vec{R} = (\vec{r}, ct)}$

$$\left.\begin{array}{l} x_1 = x \\ x_2 = y \\ x_3 = z \\ x_4 = ct \end{array}\right\} \xrightarrow[\text{TRANSFORM}]{R \rightarrow R'} \begin{array}{l} x_1' = \gamma(x_1 - \beta x_4) \\ x_2' = x_2 \\ x_3' = x_3 \\ x_4' = \gamma(x_4 - \beta x_1) \end{array}$$

DEFINE: $\vec{A} = (A_1, A_2, A_3, A_4)$ is a 4-vector if transforms like: $\vec{A} = (A_1, A_2, A_3, A_4) \rightarrow$ $A_1' = \gamma(A_1 - \beta A_4)$, $A_2' = A_2$, $A_3' = A_3$, $A_4' = \gamma(A_4 - \beta A_1)$

SCALAR PRODUCT: $\vec{A}\cdot\vec{B} = A_4B_4 - A_1B_1 - A_2B_2 - A_3B_3$

MAGNITUDE: $\|\vec{A}\| = \sqrt{\vec{A}\cdot\vec{A}} = \sqrt{A_4^2 - A_1^2 - A_2^2 - A_3^2}$

It's easy to show $\vec{A}\cdot\vec{B} = \vec{A}'\cdot\vec{B}'$ → scalar product is invariant!

Now we have to define all the "old" physics in terms of this new quantities!

What is velocity? $\vec{u} = \frac{d\vec{r}}{d\tau} = \frac{d\vec{r}}{dt}\frac{dt}{d\tau} = \gamma(v)\vec{v}$ → classical velocity

IN 3-D → proper time (used here because it is an invariant - look previous page)

In 4-D:

$$\vec{U} = \frac{d\vec{R}}{d\tau} = \begin{cases} dx_1/d\tau \\ dx_2/d\tau \\ dx_3/d\tau \\ dx_4/d\tau = c\,dt/d\tau = c\gamma(v) \end{cases}$$

→ it is obvious that $\vec{u}$ is a 4-vector

Modulus of 4-vector velocity: $\|U\|^2 = U_4^2 - U_1^2 - U_2^2 - U_3^2 = \frac{1}{(d\tau)^2}\left[dx_4^2 - dx_1^2 - dx_2^2 - dx_3^2\right] = \frac{ds^2}{d\tau^2} = c^2$

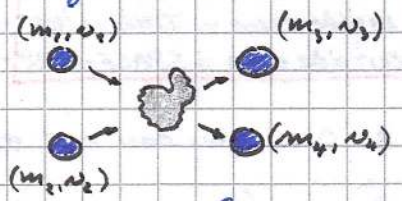
4-vector acceleration: $G_i = \frac{dU_i}{d\tau} = \frac{d^2x_i}{d\tau^2}$

Now... make scalar product $\vec{U}\cdot\vec{G} = U_4\frac{dU_4}{d\tau} - U_1\frac{dU_1}{d\tau} - U_2\frac{dU_2}{d\tau} - U_3\frac{dU_3}{d\tau} = \frac{1}{2}\frac{d}{d\tau}(\underbrace{U\cdot U}_{c^2}) = \underline{\underline{0}}$ → c² → odvod konstante

So in relativity is always... $\boxed{\vec{U}\cdot\vec{G} = 0}$ ... perpendicular!

Now we focus on kinematics... first we take a look at momentum!

Classical: $\vec{p} = m\vec{v}$



→ in R': $m_1v_{1x}' + m_2v_{2x}' = m_3v_{3x}' + m_4v_{4x}'$

... $R - R'$; $\vec{v}' = \vec{v} - \vec{V}$

So... $m_1v_{1x} + m_2v_{2x} - m_3v_{3x} - m_4v_{4x} - V(m_1 + m_2 - m_3 - m_4) = 0$

But V is arbitary $\Longrightarrow \begin{cases} m_1v_{1x} + m_2v_{2x} = m_3v_{3x} + m_4v_{4x} \\ m_1 + m_2 = m_3 + m_4 \end{cases}$

What about in new frame of 4-vectors? Can we use 4-vector velocity $\vec{U}$?

Define moment... first in 3-D: $\boxed{\vec{p} = m\vec{u} = m\gamma(v)\vec{v} = m\vec{v}/\sqrt{1 - v^2/c^2}}$

But we want 4-D... define: $\boxed{\vec{P} = mc\vec{U} = \left(c\vec{p},\ mc^2/\sqrt{1 - v^2/c^2}\right)}$ ... 4-VECTOR ENERGY-MOMENTUM

We want to demonstrate that 2nd term is energy...

Modulus of $\vec{P}$: $\|\vec{P}\|^2 = P_4^2 - P_1^2 - P_2^2 - P_3^2 = \frac{m^2c^4}{1 - v^2/c^2} - \frac{c^2m^2v^2}{1 - v^2/c^2} = m^2c^2(c^2 - v^2)\cdot\frac{1}{1 - v^2/c^2} = m^2c^4$

Look at... $P_4^2 = m^2c^4 + c^2p^2$ → derivative: $P_4\frac{dP_4}{dt} = c^2p\frac{dp}{dt} = c^2\vec{p}\cdot\frac{d\vec{p}}{dt}$

$P_4^2 = \|P\|^2 + \sum_{i=1}^{3} P_i^2$

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$$\left.\begin{aligned} P_4 &= m\gamma(v)\,c^2 \\ \vec{p} &= m\gamma(v)\,\vec{v} \end{aligned}\right\} \text{ put into } \rightarrow P_4\frac{dP_4}{dt} = c^2\vec{p}\,\frac{d\vec{p}}{dt} \longrightarrow \cancel{m\gamma}\,\cancel{c^2}\,\frac{dP_4}{dt} = \cancel{c^2}\,\cancel{m\gamma}\,\vec{v}\,\overbrace{\frac{d\vec{p}}{dt}}^{\text{FORCE!}} \Rightarrow \frac{dP_4}{dt} = \vec{v}\cdot\vec{f} = \text{POWER}$$

So the time derivative of P_4 is power. $\Rightarrow$ P_4 is ENERGY! $\boxed{E = \gamma mc^2\,;\ (E)_{v=0} = mc^2}$

$$\boxed{\|\vec{P}\|^2 = E^2 - c^2p^2 = m^2c^4} \qquad \boxed{E\vec{v} = c^2\vec{p}}$$

$$\boxed{\vec{F} = \frac{1}{c}\frac{d\vec{P}}{d\tau}} \text{ 4-VECTOR FORCE} \rightarrow \boxed{\vec{F} = \frac{1}{c}\frac{d}{d\tau}(mc\vec{U}) = m\frac{d\vec{U}}{d\tau} = m\vec{G}} \xrightarrow{\text{invariant}} \vec{F}' = m\vec{G}'$$

τ ← proper time

Let now demonstrate that Maxwell eq. are invariant under Lorentz transform!

First we have to re-define the operators for 4-D space-time...

DEL: $\vec{\nabla}_4 = \left(-\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}, \frac{\partial}{\partial(ct)}\right) = \left(-\vec{\nabla}_3, \frac{\partial}{\partial(ct)}\right)$ ... we can demonstrate that ∇_4 is behaving like 4-vector.

? means ati phm ?

excesise: demonstrate it!

DIVERGANCE: $\vec{\nabla}_4\cdot\vec{A} = -\left(-\frac{\partial A_1}{\partial x} - \frac{\partial A_2}{\partial y} - \frac{\partial A_3}{\partial z}\right) + \frac{\partial A_4}{\partial(ct)}$

D'ALAMBERTIAN: $\Box^2 = -\frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \nabla_3^2$

$\rho = \frac{dQ}{dV}\,;\ \vec{J} = \rho\vec{v} \longrightarrow \boxed{\vec{J} = (\vec{J}, c\rho)}$ 4-VECTOR CURRENT DENSITY

Continuity equation: $\frac{\partial\rho}{\partial t} + \vec{\nabla}_3\cdot\vec{J} = 0 \longrightarrow \vec{\nabla}_4\cdot\vec{J} = 0$ in $R \rightarrow R'$: $\vec{\nabla}_4'\cdot\vec{J}' = 0$ ✓ ok.

Maxwell:

$$\left.\begin{aligned} &\vec{\nabla}\cdot\vec{E} = \rho/\varepsilon_0 \qquad \vec{\nabla}\cdot\vec{B} = 0 \\ &\vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t} \qquad \vec{\nabla}\times\vec{B} = \mu_0\vec{J} + \mu_0\varepsilon_0\frac{\partial\vec{E}}{\partial t} \\ &\text{potentials: } \vec{B} = \vec{\nabla}\times\vec{A}\ ;\ \vec{E} = -\nabla v - \frac{\partial\vec{A}}{\partial t} \end{aligned}\right\} \longrightarrow \begin{aligned} &\Box^2\vec{A} = -\mu_0\vec{J} \\ &\Box^2 v = -\rho/\varepsilon_0 \end{aligned}$$

equivalen to Maxwell ... this means that is enough to demonstrate invariance of this

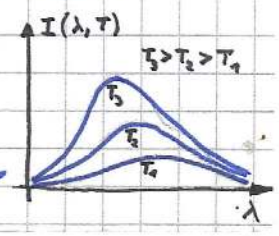
DEFINE 4-D POTENTIAL: $\boxed{\vec{A} = \left(\vec{A}, \frac{1}{c}v\right)} \longrightarrow \boxed{\Box^2\vec{A} = \mu_0\vec{J}}$ $R \rightarrow R'$ $\Box'^2\vec{A}' = \mu_0\vec{J}'$

INVARIANT

Here we will finish the relativity theory ... all physics until now is determenistic... knowing the properties of some system we can predict the future evolution of the system. All is divided in two big parts... the particle and the wave!

But technological advances made possible new experiments to be made... and new phenomena was discovered (like kathod rays (e^-); radioactivity, atom...)

First problems in physics that were giving hints of "new" physics were experiment like spectral distribution of black-body radiation!



Theoretical prediction for BB radiation of that time was: $I(\lambda, T) = \frac{2\pi k T}{\lambda^4}$

Note: $I \rightarrow \infty$ when $\lambda \rightarrow 0$ $\Rightarrow$ infinite energy!

experimental

... then Max Planck made assumption that the multitud of oscillators can be excited just at certain energies and that they emit energy just at certain levels...
In paralel with this the photo-electric effect was observed... using both things Einstein made the prediction that EM-wave is realy like a particle!
But to explain interference and diffraction we must let the light to be a wave... here comes the wave-particle duality! (The end of classical physics!)

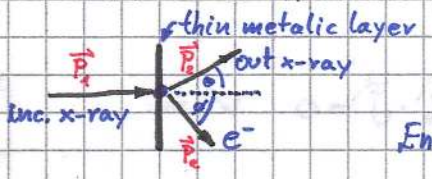
Let's assume now that light consists of particles (photons) with energy...

$\boxed{E = h\nu = \hbar\omega}$ ... but particle has momentum... use relativity and 4-vector ENERGY-MOMENTUM to find momentum... we know from relativity: $E\vec{v} = c^2\vec{p} \overset{v=c}{\Longrightarrow} Ec = c^2 p \Longrightarrow \boxed{p = \frac{E}{c} = \frac{h\nu}{c}}$

So... 4-vector ENERGY-MOMENTUM for photon: $\boxed{\vec{P} = (c\vec{p}, E) = \hbar c\left(\vec{k}, \frac{\omega}{c}\right)}$

where $\boxed{\vec{k} = \frac{2\pi\nu}{c}\cdot\hat{u}}$ → $\hat{u}$ is allong the direction of propogation of photon.

COMPTON SCATTERING



$\vec{P}_1, \vec{P}_2, \vec{P}_e$ are corresponding 4-vector ENERGY-MOMENTUM vectors!

Energy conservation (suppose e^- is at rest initialy)!

$$h\nu_1 + mc^2 = h\nu_2 + c\left(p_e^2 + m^2c^2\right)^{1/2} \rightarrow \text{energy conservation}$$

$$\vec{p}_1 = \vec{p}_2 + \vec{p}_e \rightarrow p_e^2 = p_1^2 + p_2^2 - 2p_1p_2\cos\theta \rightarrow \text{momentum conservation}$$

Let's put this together (use: $p_1 = h\nu_1/c$; $p_2 = h\nu_2/c$):

$$h\nu_1/c + mc = h\nu_2/c + \left[(h\nu_1/c)^2 + (h\nu_2/c)^2 - (2h^2\nu_1\nu_2/c^2)\cdot\cos\theta + m^2c^2\right]^{1/2}$$ ... solve this for ν-diff.

we get... $\nu_2 - \nu_1 = \frac{h\nu_1\nu_2}{mc^2}(1-\cos\theta)$ ⊕ use: $\nu = c/\lambda \Longrightarrow \boxed{\Delta\lambda = \lambda_2 - \lambda_1 = \frac{2h}{mc}\cdot\sin^2\frac{\theta}{2}}$

Now focus on this(..), expres ν_2: $\nu_2 = \nu_1 \Big/ \left[1 + \left(\frac{h\nu_1}{mc^2}\right)(1-\cos\theta)\right]$ ... and imagine that light is back-scattered ($\theta = \pi$)! → $\nu_2 = \nu_1 \Big/ \left[1 + \frac{2h\nu_1}{mc^2}\right]$ ... now look for example we send in light in band [0'5 MeV, 1 MeV] → [~0'17 MeV, ~0'2 MeV] → we get this light back-scattered... we can see that band-width is much smaller! This means we can use this phenomena as mono-chromator!

Note.. we send in light with: $h\nu_1 >> \frac{1}{2}mc^2 \Longrightarrow h\nu_2 \approx \frac{1}{2}mc^2 \sim 0'25\,\text{MeV}$ → again works like mono-chrom

energy much larger than half rest-energy of e^-

CHERNIKOV EFFECT ... charged particle moves with speed bigger than speed of light (IN MEDIUM)

speed of light in some medium: $v_l = c/n$ ... $v > c/n \rightarrow v$ = speed of particle

$\vec{P}_1$ = 4 vector Energy-Momentum of e^- before emission / $\vec{P}_2 = (\dots)$ of e^- after emission

MOMENT CONSERV: $\vec{P}_1 = \vec{P}_2 + \vec{P}_3$; $\vec{P}_3$ = 4 vector Energy-Momentum of photon emited by e^-

$\Rightarrow \vec{P}_1 - \vec{P}_3 = \vec{P}_2 \rightarrow (\vec{P}_1 - \vec{P}_3)\cdot(\vec{P}_1 - \vec{P}_3) = \vec{P}_2 \cdot \vec{P}_2$ ... we know: $P_1^2 = P_2^2 = m^2c^4 \Rightarrow$ we get...

... $\Rightarrow P_3^2 = 2\vec{P}_1 \cdot \vec{P}_3$ (some algebra was between!) ... now remember also that we are in some media (so $c \rightarrow c/n$): $E\frac{c}{n} = p\left(\frac{c}{n}\right)^2 \rightarrow \vec{p} = \frac{n}{c} h\nu \hat{v}$ and $\vec{P}_3 = (c\vec{p}, E) = (nh\nu\hat{v}, h\nu)$

So we have: $P_3^2 = h^2\nu^2(1-n^2)$ ... and then $2\vec{P}_1\cdot\vec{P}_3 = 2m\gamma(v)c^2h\nu\left(1 - \frac{n}{c}v\cos\Theta\right)$

Using equation from before: $P_3^2 = 2\vec{P}_1\cdot\vec{P}_3 \rightarrow$ we can express $\cos\Theta$ and compare with experiment: $\boxed{\cos\Theta = \frac{c}{nv}\left(1 + \frac{h\nu}{2mc^2}\cdot\frac{n^2-1}{\gamma(v)}\right)}$ $\longrightarrow$ LOW-ENERGY PHOTONS: $\cos\Theta \approx c/nv$

Ex: Find the minimum electron energy to produce Chernikov radiation in H_2O ($n \sim 4/3$)!

... next physical problem was the discrete spectra of light emited from matter and also that atoms should not be stable ... electrons should emit (e^- in orbit of p^+) countinous spectra and lose energy $\rightarrow$ fall to nucleus on a spiral ... there was formula for light from excited hydrogen atom: $\nu = \overset{\text{CONST.}}{R}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$; $m > n$; $m, n \in \mathbb{N}$

This sugested to Bohr "are energy levels in atom discrete and there exists some fundamental state"! $\rightarrow e^-$ can jump from level $E_i \rightarrow E_j$ if $h\nu = E_j - E_i \Rightarrow E_l = -h\frac{R}{l^2}$!

All mentioned things sugerst that we need some new theory to describe micro-scopic world ... theory should "limit" to classical physics for macro-scopic scale!

De-Brogie assumed in his thesis that we should adopt the wave-particle duality also to particles ... $\overset{\text{ENERGY}}{\mathcal{E}} = \hbar\omega$; $\vec{p} = \hbar\vec{k}$ $\left(\vec{k} = \frac{2\pi}{\lambda}\cdot\hat{v}\right)$ ... experimental evidence came few years later $\rightarrow$ Davisson and Germer observed interference of e^-!

We will need wave-packet mathematics for describing ... we will now review ... $\mathcal{E} = \hbar\omega$; $\vec{p} = \hbar\vec{k} \longrightarrow$ Wave-packet: $\psi(\vec{r}) = \int g(\vec{k})\exp[i(\vec{k}\cdot\vec{r} - \omega t)]\,d\vec{k}$

How can we link this mathematical object to real particle?

Lets concentrate just to 1-D! $\rightarrow$

1D: $\underset{\text{COMPLEX}}{f(k)} = \underset{\text{REAL}}{A(k)}\, e^{i\alpha(k)} \longrightarrow \psi(x,t) = \int_{-\infty}^{+\infty} A(k)\, e^{i\varphi(k)}\, dk$; where $\varphi(k) = kx - \omega t + \alpha(k)$

To have this significantly different than zero $\rightarrow$ $A(k) \neq 0$ in region Δk

$|\Delta\varphi| \approx \Delta k \left|\frac{d\varphi}{dk}\right| \leq \pi$ $\rightarrow$ condition for localized sum (da ne pride do destructive interference)

$\frac{d\varphi}{dk} = x - t\frac{d\omega}{dk} + \frac{d\alpha}{dk} \rightarrow x + \beta(k)$

$\left(\beta(k) = \frac{d\alpha(k)}{dk} - t\frac{d\omega}{dk}\right)$

$|x + \beta(k)| \leq \pi/\Delta k$

So... $x_{max} + \beta(k) \simeq \frac{\pi}{\Delta k}$; $x_{min} + \beta(k) \simeq -\pi/\Delta k$

We can: $\Delta x = x_{max} - x_{min} \simeq 2\pi/\Delta k \Rightarrow \Delta x \Delta k \simeq 2\pi$

$\rightarrow$ Remember that k is related to "particle" momentum (de Broglie equations)

We can see that we can not determine the position sharply as in classical physics...

What about velocity... where is maximum of wave packet $\rightarrow$ max: $\frac{d\varphi}{dk} = 0$ - condition for max. of wave-p.

$\frac{d\varphi}{dk} = x - t\frac{d\omega}{dk} + \frac{d\alpha}{dk} = 0 \Rightarrow x_m = t\frac{d\omega}{dk} - \frac{d\alpha}{dk}$ $\rightarrow$ here is the wave-pocket velocity

Than $\rightarrow$ Group velocity: $v_g = \frac{d\omega}{dk}$

(classical velocity of particle)

But remember... for free particle: $E = p^2/2m \Rightarrow v = \frac{dE}{dp}$ $\rightarrow$ how is this related to $v_g = \frac{d\omega}{dk}$

So: $v_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} = \frac{dE}{dp} \Rightarrow p = \hbar k$ $\rightarrow$ consistent with deBroglie!

So it looks that description with wave-pocket is consistent with what we know...

How should new equation that describes micro-world look ... it should be differential equation of 1st order with respect to time! $\rightarrow$ Why? ... we have to introduce Hamiltonian!

System: R degrees of freedom $\Longrightarrow$ we need: $q_1, q_2 \dots q_R$ coordinates

$p_1, p_2 \dots p_R$ "conjugate" momentum

We call HAMILTONIAN: $\boxed{H(q_1, q_2 \dots q_R; p_1 \dots p_R; t)}$ HAMILTONIAN

Such function that: $\boxed{\dot{q}_r = \frac{\partial H}{\partial p_r} \text{ and } \dot{p}_r = -\frac{\partial H}{\partial q_r}}$ $(r = 1, 2, \dots, R)$ HAMILTON EQUATIONS

Normaly Hamiltonian is just the energy $\rightarrow$ $\boxed{H = T + V}$ (kinetic + potential energy)

Lets look at derivative of Hamiltonian with respect to time!...

So: $\dot{H} = \frac{dH}{dt} = \sum \frac{\partial H}{\partial q_R}\dot{q}_R + \sum \frac{\partial H}{\partial p_R}\dot{p}_R + \frac{\partial H}{\partial t}$ $\rightarrow$ (use Hamilton equations) $\rightarrow \cancel{\sum \frac{\partial H}{\partial q_r}\frac{\partial H}{\partial p_r}} - \cancel{\sum \frac{\partial H}{\partial p_r}\frac{\partial H}{\partial q_r}} + \frac{\partial H}{\partial t}$

That means that $\dot{H} \neq 0$ only if Hamiltonian explicitly depends on time!

Example: Hamiltonian of e^- orbiting proton (classical Hydrogen atom)

$H = T - V = \frac{p^2}{2m} - \frac{e^2}{r}$

$$\left.\begin{aligned} \frac{\partial \vec{r}}{\partial t} &= \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p}}{m} \\ \frac{\partial \vec{p}}{\partial t} &= -\frac{\partial H}{\partial \vec{r}} = -\frac{e^2}{r^2}\hat{r} \end{aligned}\right\} \text{used Hamilton equations}$$

Hamiltonian of harmonic osc $\rightarrow$ $H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \rightarrow \dot{x} = \frac{\partial H}{\partial p} = p/m$; $\dot{p} = -\frac{\partial H}{\partial x} = -kx$

Other constrain on new equation is that it must be LINEAR and HOMOGENOUS!

$\Rightarrow$ wave-packet ψ_1 and ψ_2 solutions $\Rightarrow \lambda_1\psi_1 + \lambda_2\psi_2$ is solution

Other constrain $\rightarrow$ CORESPONDENCE PRINCIPLE ...

Free Particle: $\psi(\vec{r},t) = \int F(\vec{p}) \exp\left(\frac{i}{\hbar}[\vec{p}\cdot\vec{r} - Et]\right) d\vec{p}$ now de Broglie relation is used to $\vec{k} \rightarrow \vec{p}$

Free particle in quantum mechanics

$E = p^2/2m \rightarrow$ in classical (non-relativistic) physics!

To satisfy corespondence principle we should link the two descriptions!

Take time-derivative... $i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \int E\, F(\vec{p}) \exp\left(\frac{i}{\hbar}[\vec{p}\cdot\vec{r} - Et]\right) d\vec{p}$

gradient: $i\hbar\nabla\psi(\vec{r},t) = \int \vec{p}\, F(\vec{p}) \exp\left(\frac{i}{\hbar}[\vec{p}\cdot\vec{r} - Et]\right) d\vec{p}$

laplace: $-\hbar^2\nabla^2\psi(\vec{r},t) = \int p^2 F(\vec{p}) \exp\left(\frac{i}{\hbar}[\vec{p}\cdot\vec{r} - Et]\right) d\vec{p}$

SCHODINGER EQUAT. (FREE PARTICLE)

So from $E = p^2/2m \oplus$ corespondance principle $\Rightarrow$ $\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)}$

The "recept" to switch from classical $\rightarrow$ quantum mechanics ... properties in classical world becomes an operator: $\boxed{E \rightarrow i\hbar\frac{\partial}{\partial t}\ ;\ \vec{p} \rightarrow \frac{\hbar}{i}\nabla \rightarrow p^2 = -\hbar^2\nabla^2}$!

$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t)}$ GENERAL SCHRÖDINGER EQUATION (start from $E = \frac{p^2}{2m} + V$...)

In terms in Hamiltonian...

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H(\vec{r},\vec{p})\psi(\vec{r},t)$$ ...note: Hamiltonian is operator here!

Classical Hamiltonian: $E = H(q_1,..q_r, p_1..p_r) \rightarrow$ transform $E \rightarrow i\hbar\frac{\partial}{\partial t}$

$H(q_1...q_r, p_1...p_r) \rightarrow H(q_1...q_r; \frac{\hbar}{i}\frac{\partial}{\partial q_1} ... \frac{\hbar}{i}\frac{\partial}{\partial q_r})$ $\leftarrow$ $p \rightarrow \frac{\hbar}{i}\nabla$ ... we used this!

Example: Schrödinger equation for Hydrogen atom

classical Hamilton (for e^- and p^+): $H = \frac{p_p^2}{2M} + \frac{p_e^2}{2m} - \frac{e^2}{|\vec{r}_p - \vec{r}_e|}$ = energy

we use "recept" for transform:

operator acting on $\psi(\vec{r},t)$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2M}\nabla_p^2 - \frac{\hbar^2}{2m}\nabla_e^2 - \frac{e^2}{|\vec{r}_p - \vec{r}_e|}\right]\psi(\vec{r},t)$$

Now... use fact that $M >> m$ and put the origin to where p^+ is (so $\vec{r}_p = 0$)

We get: $i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}\right)\psi$ EQUATION of HYDROGEN ATOM

SOME CONSTANTS

Ps: wave-particle duality: $(\varepsilon, \vec{p}) \longleftrightarrow (\omega, \vec{k})$

$$\varepsilon = \hbar\omega;\ \vec{p} = \hbar\vec{k}$$

Look at EM-wave ... intensity vs photon density ...

$\psi(\vec{r}) \to \rho = \alpha|\psi(\vec{r})|^2$ ... but imagine only 1 photon => density → probability !

like E-field photon density intensity

=> Modulus of square of wave-packet is related to probability of finding particle there!

$p(\vec{r})\,d\tau = |\psi(\vec{r})|^2$ → probability of finding particle in volume element $d\tau$

So probability to find particle in volume V: $p(V) = \int_V |\psi(\vec{r})|^2 dV$

It is clear that to be physicaly reasonable must be → $\boxed{\int_{\text{all volume}} |\psi(\vec{r})|^2 dV = 1}$

Remember → it's linear equation => $\psi(\vec{r})$ solution => $A\psi(\vec{r})$ also solution => WE CAN NORMALIZE!

Note: look at time-derivative of total probability:

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(\vec{r},t)|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\psi(x,t)|^2 dx$$

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \frac{\partial}{\partial t}\left[\psi(x,t)\cdot\psi^*(x,t)\right] = \psi^*\frac{\partial}{\partial t}\psi + \psi\frac{\partial}{\partial t}\psi^* = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi^*}{\partial x^2}\psi\right) =$$

use Schrödinger: $\left.\begin{aligned}\frac{\partial\psi}{\partial t} &= \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{i}{\hbar}V\psi \\ \frac{\partial\psi^*}{\partial t} &= -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^*\end{aligned}\right\}$

$$= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)$$

So we got: $\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^2 dx = \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right]dx = \frac{i\hbar}{2m}\left[\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right]_{-\infty}^{\infty} = 0$

because ψ and ψ^* are 0 at $x = \pm\infty$!

That's ok ... total probability shouldn't change!

PS: All information about particle-wave is encoded in $\psi(\vec{r},t)$! Important is modulus squared $|\psi|^2$ ... which is the probability distribution. This probability is somehow diferent than probability in classical physics ... in classical we have many particles described by statistics, because we are not "powerfull" enough to describe exactly ... but in QM probability is intrinsic concept!

Note: Physical object is $|\psi|^2$ not ψ! Because we can measure only particle ... ... not the wave-function itself.

Psi ψ has to be normalized, so that $\int_{-\infty}^{\infty}|\psi|^2 dV = 1$! As we showed before, this normalization is "conserved" ... $\frac{d}{dt}\int_{-\infty}^{\infty}|\psi|^2 dV = 0$

We make measurement and find particle at point C! Where was the particle just before:

1) Realist – particle was at same point C => ψ is not enough, there are hidden variables

2) Othodox – particle was everywhere => ψ is enough, measurement has special effect

3) Agnostic – there is no sense in asking where was before, because we can not check it

Note: If we make 2nd measurement imediatly after 1st measurement we will find the system (particle) in same state as in 1st measurement. This is called "colapse of wave-function"!

EXPECTATION VALUE $\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$ → this is in 1-D! (~average x)

This is for position → now for velocity!

$$\frac{d}{dt}\langle x \rangle = \int_{-\infty}^{\infty} x \frac{\partial}{\partial t} |\psi(x,t)|^2 dx$$

Use: $\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}(\psi\psi^*) = \psi^* \frac{\partial}{\partial t}\psi + \psi \frac{\partial}{\partial t}\psi^*$

And: $\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar}V\psi$; $\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi$

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{i\hbar}{2m}\left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2}\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)\right]$$

So we get: $\frac{d}{dt}\langle x \rangle = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right] dx$ → now we do integration "per-partes"...

$$= \frac{i\hbar}{2m}\Big[\underbrace{x\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)\Big|_{-\infty}^{+\infty}}_{0 \text{...because } \psi \to 0 \text{ at } \pm\infty!} - \int_{-\infty}^{\infty} \frac{\partial x}{\partial x}\underbrace{\left(\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right)}_{\text{again 'per-partes'}} dx$$

no 2 here

$$\Rightarrow \frac{d}{dt}\langle x \rangle = \frac{i\hbar}{m}\int \psi^* \frac{\partial}{\partial x}\psi \, dx = \langle v \rangle = \text{expectation value for velocity (demonstrate?)}$$

So for momentum:

$$\langle p \rangle = m\frac{d}{dt}\langle x \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx = \int \psi^* \underbrace{\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)}_{\text{momentum operator for 1-D}} \psi \, dx$$

For position we can write in "operator" way: $\langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx = \int_{-\infty}^{\infty} \psi^*(x)\psi \, dx$

Now we can write expectation value for any observable ... because all of them can be expressed with $\langle x \rangle, \langle p \rangle$...

Observable $\boxed{Q = Q(x,p)}$ ⟶ $\boxed{\langle Q(x,p) \rangle = \int_{-\infty}^{\infty} \psi^* \underbrace{Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)}_{\text{we enclose operator of } Q \text{ between } \psi^*, \psi} \psi \, dx}$

Note that everything was written for 1-D!

Schrödinger: $i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + v(x,t)\Psi$ ... lets simplyfy $v(x,t) = v(x)$

Variable separation: $\Psi(x,t) = \psi(x)\varphi(t)$ (ansatz)

Plug in...

$$i\hbar \frac{1}{\varphi}\frac{d}{dt}\varphi = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2}{dx^2}\psi + v(x)$$ → both sides must equal to a constant $= E$

So we have:

$$\begin{cases} i\hbar \frac{1}{\varphi}\frac{d}{dt}\varphi = E \rightarrow \text{we can solve this} \rightarrow \boxed{\varphi(t) = \exp\left(-\frac{iE}{\hbar}\cdot t\right)} \\ -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2}{dx^2}\psi + v(x) = E \rightarrow \text{TIME-INDEPENDENT SCHRÖDINGER EQUATION} \end{cases}$$

PS: if we want the solution to be normalizable ⇒ constant E must be real!

What is special about "seperable solutions" ($\Psi(x,t) = \psi(x)\cdot\varphi(t)$):

1. they are STATIONARY STATES: $\Psi(x,t) = \psi(x)\exp\left(-\frac{iE}{\hbar}\cdot t\right) \Rightarrow |\Psi(x,t)|^2 = |\psi(x)|^2$...

   ... there is no time-dependence!

2. they are states with DEFINED TOTAL ENERGY: $\overset{\text{OBSERVABLE}}{H} = \frac{p^2}{2m} + V(x) \rightarrow \overset{\text{OPERATOR}}{\hat{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

   ⇒ Schrödinger equation can be written as: $\boxed{\hat{H}\psi = E\psi}$ ⇒ EIGENVALUES

   to demonstrate that total energy is defined calculate $\sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2$!

   $$\left.\begin{aligned} &\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E^2\psi \Rightarrow \langle H^2\rangle = E^2 \\ &\langle H\rangle = \int \psi^* \hat{H}\psi\, dx = E\int \psi^*\psi\, dx = E \end{aligned}\right\} \Rightarrow \sigma_H^2 = E^2 - E^2 = 0 \checkmark \text{ ok!}$$

3. general solution can be always written as LINEAR COMBINATION of seperate solu.!

   $$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x)\cdot\exp\left(-\frac{iE_n}{\hbar}\cdot t\right)}$$ → we get ∞-number of solutions (time-independent), each with it's own energy

So to solve Schrödinger we must know the potential $v(x)$ and the initial conditions... $\Psi_0(x, t=0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$ ... then we multiply each factor with temporal part: $\Psi(x,t) = \sum c_n \psi_n(x)\exp\left(-\frac{iE_n}{\hbar}\cdot t\right)$

Now we will take a look what we get in some special cases for potential!

Note: In general energy $E >$ minimum value of $V(x)$!

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar}[V(x) - E]\psi(x)$$ → if $E < \min(V) \Rightarrow V(x) - E$ is positive!

This would mean that $\frac{d^2\psi}{dx^2}$, ψ have always the same sign ⇒ can not normalize ψ!

INFINITE WELL $\quad V(x) = \begin{cases} 0; & 0 \le x \le a \\ \infty; & \text{else} \end{cases}$

$\rightarrow \psi = 0$ outside!

OUTSIDE THE BOX: $\psi = 0$

INSIDE THE BOX: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \implies \frac{d^2\psi}{dx^2} = -k^2\psi; \; k^2 = \frac{2mE}{\hbar^2}$

general solution: $\psi(x) = A\sin(kx) + B\cos(kx)$ → now use boundary conditions

boundary → $\psi(0) = \psi(a) = 0 \implies A\sin(0) + B\cos(0) = 0 \implies B = 0$

$\implies A\sin(ka) = 0 \implies ka = n\pi; \; n = 1, 2, \ldots$

PS: $A = 0$ is not solution because it's not normalizable (similar for $n = 0$)

So we get: $k = n\pi/a \implies$ energy is discrete: $\boxed{E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}}$

Solution for $\psi(x)$: $\boxed{\psi_n(x) = A\sin\left(\frac{n\pi}{a}\cdot x\right)}$

To find constant A: $\int_0^a |\psi(x)|^2 dx = \int_0^a |A|^2 \sin^2\left(\frac{n\pi}{a}\cdot x\right) dx = 1 \implies \boxed{A = \sqrt{2/a}}$

Now... any function $f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}\cdot x\right)$

To find coefficients c_n: $\int \psi_m^*(x) f(x)\, dx = \sum_{n=1}^{\infty} c_n \int \psi_m^* \psi_n \, dx = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$

So $\implies c_n = \int \psi_n^* f(x)\, dx$ ... to get time-dependent solution we now attach the temporal part: $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}\cdot t\right)$

Lets find now the expectation value of Hamiltonian! $\langle H \rangle = \int \psi^* \hat{H} \psi \, dx$

$$\langle H \rangle = \int \psi^* \hat{H} \psi \, dx = \int \left(\sum_m c_m \psi_m\right)^* \hat{H} \left(\sum_n c_n \psi_n\right) dx$$

$$= \sum_m \sum_n c_m^* c_n E_n \underbrace{\int \psi_m^* \psi_n \, dx}_{\delta_{mn}} = \sum_n |c_n|^2 E_n \quad \rightarrow \boxed{\langle H \rangle = \sum_n |c_n|^2 E_n}$$

So $|c_n|^2$ is the probability that measurement will give result E_n!

Note:

$\int |\Psi(x,0)|^2 dx = 1$ → integral over all space of initial condition must $= 1$!

$$\int \Big(\underbrace{\sum_m c_m \psi_m(x)}_{\text{initial condition as a sum}}\Big)^* \Big(\underbrace{\sum_n c_n \psi_n(x)}\Big) dx = \sum_m \sum_n c_m^* c_n \underbrace{\int \psi_m^*(x) \psi_n(x)\, dx}_{\delta_{mn}} = \ldots = \sum_n |c_n|^2 = 1$$

So → If initial condition is normalized $\implies c_n$ are also already normalized!

FINITE WELL ... imagine potential $V(x) = \begin{cases} V_0 > 0; & 0 \le x \le a \\ 0; & \text{else} \end{cases}$

We subdivide the problem into 3 regions...

REGION I & III: $\left(\frac{d^2}{dx^2} + k^2\right)\psi(x) = 0$; $k^2 = 2mE/\hbar^2$ → time-independent Schrödinger

So in region I the solution is: $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$ ~ (incoming) + (reflected)

And in region III the solution is: $\psi_{III}(x) = Ce^{ikx} + C'e^{-ikx}$ reflection $(=0)$

Assuming that particle comes from left to right we expect no reflection in region III!

REGION II: $\left(\frac{d^2}{dx^2} - \gamma^2\right)\psi(x) = 0$; $\gamma^2 = 2m(V_0 - E)/\hbar^2$

Now we have 2 possibilities... $E < V_0$ or $E > V_0$

1) $E < V_0$ ⟹ we get solution... $\psi_{II}(x) = De^{\gamma x} + Fe^{-\gamma x}$

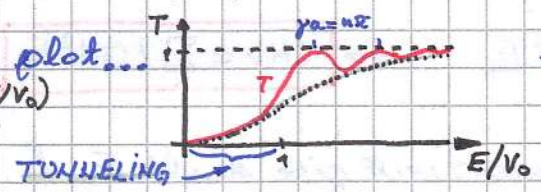
- ψ and ψ' must be continuous at $x = 0$ ⟹ $A + B = D + F$ and $ik(A - B) = \gamma(D - F)$
- Same condition for $x = a$ ⟹ $De^{\gamma a} + Fe^{-\gamma a} = Ce^{ika}$ and $\gamma(De^{\gamma a} - Fe^{-\gamma a}) = ikC\ e^{ika}$

Solving this system we get: $|C|^2 = |A|^2 \cdot 4\gamma^2 k^2 / \left[4\gamma^2 k^2 + (\gamma^2 + k^2)^2 \sinh^2(\gamma a)\right]$

2) $E > V_0$ ⟹ solution is: $\psi_{II}(x) = D'e^{i\gamma x} + F'e^{-i\gamma x}$ ... now we impose the same conditions for continuity of ψ and ψ' at both edges and solving the resulting system we get... $|C|^2 = |A|^2 \cdot 4\gamma^2 k^2 / \left[4\gamma^2 k^2 + (\gamma^2 + k^2)^2 \sin^2(\gamma a)\right]$

Note: the ratio $|C|^2/|A|^2$ is transmision probability... $T = |C|^2/|A|^2$

Now we plot... $T = T(E/V_0)$



→ we get transmision probability $T = 1$ only when $E > V_0$ and $\gamma a = n\pi$ $(n = 1, 2, \ldots)$!

Note... we have tunneling effect when $E < V_0$, but also when $E > V_0$ there is not the transmision prob. $= 1$ (except when $\gamma a = n\pi$)... particle can be reflected even when classicaly should be transmited... and when classicaly the particle should reflect (when $E < V_0$), there is some probability that particle will pass through the barier (this is TUNNELING EFFECT)!

HARMONIC OSCILLATOR

Classical Hamiltonian for H.O.: $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$ ... now make operator $\hat{H}$...

Use $p \to \frac{\hbar}{i}\frac{\partial}{\partial x}$; $x \to x$ ... so $H \to \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2$ ... note that the operator makes sense only when applied to something ...

Schrödinger: $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2} m\omega^2 x^2 \psi(x) = E\psi(x)$

We will solve this using the LADDER OPERATOR instead solving it analitically!

LADDER OPERATORS: $\boxed{Q_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i p + m\omega x\right)}$ ← Note: x and p are operators!

Look at:

$$Q_- Q_+ = \frac{1}{2\hbar m\omega}\left(p^2 + m^2\omega^2 x^2 + i m\omega p x - i m\omega x p\right)$$

$$= \frac{1}{2\hbar m\omega}\left(p^2 + (m\omega x)^2\right) - \frac{i}{2\hbar}[x, p]$$

$\boxed{[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}}$ COMUTATOR

This is COMUTATOR RELATION...

What is the effect of comutator? → $[\hat{x}, \hat{p}]g(x) = (\hat{x}\hat{p} - \hat{p}\hat{x})g(x)$

we get... $[\hat{x}, \hat{p}]g(x) = x\frac{\hbar}{i}\frac{\partial}{\partial x}g(x) - \frac{\hbar}{i}\frac{d}{dx}(x g(x)) = \cancel{\frac{\hbar}{i} x \frac{d}{dx} g(x)} - \cancel{\frac{\hbar}{i} x \frac{d}{dx} g(x)} - \frac{\hbar}{i} g(x)$

So finally... $\boxed{[\hat{x}, \hat{p}] = i\hbar \neq 0}$ → POSSITION AND MOMENTUM DO NOT COMUTE!

This means that... $Q_- Q_+ = \frac{1}{2\hbar m\omega}\left(p^2 + (m\omega x)^2\right) + \frac{1}{2} = \frac{1}{\hbar\omega} H + \frac{1}{2}$

We can write: $H = \hbar\omega\left(Q_- Q_+ - \frac{1}{2}\right)$ → Hamiltonian in terms of ladder operators...

Note: $Q_- Q_+ - Q_+ Q_- = \underline{[Q_-, Q_+] = 1}$ ⟹ also Q_- and Q_+ DO NOT COMUTE!

We can write Schrödinger equation now in terms of Q_- and Q_+ instead with H... $\boxed{\hbar\omega\left(Q_\pm Q_\mp \pm \frac{1}{2}\right)\psi = E\psi}$

Now... ψ is solution to $H\psi = E\psi$ ⟹ $a_+\psi$ is SOLUTION TO $H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$

⟹ $a_-\psi$ is SOLUTION TO $H(a_-\psi) = (E - \hbar\omega)(a_-\psi)$

We will take now a look at how to demonstrate this crucial statement.

$$H(a_+\psi) = \overbrace{\hbar\omega\left(a_+ a_- + \tfrac{1}{2}\right)}^{H}(a_+\psi) = \hbar\omega\left(a_+ a_- a_+ + \tfrac{1}{2} a_+\right)\psi =$$

$$= \hbar\omega a_+\left(a_- a_+ + \tfrac{1}{2}\right)\psi \xrightarrow{[a_-, a_+] = 1} = a_+\left[\hbar\omega\left(a_+ a_- + 1 + \tfrac{1}{2}\right)\right]\psi$$

$$= a_+\left[H + \hbar\omega\right]\psi = (E + \hbar\omega)(a_+\psi)$$

We just showed that... $H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$ ... so if we find one solution we use ladder operators to find ∞-number of other-ones!

Similarly we can show that... $H(a_-\psi) = (E - \hbar\omega)(a_-\psi)$

Note that if we keep applying "raising" operator a_+ there is no obvious problem, but if we keep applying "lowering" operator a_- we would go to NEGATIVE ENERGY...
So we should get into problem at some point applying a_-... at some point we get wave function ψ_0 that is "lowest" possible... if we apply a_- again $\rightarrow (a_-\psi_0)$ will not be normalizable any more! $(a_-\psi_0 = 0)$

$$a_-\psi_0 = 0 \rightarrow \frac{1}{\sqrt{2m\hbar\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0 \Rightarrow \int\frac{d\psi_0}{\psi_0} = -\int\frac{m\omega}{\hbar}x\,dx$$

So we get: $\ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + \text{const.} \Rightarrow \boxed{\psi_0(x) = A_0\exp(-m\omega x^2/2\hbar)}$ FUNDAMENTAL STATE

Also the minimum energy... $H\psi_0 = E_0\psi_0 \rightarrow \hbar\omega(a_+a_- + \frac{1}{2})\psi_0 = \frac{\hbar\omega}{2}\psi_0 \Rightarrow \boxed{E_0 = \frac{1}{2}\hbar\omega}$

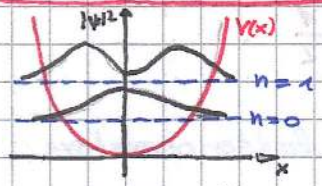
When we have this fundamental state we find other solutions just by applying raising operator. This are also all the solutions!

$$\psi_n(x) = A_n(a_+)^n\psi_0(x) \quad ; \quad E_n = (n+\tfrac{1}{2})\hbar\omega$$

To find the same solution in analytical way take a look in a book (Griffits)!

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\cdot H_n(\xi)\cdot\exp(-\xi^2/2) \quad ; \quad \xi = \sqrt{\frac{m\omega}{\hbar}}\,x}$$

... $H_0 = 1$; $H_1 = 2\xi$; $H_2 = 4\xi^2 - 2$ HERMITE POLYNOMIALS



→ Note that there is some non-zero probability to find particle outside classicly alowed region!
What is this probability? (we do for fundamental state)

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp(-\xi^2/2) \; ; \; \xi = \sqrt{\frac{m\omega}{\hbar}}\,x \; , \; d\xi = \sqrt{\frac{m\omega}{\hbar}}\,dx$$

Probability to be outside classic region...

$$P = 2\int_{x_0}^{\infty}|\psi_0(x)|^2\,dx = 2\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\int_{x_0}^{\infty}\exp(-\xi^2)\,dx = 2\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\left(\frac{\hbar}{m\omega}\right)^{1/2}\int_{x_0}^{\infty}\exp(-\xi^2)\,d\xi$$

$$= \frac{2}{\sqrt{\pi}}\int_1^{\infty}\exp(-\xi^2)\,d\xi \approx \underline{\underline{0'157}}$$ ...we used $\frac{1}{2}m\omega^2x_0^2 = E_0 = \frac{1}{2}\hbar\omega \Rightarrow x_0 = \sqrt{\frac{\hbar}{m\omega}} \Rightarrow \xi_0 = 1$

So there is almost 16% probability to find a particle out-side the classicaly allowed region (classical limit is where all energy is in the "spring")

Now we will go back and take a look at some mathematical formalizm...

What are the properties of the solutions to the Schrödinger equation?

First we define the **inner product**: $\langle f | g \rangle = \int_a^b f^*(x)\, g(x)\, dx$

Than the NORM is: $|f(x)|^2 = \int_a^b f^*(x) f(x)\, dx$ ... note: usualy $a = -\infty$, $b = \infty$

Properties of INNER PRODUCT: $|a\rangle, |b\rangle$ - vectors

1) $\langle b | a \rangle = \langle a | b \rangle^*$

2) $\langle a | a \rangle \geq 0$; $\langle a | a \rangle = 0 \Leftrightarrow |a\rangle = 0$

3) $\langle a | (\beta |b\rangle + \gamma |c\rangle) = \beta \langle a | b \rangle + \gamma \langle a | c \rangle$

SCHWARZ INEQUALITY: $\left| \int_a^b f^*(x) g(x)\, dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$

Because solutions to Schrödinger should be square integrable (=normalizable) the Schwarz inequality shows that inner product of two solutions is finite!

Now... expectation value...

$\langle Q \rangle = \int \psi^* \hat{Q} \psi\, dx = \langle \psi | \hat{Q} \psi \rangle$ ... Q is result of some measurement $\Rightarrow \langle Q \rangle \in \mathbb{R}$

$\Rightarrow \langle Q \rangle = \langle Q \rangle^* \overset{\langle f|g\rangle = \langle g|f\rangle}{\Rightarrow} \langle \psi | \hat{Q} \psi \rangle = \langle \hat{Q} \psi | \psi \rangle \Rightarrow \hat{Q}$ is HERMITIAN

Now... suppose we make many measurements of identical system of some observable Q and we get allway the same result ... $\Rightarrow \sigma^2 = \langle (Q - \langle Q \rangle)^2 \rangle = 0$ (property 2) of inner prod.) $\langle Q \rangle = q$

$\langle \psi | (Q - \langle Q \rangle)^2 \psi \rangle \overset{Q \text{ Hermit}}{=} \langle (\hat{Q} - \langle Q \rangle) \psi | (\hat{Q} - \langle Q \rangle) \psi \rangle = 0 \Rightarrow \hat{Q} \psi = \langle Q \rangle \psi = q \psi$

So $\langle Q \rangle = q$ ... expectation value of Q... is EIGENVALUE OF operator $\hat{Q}$!

$|\psi\rangle$ must be such that $\hat{Q} |\psi\rangle = q |\psi\rangle$ → we get set of eigen-functions that for a basis of Hilbert space... usualy we use Hamiltonian $\hat{H}$ to get this basis ... from any basis we can construct basis for any other ... so in principle we could use any other physical operator instead of Hamiltonian... but Hamiltonian is most practical because its eigenvalue (energy E) comes handy for time-dependent equation...

PS. After 1st measurement on system of some observable the system colapses into eigen-state ⇒ all sucesive measurements will give same result ... $\sigma^2 = 0$ ...

def: HERMITIAN OPERATOR $\boxed{\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle}$

We perform a measurement on our system. What is the probability to get certain result?

$|\psi\rangle$ = generic state of system

f_n is eigenstate correspond. to q_n

$Q\ (\to \hat{Q}) \to q_n$ with probability $|c_n|^2$ such that $\boxed{c_n = \langle f_n | \psi \rangle}$

So generic state $|\psi\rangle$ can be written as superposition of eigenstates f_n !

$|\psi\rangle$ is normalized $\Longrightarrow \boxed{\sum_n |c_n|^2 = 1}$

Proof: $1 = \langle \psi | \psi \rangle = \langle (\sum_{n'} c_{n'} f_{n'}) | (\sum_n c_n f_n) \rangle = \sum_{n'} \sum_n c_{n'}^* c_n \underbrace{\langle f_{n'} | f_n \rangle} = \sum_{n'} \sum_n c_{n'}^* c_n \delta_{n'n} = \sum_n |c_n|^2$

We used the fact that eigen-functions belonging to different eigen-values are ORTHOGONAL! ...

2 eigen-functions: (f, g); $\hat{Q} f = q f$; $\hat{Q} g = q' g$ ... use Hermitian $\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle$

$\Longrightarrow q' \langle f | g \rangle = q^* \langle f | g \rangle \overset{q=q^*}{=} q \langle f | g \rangle \Longrightarrow$ if $q \neq q' \Longrightarrow \langle f | g \rangle = 0 \to$ ORTHOGONAL

Lets show again that $q^* = q$ ... so that eigen-values of Hermitian operators are real ... $\hat{Q} f = q f$ ... we know $\hat{Q}$ is Hermitian ... $\Longrightarrow \langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle$ ... now use inner prod. properties $\Longrightarrow q \langle f | f \rangle = q^* \langle f | f \rangle \Longrightarrow q = q^*$!

Ex. Check if momentum operator is Hermitian!

$$\langle f | \hat{p} g \rangle = \int_{-\infty}^{\infty} f^* \left(\frac{\hbar}{i} \frac{d}{dx} g \right) dx = \text{"per partes"} = \cancel{\frac{\hbar}{i} f^* g \Big|_{-\infty}^{\infty}}^{\,0} + \int_{-\infty}^{\infty} \left(\frac{\hbar}{i} \frac{df}{dx} \right)^* g \, dx = \langle \hat{p} f | g \rangle \checkmark \text{ok!}$$

PS: Expectation value can be written as ... $\boxed{\langle Q \rangle = \sum_n q_n |c_n|^2}$ ... because ...

$$\ldots \langle Q \rangle = \langle \psi | \hat{Q} \psi \rangle = \langle \sum_{n'} c_{n'} f_{n'} | \hat{Q} \sum_n c_n f_n \rangle = \sum_{n'} \sum_n c_{n'}^* c_n \langle f_{n'} | \hat{Q} f_n \rangle =$$

$$= \sum_{n'} \sum_n c_{n'}^* c_n q_n \delta_{n'n} = \sum_n q_n |c_n|^2 \checkmark \text{ok!}$$

($f_{n'}, f_n$ orthogonal if $n' \neq n$)

PS. Important quantities are the expectation values ... Its what we measure!

UNCERTAINTY PRINCIPLE

Two observables (operators) ... A, B ... some system in state $|\psi\rangle$ ... and we perform observation on many identicle systems ...

$$\sigma_A^2 = \langle (A-\langle A\rangle)^2\rangle = \langle \psi | (A-\langle A\rangle)^2 \psi\rangle = \langle (A-\langle A\rangle)\psi | (A-\langle A\rangle)\psi\rangle \equiv \langle f | f\rangle$$

where: $|f\rangle = (A-\langle A\rangle)|\psi\rangle$

similarly we get: $\sigma_B^2 = \langle g | g\rangle$ ... where: $|g\rangle = (B-\langle B\rangle)|\psi\rangle$

Now ... product: $\sigma_A^2 \sigma_B^2 = ?$ → we use the Schwarz inequality and get ...

$\sigma_A^2 \cdot \sigma_B^2 = \langle f|f\rangle \cdot \langle g|g\rangle \geq |\langle f|g\rangle|^2$ ... $\langle f|g\rangle$ is complex in general!

Note ... for any $z \in \mathbb{C} \rightarrow |z|^2 = Re(z)^2 + Im(z)^2 \geq (Im(z))^2 = \left[\frac{1}{2i}(z - z^*)\right]^2$

Now we use this ... so: $|\langle f|g\rangle|^2 \geq \left[\frac{1}{2i}\left(\langle f|g\rangle - \langle g|f\rangle\right)\right]^2$

We can demonstrate that: $\langle f|g\rangle - \langle g|f\rangle = \langle [\hat{A}, \hat{B}]\rangle$ (excesise at home)

Note: $\langle f|g\rangle = \langle (A-\langle A\rangle)\psi | (B-\langle B\rangle)\psi\rangle \rightarrow$ hermitian $\rightarrow = \langle \psi | (A-\langle A\rangle)(B-\langle B\rangle)\psi\rangle =$

$$= \langle \psi | (AB - A\langle B\rangle - B\langle A\rangle + \langle A\rangle\langle B\rangle)\psi\rangle =$$

$$= \langle AB\rangle - \langle B\rangle\langle A\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle = \langle AB\rangle - \langle A\rangle\langle B\rangle$$

Similarly: $\langle g|f\rangle = \ldots = \langle BA\rangle - \langle A\rangle\langle B\rangle$

So we have: $\langle f|g\rangle - \langle g|f\rangle = \langle AB\rangle - \langle BA\rangle = \langle [\hat{A}, \hat{B}]\rangle$ ✓ OK!

So ... put all together ... $\boxed{\sigma_A^2 \sigma_B^2 \geq \left[\frac{1}{2i}\langle [\hat{A}, \hat{B}]\rangle\right]^2}$ GENERAL UNCEARTINTY PRINCIPLE

System in given state → we want to measure 2 observables ... but 1ST measurement alters the system → the order in which we perform the 2 measurements is important!

For operators that commute we can change the order ... but for operators that not commute the order in which we perform the measurements on a system matters!

Ex: $\hat{A} = x$; $\hat{B} = \frac{\hbar}{i}\frac{d}{dx}$ ... position and momentum operators ...

$$\Rightarrow \sigma_x^2 \sigma_p^2 \geq \left[\frac{1}{2i}\langle [x,p]\rangle\right]^2 = \left[\frac{1}{2i} i\hbar\right]^2 \Rightarrow \sigma_x \sigma_p \geq \frac{1}{2}\hbar$$

$[x,p] = i\hbar$

Two operators that commute also have common basis of eigen-function!

We will demonstrate now that two non-commuting operators can not have a complete set of common eigen-functions...

Now... suppose that such common set exists! $|f_1\rangle, |f_2\rangle, \dots |f_n\rangle, \dots \quad |f\rangle = \sum_n c_n |f_n\rangle$

... operators $\hat{P}, \hat{Q}$ (they do not commute $\Rightarrow [\hat{P},\hat{Q}] \neq 0$)

$$\hat{P}|f_n\rangle = p_n |f_n\rangle$$

$$\hat{Q}|f_n\rangle = q_n |f_n\rangle$$

than... $\underbrace{[\hat{P},\hat{Q}]|f\rangle}_{\neq 0} = (\hat{P}\hat{Q} - \hat{Q}\hat{P}) \sum c_n |f_n\rangle = (\overbrace{p_n q_n - q_n p_n}^{=0}) \underbrace{\sum_n c_n |f_n\rangle}_{=0} = 0$ - paradox

So... for common basis to exist the operators must commute and vice-versa!

Now... how should we prepare our system to make uncertainty as small as possible in case of position and momentum operators?

MINIMUM UNCERTAINTY WAVE PACKET (refer to previous page → derivation of general uncertainty)

... 1ST we need equality in Schwarz inequality → this is true if $g(x) = a \cdot f(x)$

... 2ND we need $\mathrm{Re}\{\langle f|g\rangle\} = 0 = \mathrm{Re}\{\langle f|f\rangle \cdot a\} \Rightarrow a \in \mathbb{C} \rightarrow a = ic;\ c \in \mathbb{R}$

$$\left(\frac{\hbar}{i}\frac{d}{dx} - \langle p\rangle\right)\psi = ia(x - \langle x\rangle)\psi \Rightarrow \psi(x) = A \underbrace{\exp\left(\frac{-a(x-\langle x\rangle)^2}{2\hbar}\right)}_{\text{GAUSSIAN}} \cdot \exp\left(\frac{i\langle p\rangle x}{\hbar}\right)$$

Remember... fundamental and 1ST excited state of harmonic oscillator are Gaussian wave-pockets!

Fundamental state of H.O. $\rightarrow \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp^{-\frac{m\omega}{2\hbar}x^2} = \alpha e^{-\xi^2/2}$

$\sigma_x \cdot \sigma_p = ?\ ;\ \sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2\ ;\ \sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2$

Note... $|\psi_0(x)|^2$ is EVEN $\Rightarrow \langle x\rangle = \int x |\psi_0(x)|^2 dx = 0$

So also for $\langle p\rangle$... $\langle p\rangle = m\frac{d}{dt}\langle x\rangle = 0$

$$\langle x^2\rangle = \alpha^2 \int x^2 \exp(-\xi^2) dx = \alpha^2 \left(\frac{\hbar}{m\omega}\right)^{3/2} \int \xi^2 \exp(-\xi^2) d\xi = \dots = \frac{\hbar}{2m\omega}$$

$$\langle p^2\rangle = \int \psi_0 \left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi_0 dx = \dots = \frac{1}{2}\hbar m\omega$$

So we have... $\sigma_x \sigma_p = \left(\frac{\hbar}{2m\omega} \cdot \frac{1}{2}\hbar m\omega\right)^{1/2} = \frac{1}{2}\hbar \rightarrow$ minimum possible value!

How can we calculate rate of change of expectation value?

$$\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle\psi|\hat{Q}\psi\rangle = \left\langle\frac{\partial\psi}{\partial t}\middle|\hat{Q}\psi\right\rangle + \left\langle\psi\middle|\frac{\partial\hat{Q}}{\partial t}\psi\right\rangle + \left\langle\psi\middle|\hat{Q}\frac{\partial\psi}{\partial t}\right\rangle$$

now use Schrödinger... $i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$ ... and we get...

Ps... minus spredaj zaradi konjugiranja

$$\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\underbrace{\langle\hat{H}\psi|\hat{Q}\psi\rangle}_{=\langle\psi|\hat{H}\hat{Q}\psi\rangle} + \frac{1}{i\hbar}\langle\psi|\hat{Q}\hat{H}\psi\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle$$

... because Hermitian!

$$\boxed{\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \cancel{\left\langle\frac{\partial Q}{\partial t}\right\rangle}}$$

... PS... $\left\langle\frac{\partial Q}{\partial t}\right\rangle$ usually $= 0$! NOT ALWAYS! npr. Hamilton with time-dependent potential.

Now... remember: $\sigma_A^2\cdot\sigma_B^2 \geq \left[\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right]^2$ and insert $\hat{A}=\hat{H}$; $\hat{B}=\hat{Q}$ ... so we have

... $\sigma_H^2\sigma_Q^2 \geq \left[\frac{1}{2i}\frac{\hbar}{i}\frac{d\langle Q\rangle}{dt}\right]^2 = \left(\frac{\hbar}{2}\right)^2\left(\frac{d\langle Q\rangle}{dt}\right)^2 \Rightarrow \sigma_H\cdot\sigma_Q \geq \frac{1}{2}\hbar\left|\frac{d\langle Q\rangle}{dt}\right|$

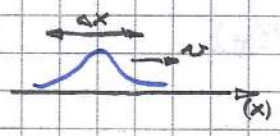
... we used previous formula here..

Denote: $\sigma_H = \Delta E$; $\Delta t = \sigma_Q \Big/ \left|\frac{d\langle Q\rangle}{dt}\right| \rightarrow \sigma_Q = \left|\frac{d\langle Q\rangle}{dt}\right|\Delta t$

So we have... $\boxed{\Delta E\cdot\Delta t \geq \frac{1}{2}\hbar}$

Ps: From relativity we might make connection from 4-vectors $\Delta x \rightarrow \Delta t$; $\Delta p \rightarrow \Delta E$ ... but this is not allowed... we are dealing with non-relativistic theory ... because when deriving Schrödinger eq. we assumed $E = p^2/2m \rightarrow$ non-relativistic case...

Ex: How much time does a free-particle wave-packet to pass a given point?



$\rightarrow$ aprox: $\Delta t = \frac{\Delta x}{v} = \frac{m\Delta x}{p}$

$\rightarrow$ energy is... $E = p^2/2m \Rightarrow \Delta E = \frac{p\Delta p}{m}$ from... $\frac{dE}{dp} = p/m$; $dE\rightarrow\Delta E$; $dp\rightarrow\Delta p$

So we have: $\Delta t\Delta E = \frac{m\Delta x}{p}\cdot\frac{p\Delta p}{m} = \Delta x\Delta p \geq \frac{1}{2}\hbar$

Lets go back to... $\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \cancel{\left\langle\frac{\partial Q}{\partial t}\right\rangle}$ $\rightarrow$ time independent!

Ex 1) $\hat{Q} = \hat{I}$ (identity)

$[\hat{H},\hat{I}] = 0$

$\frac{d}{dt}\langle I\rangle = \frac{d}{dt}\langle\psi|\psi\rangle = 0$ ~ like perservation of normalization!

Ex 2) $\hat{Q} = \hat{H} \Rightarrow [\hat{H},\hat{H}] = 0 \Rightarrow \frac{d}{dt}\langle\hat{H}\rangle = 0$ ~ conservation of energy!

Ex 3) $\hat{Q} = \hat{x}$; we need $[\hat{H},\hat{x}]$

$[\hat{x},\hat{H}] = \left[\hat{x},\frac{1}{2m}p^2 + v(x)\right]$ ... note $[\hat{x},v(x)] = 0 \rightarrow$ if $v(x)$ depends only on $x \Rightarrow 0$

$[\hat{x},\hat{p}^2] = \hat{x}\hat{p}^2 - \hat{p}^2\hat{x} = \hat{x}\hat{p}^2 - \hat{p}\hat{x}\hat{p} + \hat{p}\hat{x}\hat{p} - \hat{p}^2\hat{x} = [\hat{x},\hat{p}]\hat{p} + \hat{p}[\hat{x},\hat{p}] =$

$= i\hbar\hat{p} + \hat{p}i\hbar = 2i\hbar\hat{p}$ ... so we have: $[\hat{H},\hat{x}] = -\frac{i\hbar}{m}\hat{p} \Rightarrow \boxed{\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle}$

Ex 4) $\hat{Q} = \hat{p}$ $\qquad [\hat{p}^2, \hat{p}] = 0$

$$[\hat{H}, \hat{p}] = \left[\frac{1}{2m}\hat{p}^2 + v(x), \hat{p}\right] = [v(x), \hat{p}]$$

In general: $[\hat{f}(x), \hat{p}]\, g(x) = \left(\hat{f}(x)\frac{\hbar}{i}\frac{d}{dx}g(x) - \frac{\hbar}{i}\frac{d}{dx}\left(\hat{f}(x)g(x)\right)\right) =$

$$= \cancel{\hat{f}\frac{\hbar}{i}\frac{d}{dx}g} - \cancel{\frac{\hbar}{i}\hat{f}\frac{d}{dx}g} - \frac{\hbar}{i}g\frac{d}{dx}\hat{f} = i\hbar\frac{d\hat{f}(x)}{dx}g(x)$$

So we have: $[\hat{f}(x), \hat{p}] = i\hbar\frac{d}{dx}\hat{f}(x)$ → now we use this in Ex 4) ...

$$\Rightarrow [\hat{H}, \hat{p}] = [v(x), \hat{p}] = i\hbar\frac{dv(x)}{dx} \Rightarrow \frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\left(i\hbar\frac{\langle dv(x)\rangle}{dt}\right) \ldots$$

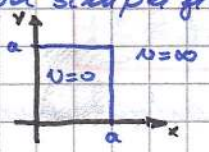
Finally → $\boxed{\frac{d}{dt}\langle p\rangle = -\frac{\langle dv(x)\rangle}{dt}}$ EHERFEST THEOREM ~ Newton law

3-D TIME INDEPENDENT SCHRÖDINGER EQ.

$$\boxed{\nabla^2\psi(\vec{r}) = \frac{2M}{\hbar^2}\left[U(\vec{r}) - E\right]\psi(\vec{r})}$$ ... remember: $\nabla^2 = \left(\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2}, \frac{\partial^2}{\partial z^2}\right)$

Lets go step by step ... first we will focus on simplified 2D case ...

2D: $v(x,y) = \begin{cases} 0; & 0 \le x \le a \text{ and } 0 \le y \le a \\ \infty; & \text{else} \end{cases}$



Schrödinger: $\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = -\frac{2M}{\hbar^2}E\psi$ ... FOR INSIDE THE SQUARE (OUTSIDE $\psi = 0$)

we seperate the variables ... $\psi(x,y) = X(x)Y(y)$ ... any other solution can be written as a sum of such solutions (look Mafia I!)

Insert seperation $\Rightarrow Y(y)X''(x) + X(x)Y''(y) = -\frac{2M}{\hbar^2}EX(x)Y(y)$

$$\Rightarrow \underbrace{\frac{1}{X}\frac{d^2X}{dx^2}}_{\text{const.}} + \underbrace{\frac{1}{Y}\frac{d^2Y}{dy^2}}_{\text{const.}} = -\frac{2ME}{\hbar^2}$$ ... each must equal a constant!

So we have: $\frac{1}{X}\frac{d^2X}{dx^2} = \text{const.} = -k_x^2 \Rightarrow X'' = -k_x^2 X \rightarrow k_x = \frac{n_x\pi}{a}$

... and for y: $\frac{1}{Y}\frac{d^2Y}{dy^2} = -k_y^2 \Rightarrow k_y = \frac{n_y\pi}{a}$

Solutions are: $X(x) = B\sin\left(\frac{n_x\pi}{a}\cdot x\right)$; $Y(y) = C\sin\left(\frac{n_y\pi}{a}\cdot y\right)$

Wave function → $\psi(x,y) = A\sin\left(\frac{n_x\pi}{a}\cdot x\right)\cdot\sin\left(\frac{n_y\pi}{a}\cdot y\right) \rightarrow \psi_{n_x,n_y}$

To get A we use normalization → $\int|\psi(x,y)|^2\,dx\,dy = 1 \Rightarrow$ get A

How ... energy → $\frac{n_x^2\pi^2}{a^2} + \frac{n_y^2\pi^2}{a^2} = \frac{2ME}{\hbar^2} \Longrightarrow E = E_{n_x,n_y} = \frac{\hbar^2\pi^2}{2Ma^2}(n_x^2 + n_y^2)$

Here we can observe DEGENERACY = 2 states have equal energy!

concept of degeneracy will be important later ...

npr. $n_x = 1$, $n_y = 2$ $\qquad$ $n_x = 2$, $n_y = 1$

$$\psi_{1,2} \neq \psi_{2,1}$$
$$E_{1,2} = E_{2,1}$$

CENTRAL FORCE: Depends only on distance from some point (centre)...

↳ central potential → $U(x,y,z) = U(r) \Rightarrow$ use Spherical coords!

Lets first study simplyfied problem: PARTICLE in 2D MOVING UNDER ACTION OF CENTRAL FOR.

We need Laplacian in Polar coords: $\nabla^2 \to \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}$

So... Schrödinger: $\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right]\psi(r,\phi) = \frac{2M}{\hbar^2}\left[U(r) - E\right]\psi(r,\phi)$

Seperation of variables: $\psi(r,\phi) = R(r)\,\Phi(\phi)$ → general ψ is a sum of this

So... $\Phi(\phi)\left[R''(r) + \frac{1}{r}R'(r)\right] + \frac{1}{r^2}R(r)\,\Phi''(\phi) = \frac{2M}{\hbar^2}\left[U(r) - E\right]R(r)\,\Phi(\phi)$

... algebra... $\underbrace{\frac{\Phi''(\phi)}{\Phi(\phi)}}_{\text{no } r \text{ dependence}} = \underbrace{\frac{-r^2R''(r) + rR'(r)}{R(r)} + \frac{2Mr^2}{\hbar^2}\left[U(r) - E\right]}_{\text{no } \phi \text{ dependence}} = -m^2$ → each side must = constant.

Angular part: $\Phi''(\phi) = -m^2\Phi(\phi) \Longrightarrow \Phi(\phi) = e^{im\phi}$

(something Quantized)

We have "geometrical" boundery con.: $\Phi(\phi) = \Phi(\phi + 2\pi) \Longrightarrow \boxed{m \in \mathbb{Z}}$ (INTEGER)

→ we fix r: $\psi(r,\phi) \sim e^{im\phi} = e^{i\left(\frac{m}{r}\right)s} \longrightarrow p = \hbar\frac{m}{r} \Longrightarrow pr = m\hbar$ ~ ANGULAR MOMENTUM

Note: e^{ikx} → represents particle with $p = \hbar k$

So fact that $m \in \mathbb{Z}$ means that Angular momentum is quantized!

Next: PARTICLE in 3D UNDER ACTION OF CENTRAL FORCE

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2\sin\Theta}\frac{\partial}{\partial\Theta}\left(\sin\Theta\frac{\partial\psi}{\partial\Theta}\right) + \frac{1}{r^2\sin^2\Theta}\frac{\partial^2\psi}{\partial\phi^2} = \frac{2M}{\hbar^2}\left[U(r) - E\right]\psi$$

We use ansatz: $\psi(r,\Theta,\phi) = R(r)\cdot\Theta(\Theta)\cdot\Phi(\phi)$

after some aglebra we get... $\frac{\Phi''}{\Phi} = (\text{function of } r \text{ and } \Theta) \Longrightarrow \Phi''(\phi) = -m^2\Phi(\phi)$

next we get something like... $(\text{func. of } \Theta) = (\text{func. of } r) = -k$

Then we get this equations: $\frac{1}{\sin\Theta}\frac{d}{d\Theta}\left(\sin\Theta\frac{d\Theta}{d\Theta}\right) + \left(k - \frac{m^2}{\sin^2\Theta}\right)\Theta = 0$ → LEGENDRA

note: independent of the potential U

$$\frac{d^2}{dr^2}(rR) = \frac{2M}{\hbar^2}\left[U(r) + \frac{k\hbar^2}{2Mr^2} - E\right](rR)$$

⇓

Solution for Φ and Θ its general for central force potential!

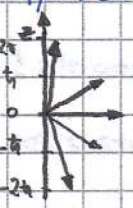
$\Phi'' = -m^2\Phi \Longrightarrow \boxed{L_z = m\hbar}$ ~ z part of angular momentum is quantized

LEGENDRA → physicaly acceptable solutions $\boxed{k = l(l+1);\ l \geq |m|}$

So: $\psi(r,\Theta,\phi) = R(r)\,\Theta_{l,m}(\Theta)\cdot e^{im\phi}$

PS: Also Total Angular Momentum is quantized → $\boxed{L = \sqrt{l(l+1)}\,\hbar}$

Npr: what are allowed L_z if total angular momentum has $l=2$!



... but because $[L_i, L_j] \neq 0$ if $i \neq j$ we have cone ...

$\vec{L}$ is anywhere on this cone

Ps. in Chemistry most important are $l=0$ and $l=1$ case ...

- Lets take a look at the simplest case ... $l=0;\ m=0$

... than the Legendra eq. $\longrightarrow \frac{d}{d\Theta}\left(\sin\Theta \frac{d\Theta}{d\Theta}\right) = 0 \implies \Theta(\Theta) = \text{const.}$

... so in this simply case our wave function is $\psi(r,\Theta,\phi) = R(r)\cdot \text{const.}$

- Now we make things slightly more complicated ... $l=1;\ m=0$

... Legendra eq. for $\Theta \longrightarrow \frac{1}{\sin\Theta}\frac{d}{d\Theta}\left(\sin\Theta\frac{d\Theta}{d\Theta}\right) + 2\Theta = 0$

... we can find that the solution for this is: $\Theta(\Theta) = A\cdot\cos\Theta$

... and so our wave-function has form: $\psi(r,\Theta,\phi) = A\,R(r)\cdot\cos\Theta$

This means that probability $|\psi|^2 \sim \cos^2\Theta \rightarrow$ highest on z-axis; zero in x-y plane

P.S.: $\boxed{\Theta_{lm}(\Theta)\, e^{im\phi} = Y_{lm}(\Theta,\phi)}$ $\rightarrow$ SPHERICAL HARMONICS

ASSOCIATED LEGENDRA FUNCTION

Until now we made general derivation for central potential ...

SCHRÖDINGER FOR 3-D CENTRAL POTENTIAL IN SPHERICAL COORDS:

Ansatz $\longrightarrow \psi(r,\Theta,\phi) = R(r)\,\Theta(\Theta)\,\Phi(\phi)$

$$\begin{cases} \Phi'' = -m^2\Phi & \implies \Phi(\phi) = e^{-im\phi};\ m = 0, \pm 1, \pm 2 \ldots \\ \frac{1}{\sin\Theta}\frac{d}{d\Theta}\left(\sin\Theta\frac{d\Theta}{d\Theta}\right) + \left(k - \frac{m^2}{\sin^2\Theta}\right)\Theta = 0 & \implies \text{LEGENDRA: } \Theta_{lm}(\Theta);\ k = l(l+1);\ l \geq |m| \\ \frac{d^2}{dr^2}(rR) = \frac{2M}{\hbar^2}\left[U(r) + \frac{k\hbar^2}{2Mr^2} - E\right](rR) & \end{cases}$$

we got 2 quantum numbers (l and m)

SPHERICAL HARMONICS: $Y_{lm}(\Theta,\phi) = \Theta_{lm}\, e^{im\phi}$

Spherical harmonics are eigen-functions for angular operators!

$L_z = m\hbar$; $L^2 = l(l+1)\hbar^2 \rightarrow$ They commute: $[L_z, L^2] = 0$

This will be demonstrated later!

Note: Only the radial equation is energy dependent! (and potential dependent)

Thats why the angular part is general $\implies$ spherical harmonics ...

Now we focus on radial equation for Hydrogen atom case...

$$\frac{d^2}{dr^2}(rR) = \frac{2M}{\hbar^2}\left[V(r) + \frac{l(l+1)\hbar^2}{2Mr^2} - E\right](rR)$$

We can see that radial eq. depends only on quantum number l, but not on m $\Rightarrow$ we expect some degeneracy (= different states with the same energy) $\Rightarrow$ there will be $(2l+1)$ degenerate states! $\rightarrow$ Because at fixed $l \rightarrow m \in \{-l, -(l-1), \dots, -1, 0, 1, \dots, (l-1), l\} \rightarrow 2l+1$ elements...

For Hydrogen: $\boxed{\frac{d^2}{dr^2}(rR) = \frac{2M}{\hbar^2}\left[\underbrace{-\frac{ke^2}{r}}_{\text{potential}} + \frac{l(l+1)\hbar^2}{2\underbrace{M}_{\text{mass of electron}}r^2} - E\right](rR)}$

Solving this eq. analytically (Mafia II) we get eq. for energy and $R(r)$:

$$E = E_r \cdot \frac{1}{n^2} \; ; \; n \in \mathbb{N} \; ; \; n > l \; ; \; E_r = -\frac{M(ke)^2}{2\hbar^2} \rightarrow \text{RYDBERG ENERGY}$$

$\hookrightarrow$ we got another quantum number $\Rightarrow$ $\boxed{(n, l, m)}$ determine state

npr.- ground state $\rightarrow (n=1, l=0, m=0)$ ... no degeneracy here

- 1st excited state $\rightarrow \left(n=2, l=\begin{cases} 0 \; ; \; m=0 \\ 1 \; ; \; m=-1,0,1 \end{cases}\right)$ ... degenerate states (4 states)

PS: in special case of Hydrogen atom the energy does not depend on quantum number l $\Rightarrow$ there are more than $(2l+1)$ degenerate states..

For Hydrogen atom there are n^2 DEGENERATE STATES ... this can be demonstraded by induction... (① True for $n=1$; ② Assume $n=N$; $1+3+\dots+(2N-1)=N^2$; ③ $N \rightarrow N+1$)

PS: Qemistry $\rightarrow$ ground state = 1s ; 1st state = 2s or 2p ... ($l=0 \rightarrow s$; $l=1 \rightarrow p$; $l=2 \rightarrow d$ ...)

Ex: Ground state $\rightarrow$ 1s or $(n=1, l=0, m=0)$

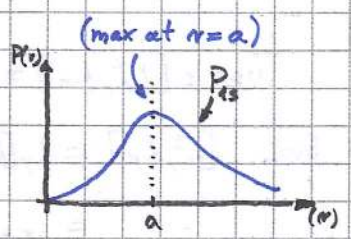
$\rightarrow$ RADIAL EQ: $\frac{d^2}{dr^2}(rR) = \frac{2M}{\hbar^2}\left[-\frac{ke^2}{r} - E_r\right](rR) \Rightarrow R_{1s}(r) = A\,e^{-r/a}$; $a = \frac{\hbar^2}{Mke^2} \rightarrow$ BOHR RADIUS

Because $l=0, m=0$ there is no angular dependence $\Rightarrow$ spherically symetric!

What is probability to find e^- between r and $r+dr$?

$|\psi|^2 dV$; $dV = 4\pi r^2 dr \rightarrow |\psi|^2 dV = P(r)dr$

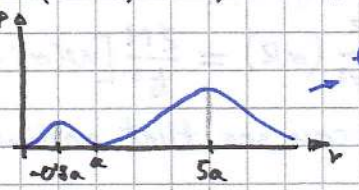
$P(r) = 4\pi r^2 |R(r)|^2 \Rightarrow P_{1s}(r) = 4\pi r^2 A^2 e^{-2r/a} \rightarrow$



Ex: First excited state → we have 4 states → consider $(n=2, l=0, m=0) = 2s$

RADIAL EQUATION $\Longrightarrow$ $R_{2s}(r) = A\left(2 - \frac{r}{a}\right) e^{-r/2a}$

$P_{2s}(r) = 4\pi r^2 |R_{2s}(r)|^2 = \dots$



→ two peaks

First excited state $(n=2, l=1, m=0)$

RADIAL EQUATION $\Longrightarrow$ $(R_{2p})_{m=0} = A r e^{-r/2a}$

WAVE FUNCTION → $\psi(r, \theta, \phi) = A r e^{-r/2a} \cdot \cos\theta$ $\quad z = r\cos\theta$

Note: wave function can be written as: $\psi = A e^{-r/2a} \cdot z$ ... but z-coord. is NOT special $\Longrightarrow$ we guess other 2 solutions $\psi_x = A e^{-r/2a} \cdot x$ and $\psi_y = A e^{-r/2a} \cdot y$

Now... PROBABILITY: $P_{2p}(r) = 4\pi r^2 |R_{2p}(r)|^2 = 4\pi A^2 r^4 e^{-r/2a}$ (peak at $\sim 4a$)

PS: ψ_x, ψ_y DO NOT CORRESPOND TO $m = \pm 1$, BUT ARE LINEAR COMBINATIONS OF THIS!

Now we go back to angular momentum...

CLASSICAL → $\vec{L} = \vec{r} \times \vec{p}$; $L_x = y p_z - z p_y$, $L_y = z p_x - x p_z$, $L_z = x p_y - y p_x$

To go to quantum case we must replace with operators!

Look at comutator → $[L_x, L_y] = [y p_z - z p_y, z p_x - x p_z]$

$$[L_x, L_y] = \underbrace{[y p_z, z p_x]}_{= y p_x [p_z, z]} - \underbrace{[y p_z, x p_z]}_{=0} - \underbrace{[z p_y, z p_x]}_{=0} + \underbrace{[z p_y, x p_z]}_{= x p_y [z, p_z]}$$

$\Longrightarrow [L_x, L_y] = y p_x [p_z, z] + x p_y [z, p_z] = y p_x (-i\hbar) + x p_y (i\hbar)$

$[L_x, L_y] = i\hbar (x p_y - y p_x) = i\hbar L_z$

By similar reasoning we get ... $\boxed{[L_x, L_y] = i\hbar L_z ; [L_y, L_z] = i\hbar L_x ; [L_z, L_x] = i\hbar L_y}$

Now:
$$[L^2, L_x] = \underbrace{[L_x^2, L_x]}_{=0} + [L_y^2, L_x] + [L_z^2, L_x]$$

use: $[L_y^2, L_x] = L_y L_y L_x - L_x L_y L_y - L_y L_x L_y + L_y L_x L_y = L_y [L_y, L_x] + [L_y, L_x] L_y$

So... $[L^2, L_x] = L_y [L_y, L_x] + [L_y, L_x] L_y + L_z [L_z, L_x] + [L_z, L_x] L_z =$

$= \dots = 0$ → they commute

$$\boxed{[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0}$$

$\Longrightarrow$ we can determine the total angular momentum and opr. z-component ... $L^2 f = \lambda f$

$L_z f = \mu f$

DEFINE : $\boxed{L_\pm = L_x \pm i L_y}$ LADDER OPERATORS

COMMUTATORS : $[L_z, L_\pm] = [L_z, L_x] \pm i [L_z, L_y] = i\hbar L_y \pm i(-i\hbar L_x) = \pm\hbar (L_x \pm i L_y)$

So $\rightarrow$ $\boxed{[L_z, L_\pm] = \pm\hbar L_\pm}$

Note $\rightarrow$ $\boxed{[L^2, L_\pm] = 0}$

Theorem: If f is an eigen-state of L^2 and L_z, so is also $(L_\pm f)$!

Proof : $L^2(L_\pm f) = L_\pm(L^2 f) = L_\pm(\lambda f) = \underbrace{\lambda(L_\pm f)}$ ✓OK! $\rightarrow$ same eigen-value for L^2!

$L_z(L_\pm f) = (L_z L_\pm - L_\pm L_z) f + L_\pm L_z f = \pm\hbar L_\pm f + L_\pm(\mu f) =$

$= \underbrace{(\mu \pm \hbar)(L_\pm f)}$ ✓OK! $\rightarrow$ new eigen-value for L_z !

So $L_\pm$ moves us up/down the possible L_z states...

Like in case of ladder operators of harmonic oscillator there should be minimum state (here also maximum state)... remember that L_z is component of L.

TOP STATE :

$L_+ f_T = 0$ ... Let $\hbar l$ be the eigen-value of L_z at this top rung

$L_z f_T = \hbar l f_T$; $L^2 f_T = \lambda f_T$

Look $\rightarrow$ $L_\pm L_\mp = (L_x \pm i L_y)(L_x \mp i L_y) = L_x^2 + L_y^2 \mp i(L_x L_y - L_y L_x) = \underbrace{L^2 - L_z^2}_{L_x^2 + L_y^2} \mp i(i\hbar L_z)$

So we can write : $\boxed{L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z}$

So $\rightarrow$ $L^2 f_T = (L_- L_+ + L_z^2 + \hbar L_z) f_T = (0 + \hbar^2 l^2 + \hbar^2 l) f_T$

$L^2 f_T = \hbar^2 l(l+1) f_T = \lambda f_T \implies \lambda = l(l+1)\hbar^2$

BOTTOM STATE :

$L_- f_B = 0$ ... Let $\hbar \bar{l}$ be eigen-value of L_z at this bottom rung

$L_z f_B = \hbar \bar{l} f_B$; $L^2 f_B = \lambda f_B$

Same as before $\rightarrow$ $L^2 f_B = (L_+ L_- + L_z^2 - \hbar L_z) f_B = (0 + \hbar^2 \bar{l}^2 - \hbar^2 \bar{l}) f_B$

$\implies L^2 f_B = \hbar^2 \bar{l}(\bar{l} - 1) f_B = \lambda f_B \implies \lambda = \bar{l}(\bar{l}-1)\hbar^2$

So we have $\rightarrow$ $l(l+1) = \bar{l}(\bar{l}-1)$ $\rightarrow$ $\cancel{\bar{l} = l+1}$ $\rightarrow$ not possible

$\rightarrow$ $\bar{l} = -l$

This tels us that applying Ladder operators we are moving : $-l, \ldots, l$

$l = -l + N \implies l = N/2$ $\longrightarrow$ ps.-orbital angular momentum has integer - half-integer is spin

bottom ladder applied N times (integer)

(Total Angular momentum) = (orbital part) $\oplus$ (spining part) $\vec{J} = \vec{L} + \vec{S}$

CLASSICALY: $\vec{J} = \vec{L} + \vec{S}$; $\underbrace{\vec{L} = \vec{r} \times \vec{p}}_{\text{in Q.M. takes integer values}}$; $\underbrace{\vec{S} = I\vec{\omega}}_{\text{in QM is } 1/2 \text{ (for } e^-, p^+)}$

SPIN:

$$\boxed{\begin{aligned} [S_x, S_y] &= i\hbar S_z \\ [S_y, S_z] &= i\hbar S_x \\ [S_z, S_x] &= i\hbar S_y \end{aligned}}$$

$$\boxed{\begin{aligned} S^2 |sm\rangle &= \hbar^2 s(s+1) |sm\rangle \\ S_z |sm\rangle &= \hbar m |sm\rangle \end{aligned}}$$

quantum number m is NOT same as previous pages

We will take more detailed look for spin $s = 1/2$ → for electrons, protons...

Possible states are: $|s = 1/2, m = 1/2\rangle$ → SPIN UP: $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$|s = 1/2, m = -1/2\rangle$ → SPIN DOWN: $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

So if you have some state $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$ → linear comb. of UP and DOWN!

We want to find representations for S^2 and S_z...

$$\begin{aligned} S^2 |s\,m\rangle &= \hbar^2 s(s+1) |s\,m\rangle \\ S_z |s\,m\rangle &= \hbar m |s\,m\rangle \end{aligned} \xrightarrow{s=1/2} \begin{cases} S^2 \chi_+ = \frac{3}{4}\hbar^2 \chi_+ \\ S^2 \chi_- = \frac{3}{4}\hbar^2 \chi_- \end{cases}$$

We can assume a matrix representation for S^2 → $S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$

So... $\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\boxed{S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

Now similar for S_z ... assume $S_z = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$

$S_z \chi_+ = \frac{1}{2}\hbar \chi_+$

$S_z \chi_- = \frac{1}{2}\hbar \chi_-$

$$\boxed{S_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

What about for S_x, S_y?

$S_+ \chi_- = \hbar \chi_+ \implies S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ RAISING OPERATOR

$S_- \chi_+ = \hbar \chi_- \implies S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ LOWERING OPERATOR

This are only for spin $1/2$!

$S_\pm = S_x \pm i S_y$

$$\boxed{\begin{aligned} S_x &= \frac{1}{2}(S_+ + S_-) = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y &= \frac{1}{2i}(S_+ - S_-) = \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{aligned}}$$

PS: We should check is this operators are Hermitian!

REMEMBER: Matrix oper. are Hermitian if $M \cdot (M^*)^T = I$ → identity matrix

You can easily check that $S_x, S_y, S_+, S_-, \ldots$ are HERMITIAN ⇒ "observable"

Suppose we have particle with state $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$ and we measure the z-component ... there are 2 possible outcomes → $+\frac{1}{2}\hbar$; $-\frac{1}{2}\hbar$!

Probabilities: $|a|^2 = (\text{probability to get } +\frac{1}{2}\hbar)$

$|b|^2 = (\text{probability to get } -\frac{1}{2}\hbar)$

Now ... what about if we measure x- or y-component?

$$S_x = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rightarrow S_x \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$= \frac{1}{2}\hbar \begin{pmatrix} \beta \\ \alpha \end{pmatrix}$$

so → $\alpha = \beta$ ... and must be $\alpha^2 + \beta^2 = 1 \Rightarrow \alpha = \beta = 1/\sqrt{2}$

So we get ... $\chi_+^{(x)} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \cdot \frac{\hbar}{2}$

$\chi_-^{(x)} = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \cdot -\frac{\hbar}{2}$

→ Like UP/DOWN but in x-direction ...

And we can write ...

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = \delta\chi_+^{(x)} + \varepsilon\chi_-^{(x)} = \left(\frac{a+b}{\sqrt{2}}\right)\chi_+^{(x)} + \left(\frac{a-b}{\sqrt{2}}\right)\chi_-^{(x)}$$

So to measure $\chi_+^{(x)}$ state (x-direction of spin) is $\left(\frac{a+b}{\sqrt{2}}\right)^2$, and for ...

Now we want to know how to sum angular momentum of 2 particles ...

Suppose we have 2 particles with spin $s = \frac{1}{2}$ (upr. e^- and p^+ in Hydrogen atom) ...

⇒ we have 4 possible states: ↑↑ ↓↓ ↓↑ ↑↓

Lets define total angular spin momentum as a sum: $\vec{S} = \vec{S}_1 + \vec{S}_2$

But ... what is the total spin angular momentum of the system?

... we have to find eigen-values / eigen-states ... $S_z \chi_1 \chi_2 = \kappa \chi_1 \chi_2$

$$S_z \chi_1 \chi_2 = (S_1^{(z)} + S_2^{(z)})\chi_1\chi_2 = (S_1^{(z)}\chi_1)\chi_2 + \chi_1(S_2^{(z)}\chi_2) = \hbar(m_1 + m_2)\chi_1\chi_2$$

operator $S_1^{(z)}$ acts only on χ_1, but not on χ_2 and vice-versa

So we have that the 4 possible states ... ↑↑ = 1 ; ↓↓ = −1 ; ↓↑ = 0 ; ↑↓ = 0 ...

... But we have the problem of 2 states with total spin zero ...

Lets do this ... $S_- \uparrow\uparrow = (S_-^{(1)} + S_-^{(2)})\uparrow\uparrow = \hbar(\downarrow\uparrow + \uparrow\downarrow)$

In reality we have 3 states ...

$$\begin{cases} |1,1\rangle = \uparrow\uparrow \\ |1,0\rangle = \frac{1}{\sqrt{2}}(\downarrow\uparrow + \uparrow\downarrow) \\ |1,-1\rangle = \downarrow\downarrow \end{cases}$$

... ⊕ 1 more!

$|0,0\rangle = \frac{1}{\sqrt{2}}(\downarrow\uparrow - \uparrow\downarrow)$

$s = 1$, $m = 1, 0, -1$

PS: TRIPLET is symetric if you change particles! →

TRIPLET STATE

PS: Not symetric →

SINGLET STATE

$s = 0$, $m = 0$

How can we notice that the particle has spin?

Lets start with orbital angular momentum...

torque $\rightarrow \vec{M} = \vec{\mu} \times \vec{B}$; $\vec{B}$ = external B-field ; $\vec{\mu} = i\vec{A}$ = magnetic moment (i → current, $\vec{A}$ → area)

Like in electro-dynamics lets take a look at energy of the system...

$$dW = -\Gamma d\Theta \Rightarrow W = -\int \Gamma d\Theta = -\int \mu B \sin\Theta d\Theta = \mu B \cos\Theta + const.$$ = work done by B-field

Energy $\rightarrow U = -W = -\mu B \cos\Theta = -\vec{\mu}\cdot\vec{B}$ → MINIMUM when $\vec{\mu}, \vec{B}$ are aligned!

Lets find the connection between angular momentum L and the magnetic moment μ... consider e^- circulating around nucleus p^+...

$i = e/T = ev/2\pi r$ → "current" ; $\mu = iA = \frac{1}{2} ev r$

now we use $L = m_e v r$ ... so we have $\mu/L = e/2m_e \Rightarrow \boxed{\vec{\mu} = \frac{-e}{2m_e}\vec{L}}$ (e^- has negative charge)

PS: This is due to orbital angular momentum, spin is neglected for the moment.

ZEEMAN EFFECT → because of mag. moment in external B-field...

Lets first consider Helium atom with electron in SINGLET STATE ... so that the spin contribution to mag. moment is zero... ($S = 0$)

If no external $\vec{B}$-field is present → $\vec{B} = 0$

↳ we have $l = 2$ → possible $m = 0, \pm 1, \pm 2 \Rightarrow$ 5 degenerate state $\sim (2l+1)$

How we switch $\vec{B}$-field on → $\vec{B} \neq 0$

↳ energy level from before → E_0, will split into 5 levels...

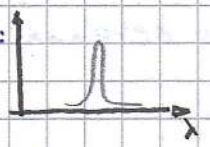
$$\Delta E = -\vec{\mu}\cdot\vec{B} = \left(\frac{e}{2m_e}\right)\vec{L}\cdot\vec{B}$$ ...let $\vec{B} = B\vec{k}$ ...

so $\Delta E = \left[\frac{e\hbar}{2m_e}\right] m B$ → here $\left[\frac{e\hbar}{2m_e}\right]$ → BOHR MAGNETON = μ_B

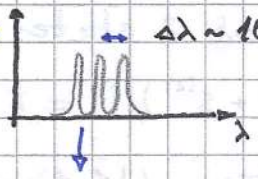
For feeling... the seperation of levels is of order $\sim 10^{-5}$ eV

Ex → we perform experiment...

$\vec{B} = 0$: $l=1; m=0,\pm1$ E_1 ↓ ~ 21 eV E_0

spectrum: 

$\vec{B} \neq 0$: $l=1$, $m=1$, $m=0$, $m=-1$, E_0

spectrum:  $\Delta\lambda \sim 10^{-4}$ nm

P.S.: Usefull for measuring B-field in astronomy!

Lets take into account the spin ... $\vec{\mu} \propto \vec{S}$; $\vec{\mu}_{SPIN} = \gamma \vec{S}$

This law is "guessed" and tested experimentaly ... and we get → $\boxed{\vec{\mu}_{SPIN} = -\frac{e}{m_e}\vec{S}}$

So the total magnetic moment is → $\boxed{\vec{\mu} = \vec{\mu}_{ORB} + \vec{\mu}_{SPIN} = -\frac{e}{2m_e}(\vec{L} + 2\vec{S})}$

ANOMALUS ZEEMAN EFFECT

Lets consider Hydrogen atom with $l=0$ ⇒ no angular momentum ...

so we have only spin contribution ... $\vec{\mu} = \vec{\mu}_{SPIN} = -\frac{e}{m_e}\vec{S}$

$\vec{B} \neq 0$ ⇒ energy $= -\vec{\mu}_{SPIN} \cdot \vec{B}$

BOHR MAGNETON

remember $\vec{B} = B\vec{k}$; $S_z = \pm\frac{1}{2}$ ⇒ $\Delta E = 2\frac{e\hbar}{2m_e} \cdot B = 2\mu_B B$

PAULI EXCLUSION PRINCIPLE → no two electrons can occupy the same quantum state

mpr. Helium E_0 ↑↑ → not possible E_0 ↑↓ OK! ✓

Suppose we have two identical particles that can not be distinguished ...

Wave function → $|\psi(1,2)|^2 = |\psi(2,1)|^2$ ⇒ we can not see the difference if we exchange the particles ... $\psi(1,2) = k\,\psi(2,1) = \pm\psi(2,1)$ ($k = \pm 1$)

If we choose ⊕ ⇒ BOSONS (spin integer) → symetric wave function

If we choose ⊖ ⇒ FERMIONS (spin = half integer) → anti-symetric wave function

→ from here the Pauli Exclusion Principle comes from ...

Ex... suppose we have 2 electrons ... initialy very far apart → one e^- → $\phi(1)$; one e^- → $\chi(2)$

How to combine the wave function when they come close?

$\psi(1,2) \neq \phi(1)\chi(2)$ → NO! ... like this would be distinguishable

$\psi(1,2) = \phi(1)\chi(2) - \chi(1)\phi(2)$ → OK! ✓

In H atom ... suppose e^- are in same state ⇒ $1=2$ ⇒ $\psi = 0$ → not normal. ⇒ not possible

Note : $\psi(1,2) = \phi(1)\chi(2) - \chi(1)\phi(2)$ → FERMIONS ($1=2$ not possible)

$\psi(1,2) = \phi(1)\chi(2) + \chi(1)\phi(2)$ → BOSONS ($1=2$ is possible)

Ex: Suppose we have 2 particles (in 1-D), one in state $\psi_a(x)$ and other in state $\psi_b(x)$ and suppose that both wave-functions are normalized and orthogonal! If particles can be distinguished (like classical case)

1) $\rightarrow \psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$ (DISTINGUISHABLE)

But if the 2 particles can not be distinguished between...

2.) $\rightarrow \psi_+(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1)\right]$ (SYMETRIC NON-DISTINGUISHABLE)

3.) $\rightarrow \psi_-(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_a(x_1)\psi_b(x_2) - \psi_a(x_2)\psi_b(x_1)\right]$ (ANTI-SYMETRIC NOT-DISTINGUISHABLE)

Lets calculate expectation value $\langle (x_2 - x_1)^2 \rangle$ for all 3 cases!

1.) $|\psi(x_1, x_2)|^2 = (\psi_a(x_1)\psi_b(x_2))(\psi_a^*(x_1)\psi_b^*(x_2)) = |\psi_a(x_1)|^2 |\psi_b(x_2)|^2$

$\Rightarrow \langle x_1^2 \rangle = \int x_1 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_a$

$\Rightarrow \langle x_2^2 \rangle = \int |\psi_a(x_1)|^2 dx_1 \int x_2 |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_b$

$\Rightarrow \langle x_1 x_2 \rangle = \int x_1 |\psi_a(x_1)|^2 dx_1 \int x_2 |\psi_b(x_2)|^2 dx_2 = \langle x \rangle_a \langle x \rangle_b$

So $\rightarrow \langle (x_2 - x_1)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b$

2.) & 3.) $|\psi_\pm(x_1, x_2)|^2 = \frac{1}{2}\left[\psi_a(x_1)\psi_b(x_2) \pm \psi_b(x_1)\psi_a(x_2)\right] \cdot \left[\psi_a^*(x_1)\psi_b^*(x_2) \pm \psi_b^*(x_1)\psi_a^*(x_2)\right]$

...after some computation we get following result...

$$\langle (x_2 - x_1)^2 \rangle_\pm = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x_b \rangle \underbrace{\mp 2 |\langle x \rangle_{ab}|^2}_{\text{we got additional term}}$$

where $\rightarrow \langle x \rangle_{ab} = \int x \psi_a^*(x) \psi_b(x) dx$

We can write: $\boxed{\langle (\Delta x)^2 \rangle_\pm = \langle (\Delta x)^2 \rangle_{DISTING.} \mp 2 |\langle x \rangle_{ab}|^2}$ "EXCHANGE FORCE"

From equation for $\langle x \rangle_{ab}$ we can see that this term is NON-ZERO only if the two wave-function OVERLAP... with no overlap we go back to classical case... we call this term EXCHANGE FORCE!

Consider Hydrogen molecule H_2!

$\rightarrow$ this is only possible if case 2.) is true (e^- are closer) $\Rightarrow$ this is for e^- possible only if we multiply state 2.) with SINGLET SPIN case!

We will make now short introduction to solid-state physics ...

SOLID-STATE PHYSICS

Simple model → electrons do not interact with each other but can not escape from the piece of material ⇒ infinite well

$$V(x,y,z) = \begin{cases} 0, & 0<x<l_x \\ & 0<y<l_y \\ & 0<z<l_z \\ \infty, & \text{else} \end{cases}$$

We can focus on solving only for one e^-, because they do not interact!

⇒ FOR 1 e^- : $-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$ → we seperate into 3 equations!

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} = E_x X \longrightarrow X(x) = A_x \sin(k_x x) + B_x \cos(k_x x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2Y}{dy^2} = E_y Y \longrightarrow Y(y) = A_y \sin(k_y y) + B_y \cos(k_y y)$$

$$-\frac{\hbar^2}{2m}\frac{d^2Z}{dz^2} = E_z Z \longrightarrow Z(z) = A_z \sin(k_z z) + B_z \cos(k_z z)$$

Now we impose boundary cond. → $X(0) = Y(0) = Z(0) = 0 \Rightarrow B_x = B_y = B_z = 0$

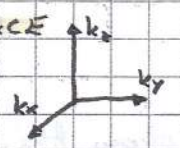
→ $X(l_x) = Y(l_y) = Z(l_z) = 0 \Rightarrow k_x l_x = \frac{n_x}{\pi}$; $k_y l_y = \frac{n_y}{\pi}$; $k_z l_z = \frac{n_z}{\pi}$

So we have → $\psi(x,y,z) = \sqrt{\frac{8}{l_x l_y l_z}} \sin\left(\frac{n_x \pi}{l_x}\cdot x\right) \sin\left(\frac{n_y \pi}{l_y}\cdot y\right) \sin\left(\frac{n_z \pi}{l_z}\cdot z\right)$

And for energy → $E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2}\right) = \frac{\hbar^2 k^2}{2m}$

Now we move into k-space ...

k-SPACE



planes at: $k_x = \frac{\pi}{l_x}, \frac{2\pi}{l_x}, \frac{3\pi}{l_x} \dots$

$k_y = \frac{\pi}{l_y}, \frac{2\pi}{l_y}, \frac{3\pi}{l_y} \dots$

$k_z = \frac{\pi}{l_z}, \frac{2\pi}{l_z}, \frac{3\pi}{l_z} \dots$

Each state occupies the volume $\frac{\pi^3}{l_x l_y l_z}$

Now... we have N atoms ($N \sim 10^{23}$), each atom contributes q electrons ...

Electrons can occupy only the states at intersection of planes ... because all k_x, k_y, k_z are positive ⇒ all electrons are in 1ST quadrant of k-space.

We aproximate the volume they occupy with the sphere ...

Radius of sphere k_f → $\frac{1}{8}\left(\frac{4}{3}\pi k_f^3\right) = \frac{Nq}{2}\left(\frac{\pi^3}{l_x l_y l_z}\right)$

→ because of spin (each state has two e^-)

So ⇒ $k_f = (3\rho\pi^2)^{1/3}$; $\rho = Nq/V$

The surface of this "sphere" is called FERMI SURFACE

FERMI ENERGY: $E_F = \frac{\hbar^2}{2m}(3\rho\pi^2)^{2/3}$ = energy of e^- on Fermi surface ...

We can also calculate the total energy ...

Total energy of electrons: - a shell of thickness dk : $\frac{1}{8}(4\pi k^2)\,dk$

- the number of e^- states in shell is: $\dfrac{\overset{\text{SPIN}}{2}\left[\frac{1}{2}\pi k^2 dk\right]}{\pi^3/V} = \dfrac{V}{\pi^2}k^2 dk$

- each state carries an energy $\frac{\hbar^2 k^2}{2m}$ $\Longrightarrow$ energy of shell: $dE = \frac{\hbar^2 k^2}{2m}\frac{V}{\pi^2}k^2 dk$

So the total energy: $$E = \frac{\hbar^2 V}{2\pi^2 m}\int_0^{k_8} k^4 dk = \frac{\hbar^2 k_8^5 V}{10\pi^2 m} = \frac{\hbar^2 (3\pi^2 N q)^{5/3} V^{-2/3}}{10\pi^2 m}$$

We have like some pressure due to the this free electron gas!

we try to squeze solid $\Longrightarrow \Delta E = -\frac{2}{3}\frac{\hbar^2(3\pi^2 N q)^{5/3}}{10\pi^2 m}V^{-5/3}dV = -\frac{2}{3}\frac{E}{V}dV$

remember thermodynamics $\rightarrow dW = PdV$

Than the pressure is: $\boxed{P = \frac{2}{3}\frac{E}{V}}$ DEGENERACY PRESSURE

This is just due to anti-symetric wave-function, not due to repulsion of e^-!

Now we improve the model! The electrons will now feel the potential due to nucleus latice $\Longrightarrow$ periodic potential!

BLOEH'S THEOREM

$V(x+a) = V(x) \rightarrow$ periodic potential (in 1-D)

than $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$ has solution $\psi(x+a) = e^{ika}\psi(x)$

where k = constant. (not dependent on x)

Proof: we introduce DISPLACEMENT OPERATOR $D \rightarrow D f(x) = f(x+a)$

↳ we can show that commutes with Hamilton $[D, H] = 0$ ... to show this we must show: $\left[D, \overset{\text{momentum}}{\frac{d^2}{dx^2}}\right] f(x) = D f''(x) - \frac{d}{dx^2} f(x+a) = 0$ $\qquad v(x) = v(x+a)$

$$[D, \overset{\text{potential}}{V}] f(x) = D(v(x) f(x)) - v(x)(D f(x)) = v(x+a) f(x+a) - v(x) f(x+a) = 0$$

So we can choose eigen-function of H (solutions to Schrödinger) ψ which are also eigen-functions for D: $D\psi(x) = \lambda\psi(x) \Longrightarrow \psi(x+a) = \lambda\psi(x)$; $\lambda = e^{ika}$

Note: To avoid problems at boundaries assume $\psi(x + \overset{\text{\# of atoms}}{N}a) = \psi(x)$ (CIRCULAR BOUNDARY)

So... if we apply Bloch's theorem $\rightarrow e^{iNka}\psi(x) = \psi(x) \Longrightarrow k \in \mathbb{R}$

The simplest potential to describe potential due to stacionary atomic nuclea is $\rightarrow V(x) = \alpha \sum_{j=0}^{N-1} \delta(x-ja)$

Now we solve Schrödinger for $0<x<a$ (free particle) and we get known solution: $\psi(x) = A\sin(kx) + B\cos(kx)$; where $k = \sqrt{2mE}/\hbar$ ... we have to include bounderies now... in region before $-a<x<0$ we use Bloch's theorem to find $\psi(x) = e^{-ika}\left[A\sin(k[x+a]) B\cos(k[x+a])\right]$

At $x=0$ the wave-function $\psi(x)$ must be countinous... from this we get $B = e^{-ika}\left[A\sin(ka) + B\cos(ka)\right]$ (*)

But we have problem because ψ' is not countinous at $x=0$... we integrate whole equation: $-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2}dx + \int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)dx = \int_{-\varepsilon}^{\varepsilon} E\psi(x)dx$ and $\varepsilon \rightarrow 0$

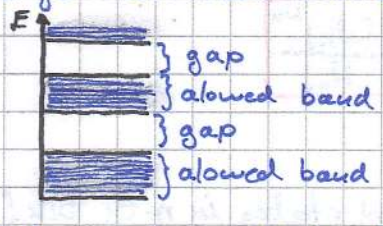
$$\Rightarrow \lim_{\varepsilon\to 0}\left(\psi'|_{+\varepsilon} - \psi'|_{-\varepsilon}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)dx = \frac{2m\alpha}{\hbar^2}\overbrace{\psi(0)}^{=B} = 2m\alpha B/\hbar^2$$

So we get: $KA - e^{-ika}K\left[A\cos(ka) + B\cos(ka)\right] = 2m\alpha B/\hbar^2$ (**)

Combining both equations (*) & (**) we get: $\cos(Ka) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)$

Define $z = ka$; $\beta = m\alpha a/\hbar^2 \Longrightarrow f(z) = \cos(z) + \beta\frac{\sin(z)}{z}$

Look at the book to see the plot of this function ... we can see that we get alowed bands seperated by gaps that are not alowed!



→ Because N is very big (# of atoms) the energy levels in alowed bands are very close → continuum! $k_a = \frac{2\pi a}{N}$

If band is partialy filled → CONDUCTOR

If band is fully filled → INSULATOR (because we need big energy to "push" electron over the gap into the next alowed band)

This topic will be described in more detail at Solid State Physics course...

V enačbah je vektor K in nanje → glej knjigo o ez signalu

QUANTUM STATISTICAL MECHANICS

Here we will be dealing with multitude of particles ... thats why we need statistics to describe this!

Consider arbitary potential ... for which one-particle energy levels are:

$E_1, E_2, E_3 \ldots$ = energy levels for one-particle

$d_1, d_2, d_3 \ldots$ = degeneracies of energy levels for one-particle

Now → Suppose we put N particles into this potential. We are intrested in the configuration $(\overset{\text{energy } E_1}{N_1}, \overset{E_2}{N_2}, \overset{E_3}{N_3} \ldots) \ldots$? ps: $\sum N_i = N$

How many distinct states correspond to this configuration?

Lets find the function $Q(N_1, N_2, N_3 \ldots)$ = (# of states) ...

① DISTINGUISHABLE PARTICLES

How many ways are to select N_1 particles from total of N particles → $\binom{N}{N_1} = \frac{N!}{N_1!(N-N_1)!}$ because they are distinguishable

Because of degeneracy we must multiply by $(d_1)^{N_1}$ ... so there are in total $\binom{N}{N_1} d_1^{N_1}$ ways to put into 1ST bin!

Now for 2ND bin ... there are $\frac{(N-N_1)!}{N_2!(N-N_1-N_2)!} d_2^{N_2}$ ways ... and so on!

So → $Q(N_1, N_2, N_3) = \frac{N!\, d_1^{N_1}}{N_1!\,(N-N_1)!} \cdot \frac{(N-N_1)!\, d_2^{N_2}}{N_2!\,(N-N_1-N_2)!} \cdot \frac{(N-N_1-N_2)!\, d_3^{N_3}}{N_3!\,(N-N_1-N_2-N_3)!} = \frac{N!\, d_1^{N_1} d_2^{N_2} d_3^{N_3} \ldots}{N_1!\, N_2!\, N_3! \ldots}$

We write this in this form: $\boxed{Q(N_1, N_2, N_3 \ldots) = N! \prod_{n=1}^{\infty} \frac{(d_n)^{N_n}}{N_n!}}$

② FERMIONS

For fermions there are $\binom{d_n}{N_n}$ ways to choose N_n occupied states in n-th bin!

So → $\boxed{Q(N_1, N_2, N_3 \ldots) = \prod_{n=1}^{\infty} \frac{d_n!}{N!\,(d_n - N_n)!}}$ ... ps: we can not put more fermions than is degeneracy

③ BOSONS

We get → $\boxed{Q(N_1, N_2, N_3 \ldots) = \prod_{n=1}^{\infty} \frac{(N_n + d_n - 1)!}{N_n!\,(d_n - 1)!}}$

Now we are intrested in maximizing this Q functions → we want to find the most probable ones ...

We must use the method of Lagrangian Multipliers ... because there are some constrains!

$\Rightarrow$ Maximize $Q(N_1, N_2, N_3 \dots)$ with constrains: (1) $\sum_{n=1}^{\infty} N_n = N$ & (2) $\sum_{n=1}^{\infty} N_n E_n = E$

Lagran. Multi.: we have $F(x_1, x_2, \dots)$ subject to constrains $f_1(x_1, x_2 \dots) = 0$ and $f_2(x_1, x_2 \dots) = 0$

and we want to maximize $\Rightarrow G(x_1, x_2 \dots \lambda_1, \lambda_2) = F + \lambda_1 f_1 + \lambda_2 f_2 \rightarrow$ we maximize $G \Rightarrow \frac{\partial G}{\partial x_n} = 0$ and $\frac{\partial G}{\partial \lambda_n} = 0$!

In our case we will work with logaritms to get rid of the multiplications in $Q \Rightarrow$ we define: $G = \ln(Q) + \alpha\left[N - \sum_{n=1}^{\infty} N_n\right] + \beta\left[E - \sum_{n=1}^{\infty} N_n E_n\right]$

① DISTHINGUISHABLE PARTICLES

$\hookrightarrow G = \ln(N!) + \sum_{n=1}^{\infty}\left[N_n \ln(d_n) - \ln(N!)\right] + \alpha\left[N - \sum_{n=1}^{\infty} N_n\right] + \beta\left[E - \sum_{n=1}^{\infty} N_n E_n\right]$

We will use Stirling aproximation: $\ln(z!) \approx z\ln(z) - z$; $z >> 1$

So: $G \approx \sum_{n=1}^{\infty}\left[N_n \ln(d_n) - N_n \ln(N_n) + N_n - \alpha N_n - \beta E_n N_n\right] + \ln(N!) + \alpha N + \beta E$

Now we look for extremes: $\frac{\partial G}{\partial N_n} = \ln(d_n) - \ln(N_n) - \alpha - \beta E_n = 0$

We get: $\boxed{N_n = d_n e^{-(\alpha + \beta E_n)}}$ $\rightarrow$ most probable occupation number for n-th bin

② FERMIONS

$\hookrightarrow G = \sum_{n=1}^{\infty}\left\{\ln(d_n!) - \ln(N_n!) - \ln([d_n - N_n]!)\right\} + \alpha\left[N - \sum N_n\right] + \beta\left[E - \sum N_n E_n\right]$

We assume $d_n >> N_n$ so that we use Stirling aprox. for all $\ln()$ terms.

$\Rightarrow G \approx \sum_{n=1}^{\infty}\left[\ln(d_n!) - N_n \ln(N_n) + N_n - (d_n - N_n)\ln(d_n - N_n) + (d_n - N_n) - \alpha N_n - \beta E_n N_n + \alpha N + \beta E\right]$

Now extremes: $\frac{\partial G}{\partial N_n} = -\ln(N_n) + \ln(d_n - N_n) - \alpha - \beta E_n = 0$

We get: $\boxed{N_n = d_n / \left(e^{\alpha + \beta E_n} + 1\right)}$

③ BOSONS

$\hookrightarrow$ Finally we get: $\boxed{N_n = d_n / \left(e^{\alpha + \beta E_n} - 1\right)}$ (we need to know E_n)

Now we should determine α & β ... to do this we must specify potential!

For example we will consider ideal gas in 3-D ... (gas of electrons!)

we know the solution: $E_k = \frac{\hbar^2}{2m} k^2$, $\vec{k} = \left(\frac{\pi n_x}{l_x}, \frac{\pi n_y}{l_y}, \frac{\pi n_z}{l_z}\right)$

We need degeneracy $\rightarrow$ for a bin (with energy E) we take a spherical shell in 1ST octant in k-space: we need a number of states in this shell $\rightarrow$ $d_k = \frac{1}{8}\frac{4\pi k^2 dk}{\pi^3/V} = \frac{V}{2\pi^2} k^2 dk$

$\hookrightarrow$ we did not take into acount the spin

Now we use constrains: $\sum_n N_n = N$ (I) & $\sum_n N_n E_n = E$ (II)

$$(I) \Longrightarrow N = \frac{V}{2\pi^2} e^{-\alpha} \int_0^\infty e^{-\beta \frac{\hbar^2 k^2}{2m}} k^2 dk = V e^{-\alpha} \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \Longrightarrow e^{-\alpha} = \frac{N}{V}\left(\frac{2\pi\beta\hbar^2}{m}\right)^{3/2}$$

$$(II) \Longrightarrow E = \frac{V}{2\pi^2} e^{-\alpha} \frac{\hbar^2}{2m} \int_0^\infty e^{-\beta \frac{\hbar^2 k^2}{2m}} k^4 dk = \frac{3V}{2\beta} e^{-\alpha} \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \Longrightarrow E = \frac{3N}{2\beta}$$

REMEMBER: for classical gas ... average energy of particle (kinetic en)

$$\frac{E}{N} = \frac{3}{2} k_B T$$ → classical formula for average kinetic energy of gas at temp. T!

So our β is related to temperature: $\boxed{\beta = 1/k_B T}$ k_B = Boltzmann konstant

For α we define Chemical potential: $\boxed{\mu(T) = -\alpha k_B T}$

→ Most probable number of particles in a particular (one-particle) state of energy ε ... lets denote this by $u(\varepsilon)$

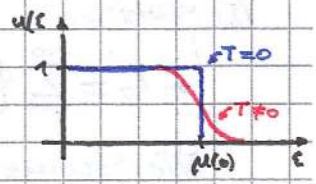
$u(\varepsilon) = \exp[-(\varepsilon-\mu)/k_B T]$ Maxwell-Boltzmann

$u(\varepsilon) = 1/(\exp[(\varepsilon-\mu)/k_B T] + 1)$ Fermi-Dirac

$u(\varepsilon) = 1/(\exp[(\varepsilon-\mu)/k_B T] - 1)$ Bose-Einstein

Now → for Fermi-Dirac distribution...

note: $e^{(\varepsilon-\mu)/k_B T} \longrightarrow \begin{cases} 0 & \text{if } \varepsilon < \mu(0) \\ \infty & \text{if } \varepsilon > \mu(0) \end{cases} \Longrightarrow u(\varepsilon) \longrightarrow \begin{cases} 1; & \varepsilon < \mu(0) \\ 0; & \varepsilon > \mu(0) \end{cases}$



VAJE KVANTNA MEHANIKA

20/04/2015

① At what speed does a meter stick move if it's length is observed to shrink to 0'5m?

$$x' = \gamma(x - vt) \; ; \; \gamma = 1/\sqrt{1 - v^2/c^2}$$

we know that $x' = \gamma(x - vt)$, where x' is measured in S' frame in which the stick is at rest (S' moving with v) and x measured in S (which is at rest)

$\Delta x' = \gamma(\Delta x - v\Delta t)$ ... here Δx is measured by stationary observer at $\Delta t = 0$!

$$\Rightarrow \Delta x' = \gamma \Delta x \Rightarrow \gamma = \frac{\Delta x'}{\Delta x} = \frac{1}{0'5} = 2 \Rightarrow \gamma^2 = 4 = \frac{1}{1-\beta^2} \Rightarrow \beta = \sqrt{0'75} \approx 0'866$$

$$\Rightarrow \boxed{v \approx 0'866 \cdot c}$$

② At what speed does a clock move if it runs at a rate which is one-half the rate of a clock at rest?

$$t = \gamma\left(t' + \frac{v}{c^2}x'\right) \rightarrow \Delta t = \gamma\left(\Delta t' + \frac{v}{c^2}\Delta x'\right) \; ; \; \gamma = 1/\sqrt{1-\beta^2} \; ; \; \beta = \frac{v}{c}$$

$\Delta t'$ = time interval measured by an observer at rest in S' and $\Delta x' = 0$!

So $\Delta t = \gamma \Delta t'$ and $\frac{\Delta t'}{\Delta t} = \frac{1}{2} \Rightarrow \gamma = 2 \Rightarrow \ldots \boxed{v \approx 0'866 \cdot c}$

③ The average half-time of π-meson in its own frame of reference is 26'0 us (this is proper lifetime). If the π-meson moves with speed 0'95c with respect to the Earth, what is its life time as measured by observer at rest on Earth? What is the average distance it travels before decaying as measured by an observer at rest on Earth?

$$\Delta t = \gamma(\underbrace{\Delta t'}_{\text{proper time (in meson's system} \Rightarrow \Delta x' = 0)} + \frac{v}{c^2}\Delta x') \Rightarrow \Delta t = \gamma \Delta t' \rightarrow \Delta t = \frac{1}{\sqrt{1-0'95^2}} \cdot 26'0\,us = \boxed{83'3\,us}$$

Average distance ... $= v \cdot \Delta t = 0'95 \cdot 83'3\,us \cdot c = \boxed{23'7\,m}$

④ A muon travelling through laboratory at 0'6c. How long does it last? Proper life-time of muon is 2×10^{-6} s. $\Delta t = \gamma \cdot \Delta t' = \ldots = \boxed{2'5 \times 10^{-6}\,s}$

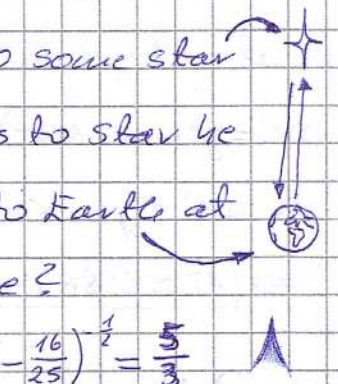
(5.) If the particle's kinetic energy is n times its rest energy ($E=mc^2$), what is its speed? PS. Total energy $= \gamma mc^2 =$ (rest En. + kinetic En.)

Kinetic energy $= nmc^2 = \gamma mc^2 - mc^2 = (\gamma - 1)mc^2 \Rightarrow n = \gamma - 1$

$$\Rightarrow \gamma^2 = \frac{1}{1-\beta^2} = (n+1)^2 \Rightarrow \beta^2 = 1 - \frac{1}{(n+1)^2} = \frac{(n+1)^2-1}{(n+1)^2} \Rightarrow v = \frac{\sqrt{n(n+2)}}{(n+1)} \cdot c$$

24/04/2015

(1.) On 21 birthday one twin gets on a moving sidewalk to some star moving with $\frac{4}{5}c$; his twin stys home. When twin gets to star he imediaty gets to return at same speed and arrives back to Earth at 39th birthday. How old is the twin that stayed at home?



proper time of moving twin $\Delta\tau = 18$ years; $\gamma = (1-\beta^2)^{-\frac{1}{2}} = \left(1-\frac{16}{25}\right)^{-\frac{1}{2}} = \frac{5}{3}$

$\Rightarrow \Delta t = \gamma \Delta\tau = \frac{5}{3} \cdot 18$ years $= \underline{30}$ years $\Rightarrow$ $\boxed{\text{Other twin is 51 years old!}}$

P.S.

Star is 15 years $\cdot \frac{4}{5}c = 12$ light years away!

↳ Vzamem kolko časa se je gibal za tistega na Zemljo!

Call the outbound side-walk system $\bar{S}$ and the inbound one $\tilde{S}$ (the Earth system is S). All three systems set their master clocks, and choose their origins, so that $x = \bar{x} = \tilde{x} = 0$; $t = \bar{t} = \tilde{t} = 0$, at the moment of departure. What are the co-ordinates (x,t) on the jump between side-walks?

$\Rightarrow$ $\boxed{x = 12 \text{ ly}}$ and $\boxed{t = 15 \text{ years}}$!

What are the co-ordinates $(\bar{x}, \bar{t})$ of the jump?

$\Rightarrow$ Obviously $\boxed{\bar{x} = 0}$; $\boxed{\bar{t} = 9 \text{ years}}$!

$$w = \frac{0+v}{1+\frac{0 \cdot v}{c^2}} = \frac{\frac{4}{5}c + \frac{4}{5}c}{1+\frac{16}{25}} = \frac{\frac{8}{5}c}{\frac{41}{25}} = \frac{\cancel{25}^{5} \cdot 8}{\cancel{5} \cdot 41} = \frac{40}{41}c = w$$

hitrost $\bar{S}$ gledem $\tilde{S}$

What are co-ordinates $(\tilde{x}, \tilde{t})$ of the jump?

$$\tilde{x} = \gamma(w)\left[\underset{0}{\bar{x}} - w\bar{t}\right] = +\underset{4'55}{\gamma(w)}\, w\bar{t} = +4'55 \cdot \frac{40}{41} \cdot c \cdot 9 \text{ years} = \boxed{+40 \text{ light years}}$$

$$\tilde{t} = \gamma(w)\left[\bar{t} - \frac{w}{c^2}\underset{0}{\bar{x}}\right] = 4'55 \cdot 9 \text{ years} \approx \cancel{40'96 \text{ years}} = \boxed{41 \text{ years}}$$

If the traveling twin wanted her watch to agree with the clock in $\tilde{S}$, how would have to be reset the clock imediatly after the jump.

Before the jump (just before) ... clock = 9 years

Just after the jump ... we want the clock = 41 years $\Rightarrow$ $\boxed{32 \text{ years } \oplus}$

If the clock is reset as before written, what would clock show when returned to Earth $\rightarrow$ Jump $\rightarrow$ clock = 41 years $\oplus$ 9 years to Earth

$\Rightarrow$ clock at Earth = $\boxed{50 \text{ years}}$

29.04.15

① A neutral pion of rest-mass m and relativistic momentum $p = \frac{3}{4}mc$ decays into two photons. One of the photons is emited in same direction as original pion, and other in oposite direction. Find the relativistic energy of each photon!

energy of pion: $E^2 = p^2c^2 + m^2c^4 \Rightarrow E^2 = \frac{9}{16}m^2c^4 + m^2c^4 = \frac{25}{16}m^2c^4 \Rightarrow \boxed{E = \frac{5}{4}mc^2}$

energy of photons: E_A and E_B (mass of photon = 0)

$\Rightarrow$ by conservation of energy $\Rightarrow \boxed{E_A + E_B = \frac{5}{4}mc^2}$

$\Rightarrow$ since photon has no mass $\Rightarrow p_A = \frac{E_A}{c}$ and $p_B = \frac{-E_B}{c}$ (−) because of opposite direction)

$\rightarrow$ by conservation of momentum $\Rightarrow \boxed{p_A + p_B = \frac{E_A - E_B}{c} = \frac{3}{4}mc}$

So we have: $\left.\begin{aligned} E_A + E_B &= \frac{5}{4}mc^2 \\ E_A - E_B &= \frac{3}{4}mc^2 \end{aligned}\right\} \Rightarrow \boxed{E_A = \frac{4}{4}mc^2 = mc^2}$ and $\boxed{E_B = \frac{1}{4}mc^2}$

②

$$\begin{cases} E_x' = E_x \\ E_y' = \gamma(E_y - vB_z) \\ E_z' = \gamma(E_z + vB_y) \end{cases} \qquad \begin{cases} B_x' = B_x \\ B_y' = \gamma(B_y + \frac{v}{c^2}E_z) \\ B_z' = \gamma(B_z - \frac{v}{c^2}E_y) \end{cases}$$

Show that $\vec{E}\cdot\vec{B}$ is relativisticly invariant! $\rightarrow$ show $\vec{E}'\cdot\vec{B}' = \vec{E}\cdot\vec{B}$

$$\rightarrow \boxed{\vec{E}'\cdot\vec{B}'} = (E_x, \gamma E_y - \gamma v B_z, \gamma E_z + \gamma v B_y)\cdot(B_x, \gamma B_y + \frac{\gamma v}{c^2}E_z, \gamma B_z - \frac{\gamma v}{c^2}E_y) =$$

$$= E_x B_x + \gamma^2 E_y B_y + \cancel{\gamma^2 \frac{v}{c^2} E_y E_z} - \cancel{\gamma^2 v B_y B_z} - \gamma^2 \frac{v^2}{c^2} E_z B_z + \gamma^2 E_z B_z -$$

$$- \cancel{\gamma^2 \frac{v}{c^2} E_y E_z} + \cancel{\gamma^2 v B_y B_z} - \gamma^2 \frac{v^2}{c^2} E_y B_y =$$

$$= E_x B_x + E_y B_y \underbrace{\left(\gamma^2\left(1 - \frac{v^2}{c^2}\right)\right)}_{1} + E_z B_z \left(\gamma^2\left(1 - \frac{v^2}{c^2}\right)\right) = E_x B_x + E_y B_y + E_z B_z = \vec{E}\cdot\vec{B} \checkmark$$

(use $\gamma^2 = \left(1 - \frac{v^2}{c^2}\right)^{-1}$)

③ A pion at rest decays into muon and neutrino. Find the energy of the outgoing muon, in terms of the two masses, m_π and m_μ. (Assume $m_\nu = 0$!)

$E_\pi = m_\pi c^2$; $E_\mu^2 = p_\mu^2 c^2 + m_\mu^2 c^4$; $E_\nu = 0$ (since $m_\nu = 0$)

$p_\pi = 0$; $p_\mu = \dots = -p_\nu$ (conservation of momentum $\Rightarrow p_\mu + p_\nu = 0$)

conservation of energy: $m_\pi^2 c^4 = p_\mu^2 c^2 + m_\mu^2 c^4 + E_\nu \Rightarrow \boxed{p_\mu = c\sqrt{m_\pi^2 - m_\mu^2}}$

$\rightarrow E_\mu + E_\nu = m_\pi c^2$

For neutrino $E_\nu^2 = p_\nu^2 c^2$

For muon $E_\mu^2 = p_\mu^2 c^2 + m_\mu^2 c^4$

$\Rightarrow p_\nu^2 c^2 + p_\mu^2 c^2 + m_\mu^2 c^4 = m_\pi^2 c^4$ ⊕ use $p_\nu^2 = p_\mu^2$

$\Rightarrow 2 p_\mu^2 + m_\mu^2 c^2 = m_\pi^2 c^2$

So $p_\mu^2 = \frac{1}{2}(m_\pi^2 - m_\mu^2) c^2$

So energy of muon: $\boxed{E_\mu^2 = p_\mu^2 c^2 + m_\mu^2 c^4 = \frac{1}{2} m_\pi^2 c^4 - \frac{1}{2} m_\mu^2 c^4 + m_\mu^2 c^4 = \frac{1}{2}(m_\pi^2 + m_\mu^2) c^4}$

2 – daj že 1x

03.05.2015

① a) Write the special relativistic relation between energy E and the momentum p for a particle of mass m. Express speed! (with E, p)

b) Associating the pulsation ω and wave vector k to its energy and momentum, obtain the relativistic relation of dispersion and expression of particle speed in terms of ω and k!

c) Express the phase velocity from the disperssion relation for a relativistic particle. How does it compare to the speed of light?

d) Express the group velocity from disperssion relation for a relativistic particle! How does the ~~phase~~ group velocity compare to the velocity of a particle?

a) $E^2 = p^2c^2 + m^2c^4$ ... $\beta = \frac{v}{c} = \frac{mv}{mc} = \frac{pc}{mc^2} = \frac{pc}{E_0} \Rightarrow \boxed{v = pc^2/E_0}$

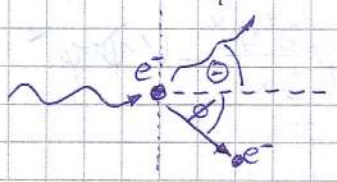
b) use $E = \hbar\omega$, $p = \hbar k$ ⊕ $E^2 = p^2c^2 + m^2c^4 \Rightarrow \hbar^2\omega^2 = \hbar^2k^2c^2 + m^2c^4 \Rightarrow \boxed{\omega = \sqrt{k^2c^2 + \frac{1}{\hbar^2}m^2c^4}}$

c,d) phase velocity $= \frac{\omega}{k} \rightarrow v_p = \frac{\omega}{k} = \sqrt{c^2 + \frac{m^2c^4}{\hbar^2k^2}} = \underbrace{\sqrt{c^2 + \frac{m^2c^4}{p^2}}}_{\text{can be bigger than } c} = \frac{1}{p}\sqrt{p^2c^2 + m^2c^4} = \overset{\text{total energy}}{E}/p$

group velocity $= \frac{d\omega}{dk} \rightarrow v_g = \frac{d\omega}{dk} = \frac{1}{\cancel{2}\omega\dots}\cancel{2}kc^2 = \frac{kc^2}{\omega} = \frac{c^2}{v_p}$

$\rightarrow \frac{\hbar k c^2}{\hbar\omega} = \frac{pc^2}{E_0 \rightarrow mc^2} \rightarrow v$ equals to particle speed

② A photon of energy E_0 "~~becomes~~ bounces" of an electron initialy at rest. Find the energy E of the outgoing photon, as a function of the scattering angle Θ. Show that the change in wavelength ($\Delta\lambda$) is independent of the incident wavelength λ.



Before: $\vec{p}_{tot} = \hbar\vec{k}$; $E_{tot} = E_0 = \hbar\omega$ } momentum and

After: $p_{tot} = p_e + p_\gamma$; $E_{tot} = E_\gamma + E_{e^-} = E_0$ } energy conservation!

MOMENTUM CONSERVE:

Vertical: $p_e \sin\phi = p_\gamma \sin\Theta$; $p_\gamma = E/c$ $\Rightarrow \sin\phi = \frac{E}{p_e c}\cdot\sin\Theta$

Horizontal: $\frac{E_0}{c} = \frac{E}{c}\cos\Theta + p_e\cos\phi = \frac{E}{c}\cos\Theta + p_e\sqrt{1-\sin^2\phi} =$

$$= \frac{E}{c}\cos\Theta + p_e\sqrt{1-\frac{E^2}{p_e^2c^2}\sin^2\Theta} = \frac{E}{c}\cos\Theta + \frac{1}{c}\sqrt{p_e^2c^2 - E^2\sin^2\Theta}$$

$$\Rightarrow E_0 = E\cos\Theta + \sqrt{p_e^2c^2 - E^2\sin^2\Theta} \quad /^2 \Rightarrow$$

$$\Rightarrow p_e^2c^2 - E^2\sin^2\Theta = E_0^2 + E^2\cos^2\Theta - 2EE_0\cos\Theta$$

$$\Rightarrow \boxed{E^2 + E_0^2 - 2EE_0\cos\Theta = p_e^2c^2}$$

ENERGY CONSERV:

$$E_0 + mc^2 = E + \sqrt{p_e^2c^2 + m^2c^4}$$

$$\Rightarrow \boxed{p_e^2c^2 + \cancel{m^2c^4} = (E_0 - E + mc^2)^2 = (E_0-E)^2 + 2(E_0-E)mc^2 + \cancel{m^2c^4}}$$

ENERGY & MOMENTUM CONSERVE!

$$E^2 + E_0^2 - 2EE_0\cos\Theta = (E_0-E)^2 + 2(E_0-E)mc^2$$

$$\cancel{E^2} + \cancel{E_0^2} - 2EE_0\cos\Theta = \cancel{E_0^2} + \cancel{E^2} - 2EE_0 + 2(E_0-E)mc^2$$

$$\Rightarrow \cancel{2}EE_0(1-\cos\Theta) = \cancel{2}(E_0-E)mc^2 \quad /:E_0mc^2$$

$$\Rightarrow \frac{E(1-\cos\Theta)}{mc^2} = 1 - \frac{E}{E_0} \rightarrow \boxed{E\left[\frac{(1-\cos\Theta)}{mc^2} + \frac{1}{E_0}\right] = 1}$$

So: $\boxed{E = \left[\frac{(1-\cos\Theta)}{mc^2} + \frac{1}{E_0}\right]^{-1}}$ now use $E = \frac{hc}{\lambda}$ and $E_0 = \frac{hc}{\lambda_0}$

$$\Rightarrow \frac{\lambda}{hc} = \frac{(1-\cos\Theta)}{mc^2} + \frac{\lambda_0}{hc} \rightarrow \frac{(\lambda-\lambda_0)}{hc} = \frac{(1-\cos\Theta)}{mc^2}$$

$$\Rightarrow \boxed{\Delta\lambda = \lambda - \lambda_0 = \frac{h}{mc}\underbrace{(1-\cos\Theta)}_{\left(2\sin^2\frac{\Theta}{2}\right)}} \rightarrow \text{indipendent of } \lambda_0$$

$\Downarrow$

indipendent of E_0

$$\Rightarrow \boxed{\Delta\lambda = \frac{2h}{mc}\sin^2\frac{\Theta}{2}}$$

(3.) Consider a 1-D bound particle. Show that $\frac{d}{dt}\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = 0$!

$$\left.\begin{aligned} &(1)\ i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \\ &(2)\ -i\hbar\frac{\partial}{\partial t}\Psi^* = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + V\Psi^* \end{aligned}\right\}\ \text{Now do } \Psi^*\cdot(1) - (2)\cdot\Psi\ !$$

because is conjugate!

we get: $\underbrace{i\hbar\Psi^*\frac{\partial\Psi}{\partial t} + i\hbar\Psi\frac{\partial\Psi^*}{\partial t}} = -\frac{\hbar^2}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2} + \cancel{V\Psi\Psi^*} + \frac{\hbar^2}{2m}\Psi\frac{\partial^2\Psi^*}{\partial x^2} - \cancel{V\Psi\Psi^*}$

$$\Rightarrow \boxed{i\hbar\frac{\partial}{\partial t}(\Psi^*\Psi) = -\frac{\hbar^2}{2m}\left[\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2}\right]}$$

$$\Rightarrow \boxed{i\hbar\frac{\partial}{\partial t}(\Psi^*\Psi) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]}$$

now $\frac{d}{dt}\int_{-\infty}^{\infty}\Psi^*\Psi\,dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}(\Psi^*\Psi) = -\frac{\hbar}{2im}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]dx$

integral odvoda po x po x

$$= \frac{i\hbar}{2m}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]_{-\infty}^{\infty} = 0$$

because $\Psi = 0$ at $x = \pm\infty$

11/05/15

(1) If $V(x)$ is even function, than $\Psi(x)$ can always be taken to be either even or odd!

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x)\ ;\ x \to (-x)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{d(-x)^2}\Psi(-x) + \underbrace{V(-x)}_{V(x)\ \text{because its EVEN!}}\Psi(-x) = E\Psi(-x)\ ;\ \text{use}\ \frac{d^2}{d(-x)^2} = \frac{d^2}{dx^2}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(-x) + V(x)\Psi(-x) = E\Psi(-x) \Rightarrow \Psi(-x) = \pm\Psi(x)\ \text{SOLVES eq!}$$

$\Rightarrow \Psi_+(x) = \Psi(x) + \Psi(-x)$ is solution, and $\Psi_+(-x) = \Psi(-x) + \Psi(x)$ is equal

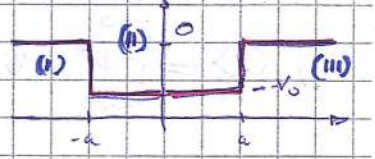
$\Rightarrow \Psi_+$ is EVEN function!

Similarly for $\Psi_-(x) = \Psi(x) - \Psi(-x)$; $\Psi_-(-x) = \Psi(-x) - \Psi(x) = -\Psi_-(x)$

is solution and is ODD function!

Note $\Psi(x) = \frac{1}{2}(\Psi_+(x) + \Psi_-(x)) \Rightarrow$ any solution $\Psi(x)$ can be written as linear combination of EVEN and ODD function!

② **Finite square well problem** ... $V(x) = \begin{cases} -V_0 ; & |x| \leq a \\ 0 ; & |x| > a \end{cases}$



We have 3 regions ... (I), (II), (III)

Region (I) ... $V(x)=0 \Longrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \rightarrow \frac{d^2\psi}{dx^2} = k^2\psi \; ; \; k^2 = -\frac{2mE}{\hbar^2}$

So solution is $\psi_1(x) = Ae^{kx} + Be^{-kx}$

B.C.: for $x \to -\infty$, $\psi_1 \to 0 \Longrightarrow \boxed{B=0} \Longrightarrow \boxed{\psi_1(x) = Ae^{kx}}$!

Region (II) ... $V(x) = -V_0$

$$\Longrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \Longrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E+V_0)\psi \Longrightarrow \frac{d^2\psi}{dx^2} = -l^2\psi ; \; l^2 = \frac{2m(E+V_0)}{\hbar^2}$$

$$\Longrightarrow \boxed{\psi_2(x) = C\sin(lx) + D\cos(lx)} \; !$$

Region (III) ... $V(x)=0$ ... similar as region (I) $\Longrightarrow \psi_3(x) = \overset{=0 \to \text{B.C. } x\to\infty;\, \psi\to 0}{Fe^{kx}} + Ge^{-kx} \Longrightarrow \boxed{\psi_3(x) = Ge^{-kx}}$!

Now ... due to ex. ① we have even potential $V(x) \rightarrow$ we take ψ to be even!

So ...

$$\psi(x) = \begin{cases} Ge^{-kx} & ; x > a \\ D\cos(lx) & ; 0 < x < a \\ \psi(-x) & ; x < 0 \end{cases} \quad \oplus \text{ continuity of } \frac{d\psi}{dx} \text{ at } x = a$$

continuity ...

$$\left.\begin{aligned} -kGe^{-ka} &= -lD\sin(la) \\ Ge^{-ka} &= D\cos(la) \end{aligned}\right\} \Longrightarrow -k = -l\tan(la) \Longrightarrow \text{allowed energies}$$

$$\Longrightarrow \tan^2(la) = \frac{E}{E+V_0} \; ?$$

③ Consider wave-function $\psi(x,t) = Ae^{-\lambda|x|}e^{-i\omega t}$; where A, λ and ω are positive real constants. Normalize ψ! Determine expectation value for $\langle x \rangle, \langle x^2 \rangle$! Find σ_x; sketch $|\psi(x)|^2$ $\oplus$ mark points $(\langle x \rangle \pm \sigma)$ to illustrate the sense in which σ represents the spread of x. What is the probability that particle is found outside this range?

a) Normalize $\rightarrow \int_{-\infty}^{\infty} |\psi|^2 dx = 1$ ~~$A^2e^{-2i\omega t}\int_{-\infty}^{\infty} e^{-2\lambda|x|}dx = 2A^2e^{-2i\omega t}\int_0^{\infty} e^{-2\lambda x}dx$~~

$\Downarrow$

~~$= 2A^2e^{-2i\omega t}$~~

$$\int_{-\infty}^{\infty} \psi\psi^* dx = A^2\int_{-\infty}^{\infty} e^{-2\lambda|x|}e^{-i\omega t}e^{+i\omega t}dx = A^2\int_{-\infty}^{\infty} e^{-2\lambda|x|}dx = 2A^2\int_0^{\infty} e^{-2\lambda x}dx$$

$$\Longrightarrow 2A^2\frac{1}{-2\lambda}\left[e^{-2\lambda x}\right]_0^{\infty} = \frac{A^2}{\lambda} = 1 \Longrightarrow \boxed{A = \sqrt{\lambda}} \; !$$

b) $\langle x\rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx = \int_{-\infty}^{\infty} A e^{-\lambda|x|} \cancel{e^{+i\omega t}} \cdot x \cdot A e^{-\lambda|x|} \cancel{e^{-i\omega t}} dx = A^2 \int_{\infty}^{\infty} e^{-2\lambda|x|} x \, dx = 0$

(even) · (ODD) = ODD

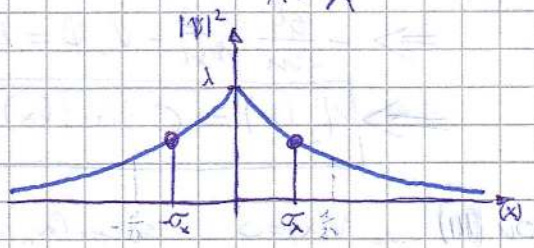
$\langle x^2\rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi \, dx = \int_{-\infty}^{\infty} A e^{-\lambda|x|} \cancel{e^{+i\omega t}} \cdot x^2 \cdot A e^{-\lambda|x|} \cancel{e^{-i\omega t}} dx = \cancel{0}$

$= A^2 \int_{-\infty}^{\infty} \underbrace{x^2 e^{-2\lambda|x|}}_{\text{(even)}} dx = 2A^2 \int_0^{\infty} x^2 e^{-2\lambda x} dx = 2A^2 \left[e^{-2\lambda x} \left(-\frac{x^2}{2\lambda} - \frac{2x}{4\lambda^2} - \frac{2}{8\lambda^3} \right) \right|_0^{\infty} =$

$\int x^2 e^{cx} dx = e^{cx}\left(\frac{x^2}{c} - \frac{2x}{c^2} + \frac{2}{c^3}\right)$ $\quad = 2A^2 \frac{1}{+4\lambda^3} = + \boxed{\frac{1}{2\lambda^2}}$

$A^2 = \lambda$

$\Rightarrow \boxed{\langle x^2\rangle = \frac{1}{2\lambda^2}}$



$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{1}{2\lambda^2} - 0 \Rightarrow \cancel{\sigma_x = 1/2\lambda^2}$

$\boxed{\sigma_x = 1/\lambda\sqrt{2}}$

$P(\text{outside}) = 1 - P(\text{inside})$

$P(\text{inside}) = 2A^2 \int_0^{\sigma_x} \psi^* \psi \, dx = 2A^2 \int_0^{1/\lambda\sqrt{2}} e^{-2\lambda x} dx = -\frac{2A^2}{2\lambda} \left[e^{-2\lambda x} \right|_0^{1/\lambda\sqrt{2}} = \frac{A^2}{\lambda}\left(1 - e^{-\sqrt{2}}\right) = \boxed{1 - e^{-\sqrt{2}}}$ $\quad A^2 = \lambda$

So $P(\text{outside}) = 1 - (1 - e^{-\sqrt{2}}) = e^{-\sqrt{2}} \cong \boxed{0.2431}$

15/5/15

① Consider 1D time-independent Schrödinger eq. for some arbitary potential $v(x)$. Prove that is solution ψ has property $\psi(x) \to 0$ when $x \to \pm\infty$, than the solution must be non-degenerate and therefore real. Apart from a possible overall phase factor!

→ suppose that exists another fun. $\phi(x)$ that solves same Schrödinger! (for the same energy E as for $\psi(x)$)!

also for ϕ holds that $\lim_{x\to\pm\infty} \phi(x) = 0$!

We have to prove that $\psi(x) \propto \phi(x)$ → (proportional)

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

Similarly we get... $\boxed{\frac{\phi''}{\phi} = -\frac{2m}{\hbar^2}(E-V)}$

SO WE HAVE: $\frac{\psi''}{\psi} = \frac{\phi''}{\phi} \Rightarrow \psi''\phi - \phi''\psi = 0 \Rightarrow \boxed{\frac{\partial}{\partial x}(\psi'\phi - \phi'\psi) = 0}$

FROM: $\frac{\partial}{\partial x}(\psi'\phi - \phi'\psi) = 0 \Longrightarrow \boxed{\psi'\phi - \phi'\psi = \text{const}}$

the boundary condition at $x \to \pm\infty$ is $\psi, \phi = 0 \Longrightarrow \boxed{\text{constant} = 0}$

So: $\psi'\phi = \phi'\psi \Longrightarrow \frac{\psi'}{\psi} = \frac{\phi'}{\phi}$ → now we integrate $\Longrightarrow$

$\Longrightarrow \ln\psi = \ln\phi + (\text{const}) \Longrightarrow \boxed{\psi = (\text{const.})\cdot\phi} \Longrightarrow$ { they represent the same solution $\Longrightarrow$ NON-DEGENERATE

When $V(x)$ is REAL; ψ^* and ψ satisfy same equation with same energy and same B.C. $\lim_{x\to\pm\infty}\psi^* = 0$ ... Hence $\psi^* = c\psi$; $c = \text{const.}$

$\Longrightarrow \psi = c^*\psi^*$

now $\psi^*\psi = 1 \Longrightarrow |c|^2 = 1 \Longrightarrow \boxed{c = \exp(i\delta)}$ → PHASE ($\delta \in \mathbb{R}$)

If we choose $\delta = 0 \Longrightarrow c = 1$ ... then ψ is a REAL FUNCTION!

(2.) The ground state of harmonic osc. is $\psi_0(x) = \alpha e^{-\xi^2/2}$; where $\alpha = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$ and $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$ ...

a) Compute $\langle x\rangle, \langle p\rangle, \langle x^2\rangle, \langle p^2\rangle$ for the state ψ_0

b) Check the uncertainty principle

c) Compute the average kinetic energy $\langle T\rangle$ and average poten. ene. $\langle V\rangle$

Is their sum what you would expect?

→ a) $\langle x\rangle = \int_{-\infty}^{\infty}\psi^*\hat{x}\psi\,dx = \int_{-\infty}^{\infty}\alpha^2 x e^{-\xi^2}dx = \alpha^2\int_{-\infty}^{\infty} x e^{-\frac{m\omega}{\hbar}x^2}dx = 0$ → ODD FUNCTION

$\langle p\rangle = \int\psi^*\frac{\hbar}{i}\frac{d}{dx}\psi\,dx = \alpha^2\int e^{-\frac{m\omega}{2\hbar}x^2}\frac{\hbar}{i}\frac{d}{dx}\left(e^{-\frac{m\omega}{2\hbar}x^2}\right)dx =$

$= -i\hbar\alpha^2\int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2}\cdot e^{-\frac{m\omega}{2\hbar}x^2}\cdot\left(-\frac{m\omega}{\hbar}x\right)dx = im\omega\alpha^2\underbrace{\int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2}x\,dx}_{=0}$ ODD FUNCTION

$\langle x^2\rangle = \int_{-\infty}^{\infty}\psi^* x^2\psi\,dx = \alpha^2\int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2}dx = 2\alpha^2\int_0^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2}dx =$

ps. $\int_0^{\infty} x^2 e^{-ax^2}dx = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}$; for $a \geq 0$

$= 2\alpha^2\cdot\frac{1}{4}\sqrt{\frac{\pi\hbar^3}{m^3\omega^3}} = \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}\cdot\frac{\pi\hbar^3}{m^3\omega^3}} =$

$\boxed{\langle x^2\rangle = \frac{1}{2}\frac{\hbar}{m\omega}}$

$\langle p^2\rangle = \int_{-\infty}^{\infty}\psi^*\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi\,dx = -\alpha^2\int e^{-\frac{m\omega}{2\hbar}x^2}\hbar^2\frac{d^2}{dx^2}\left(e^{-\frac{m\omega}{2\hbar}x^2}\right)dx =$

$= -\hbar^2\alpha^2\int e^{-\frac{m\omega}{2\hbar}x^2}e^{-\frac{m\omega}{2\hbar}x^2}\left(\frac{m^2\omega^2}{\hbar^2}x^2 - \frac{m\omega}{\hbar}\right)dx = -\hbar^2\alpha^2\int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2}\left(\frac{m^2\omega^2}{\hbar^2}x^2 - \frac{m\omega}{\hbar}\right)dx$

$$\langle p^2\rangle = -\hbar^2\alpha^2\int_{-\infty}^{\infty}\frac{m^2\omega^2}{\hbar^2}x^2 e^{-\frac{m\omega}{\hbar}x^2} + \hbar^2\alpha^2\int_{-\infty}^{\infty}\frac{m\omega}{\hbar}e^{-\frac{m\omega}{\hbar}x^2}dx =$$

$$\boxed{\text{PS } \int_0^{\infty} e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} \quad a>0}$$

$$= \underbrace{-2\hbar^2\alpha^2\int_0^{\infty}\frac{m^2\omega^2}{\hbar^2}x^2 e^{-\frac{m\omega}{\hbar}x^2}} + \underbrace{2\alpha^2 m\omega\hbar\int_0^{\infty}e^{-\frac{m\omega}{\hbar}x^2}dx}$$

$$-2\hbar^2\alpha^2\frac{m^2\omega^2}{\hbar^2}\cdot\frac{1}{4}\sqrt{\frac{\pi\hbar^3}{m^3\omega^3}} + 2\alpha^2 m\omega\hbar\frac{1}{2}\sqrt{\frac{\pi\hbar}{m\omega}} =$$

$$= -\frac{\hbar^2 m^2\omega^2}{2\hbar^2}\sqrt{\frac{m\omega}{\pi\hbar}\cdot\frac{\pi\hbar^3}{m^3\omega^3}} + \hbar m\omega\sqrt{\frac{m\omega}{\pi\hbar}\cdot\frac{\pi\hbar}{m\omega}} = \boxed{\frac{1}{2}m\omega\hbar = \langle p^2\rangle}$$

b) $\sigma_x\sigma_p \geq \frac{1}{2}\hbar$?

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{\hbar}{2m\omega} \quad ; \quad \sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2 = \frac{1}{2}\hbar m\omega$$

$$\Rightarrow \sigma_x^2\sigma_p^2 = \frac{\hbar}{2m\omega}\cdot\frac{1}{2}\hbar m\omega = \frac{1}{4}\hbar^2 \Rightarrow \boxed{\sigma_x\sigma_p = \frac{1}{2}\hbar} \checkmark \text{ OK.}$$

c) $\langle T\rangle = \frac{\langle p^2\rangle}{2m} = \frac{1}{4}\hbar\omega$

$\langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle = \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega} = \frac{1}{4}\hbar\omega$

$$\boxed{\langle T\rangle + \langle V\rangle = \frac{1}{2}\hbar\omega} = E_0 \checkmark \text{ ok!}$$

3. a) Show that the sum of 2 Hermitian operators is Hermitian!

Def. of Hermit: $\langle f|\hat{Q}g\rangle = \langle\hat{Q}f|g\rangle \Rightarrow \hat{Q}$ is Hermit!

Suppose $\hat{H}$ and $\hat{K}$ are 2 Hermit operators ...

$\Rightarrow \langle f|\hat{H}g\rangle = \langle\hat{H}f|g\rangle$ and $\langle f|\hat{K}g\rangle = \langle\hat{K}f|g\rangle$

Now $\rightarrow \langle f|(\hat{H}+\hat{K})g\rangle = \langle f|\hat{H}g\rangle + \langle f|\hat{K}g\rangle = \langle\hat{H}f|g\rangle + \langle\hat{K}f|g\rangle =$

$= \langle(\hat{H}+\hat{K})f|g\rangle \Rightarrow$ sum $(\hat{H}+\hat{K})$ is HERMIT!

b) Suppose $\hat{Q}$ is Hermit, and α is a complex number. Under what condition (on α) is $\alpha\hat{Q}$ Hermitian?

$\Rightarrow \hat{Q}$ is Hermit $\Leftrightarrow \langle f|\hat{Q}g\rangle = \langle\hat{Q}f|g\rangle$

$$\left.\begin{array}{l}\langle f|\alpha\hat{Q}g\rangle = \langle\alpha\hat{Q}f|g\rangle = \alpha^*\langle\hat{Q}f|g\rangle \\ \quad\quad\quad\quad \| \\ \quad\quad\quad \alpha\langle f|\hat{Q}g\rangle\end{array}\right\} \Rightarrow \alpha = \alpha^* \Rightarrow \boxed{\alpha \in \mathbb{R}}!$$

[α should be Real!]

c) when is the product of 2 Hermit operators again Hermit?

$\rightarrow \langle f|\hat{H}\hat{K}g\rangle = \langle \hat{H}f|\hat{K}g\rangle = \langle \hat{K}\hat{H}f|g\rangle \Rightarrow$ to be Hermit must be true that $\hat{K}\hat{H} = \hat{H}\hat{K} \Rightarrow \boxed{[\hat{H},\hat{K}]=0}$ $\rightarrow$ COMUTATOR MUST BE ZERO!

d) show that the position operator ($\hat{x} = x$) and the Hamiltonian operator ($\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$) are Hermitian operators!

$\rightarrow \langle f|\hat{x}g\rangle = \int f^* x g\, dx = \int (xf)^* g\, dx = \langle \hat{x}f|g\rangle \Rightarrow \hat{x}$ is HERMIT!

$\rightarrow$ we can do this because x is REAL

$$\rightarrow \langle f|\hat{H}g\rangle = \int f^*\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right) g\, dx = \int f^*\left(-\frac{\hbar^2}{2m}\frac{d^2 g}{dx^2}\right)dx + \int f^* U(x) g(x)\, dx$$

now: $\int_{-\infty}^{\infty} f^* \frac{d^2 g}{dx^2} dx \rightarrow$ "per partes" $\rightarrow f^*\frac{dg}{dx}\Big|_{-\infty}^{\infty} - \int \frac{df^*}{dx}\frac{dg}{dx} dx =$

$$= \underbrace{f^*\frac{dg}{dx}\Big|_{-\infty}^{\infty}}_{=0} - \underbrace{\frac{df^*}{dx} g\Big|_{-\infty}^{\infty}}_{=0} + \int_{-\infty}^{\infty}\frac{d^2 f^*}{dx^2} g\, dx = \int_{-\infty}^{\infty}\frac{d^2 f^*}{dx^2}\cdot g\, dx$$

$\rightarrow$ because $\lim_{x\to\pm\infty} f, g = 0$

and: $\int f^* U(x) g\, dx = \int (U(x) f)^* g\, dx \rightarrow$ since $U(x)$ is REAL

$\Rightarrow \langle f|\hat{H}g\rangle = \langle \hat{H}f|g\rangle \Rightarrow$ HAMILTON is HERMIT!

19/5/15

① Consider the infinite square well of width a! Calculate the momentum representations $\phi_n(p)$ of the stationary states. Manipulate the expression so as to make it appear as a sum of two sin() functions.

$$\phi_n(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_0^a \phi_n(x)\exp[-ipx/\hbar]\, dx \quad ; \phi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

$$\Rightarrow \phi_n(p) = \frac{1}{\sqrt{\hbar}}\int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) e^{-ipx/\hbar} dx =$$

$$= \frac{\sqrt{2}}{\sqrt{ha}}\int_0^a \frac{1}{2i}\left[e^{i\frac{n\pi x}{a}} - e^{-i\frac{n\pi x}{a}}\right] e^{-ipx/\hbar} dx =$$

$$= \sqrt{\frac{2}{ha}}\cdot\frac{1}{2i}\int_0^a\left(\exp\left[i\left(\frac{n\pi}{a}-\frac{p}{\hbar}\right)x\right] - \exp\left[-i\left(\frac{n\pi}{a}+\frac{p}{\hbar}\right)x\right]\right)dx = \dots$$

$$\dots = \frac{\exp\left[i\left(\frac{n\pi}{2}-\frac{pa}{2\hbar}\right)\right]}{2i\sqrt{ha/2}}\left[\frac{\sin\left(\frac{\pi a}{2}-\frac{pa}{2\hbar}\right)}{\frac{n\pi}{2a}-\frac{pa}{2\hbar}} + (-1)^{n+1}\frac{\sin\left(\frac{n\pi}{2}+\frac{pa}{2\hbar}\right)}{\frac{n\pi}{2a}+\frac{pa}{2\hbar}}\right]$$

(2.) Prove the "uncertainty principle" relating the uncertainty in position ($\hat{A}=\hat{x}$) to the uncertainty in energy ($\hat{B}=\frac{\hat{p}^2}{2m}+V$)

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2$$

$$[\hat{A},\hat{B}] = \left[x, \frac{p^2}{2m}+V\right] = \left[x,\frac{p^2}{2m}\right]+[x,V] = \frac{1}{2m}[x,p^2]+[x,V]$$

$$[x,p^2] = xp^2-p^2x = xp^2-pxp+pxp-p^2x =$$

$$= (xp-px)p+p(xp-px) = \overbrace{[x,p]}^{=i\hbar}p+p\overbrace{[x,p]}^{=i\hbar}$$

$$= 2i\hbar p$$

So $[\hat{A},\hat{B}] = \frac{1}{2m}\cdot 2i\hbar p = \frac{1}{m}\cdot i\hbar p$

position (x) - energy (H) ?

$$\Rightarrow \langle[\hat{A},\hat{B}]\rangle = \frac{i\hbar}{m}\langle p\rangle \quad \Rightarrow \sigma_A^2\sigma_B^2 = \frac{1}{4\cancel{i^2}}\cdot\frac{\cancel{i^2}\hbar^2}{m^2}\langle p\rangle^2 \Rightarrow \boxed{\sigma_x\sigma_H = \frac{\hbar}{2m}|\langle p\rangle|}$$

20/5/15

(1.) An ANTI-HERMITIAN operator is equal to minus its hermitian conjugate $\hat{Q}^\dagger = -\hat{Q}$

a) show that the expectation value of anti-hermit is imaginary

b) show that the commutator of two hermit operators is anti-hermit. How about the commutator of two anti-hermit?

(a) $\rightarrow \langle Q\rangle = \langle\psi|Q\psi\rangle = \langle Q^\dagger\psi|\psi\rangle = -\langle Q\psi|\psi\rangle = -\langle\psi|Q\psi\rangle^*$

$\Rightarrow \langle Q\rangle = -\langle Q\rangle^* \rightarrow$ only possible if IMAGINARY!

(b) $\rightarrow [P,Q]^\dagger = (PQ-QP)^\dagger = (PQ)^\dagger-(QP)^\dagger = Q^\dagger P^\dagger - P^\dagger Q^\dagger = QP-PQ$

$= -(PQ-QP) = -[P,Q] \Rightarrow [P,Q]^\dagger = -[P,Q] \Rightarrow$ ANTI-HERMIT

$\rightarrow$ now P, Q are anti-hermit

$[P,Q]^\dagger = (PQ-QP)^\dagger = (PQ)^\dagger-(QP)^\dagger = Q^\dagger P^\dagger - P^\dagger Q^\dagger = QP-PQ = -[P,Q]$

$\Rightarrow$ commutator its again ANTI-HERMIT

② What is the most probable value of r in the ground state of Hydrogen?

$$\psi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

$$\rightarrow P(r, r+dr) = |\psi|^2 \cdot \overbrace{4\pi r^2 dr}^{=dV} = \frac{1}{\pi a^3} \cdot 4\pi r^2 \cdot e^{-2r/a} \Rightarrow p(r) = \frac{4r^2}{a^3} \cdot e^{-2r/a}$$

$$\frac{dp}{dr} = 0 \Rightarrow \frac{d}{dr}\left[\frac{4r^2}{a^3} e^{-2r/a}\right] = \frac{8r}{a^3} e^{-2r/a} + \frac{4r^2}{a^3} \cdot e^{-2r/a} \cdot \left(-\frac{2}{a}\right) =$$

$$0 = \left(\frac{8r}{a^3} - \frac{8r^2}{a^4}\right) \cdot e^{-2r/a} \Rightarrow \frac{r}{a^3} = \frac{r^2}{a^4} \Rightarrow \boxed{r = a} \; !$$

③ Show: Starting with canonical commputation relation for position and momentum, work out the following commutators! remember: $\boxed{[x, p_x] = i\hbar}$

$[L_z, x] = i\hbar y$; $[L_z, y] = -i\hbar x$; $[L_z, z] = 0$

$\vec{L} = \vec{r} \times \vec{p} \Rightarrow \boxed{L_z = x p_y - y p_x}$ ... we get this from $\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$

So... $[L_z, x] = [x p_y - y p_x, x] = [x p_y, x] - [y p_x, x]$

we apply $\rightarrow \boxed{[AB, C] = [A, C]B + A[B, C]}$

$$\Rightarrow [L_z, x] = \ldots = [x p_y, x] - [y p_x, x] = \underbrace{[x, x]}_{=0} p_y + x \underbrace{[p_y, x]}_{=0} - \underbrace{[y, x]}_{=0} p_x - y[p_x, x] =$$

$$= -y[p_x, x] = y[x, p_x] = i\hbar y \checkmark \text{ok!}$$

$$\rightarrow [L_z, y] = [x p_y - y p_x, y] = [x p_y, y] - [y p_x, y] =$$

$$= \overbrace{[x, y]}^{=0} p_y + x[p_y, y] - \overbrace{[y, y]}^{=0} p_x - y\overbrace{[p_x, y]}^{=0} = x[p_y, y] = -i\hbar x \checkmark \text{ok!}$$

$$\rightarrow [L_z, z] = [x p_y - y p_x, z] = [x p_y, z] - [y p_x, z] =$$

$$= \overbrace{[x, z]}^{=0} p_y + x\overbrace{[p_y, z]}^{=0} - \overbrace{[y, z]}^{=0} p_x - y\overbrace{[p_x, z]}^{=0} = 0 \checkmark \text{ok!}$$

now for:

1) $[L_z, p_x] = [x p_y - y p_x, p_x] = [x p_y, p_x] - [y p_x, p_x] =$

$$= [x, p_x] p_y + x\overbrace{[p_y, p_x]}^{=0} - \overbrace{[y, p_x]}^{=0} p_x - y\overbrace{[p_x, p_x]}^{=0} = +i\hbar p_y$$

2) $[L_z, p_y] = [x p_y - y p_x, p_y] = [x p_y, p_y] - [y p_x, p_y] =$

$$= \overbrace{[x, p_y]}^{=0} p_y + x\overbrace{[p_y, p_y]}^{=0} - [y, p_y] p_x - y\overbrace{[p_x, p_y]}^{=0} = -i\hbar p_x$$

3) $[L_z, p_z] = \ldots = 0$

Use this results to obtain $[L_z, L_x] = i\hbar L_y$

$$[L_z, L_x] = [L_z, y p_z - z p_y] = [L_z, y p_z] + [z p_y, L_z] =$$

$$= \underbrace{[L_z, y]}_{-i\hbar x} p_z + y\overbrace{[L_z, p_z]}^{=0} - \overbrace{[L_z, z]}^{=0} p_y - z\underbrace{[L_z, p_y]}_{-i\hbar p_x} = -i\hbar x p_z + i\hbar z p_x = i\hbar L_y \checkmark \text{ok!}$$

Evaluate the commutators $[L_z, r^2]$ and $[L_z, p^2]$; use: $r^2 = x^2 + y^2 + z^2$; $p^2 = p_x^2 + p_y^2 + p_z^2$

$\rightarrow$

$$[L_z, r^2] = [L_z, x^2] + [L_z, y^2] + \overbrace{[L_z, z^2]}^{=0} = -\overbrace{[x, L_z]}^{=-i\hbar y} x - x\overbrace{[x, L_z]}^{=i\hbar x} - \overbrace{[y, L_z]}^{=} y - y\overbrace{[y, L_z]}^{=}$$

$$= i\hbar y x + i\hbar x y - i\hbar x y - i\hbar y x = i\hbar \overbrace{[y, x]}^{=0} + i\hbar \overbrace{[x, y]}^{=0} = 0 + 0 = 0 \checkmark \text{OK!}$$

$$[L_z, p^2] = [L_z, p_x^2] + [L_z, p_y^2] + \overbrace{[L_z, p_z^2]}^{=0} = -\overbrace{[p_x, L_z]}^{=-i\hbar p_y} p_x - p_x \overbrace{[p_x, L_z]}^{=} - \overbrace{[p_y, L_z]}^{=i\hbar p_x} p_y - p_y \overbrace{[p_y, L_z]}^{=}$$

$$= i\hbar p_y p_x + i\hbar p_x p_y - i\hbar p_x p_y - i\hbar p_y p_x = 0 \checkmark \text{OK!}$$

Show that the Hamiltonian $H = \frac{1}{2m} p^2 + V$ commutes with all three components of $\underline{L}$!

because V is function of r^2 and $[L_x, r^2] = 0$!

$$[L_x, H] = \frac{1}{2m} \overbrace{[L_x, p^2]}^{=0} + \overbrace{[L_x, V]}^{=0} = \ldots = 0$$

so H, L_z, L^2 are mutually compatible observables!

(4.) Consider ∞-$\square$ well of width a and the wave-function $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\left[|\phi_1\rangle + |\phi_2\rangle\right]$

a) write $|\psi(t)\rangle$ using the Bohr frequency $\rightarrow \omega_{21} = \frac{E_2 - E_1}{\hbar}$

$$\rightarrow |\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{-iE_1 t/\hbar}|\phi_1\rangle + e^{-iE_2 t/\hbar}|\phi_2\rangle\right] =$$

$$= \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar}\left[|\phi_1\rangle + e^{-i(E_2 - E_1)t/\hbar}|\phi_2\rangle\right] = \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar}\left[|\phi_1\rangle + e^{-i\omega_{21} t}|\phi_2\rangle\right]$$

now: $|\phi_1\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$; $|\phi_2\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$

b) Calculate $\langle x\rangle(t)$! (start with $\langle x - \frac{a}{2}\rangle = \langle x\rangle - \frac{a}{2}$)

$$\langle x - \tfrac{a}{2}\rangle = \langle\psi|x - \tfrac{a}{2}|\psi\rangle = \frac{1}{2}\Big(\overbrace{\langle\phi_1|x - \tfrac{a}{2}|\phi_1\rangle}^{=0} + \overbrace{\langle\phi_2|x - \tfrac{a}{2}|\phi_2\rangle}^{=0} +$$

$$+ \langle\phi_1|(x - \tfrac{a}{2})e^{-i\omega_{21}t}|\phi_2\rangle + \langle\phi_2|e^{i\omega_{21}t}(x - \tfrac{a}{2})|\phi_1\rangle\Big)$$

Now...

$$\langle\phi_1|x - \tfrac{a}{2}|\phi_1\rangle \sim \int_0^a (x - \tfrac{a}{2}) \sin^2\left(\tfrac{\pi x}{a}\right) dx = 0 \rightarrow \text{integrant is ODD w.r.t. } a/2$$

$$\langle\phi_2|x - \tfrac{a}{2}|\phi_2\rangle \sim \int_0^a (x - \tfrac{a}{2}) \sin^2\left(\tfrac{2\pi x}{a}\right) dx = 0$$

$$\text{So} \rightarrow \langle x - \tfrac{a}{2}\rangle = \frac{2}{a}\int_0^a \left\{\sin\left(\tfrac{\pi x}{a}\right)(x - \tfrac{a}{2}) e^{-i\omega_{21}t} \sin\left(\tfrac{2\pi x}{a}\right) + \sin\left(\tfrac{2\pi x}{a}\right) e^{i\omega_{21}t}(x - \tfrac{a}{2}) \sin\left(\tfrac{\pi x}{a}\right)\right\} dx =$$

$$= \frac{4}{a}\int_0^a \sin\left(\tfrac{\pi x}{a}\right)\sin\left(\tfrac{2\pi x}{a}\right)(x - \tfrac{a}{2})\cos(\omega_{21}t)\, dx =$$

$$= \frac{4}{a}\cos(\omega_{21}t)\left[\int_0^a x \sin\left(\tfrac{\pi x}{a}\right)\sin\left(\tfrac{2\pi x}{a}\right) dx - \frac{a}{2}\underbrace{\int_0^a \sin\left(\tfrac{\pi x}{a}\right)\sin\left(\tfrac{2\pi x}{a}\right) dx}_{=0}\right] =$$

$$= \frac{4}{a}\cos(\omega_{21}t)\int_0^a x \sin\left(\tfrac{\pi x}{a}\right)\sin\left(\tfrac{2\pi x}{a}\right) dx =$$

$$= \frac{4}{a}\cos(\omega_{21}t)\int_0^a x\left(e^{i\pi x/a} - e^{-i\pi x/a}\right)\left(e^{i2\pi x/a} - e^{-i2\pi x/a}\right)\frac{1}{-4}\, dx =$$

$$= -\frac{1}{a}\cos(\omega_{21}t)\int_0^a x\left(e^{3i\pi x/a} + e^{-3i\pi x/a} - e^{i\pi x/a} - e^{-i\pi x/a}\right) dx =$$

$$= -\frac{1}{a}\cos(\omega_{21}t)\cdot 2\cdot\int_0^a x\left[\cos\left(\tfrac{3\pi x}{a}\right) - \cos\left(\tfrac{\pi x}{a}\right)\right] dx$$

we get... $\langle x - \frac{a}{2}\rangle = \frac{32a}{9\pi^2}\cos(\omega_{21}t) \implies \langle x\rangle(t) = \frac{32a}{9\pi^2}\cos(\omega_{21}t) + \frac{a}{2}$

c) Calculate $\langle H\rangle$ and $\langle H^2\rangle$ to estimate ΔH ... the standard deviation of the energy. Then calculate $\Delta H \cdot \frac{2\pi}{\omega}$!

$$\rightarrow \langle H\rangle = \langle\psi|H|\psi\rangle = \frac{1}{2}\Big[\underbrace{\langle\phi_1|H|\phi_1\rangle}_{=E_1} + \underbrace{\langle\phi_2|H|\phi_2\rangle}_{=E_2} + \underbrace{\langle\phi_1|H|\phi_2\rangle}_{=0} + \underbrace{\langle\phi_2|H|\phi_1\rangle}_{=0}\Big] =$$

$$= \frac{1}{2}\left[E_1 + E_2\right]$$

$$\rightarrow \langle H^2\rangle = \ldots = \frac{1}{2}\left[E_1^2 + E_2^2\right]$$

$$\rightarrow \Delta H^2 = \langle H^2\rangle - \langle H\rangle^2 = \frac{1}{2}\left[E_1^2 + E_2^2 - \frac{1}{2}E_1^2 - \frac{1}{2}E_2^2 - \frac{2}{2}E_1E_2\right] = \cancel{-E_1E_2}, \ \cancel{\Delta H = \sqrt{\Delta H^2}}$$

$$= \frac{1}{2}\left[\frac{1}{2}E_1^2 + \frac{1}{2}E_2^2 - E_1E_2\right]$$

we know for this case that $E_n \sim n^2 \Rightarrow E_2 = 4E_1$

So $\Delta H = \left[\frac{1}{4}E_1^2 + \frac{16}{4}E_1^2 - \frac{4E_1^2}{2}\right]^{1/2} = \ldots = \frac{3}{2}E_1$

Now... $\Delta H \cdot \frac{2\pi}{\omega} = \frac{3}{2}E_1 \cdot 2\pi \cdot \frac{\hbar}{\underbrace{E_2 - E_1}_{=3E_1}} = \frac{3}{2}E_1 \frac{2\pi\hbar}{3E_1} = \frac{1}{2}h$

25/5/15

① Find $\langle r\rangle$ and $\langle r^2\rangle$ for e^- in H atom ground state! Express in terms of Bohr radius. $\psi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$

$$\Rightarrow \langle r\rangle = \int_0^\infty \psi^* r \psi \, dV = \frac{1}{\pi a^3}\int_0^\infty r e^{-2r/a} dV = \frac{1}{\pi a^3}\int e^{-2r/a} r^3 \overbrace{\sin\theta \, d\theta \, d\phi}^{4\pi} dr =$$

$$= \frac{1}{\pi a^3}\cdot 4\pi \int_0^\infty r^3 e^{-2r/a} = \frac{4}{a^3}\underbrace{\Gamma(4)}_{3!=6}\cdot\left(\frac{a}{2}\right)^4 = \boxed{\frac{3}{2}a} = \langle r\rangle$$

use $\Gamma(n) = \int_0^\infty x^{n-1}e^{-x}dx$

$$\rightarrow \langle r^2\rangle = \frac{1}{\pi a^3}\cdot 4\pi\int_0^\infty r^4 e^{-2r/a} dr = \frac{4}{a^3}\cdot\underbrace{\Gamma(5)}_{4!=24}\left(\frac{a}{2}\right)^5 = \boxed{3a^2} = \langle r^2\rangle$$

b) Find $\langle x\rangle$ and $\langle x^2\rangle$ for e^- in ground state of hydrogen!

$\langle x\rangle = 0 \rightarrow$ because integrand will be odd function

$\langle x^2\rangle = \frac{1}{3}\langle r^2\rangle = a$

c) Find $\langle x^2\rangle$ in state $n=2; l=1; m=1$ ... $\psi_{211} = \frac{1}{\sqrt{\pi a}}\frac{1}{8a^2} r e^{-r/2a} \sin\theta \, e^{i\phi}$

use $x = r\sin\theta\cos\phi$ (in spherical coords)

$$\langle x^2\rangle = \frac{1}{\pi a}\frac{1}{(8a^2)^2}\int\left(r^2 e^{-2r/2a}\sin^2\theta\right) r^2\sin^2\theta\cos^2\phi \, r^2\sin\theta \, d\theta \, d\phi \, dr =$$

$$= \frac{1}{64\pi a^5}\int_0^\infty r^6 e^{-r/a} dr \int_0^\pi \sin^5\theta \, d\theta \int_0^{2\pi}\cos^2\phi \, d\phi =$$

$$= \frac{1}{64\pi a^5}\left[6!\, a^7\right]\cdot\left[\frac{16}{15}\right]\left[\pi\right] = \boxed{12a^2}$$

② Prove $[AB, C] = A[B,C] + [A,C]B$

$\rightarrow [AB,C] = ABC - CAB = ABC - ACB + ACB - CAB = A(BC-CB) + (AC-CA)B$ ✓

Show $[x^n, p] = i\hbar n x^{n-1}$ $\quad p = -i\hbar \frac{\partial}{\partial x}$

$\rightarrow [x^n, p]g = x^n p g - p x^n g = -x^n i\hbar \frac{dg}{dx} + i\hbar \frac{d}{dx}(x^n g) =$

$= -i\hbar x^n \cancel{\frac{dg}{dx}} + \cancel{i\hbar x^n \frac{dg}{dx}} + i\hbar n x^{n-1} g$ ✓ ok

Show $[f(x), p] = i\hbar \frac{df}{dx}$

$\rightarrow [f(x), p]g = -f(x) i\hbar \frac{dg}{dx} + i\hbar \frac{d}{dx}(fg) = \cancel{-i\hbar f g'} + \cancel{i\hbar f g'} + i\hbar \frac{df}{dx} g$ ✓

③ Show $\frac{d}{dt}\langle \hat{Q} \rangle = \frac{i}{\hbar}\langle [H, Q] \rangle + \langle \frac{\partial Q}{\partial t} \rangle$

$\rightarrow \frac{d}{dt}\langle \hat{Q} \rangle = \frac{d}{dt}\langle \psi | Q \psi \rangle = \langle \frac{\partial \psi}{\partial t} | Q\psi \rangle + \langle \psi | \frac{\partial Q}{\partial t} \psi \rangle + \langle \psi | Q \frac{\partial \psi}{\partial t} \rangle$

we use also schrödinger $H\psi = i\hbar \frac{\partial \psi}{\partial t}$

$\Rightarrow = -\frac{1}{i\hbar}\langle H\psi | Q\psi \rangle + \langle \psi | \frac{\partial Q}{\partial t} \psi \rangle + \langle \psi | Q H \psi \rangle \frac{1}{i\hbar}$

conjugate

$= -\frac{1}{i\hbar}\langle \psi | H Q \psi \rangle + \frac{1}{i\hbar}\langle \psi | Q H \psi \rangle + \langle \psi | \frac{\partial Q}{\partial t} \psi \rangle =$

$= -\frac{1}{i\hbar}\langle \psi | (HQ - QH)\psi \rangle + \langle \frac{\partial Q}{\partial t} \rangle = \frac{i}{\hbar}\langle [H, Q] \rangle + \langle \frac{\partial Q}{\partial t} \rangle$ ✓

④ A H atom starts out in following lin. comb of two states.

$n=2;\ l=1;\ m=1$ and $n=2;\ l=1;\ m=-1$

$\psi(r,0) = \frac{1}{\sqrt{2}}(\psi_{211} + \psi_{21-1})$

a) construct $\psi(r,t)$

b) find the expectation value for potential energy $\langle V \rangle$

a) $\rightarrow \psi(r,t) = \frac{1}{\sqrt{2\pi a}} \frac{1}{4a^2} N e^{-r/2a} \sin\theta \sin\phi\, e^{-iE_2 t/\hbar}$

b) $\rightarrow V = -e^2/4\pi\varepsilon r$

$\langle V \rangle = \int |\psi|^2 \left(-\frac{e^2}{4\pi\varepsilon r}\right) d^3r = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{2\pi a}\frac{1}{(4a^2)^2}\int N e^{-r/a} \sin^2\theta \sin^2\phi\, N^2 \sin\theta\, d\theta\, d\phi\, dr$

$a = \frac{4\pi\varepsilon_0 \hbar^2}{me^2}$

$\langle V \rangle = \frac{1}{32\pi a^5}\left(-\frac{\hbar^2}{am}\right)\underbrace{\int_0^\infty r^3 e^{-r/a} dr}_{(3!\,a^4)}\underbrace{\int_0^\pi \sin^3\theta\, d\theta}_{(4/3)}\underbrace{\int_0^{2\pi} \sin^2\phi\, d\phi}_{(\pi)}$

$\langle V \rangle = -\frac{\hbar^2}{32\pi m a^6} \cdot 3!\, a^4 \cdot \frac{4}{3} \cdot \pi \Longrightarrow \boxed{\langle V \rangle = -\frac{\hbar^2}{4\pi a^2}}$

Note: $E_1 = -\frac{\hbar^2}{8ma^2}$

$\Downarrow$

$\boxed{\langle V \rangle = -\frac{1}{2}E_1} = -6.8\,eV$

29/05/2015

① The Hamilton for a certain 3-level system is represented by the matrix: $H = \begin{pmatrix} a & 0 & b \\ 0 & c & 0 \\ b & 0 & a \end{pmatrix}$, where $a, b, c \in \mathbb{R}$ and $(a-c) \neq \pm b$!

a) If the system starts out in state $|s(0)\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, what is $|s(t)\rangle$?

$\Rightarrow$ we have to find eigen-value of this matrix!

The eigen-values of H are $\boxed{E_1 = c;\ E_2 = a+b;\ E_3 = a-b}$

Now for eigen-vectors $H\lambda = E\lambda$ where $\lambda = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow$

$\Rightarrow$ normalized eigen-vectors are $\boxed{|s_1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix};\ |s_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix};\ |s_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}}$

So system starts in $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ state $\Rightarrow |s_1\rangle$ state $\Rightarrow E_1 = c$! $\quad |s(0)\rangle = |s_1\rangle$

$\Rightarrow \cancel{|s(t)\rangle = |s_1\rangle}\ \boxed{|s(t)\rangle = e^{-ict/\hbar}|s_1\rangle} = e^{-ict/\hbar}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

b) If the system starts in $|s(0)\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, what is $|s(t)\rangle$?

Note: $\boxed{|s(0)\rangle = \frac{1}{\sqrt{2}}\left(|s_2\rangle - |s_3\rangle\right)}$

$$\Rightarrow |s(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_2t/\hbar}|s_2\rangle - e^{-iE_3t/\hbar}|s_3\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-i(a+b)t/\hbar}|s_2\rangle - e^{-i(a-b)t/\hbar}|s_3\rangle\right) =$$

$$= \frac{1}{2}\left[e^{-i(a+b)t/\hbar}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} - e^{-i(a-b)t/\hbar}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}\right]$$

$$\Rightarrow |s(t)\rangle = \frac{1}{2}e^{-iat/\hbar}\begin{pmatrix} e^{-ibt/\hbar} - e^{+ibt/\hbar} \\ 0 \\ e^{-ibt/\hbar} + e^{+ibt/\hbar} \end{pmatrix} = \frac{1}{2}e^{-iat/\hbar}\begin{pmatrix} -i\sin(bt/\hbar) \\ 0 \\ \cos(bt/\hbar) \end{pmatrix}$$

② Suppose a spin $\frac{1}{2}$ particle in state $\chi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix}$ ... what are the probabilities of getting $+\hbar/2$ and $-\hbar/2$ if we measure S_z?

~~remark~~ $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \end{pmatrix} = a\chi_+ + b\chi_-$

$S_z\chi_+ = +\frac{\hbar}{2}\chi_+$ and $S_z\chi_- = -\frac{\hbar}{2}\chi_-$ ... so probability of getting $+\frac{\hbar}{2}$ is $|a|^2$ and of getting $-\frac{\hbar}{2}$ is $|b|^2$ ...

Now $\chi = \frac{1+i}{\sqrt{6}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{\sqrt{2}}{\sqrt{3}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow a = \frac{1+i}{\sqrt{6}}$ and $b = \frac{\sqrt{2}}{\sqrt{3}}$

So for $+\frac{\hbar}{2} \rightarrow$ probability is $\left(\left|\frac{1+i}{\sqrt{6}}\right|\right)^2 = \frac{1}{3}$

and for $-\frac{\hbar}{2} \rightarrow$ probability is $= \frac{2}{3}$

PS: you must into account that must be normalized!

③ Prove that for a particle in potential $v(\vec{r})$ the rate of change of expectation value for angular momentum $\vec{L}$ is equal to expectation value of torque $\rightarrow \frac{d}{dt}\langle L\rangle = \langle N\rangle$; where $\vec{N} = \vec{r}\times(-\nabla v)$!

remember: $\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [H, Q]\rangle + \langle \frac{\partial Q}{\partial t}\rangle$

$\rightarrow \frac{d}{dt}\langle L_x\rangle = \frac{i}{\hbar}\langle [H, L_x]\rangle$

$[H, L_x] = [\frac{p^2}{2m} + V, L_x] = \underbrace{[\frac{p^2}{2m}, L_x]}_{0} + [V, L_x] = [V, yp_z - zp_y] =$

$= [V, yp_z] - [V, zp_y] = i\hbar\left[y\frac{\partial V}{\partial z} - z\frac{\partial V}{\partial y}\right] = i\hbar\left[\vec{r}\times(\nabla v)\right]_x$

So: $\frac{d}{dt}\langle L_x\rangle = -\langle [\vec{r}\times(\nabla v)]_x\rangle$

Similar ... so $\frac{d}{dt}\langle L\rangle = \langle \vec{r}\times(-\nabla v)\rangle = \langle \vec{N}\rangle$ ✓ OK!

b) Show that $\frac{d}{dt}\langle L\rangle = 0$ for any spherically symetric potential!

(this one form of quantum statment of conservation of angular momentum)!

So $V(\vec{r}) = v(r) \Longrightarrow \boxed{\nabla v = \frac{\partial v}{\partial r}\hat{r}}$

So torque: $\langle N\rangle = (\vec{r}\times\hat{r}\frac{\partial v}{\partial r}) = 0 \Longrightarrow \frac{d}{dt}\langle L\rangle = 0$ by previous result!

④ An operator $\hat{A}$, representing observable A, has two normalized eigen-states ψ_1 and ψ_2, with eigen-values a_1 and a_2! Operator $\hat{B}$ (observable B) has 2 normalized eigen-states ϕ_1 and ϕ_2, with eigen-values b_1 and b_2! The eigen-states are related by $\psi_1 = (3\phi_1 + 4\phi_2)/5$ and $\psi_2 = (4\phi_1 - 3\phi_2)/5$ ..

a) observable A is measured and we got a_1 ... what is the state of system immediaty after?

↳ because we measured a_1 the system must be in ψ_1 state!

b) if B is now measured, what are the possible results and their probabilities?

↳ system is in $\psi_1 = \frac{3\phi_1 + 4\phi_2}{5}$ state $\Longrightarrow$ we can get b_1 or b_2

$\Longrightarrow$ for $b_1 \rightarrow \phi_1$ state $\rightarrow$ probability is $\left(\frac{3}{5}\right)^2 = \boxed{9/25}$

$\Longrightarrow$ for $b_2 \rightarrow \phi_2$ state $\rightarrow$ probability is $\left(\frac{4}{5}\right)^2 = \boxed{16/25}$

c) imediaty after we measure A again ... what are probabilities for a_1, a_2

(algebra) ... $\phi_1 = \frac{3}{5}\psi_1 + \frac{4}{5}\psi_2$; $\phi_2 = \frac{4}{5}\psi_1 - \frac{3}{5}\psi_2$

if the system was before in ϕ_1 state $\Rightarrow P_{\phi_1}(a_1) = 9/25$; if was in ϕ_2 state $\Rightarrow P_{\phi_2}(a_1) = 16/25$

$\rightarrow P(a_1) = P(\text{in}\,\phi_1)\cdot P_{\phi_1}(a_1) + P(\text{in}\,\phi_2)\cdot P_{\phi_2}(a_1) = \frac{9}{25}\cdot\frac{9}{25} + \frac{16}{25}\cdot\frac{16}{25} = 327/625 \approx 0'5232$

(5) An electron is in the state $\chi = A\begin{pmatrix}3i\\4\end{pmatrix}$.

a) Determine the normalization coefficient A!

b) Find the expectation value for S_x, S_y and S_z!

a) $\rightarrow A = 1/5$ ... because $\chi^*\chi = 1 \Rightarrow |A|^2 (-3i, 4)\cdot\begin{pmatrix}3i\\4\end{pmatrix} =$

$$= |A|^2(9+16) = |A|^2\cdot 25 = 1 \Rightarrow |A|^2 = \frac{1}{25} \Rightarrow |A| = 1/5$$

b) REMEMBER: $S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$; $S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}$; $S_z = \frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$$\Rightarrow \langle S_x\rangle = \chi^* S_x \chi = \frac{1}{25}\cdot\frac{\hbar}{2}\cdot(-3i, 4)\begin{pmatrix}0&1\\1&0\end{pmatrix}\cdot\begin{pmatrix}3i\\4\end{pmatrix} =$$

$$= \frac{\hbar}{50}(-3i, 4)\cdot\begin{pmatrix}4\\3i\end{pmatrix} = \frac{\hbar}{50}[-12i + 12i] = \boxed{0}!$$

$$\Rightarrow \langle S_y\rangle = \chi^* S_y \chi = \frac{1}{25}\frac{\hbar}{2}(-3i, 4)\begin{pmatrix}0&-i\\i&0\end{pmatrix}\begin{pmatrix}3i\\4\end{pmatrix} =$$

$$= \frac{\hbar}{50}(-3i, 4)\cdot\begin{pmatrix}-4i\\-3\end{pmatrix} = \frac{\hbar}{50}[-12 - 12] = -\frac{24}{50}\hbar = \boxed{-\frac{12}{25}\hbar}!$$

$$\Rightarrow \langle S_z\rangle = \chi^* S_z \chi = \frac{1}{25}\frac{\hbar}{2}(-3i, 4)\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}3i\\4\end{pmatrix} =$$

$$= \frac{\hbar}{50}(-3i, 4)\cdot\begin{pmatrix}3i\\-4\end{pmatrix} = \frac{\hbar}{50}[9-16] = \boxed{-\frac{7}{50}\hbar}!$$