Chapter 5

Multiple Particle Systems, Identical Particles, & The Symmetrization Principle

Hm, tricky.

1) Generalizing the Sch. Eq. for Multiple Particles

— How to do this is another one of those micropostulates of QM.

My term for those tricks needed to develop QM beyond the 6 or so postulates that some QM books start out with (e.g., CT-215-222). Some are NOT ~~so minor~~ micro — like the symmetrization postulate (symmetrization principle) (CT-1386)

Well every particle gets its own label. For n particles

e.g., 1, 2, ... , n

If the particles are distinct, you really can identify them ~~and say this~~ experimentally and say this is particle 1 or particle 2.

If identical particles, you can if they are dynamically distinct (i.e., their wave functions do NOT overlap).

If they are identical and their wave functions overlap, you cannot really identify them (the symmetrization principle itself rules this out).

But we can still "formally" label them.

By can "formally", I mean when you do this the formalism works (i.e., it predicts the right behavior).

The Sch. eqn.

becomes

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

where

$$\Psi = \Psi(\underset{\sim}{r}_1 m_1, \underset{\sim}{r}_2 m_2, \ldots, \underset{\sim}{r}_N m_N)$$

digress on spin to p. 5-8

This is the spatial representation of the state

spatial coordinate of particle 1

spin coordinate of particle 1

Say you have a spin s particle

s is the spin quantum number

the total spin angmom. squared is $s(s+1)\hbar^2$

which is an invariant for the particle.

e.g., for an electon $s = \frac{1}{2}$

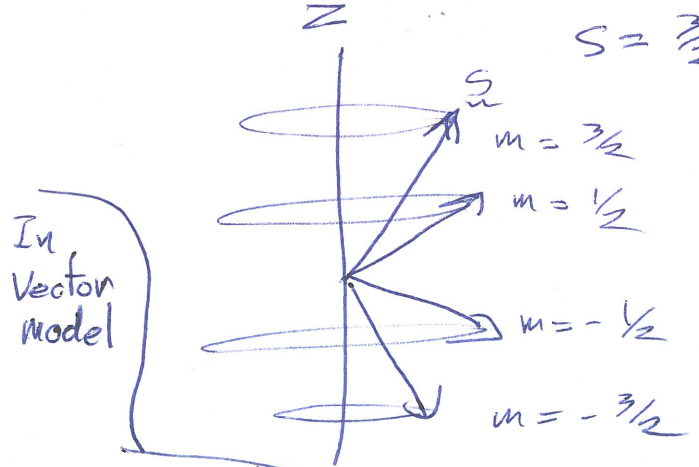
and $s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$

If you've chosen a z-axis, then spin z eigenstates have possible values

$m = -s, -s+1, \ldots, s-1, s$

or $2s+1$ values in total.

In the vector model of ang. mom. (ER-258, 283) which is useful for understanding QM ang mom, e.g.



$$\left| m_{\substack{(max)\\(min)}} \right| = s < \sqrt{s(s+1)}$$

So having $\underline{s}$ aligned with z-axis is NOT an allowed QM state.

So a spin 1/2 up state is ~~up~~ not totally up. ~~up~~

$\theta = \sin^{-1}(1/\sqrt{3}) \cong 35^\circ$ $\quad \frac{1}{2}$ $\quad \sqrt{\theta}$ $\quad \sqrt{3/4} = \sqrt{3}/2$

Which is a remarkable QM feature.

Recall also that if you are in z-axis m eigenstate, you have a definite z-component of angular momentum, but you can't then be in a definite x- or y-component of angular momentum (ie, be in a ~~definite~~ pure x or y ang. mom. eigenstate)

J_x, J_y, J_z

generic ang. mom. observables

L_x, L_y, L_z for orbital angular mom.

S_x, S_y, S_z for spin angular mom.

are incompatible observables.

They do NOT commute

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and have uncertainty relations

(CT-645)

$$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k$$

not an index — the imaginary unit

Einstein summation on k (sum on repeated index is the Einstein summation rule. The summation is suppressed. It's very elegant an essential in General Relativity)

The Fact that we use the z-axis eigenstates does NOT mean we cannot give any spin state in terms of the z-axis eigenstates.

They are a complete set.

Consider spin 1/2 particles and spinor representation

$$\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Any spinor χ can be expanded in this two

$$\chi = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

An angle in 3-d space is specified by 2-coordinates (θ, ϕ) and so spin of a given size can have its orientation specified by two unit vectors.

So for instance, eigenstates of x-axis & y-axis can be represented by $\chi_{\frac{1}{2}}$ and $\chi_{-\frac{1}{2}}$ in linear combination.

end digression on spin

Sch. eq. again

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t} .$$

Curly brackets mean = set of "

What's H?

$$H = \sum_i -\frac{\hbar^2}{2m_i} \nabla_i^2 + V(\{r_i\})$$

Each particle i gets its own kinetic energy operator

$$-\frac{\hbar^2}{2m_i}\nabla_i^2$$

m_i: mass of particle i

∇_i^2: Laplacian for particle i (Wik)

$V(\{\underset{\sim}{r}_i\})$ is the joint potential.

— which in general can be immensely complex

— all kinds of interparticle forces and external forces too.

I've suppressed any spin energy operators for simplicity.

The wave function

$$\psi(\underset{\sim}{r}_1 m_1, \ldots \underset{\sim}{r}_n m_n)$$

is as always a probability amplitude

$$|\psi(\underset{\sim}{r}_1, m_1, \ldots, \underset{\sim}{r}_n m_n)|^2$$

is the probability density

for "measuring"

particle 1 at $\underset{\sim}{r}$ in z-state m_1

particle 2 at $\underset{\sim}{r}$ in z-state m_2

⋮

need to multiply by $dx_1 dx_2 \ldots$ to get probability for the "hyper box" $dx_1 dy_2 \ldots dz_n$

I put "measuring" in quotes because "measurement" is funny in QM as we all know.

If you could actually carry out

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such a simultaneous measurement, then afterward the wave function would have collapsed so that particle 1 would be in the vicinity of $\vec{r}_1$ with $\uparrow$-spin state m_1, particle 2 would be ... etc.

Amplification of microscopic probabilism affects macroworld. Cobbe experiment – a radioactive source gives 10 decays/s on average, but how many occur is dictating by pure probabilism in QM theory. So you bet yourself you'll get a collie if you count more than 10 decays in a second — The whole future of human kind is now dependent on ~~on~~ ~~coin~~ an intrinsically random process – Such amplification of QM randomness probably goes on all the time – even in our brains.

You had to use new forces to bring about the wave function collapse

Wave function collapse being one of the mysteries of QM.

— It makes QM probabistic.

— The Sch. eq. itself is pure deterministic.

Quantum decoherence theory (which we will NOT go into)

Environmental perturbations cause interference (or entanglement) between states to damp out. The non-interfering states continue to evolve without collapse. One has the many-worlds hypothesis in which a quasi-infinity of parallel worlds come into existence every instant. But we were totally disconnected from all but the one we are in. Wave function collapse could be added to decoherence to kill off alternative worlds.

- explains how wave function collapse appears to happen.
- I believe the theory is now consensus accepted theory. (Could be wrong)
- But it doesn't actually say if wave function collapse happens or not.

Maybe it never does — the many worlds hypothesis.

- In usual practice ~~general~~, I think experience tells you when to break off a Sch. eqn. calculation and calculate probabilities.
- Decoherence theory probably allows you to know when → if you could solve it.

But even without collapse the probality density is still very useful.

↳ In usual QM interpretation a particle is in a continuum superposition of positions and discrete ~~spin~~ ~~state~~ superposition of spin states.

↳ the probability density allows one to calcalate the effects of this spread-outedness.

— e.g., the charge distribution in an atom which is needed to calcalate the potential in the atom which is needed to calculate

the atomic wave function
which is needed to ....
and so on.

High accuracy
↳ Solutions of atoms beyond hydrogen require iterative calculations ⟶ you assume initial wave function, calculate the potential, calculate the new wave functions, and so on until a self consistent solution emerges.

Such a self-consistent solution just assuming the Pauli exclusion principle (which we'll get too soon)

is a Hartree calculation (ER-320)

- assuming full symmetrization is a Hartree-Fock calcution (ER-322)

I don't think either obtain the highest accuracy of modern many-body theory (Lindmilla?)

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As always the wave function must be normalized.

— the totall probability of finding all the particles somewhere in some spin state must be 1

Probability density for measuring particle 1 at $\vec{r}_1$ with m_1 in $\rho = \sum_{m_2 m_3 \cdots m_n} \int |\psi|^2 d\tau_2 \cdots d\tau_n$

$$\sum_{m_1 m_2 m_3 \cdots m_n} \int_1 \int_2 \cdots |\psi(\vec{r}_1, m_1, \ldots \vec{r}_n m_n)|^2 d\tau_1 \cdots d\tau_n$$

(Baym - 390)

summing over spin coordinates is rather tedious which is why among many other good reasons people like to use the spinor representation

I have to confess, I'm ignorant of how one

uses spinor representation
for general wavefunctions

But if you can represent
the wave function as
a product of single particle
wave functions
or a sum of products
of single particle
wave functions

(and CT-1378 hints
that you can, but grows
coy as QM textbook authors
often do on obvious
~~Poss~~ questions)

then using spinors to
evaluate probabilities and
expectation values
is straightforward.

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Example consider one spin 1/2 particle.

One could write the wave function

$$\Psi(\underset{\sim}{r}, m) = \begin{cases} \Psi(\underset{\sim}{r}, \frac{1}{2}) & \text{up state part} \\ \Psi(\underset{\sim}{r}, -\frac{1}{2}) & \text{down state part} \end{cases}$$

In spinor form

$$\underset{\sim}{\Psi} = \begin{pmatrix} \Psi_{\uparrow}(\underset{\sim}{r}) \\ \Psi_{\downarrow}(\underset{\sim}{r}) \end{pmatrix}$$

If the spin state is position-independent

$$\underset{\sim}{\chi} = \Psi(\underset{\sim}{r}) \begin{pmatrix} a \\ b \end{pmatrix}$$

and if ~~def~~ pure up or down

$$\Psi(\underset{\sim}{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \Psi(\underset{\sim}{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

So

$$|\underset{\sim}{\psi}|^2 = \underset{\sim}{\psi}^\dagger \cdot \underset{\sim}{\psi}$$

$$= \left(\psi_\uparrow^*(\underset{\sim}{r}),\ \psi_\downarrow^*(\underset{\sim}{r})\right) \begin{pmatrix} \psi_\uparrow(\underset{\sim}{r}) \\ \psi_\downarrow(\underset{\sim}{r}) \end{pmatrix}$$

$$= |\psi_\uparrow|^2 + |\psi_\downarrow|^2$$

same as sum on m_s

$$1 = \int \left(|\psi_\uparrow|^2 + |\psi_\downarrow|^2\right) d\underset{\sim}{r}$$

Example 1 with a sum on single particle states.

$$\underset{\sim}{\psi} = a\,\psi_a(\underset{\sim}{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\,\psi_b \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\underset{\sim}{\psi}|^2 = |a|^2 |\psi_a|^2 + a^* b \psi_a^* (1\ 0) \cdot \psi_b \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$+ b^* a\, \psi_b^* (0\ 1) \cdot \psi_a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + |b|^2 |\psi_b|^2$$

$$= |a|^2 |\psi_a|^2 + |b|^2 |\psi_b|^2$$

since the up and down states are orthonormal

$$\int |\underset{\sim}{\psi}|^2 dv = |a|^2 + |b|^2$$

assuming ψ_a and ψ_b are normalized.

For $\underset{\sim}{\psi}$ to be normalized

$$|a|^2 + |b|^2 = 1$$

Example 2

Consider the product state

$$\underset{\sim}{\psi}(\underset{\sim}{r}_1, \underset{\sim}{r}_2) = \psi_a(\underset{\sim}{r}_1)\begin{pmatrix} a \\ a' \end{pmatrix}_1 \psi_b(\underset{\sim}{r}_2)\begin{pmatrix} b \\ b' \end{pmatrix}_2$$

The 1-spinor always ~~dot product~~ inner products with the 1-spinor and the 2-spinor with the 2-spinor.

This is how the sums on each spin coordinate are done in spinor representation.

$$|\underline{\Psi}(\underline{r}_1, \underline{r}_2)|^2 = |\Psi_a|^2 (a^*, a'^*) \begin{pmatrix} a \\ a' \end{pmatrix} |\Psi_b|^2 (b^* b'^*) \begin{pmatrix} b \\ b' \end{pmatrix}$$

assume normalized

$$= |\Psi_a|^2 |\Psi_b|^2$$

$$\iint |\Psi_a(\underline{r}_1)|^2 |\Psi_b(\underline{r}_2)|^2 d\underline{r}_1 d\underline{r}_2$$

$$= \int |\Psi_a(\underline{r}_1)|^2 d\underline{r}_1 \int |\Psi_b(\underline{r}_2)|^2 d\underline{r}_2$$

$$= 1 \cdot 1 = 1$$

if Ψ_a and Ψ_b are both normalized.

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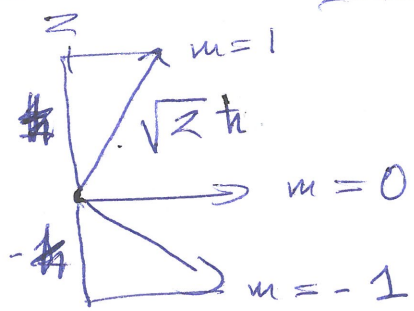
Example 3 A sum of product states.
(assuming space & spin states decoupled)

$$\psi = \psi_a(\underline{r}_1)\psi_b(\underline{r}_2)\frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 \pm \begin{pmatrix}0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2\right]$$

Vector Model + case is the ~~m = 0~~ $s=1,\ m=0$ solution of the triplet solution of adding two spins (Gr - 185)



- case is the $s=0,\ m=0$ or singlet solution of adding two spins.

What makes two spins "add".

- Some interaction between spins (usually there magnetic moments) will give singlet & triplet solutions different energies
- they are ~~eigenstates~~ stationary states of that interaction with different energies

~~Some~~

- pretty often it seems perturbations cause mixed states to decay stationary states

→ vague but then ~~some~~ textbooks grow coy on this obvious question.

- An external ~~potential~~ potential may define a z-axis and make the triplet states energy ~~dif~~ separated ~~energy~~ stationary states.

and then the system often like to sit in one triplet state or another.

If there are no interactions at all, the triplet-singlet solutions still form a complete set for the 4-dimensional ~~state~~ space and

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random state the spins are in can be expanded in the triplet-singlet solutions

$$|\psi|^2 = |\psi_a(\underset{\sim}{r}_1)|^2 |\psi_b(\underset{\sim}{r}_2)|^2$$

$$* \frac{1}{2}\Big[(1,0)_1 \begin{pmatrix}1\\0\end{pmatrix}_1 (0,1)_2 \begin{pmatrix}0\\1\end{pmatrix}_2$$

vanish by orthogonality

$$\left\{ \begin{array}{l} \pm (1,0)_1 \begin{pmatrix}0\\1\end{pmatrix}_1 (0\ 1)_2 \begin{pmatrix}1\\0\end{pmatrix}_2 \\ \pm (0,1)_1 \begin{pmatrix}1\\0\end{pmatrix}_1 (1,0)_2 \begin{pmatrix}0\\1\end{pmatrix}_2 \end{array} \right.$$

$$+ (0,1)_1 \begin{pmatrix}0\\1\end{pmatrix}_1 (1,0) \begin{pmatrix}1\\0\end{pmatrix}_2 \Big]$$

$$= |\psi_a(\underset{\sim}{r}_1)|^2 |\psi_b(\underset{\sim}{r}_2)|^2 \frac{1}{2}(1+1)$$

$$= |\psi_a(\underset{\sim}{r}_1)|^2 |\psi_b(\underset{\sim}{r}_2)|^2$$

$$\int |\underset{\sim}{\psi}|^2 d\underset{\sim}{r}_1 d\underset{\sim}{r}_2 = \int |\psi_a(\underset{\sim}{r}_1)|^2 d\underset{\sim}{r}_1 \int |\psi_b(\underset{\sim}{r}_2)|^2 d\underset{\sim}{r} = 1 \cdot 1 = 1$$

if ψ_a and ψ_b are normalized.

For expectation values for spinors you use the matrix operator.

Each particle in a system has its own individual matrix operator.

e.g. $\chi = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 \pm \begin{pmatrix}0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2\right]$

has a

$$S_{z1} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_1 \qquad \text{(Gr-174)}$$

$$S_{z2} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_2$$

To find the total z expectation value use $S_z = S_{z1} + S_{z2}$

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Each matrix acts only on its own spinor

(It's just the formalism that works — just accept it)

Actually the triplet-singlet solution are eigenvectors of S_z

$$S_z \chi = \frac{1}{\sqrt{2}} \left[S_{z_1} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 + S_{z_2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 \right.$$

$$\left. \pm S_{z_1} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \pm S_{z_2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \right]$$

$$= \frac{\hbar}{2} \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 \right.$$

$$\left. \pm (-1) \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \pm \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \right]$$

$$= \frac{\hbar}{2} \frac{1}{\sqrt{2}} \left[0 - 0 \right] = 0$$

The eigenvalue for both $s=1, m=0$ and $s=0, m=0$ states is 0 as it should be.

We could have added the spinors another way with a bit of care

~~[redacted]~~

$$\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 + \begin{pmatrix}0\\\pm 1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2 + \begin{pmatrix}-1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 + \begin{pmatrix}0\\\pm 1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2$$

↑ decided to put factor with $\begin{pmatrix}0\\1\end{pmatrix}_1$ state

$$= \begin{pmatrix}0\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}_2 + \begin{pmatrix}0\\0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}_2$$

$$= 0$$

Note there is some trickiness in adding

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spinors and products of spinors

a) one can add

$$a\begin{pmatrix}1\\0\end{pmatrix}_1 + b\begin{pmatrix}0\\1\end{pmatrix}_1$$

{ a superposition of states of different spin for 1 particle

b) Bat

$$\times \quad a\begin{pmatrix}1\\0\end{pmatrix}_1 + b\begin{pmatrix}0\\1\end{pmatrix}_2 \quad \times$$

↳ is meaningless in the formalism (i.e., it has no meaning attached)

c) Product

$$\begin{pmatrix}1\\0\end{pmatrix}_1 \begin{pmatrix}0\\1\end{pmatrix}_2$$ makes sense.

↳ The state of two particles of different spin.

d) We can add ~~2~~ such product states

$$\frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 + \begin{pmatrix}0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2\right]$$

↳ a superposition of two two-particle states

But in spinor notation
we cannot simplify
this sum of products.
— It's already as simple
as can be made.

Probably there are other
notations which are more compact,
but they are beyond
our scope (and my knowledge)

c) We can factor though

$$\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 + \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}_2$$

$$= \left[\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right]\begin{pmatrix}0\\1\end{pmatrix}_2$$

The product of spinors
and, in fact, of all states
are <u>tensor products</u>
viewed at higher level
than we'll go into (CT-153ff)

5-28
2001 jan 01

- See Wik, Quantum entanglement
- Greenstein & Zajonc, p. 131 ff

Another Note

Entanglement & entangled states

Schrödinger's own word or at least one he emphasized in 1935

Jim NO expert on even tolerably well informed

Entanglement is when the **state** of a multi-particle system **cannot** be factored.

For example, $\Psi(\underset{\sim}{r}_1, \underset{\sim}{r}_2) = \Psi_a(\underset{\sim}{r}_1)\,\Psi_b(\underset{\sim}{r}_2)$ } product state or separable state.

is factorable

and $\Psi = \frac{1}{\sqrt{2}}\left[\Psi_a(\underset{\sim}{r}_1)\Psi_b(\underset{\sim}{r}_2) \pm \Psi_a(\underset{\sim}{r}_2)\Psi_b(\underset{\sim}{r}_1)\right]$

is not **factorable**

- Cannot be written as product of states for particle 1 and particle.

In this example the single particle states

are common to both particles.

— So the particles could be identical. (~~We'll~~ patience we'll get identical particles)

But distinct particles can be entangled too

$$\Psi = c_1 \Psi_a(\underset{\sim}{r}_1)\Psi_b(\underset{\sim}{r}_2) + c_2 \Psi_c(\underset{\sim}{r}_1)\Psi_d(\underset{\sim}{r}_2)$$

Ψ_a and Ψ_c are only states of particle 1 | Ψ_b and Ψ_d are only states of particle 2

If a state is NOT entangled, then in some cases (but not all) the particles can be dealt with separately.

If a state is entangled, one cannot fully account

for the system

by dealing with the particles in isolation. — No matter how far apart they are.

The classic thought experiment

by EPR (Einstein, Podolsky, & Rosen 1935)

I'm not actually giving their coincidence which were a bit trickier

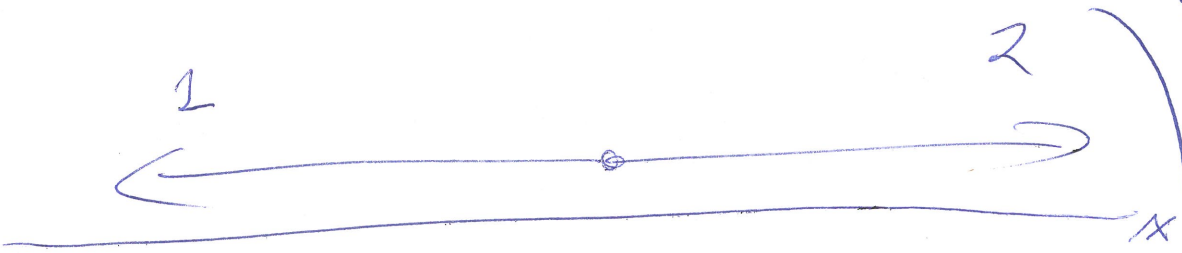
is you create two particles in an entangled spin state traveling in opposite directions

I think just writing this down is not a complete specification. One needs rules for interpreting it and some function calculus.

Spin state of system

$$\chi = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\end{pmatrix}_2 - \begin{pmatrix}0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\end{pmatrix}_2\right]$$

Singlet state $S = 0$, $m = 0$



which is a superposition state

e.g., an electron-positron pair created from 2 γ-rays.

— Before creation zero charge
zero momentum
zero ang. mom.

— after the same by conservation laws

Say you measure particle 1 spin state along some z-axis ~~on the~~ when the particles are far apart.

From the expansion itself the probability for spin up is $\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$

and that for spin down $\left(\frac{1}{\sqrt{2}}\right) = \frac{1}{2}$

If state had been $\chi = \begin{pmatrix}1\\0\end{pmatrix}_1 \begin{pmatrix}0\\1\end{pmatrix}_2$ a measurement of 1 would still have $\frac{1}{2}$ chance of being up/down. But it was up/down before before the measurement. What we have is classical ignorance of it's pre-measured state, not quantum superposition

Recall the <u>generalized Born postulate</u>.

— the expansion coefficients are the probability amplitudes

Gr-106ff

— The spatial wave function

in this general picture
is the continuous expansion
coefficient for an
expansion in
spatial eigenstates
which are Dirac Delta
functions in the ~~spatial~~ position representation itself

$$|\psi\rangle = \int d\underset{\sim}{r}' \psi(\underset{\sim}{r}') |\underset{\sim}{r}'\rangle$$

To find the coefficient for $|r\rangle$

$$\langle r|\psi\rangle = \int dr' \psi(\underset{\sim}{r}') \langle r|r'\rangle$$

$$\langle r|r'\rangle \sim \delta(x - r')$$

(CT-145)

$$= \psi(\underset{\sim}{r})$$

For discrete representations

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

and $|c_i|^2$ is the probability

of "measuring"
the system in state $|\phi_i\rangle$

- of collapsing the wave function
to that state
on a measurement
of the observable Q
of which $\Xi|\phi_i\rangle\Xi$
are the eigenstates.

- or of state $|\phi_i\rangle$
~~contributing to~~
contributing to some
effect of the uncollapsed
state.

Say particle 1 has spin up/down,
then particle 2 has spin down/up
post-wave function collapse.

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The strict QM interpretation is that before the measurement, the state the ~~was~~ was in the entangled superposition state.

Measurement of particle 1 ~~one~~ collapses it to up/down and particle 2 (unmeasured) to down/up.

instantaneous collapse in the strict QM view.

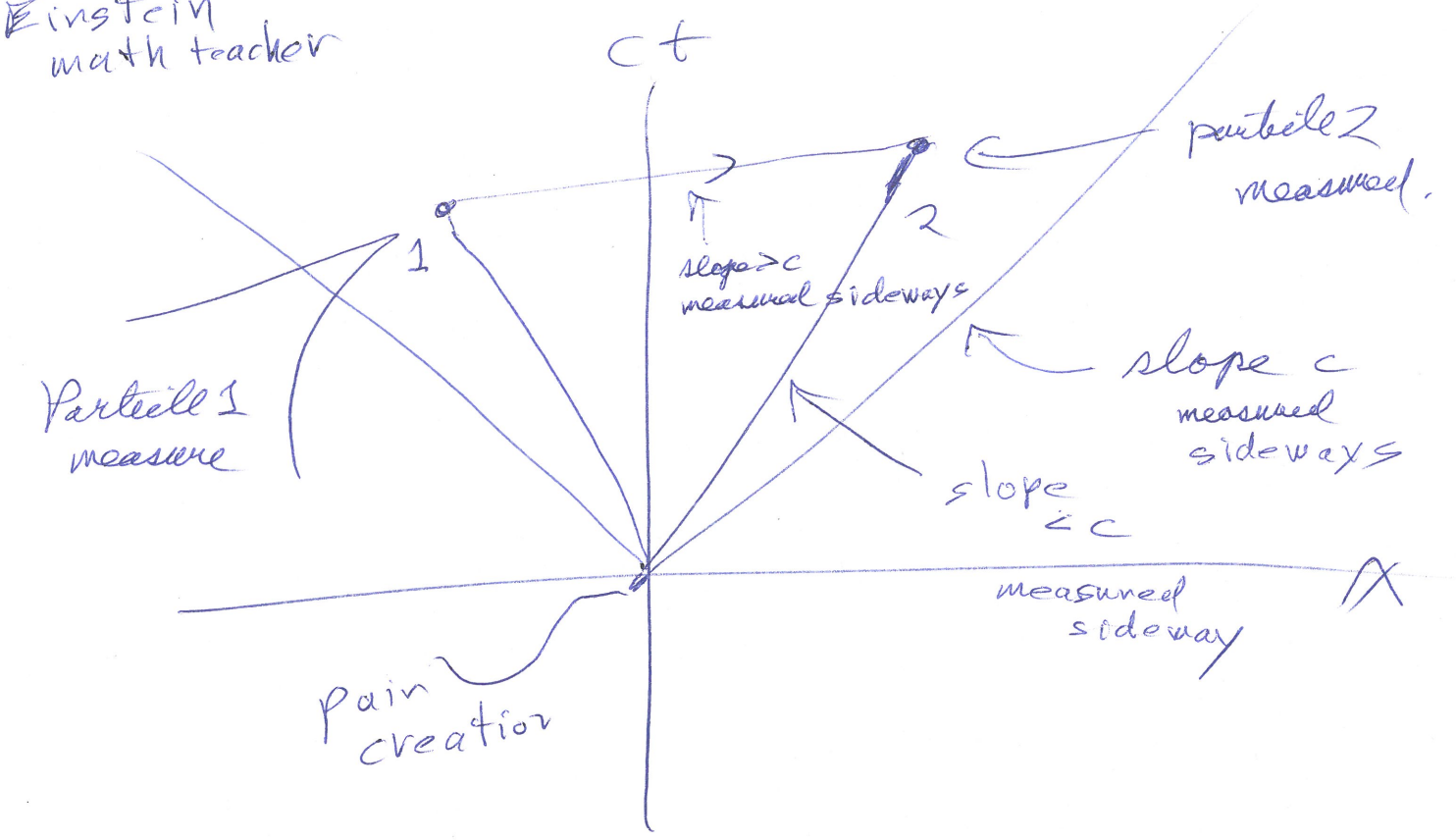
You then measure particle 2 and indeed it is down/up.

But because the particles are moving apart

their interval can be spacelike in the jargon of special relativity

Minkowski diagram

Einstein math teacher



So strict QM point of view the wave function collapse signal travels at $v = \infty$

EPR actually had some other point of interest ↓ I'm skipping some of the history, I don't know about

EPR (at least the ideal EPR maybe not the EPR of history)

that this instantaneous collapse was spooky action at a distance was spooky action at a distance (spukhafte Fernwirkung in Einstein's own words)

What they argued was yes if you measured particle 1 up/down particle 2 would be down/up

You can't know what it was and so there is still a 50-50 probability of particle 1 being up/down

but the decision to be up/down and down/up happened at the creation event

and not
thru an instantaneous
collapse at measurement
of particle 1's spin state.

~~Now at~~
At that time 1935,
there seemed no theoretical
prediction that
could distinguish the
two possibilities.
and no experiments were
done.

In the 1960s, John Bell (1928-1990)
discovered inequalities
for a more complex
variation on the EPR
experiment that
if violated

We will not go into experimental details — you can look them up.

would require
instantaneous
or at least superluminal
collapse.

At first Bell's ~~inequalities~~ Theorem (or inequalities) didn't attract a lot of attention, but in the 1970s & 1980s the experiments were done that showed that showed inequalities were violated { GZ -122

Requiring instantaneous signaling it seems.

The experimental results are incontrovertible
Now

They've been done many times with ever greater precision and distance.

Some still argue that Bell's Theorem is somehow wrong, and so the results do NOT prove instantaneous signaling.

But the consensus view of the great minds is that Bell's theorem is right.

The current record experiment (Salart et al. 2008) shows the signaling speed $v \geq 10^4 c$ which is also consistent with being instantaneous.

5-40

Given that Bell's theorem (and extensions are right) and current experiments (which must be mostly right),

— instantaneous wave function collapse of entangled states seems true.

→ and if for entangled states, no reason to doubt that wave function collapse is equally true.

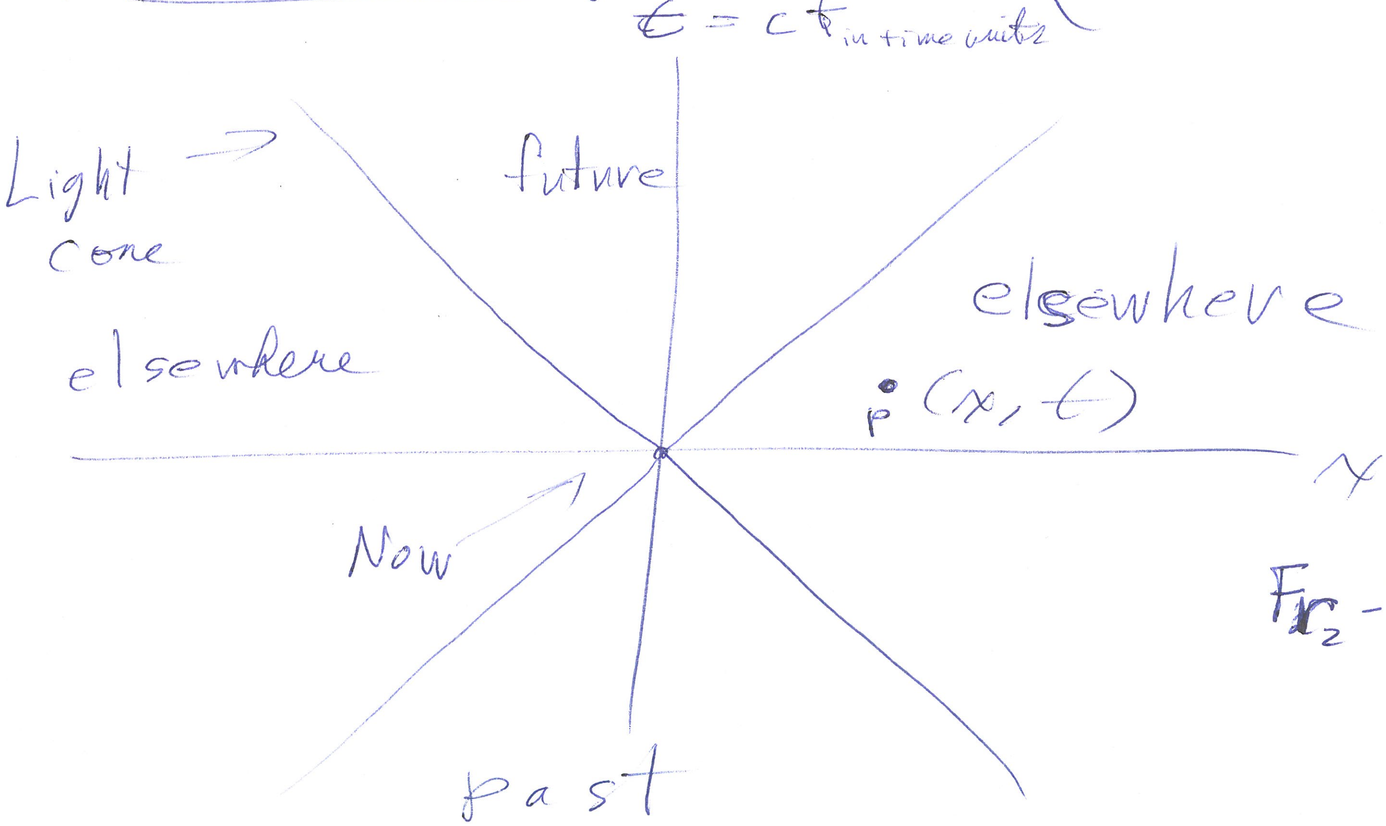
Of Course this leads to two immediate questions.

i) In what frame of reference is the collapse instantaneous or simultaneous?

Remember in special relativity (SR) simultaneity is reference frame dependent.

{ SR is so much easier if one uses $t = ct$ in time units.

<u>Minkowski diagram</u>



Fr2-118

7-92

Wkelden elsewhere

is past or future or present relative to NOW depends on the reference frame of the observer

The interval from NOW to P at (x,t) is $x^2 - t^2 = s^2 > 0$

and is space-like in SR jargon.

Well no source I can find spits out the answer explicitly; (GZ-184 bunch aside - the question with it's a no-problem answer)

{ Wik seems to fail too.

— But symmetry suggests the simultaneous collapse must be in frame of the creation event (of the 2-particle system)

ii) Is Causality violated by simultaneous collapse over space-like intervals?

The answer is No but it is tricky.

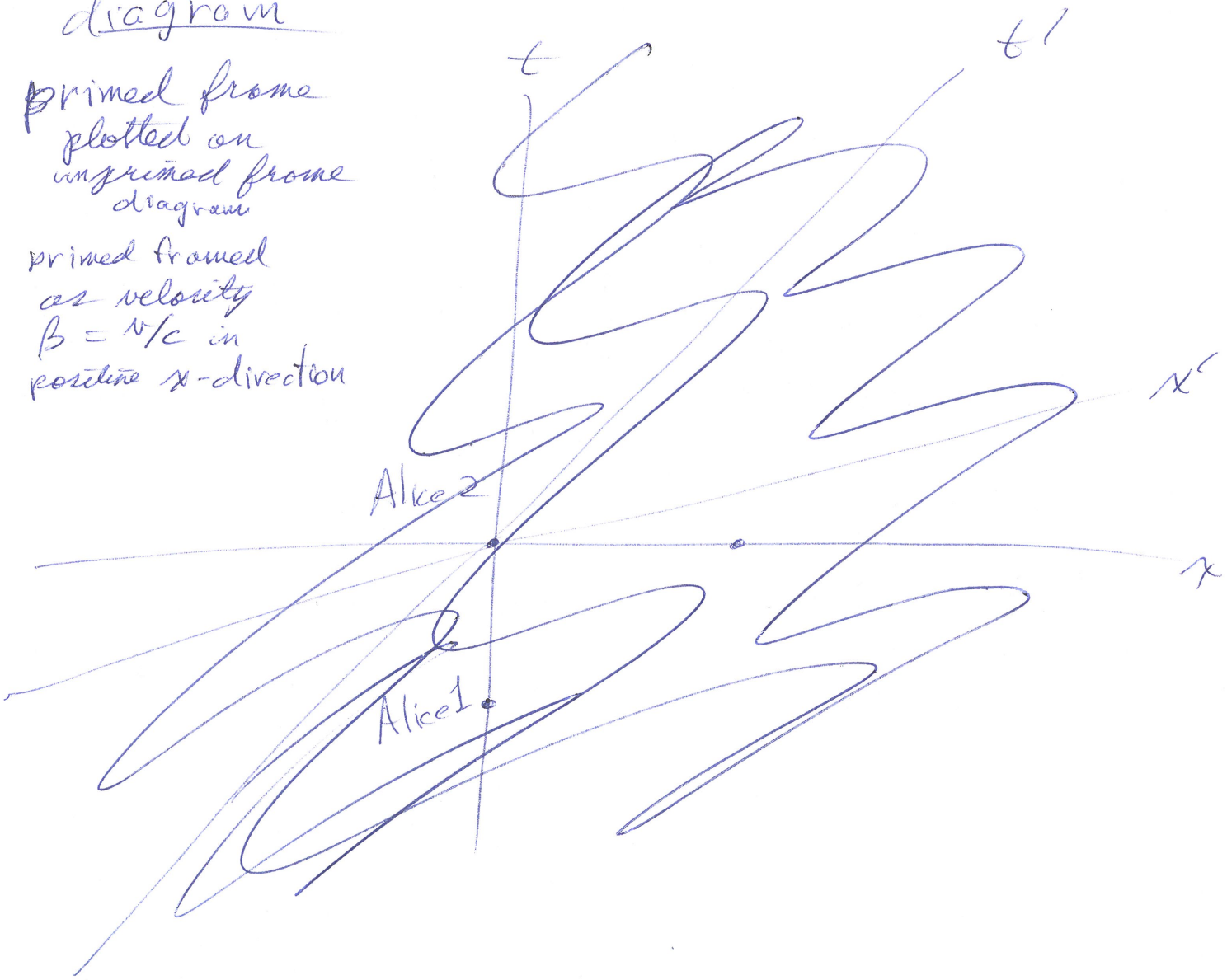
Say Alice & Bob can send send instantaneous messages in their current rest frames.

{ The two mythical experimenters of QM.

5-44

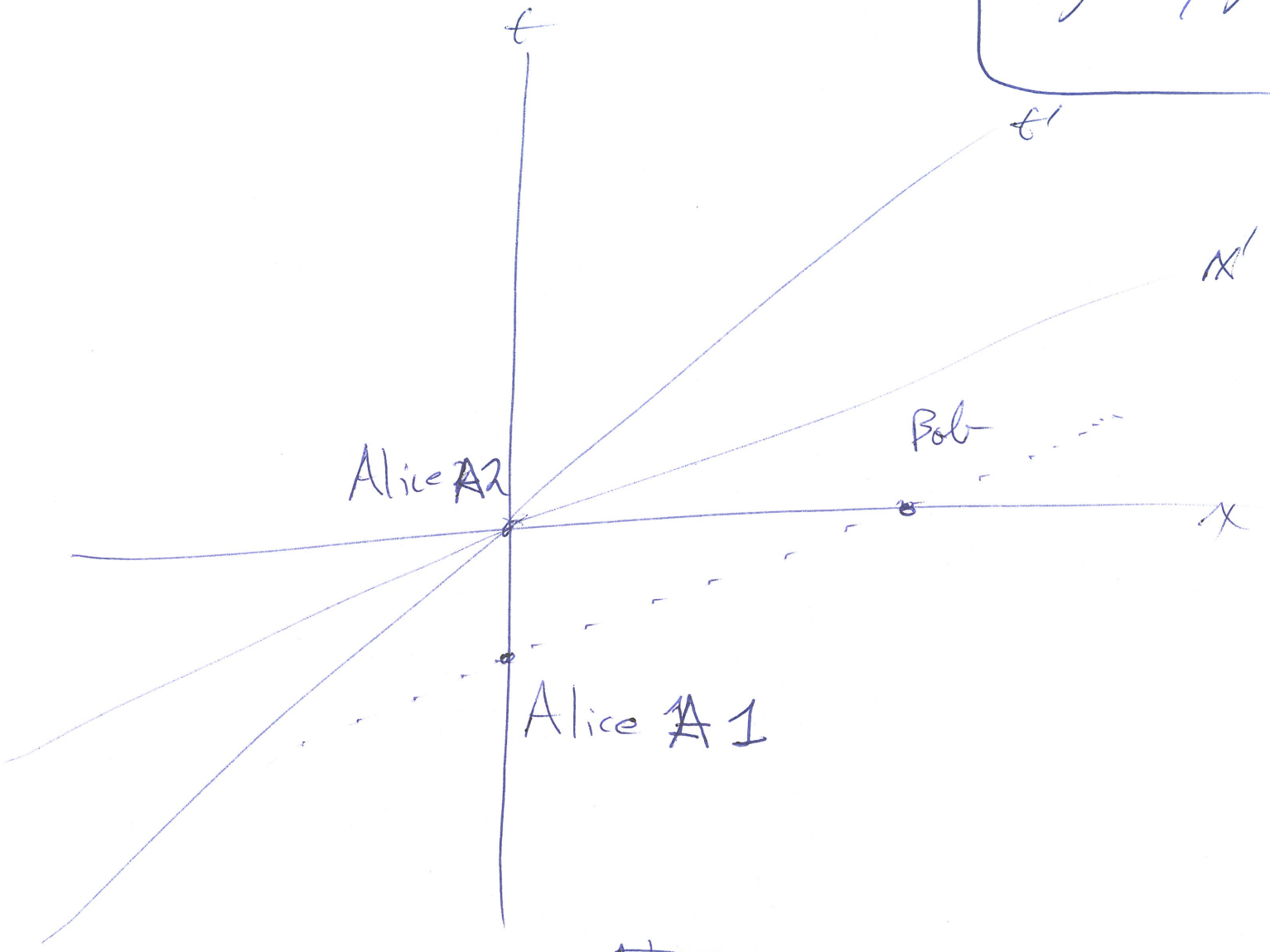
and Bob is instantaneously able to accelerate and change rest frames

Consider the following Minkowski diagram



primed frame plotted on unprimed frame diagram

primed framed as velocity $\beta = v/c$ in positive x-direction



The Scenario ~~Alice~~

a) ~~Bob~~ between A1 and A2 Alice stubs her toe badly

b) at A2 she instantly sends a message to space-like Bob "Ouch just stabbed my toe, it hurts ☹, Alice".

c) Kindly Bob jumps from the unprimed frame to the

primed frame
(or if that's too
wizard for you
forward's Alice's
message to Bob'
in the primed frame)

c) and then Bob (or Bob')
instantly sends
a message to Alice
at A1 which is
in a spacetime point
in the present of the primed frame
= Be careful you just
stubbed your toe
and it hurts," Bob"

d) Alice at A1 reads
Bob's message and
doesn't stub her
toe and doesn't send a
toe-stub message to Bob.

The effect preceding the cause

e) Later Alice
and Bob meet up
at the same point
in spacetime
and wonder
who sent the warning
message
Bob says he never received
and ~~message~~ from Alice
and never sent a warning.

Scifi writers weigh in with
possibilities

i) The stubbed Alice
& warning Bob
have been erased.

ii) The stubbed Alice and
warning Bob are
off carrying on in
an alternative universe
where Alice complains Bob
never warned her.

5-48

iii) The universe goes black on these clowns who are messing with reality.

Of course, the whole problem vanishes if we do NOT have instant messaging (actually many problems would disappear without instant messaging)

Actually (i) would seem plausible if the many-worlds hypothesis were true — bifurcations happen all the time anyway — which suggests that since we don't have instant messaging that manyworlds is false and wave function collapse is true (just saying)

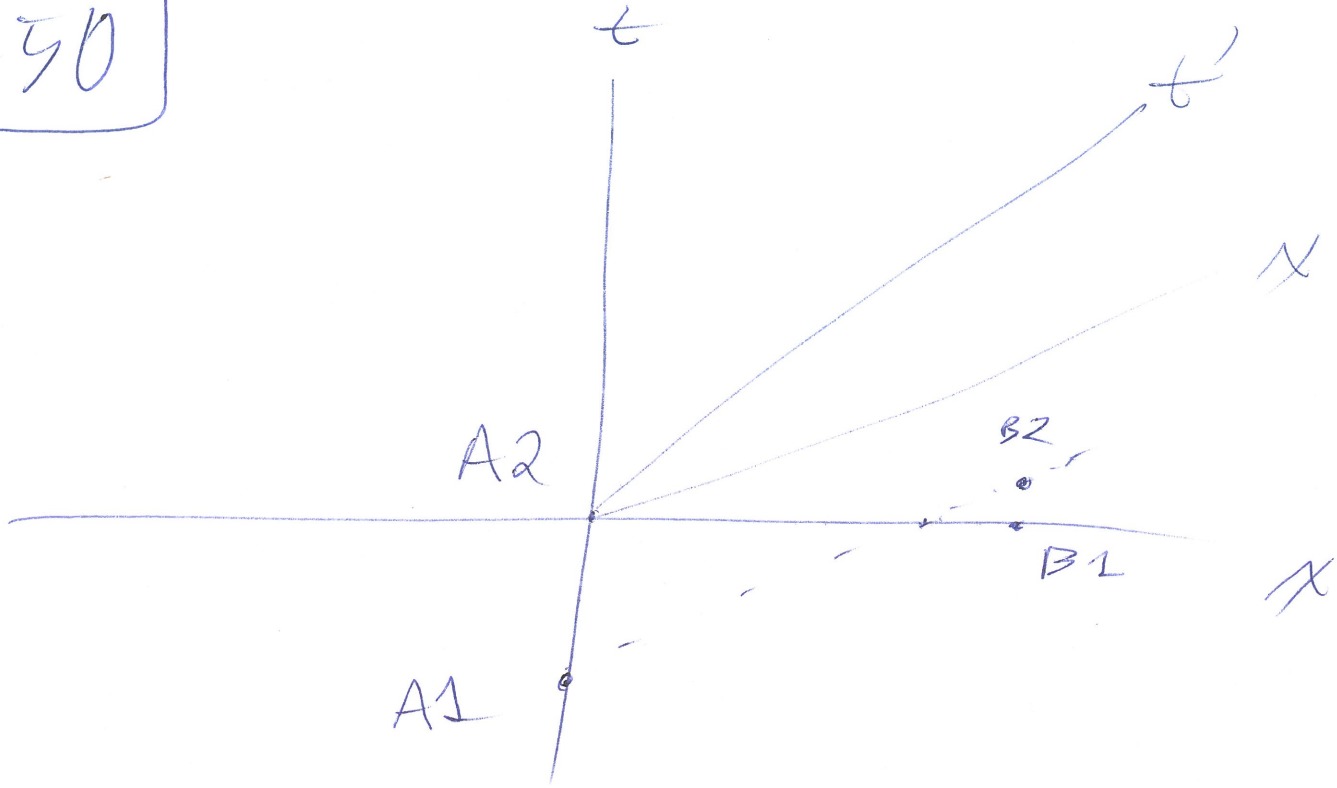
But what about with our two particle setup where ~~a not~~ an entangled state can instantly message itself.

Can causality be messed with?

No

- Remember the two-particles start out in the "PAST" since they travel at less than ~~c~~ c or c if they are photons.
- So if the particles are initiated, the measurements can be made regardless if either Bob or Alice tries to measure the spins

t-50



a) Alice at A1 measures a spin up ~~It is up.~~

b) ~~Bob~~ She knows Bob at B2 will measure spin down

Bob at B2 is in the prime frame and in that frame measures spin down at the same instant as Alice at A1

b) Alice at A2 measures spin up again and knows Bob at B1 will measure spin down.

5-91

But her measurements were had up and down with equal probability

~~Thus~~ — There is no way she could have alerted Bob at B1 that he would measure spin down at B2.

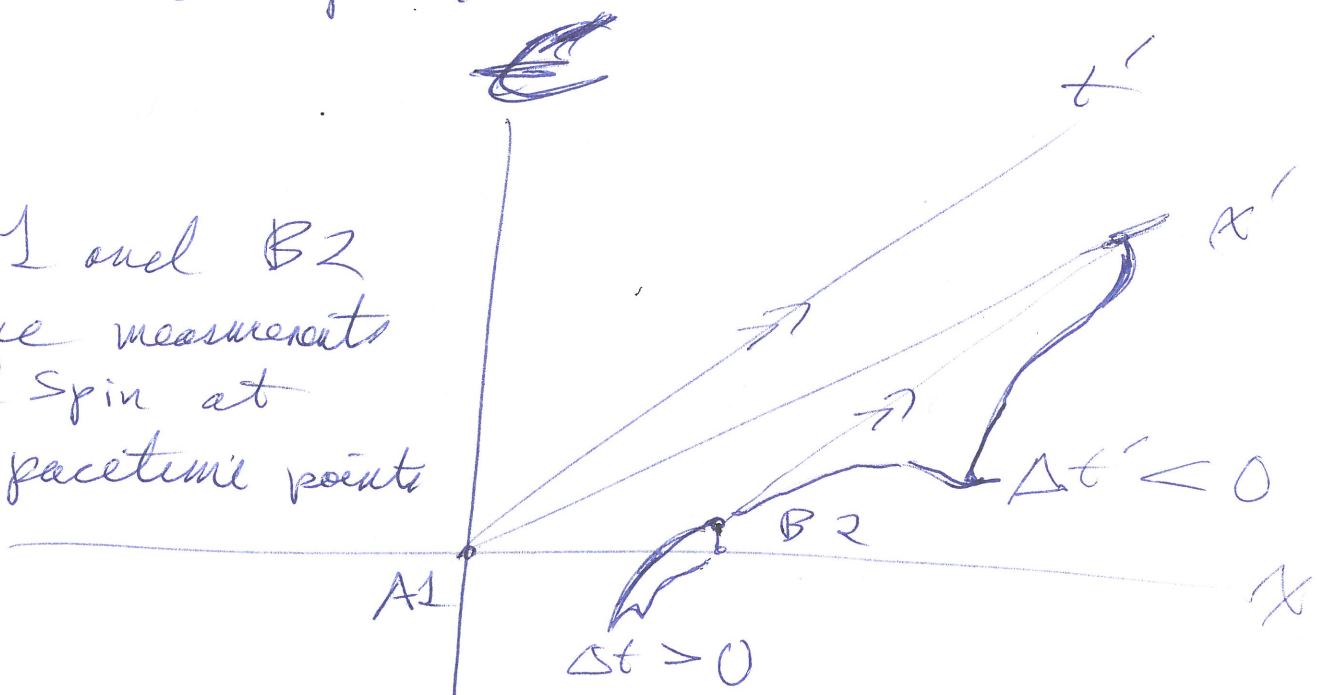
(Maybe she was desperate too. Maybe Bob had threatened suicide if measured spin down at B2.)

We could go on with such scenarios.

But others have done that.

No ways to change the past exist.

It's true though ~~that each observer~~ that sets of observers in a primed frame would come to different conclusions who initiated the collapse.



The unprimed observers see the measurement at A1 before that at B2.

The primed observers see the measurement at B2 before that at A1.

So there's a degree of causality confusion.

But Which event caused the other.

— In ordinary special relativity neither since the interval is spacelike.

a) But in the QM picture it seems like cause-and-effect can sometimes be frame dependent.

b) Note that if nonlocal entangled collapse is ruled out (by Bell's theorem shown to be wrong for example)

5-54)

then this oddity could be ~~avoided too~~ avoided (but not necessarily due to be) dismissed.

Neither measurement at A1 or B2 were causes, both were effects — the causes happened in the PAST when the particles system was created.

~~I don't feel~~

At present though Bell's theorem ~~stands~~ is thought correct.

But if Bell's theorem were ~~correct~~ incorrect, then (a) & (b) would both be possible and (b) preferred only since it seems more consistent with reality as we think we know it.

2) Solving the Sch. Eqn for Multi-Particle Systems

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

- we'll ignore spin for awhile.

- we'll consider stationary states (AKA energy eigenstates) which are the QM analog of static states classically (don't need to get beyond statics in QM.
  - Even linear superposition of stationary states which

which oscillate
a bit with time
are tame compared
to behavior with
~~chang~~ time-varying
potential.)

For stationary states

V is time-independent
and thus we can separate
time and space (and spin too)
variables.

$$\psi(\xi_{r_i}, \xi, t) = \psi(\xi_{r_i}, \xi) T(t)$$

It may seem that we are being very restrictive in eliminating from consideration all states which can't be separated.

But recall $\psi(\xi_1, \xi_2, \ldots, \xi_N)$ constitute a complete set for the space of solutions

— guaranteed mathematically in some cases (Sturm-Liouville theory Arf - 422)

— a postulate of QM (CT - 215ff more or less and CT-137 Gr - 102)

So any state (of the system space) can be constructed by a linear combination of states from the complete set.

— So there is no in principle restriction by looking for separable states first.

Substitute into Sch. Eq. and divide by $\psi(\xi_{n,i},\xi)\bar{T}(t)$ gives

$$\frac{H\psi(\xi_{n,i},\xi)}{\psi(\xi_{n,i},\xi)} = \frac{i\hbar\frac{\partial}{\partial t}\bar{T}(t)}{\bar{T}(t)}$$

Recall we assume V was time independent.

no explicit t dependence

no explicit position dependence

implicitly no position dependence

implicitly no t dependence.

Both sides equal a constant of separation which we label E and

turns out to be the eigen energies.

Question solve

$$E = i\hbar \frac{\partial \psi}{\partial t} \Big/ \psi$$

2 minutes and don't look at the answer

$$\frac{E}{i\hbar} dt = \frac{d\psi}{\psi}$$

$$\frac{E}{i\hbar} t = \ln \psi$$

$$-iE/\hbar t = \ln \psi$$

$$\psi = e^{-iEt/\hbar}$$

~~Normalized usually by convention~~

No coefficient is used by convention.

— the normalization constant goes with the position solution.

digression

Query is $t_{op} = i\hbar \frac{\partial}{\partial t}$

an observable (CT-137) or a Hermitian operator in any sense?

Well $i\hbar \frac{\partial \vec{\psi}}{\partial t} = E\vec{\psi}$

it has real eigenvalues — we know from spatial eigenproblem

The solutions aren't normalizable over all time $t \in [-\infty, \infty]$ in an ordinary sense, but neither are those of similar momentum operator

$$p_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$ (in 1-d)

(Gr - 17)

$$\langle \gamma_{E'} | \gamma_E \rangle = \int_{-\infty}^{\infty} e^{i(E'-E)t/\hbar}\, dt$$

$$= 2\pi \delta(E'-E)$$

(Av-673)

— a Dirac delta

"normalization"

— which recall has its meaning as a limiting process under an integral sign.

Hermitian? $\langle \gamma_{E'} | t_{op} | \gamma_E \rangle$

$$= \langle \gamma_E | t_{op}^{\dagger} | \gamma_{E'} \rangle^*$$

$$\langle \gamma_{E'} | \gamma_E \rangle$$

$$= \langle \gamma_E | \gamma_{E'} \rangle^*$$

$$= \left[\langle \gamma_E | \gamma_{E'} \rangle \right]^*$$

$$= \left[E' \langle \gamma_E | \gamma_{E'} \rangle \right]^*$$

since $\langle \gamma_E | \gamma_{E'} \rangle$ is a Dirac delta function E can be replaced by E'

5-62

$$= \langle \gamma_E | E' | \gamma_{E'} \rangle^*$$

$$= \langle \gamma_E | i\hbar \frac{\partial}{\partial t} | \gamma_{E'} \rangle^*$$

$$\therefore \quad t_{op}^\dagger = t_{op}$$

So in <u>some sense</u>

$$t_{op} = i\hbar \frac{\partial}{\partial t}$$

seems to be a GM observable.

<u>But</u> no one seems to mention it, so it so the "sense" may not be useful

The spatial part is the energy eigen. problem

$$H\psi = E\psi$$

E is the eigen energy

ψ are the eigenstates or for this eigen problem they have the special name of stationary states

since aside from the $e^{-iEt/\hbar}$ factor they have no time dependence.

Q M observable that corresponds to classical Hamiltonian (which is usually ~~but~~ in cases of interest, but not always the energy of a classical system. Goldstein p. 62, 339)

∴ E can be identified as the eigen-energy of the system. — dimensionally it is energy, of course.

Actually, one can proceed further in complete generality.

5-64

To proceed one must specify $V = V(\{\vec{r}_i\}, \xi)$ and most potentials yield very intractable PDEs.

Multi body problem – exact solutions exist only for a few ideal cases (e.g. Hydrogenic atom & free electron gas)

partial differential equations

But for insight and because it is an important approximation for many cases (atoms, free electron gas),

Let's assume

$$V(\{\vec{r}_i\}, \xi) = \sum_i V_i(\vec{r}_i)$$

– Every particle has it's own potential that is independent of the other particles.

Each term j depends explicitly only on $\underset{\sim}{r}_j$

and NOT on the other $\underset{\sim}{r}_i$.

But the other ~~term~~ i

(~~excluding~~ don't depend

on $\underset{\sim}{r}_j$

So the term j implicitly doesn't depend on $\underset{\sim}{r}_j$ either.

Each term i equals a constant

which it only makes sense to identify as the eigenenergy of state i.

Now $H\Psi = E\Psi$

i

$$\left[\sum_i \left(\frac{-\hbar^2}{2m_i}\nabla_i^2 + V_i(\underline{r}_i)\right)\right]\Psi = E\Psi$$

We can now separate and get the extremely useful single-particle solution.

$$\Psi(\underline{r}_1, \underline{r}_2, \ldots) = \prod_i \Psi_i(\underline{r}_i)$$

product of single particle solution.

The separation procedure yields

$$\sum_i \left[\frac{\left(\frac{-\hbar^2}{2m_i}\nabla_i^2 + V\right)\Psi_i(r_i)}{\Psi_i(\underline{r}_i)}\right] = E$$

or $$\sum_i \left[\frac{H_i \Psi_i}{\Psi_i}\right] = E$$

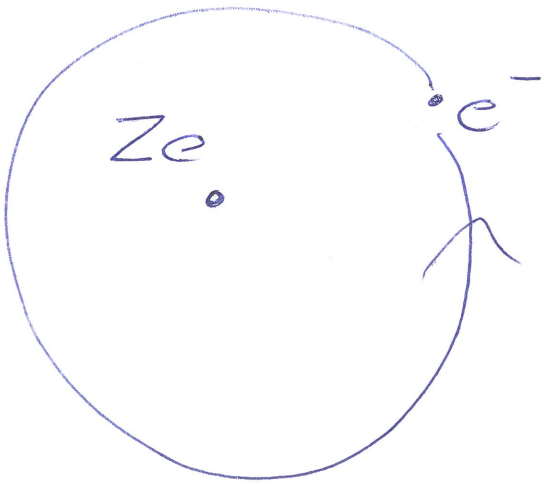
So $$\frac{H_i \psi_i}{\psi_i} = E_i$$

$$H_i \psi_i = E_i \psi_i$$

the 1-particle Sch. eqn. for particle i

- in general one has to solve each one separately.
- for the free electron gas (as we'll see later) all the Sch. eqn. for the particles are identical, and so only one set of single particle states (which is a tremendously important ideal case).

3) Hydrogenic Atom (or hydrogen-like atom) as a 2-body Problem.



a "nucleus" of charge Ze and orbiting particle of charge e^-

- examples
  - H atom itself
  - He^+ (once ionized Helium, $Z = 2$)
  - positronium
    - bound positron and electron
    - $Z = 1$
  - muonium ~~atom~~ hydrogen
    - ~~proton~~ and muon (wik)
  - muonium antimuon and an electron (wik)

protonium proton & antiproton.

Li^{2+} ion with $Z = 3$

As long as complications like spin, magnetic forces, relativistic effects maybe etc. are neglected one has the ideal hydrogenic atom for which an exact solution exists.

In earlier lectures you have probably seen this solution for the special case of

5-70)

hydrogen itself

but probably/maybe

only as a 1-body

problem

in which proton

was just regarded

as a point source

of Coulomb force

at rest in an inertial frame.

Which is an approximation

The ideal 2-body problem

with the center-of-mass

at rest in an inertial frame

is NOT much harder.

You reduce the new problem to the old problem to get the solution.

It's not too hard.

The Sch. eqn is

$$\left(-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 - \frac{Ze^2}{4\pi\varepsilon_0|\underline{r}_1 - \underline{r}_2|}\right)\psi(\underline{r}_1, \underline{r}_2) = E_{total}\,\psi(\underline{r}_1, \underline{r}_2)$$

E_{total} is the total energy of the system. I reserve E for another use.

The potential is inseparable in this case — so the separation of the variables trick does NOT work.

5-72

We assume $\underset{\sim}{v}_1$, $\underset{\sim}{v}_2$ are measured relative to an inertial frame

Question What if they aren't relative to an inertial frame?

They are relative to a non-inertial frame.

How must we change the equation

Ans. Include a non-inertial force potential. (or so I'd guess)

One key point about the Sch. eqn. is the potential only depends on the relative position of the particles

$$\underset{\sim}{r} = \underset{\sim}{r}_2 - \underset{\sim}{r}_1$$

This is just like a classical 2-body central force problem.

So we can change coordinates from $\underset{\sim}{r}_1, \underset{\sim}{r}_2$ to $\underset{\sim}{r}$ and $\underset{\sim}{R}$

Question What is $\underset{\sim}{R}$

5-74

Ans Center-of-mass coordinate.

$$\underset{\sim}{R} = \frac{m_1 \underset{\sim}{r}_1 + m_2 \underset{\sim}{r}_2}{m_1 + m_2}$$

Converting potential is easy

$$\frac{2e^2}{4\pi\varepsilon_0 |\underset{\sim}{r}_2 - \underset{\sim}{r}_1|} = \frac{2e^2}{4\pi\varepsilon_0 r}$$

But to convert the kinetic energy operators take the chain rule and a priori we might wonder if we'd get a mess.

Let's use Cartesian coordinates for getting the transformations and just consider the x ones.

The y & z ones are analogous.

Consider general wave function $\psi(x_1, x_2) = \psi(x, X)$

Question $\frac{\partial \psi(x,X)}{\partial x_i} = ?$

Ans. where i can be either 1 or 2

Answer

$$\frac{\partial \psi}{\partial x_i} = \frac{\partial \psi}{\partial x}\frac{\partial x}{\partial x_i} + \frac{\partial \psi}{\partial X}\frac{\partial X}{\partial x_i}$$

$$= \frac{\partial \psi}{\partial x}(\mp 1) + \frac{\partial \psi}{\partial X}\frac{m_i}{m}$$

where $m = m_1 + m_2$
and upper case for $i = 1$
lower case for $i = 2$

Question $\frac{\partial^2 \psi}{\partial x_i^2} = ?$

Ans. $$\frac{\partial^2 \psi}{\partial x_i^2} = \frac{\partial^2 \psi}{\partial x^2}(\mp 1)^2 + \frac{\partial^2 \psi}{\partial X \partial x}\frac{m_i}{m}(\mp 1)$$

$$+ \frac{\partial^2 \psi}{\partial X \partial X}(\mp 1)\frac{m_i}{m} + \frac{\partial^2 \psi}{\partial X^2}\left(\frac{m_i}{m}\right)^2$$

5-76 Question

Now what is $\frac{1}{m_1}\frac{\partial^2 \psi}{\partial x_1^2} + \frac{1}{m_2}\frac{\partial^2 \psi}{\partial x_2^2}$

in terms of x and X variables.

Ans

$$\frac{1}{m_1}\frac{\partial^2 \psi}{\partial x_1^2} + \frac{1}{m_2}\frac{\partial^2 \psi}{\partial x_2^2}$$

$$= \frac{1}{m_1}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{m_2}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{m_1}$$

$$= \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\frac{\partial^2 \psi}{\partial x^2} + 0 + 0 + \left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

$$+ \frac{1}{m_1}\frac{\partial^2 \psi}{\partial X^2}\left(\frac{m_1}{m}\right)^2$$

$$+ \frac{1}{m_2}\frac{\partial^2 \psi}{\partial X^2}\left(\frac{m_2}{m}\right)^2$$

$$= \frac{1}{\mu}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{m}\frac{\partial^2 \psi}{\partial X^2}$$

where $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$

or $\mu = \begin{cases} \dfrac{m_1 m_2}{m_1 + m_2} \text{ is the reduced mass of relative particle} \\ \dfrac{m_1}{2} \text{ if } m_1 = m_2 \text{ or electron} \\ \dfrac{m_1}{1 + m_1/m_2} \cong m_1\left(1 - \dfrac{m_1}{m_2}\right) \text{ if } m_1 << m_2. \end{cases}$

$\mu_{\text{electron in H}} = m_e\left(1 - \frac{m_e}{m_p}\right) \cong m_e\left(1 - \frac{1}{2000}\right)$

$\mu_{\text{positronium}} = \frac{m_e}{2}$

Now our Sch. Eqn for the hydrogenic atom is

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{\hbar^2}{2m}\nabla^2_{cm} - \frac{Ze^2}{4\pi\varepsilon_0 r}\right]\psi(x,y) = E\,\psi(x,y)$$

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

which can be converted to spherical polar form and is to solve the problem.

Since the potential doesn't depend on R we can do the old separation of variables trick to get

$$\frac{\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{2e^2}{4\pi\varepsilon_0 r}\right)\psi(x)}{\psi(x)} + \frac{\left(\frac{-\hbar^2}{2M}\nabla_{cm}^2\right)\psi_{cm}(R)}{\psi_{cm}(R)} = E_{total}$$

Both must equal constants which we identify as the relative energy E and CM energy E_{cm}

$$E + E_{cm} = E_{total}$$

a) The CM equation is

$$-\frac{\hbar^2}{2M}\nabla_{cm}^2\psi_{cm} = E_{cm}\psi_{cm}$$

which is just the free particle wave function.

Eigen solution?

- We can separate into x, y, z parts. We only need to look at x part
  - y & z are similar mutatis mutandis

x-part $\quad -\frac{\hbar^2}{2M}\frac{\partial^2\psi_{cm}(x)}{\partial x^2} = E_{x\,cm}\psi_{cm}(x)$

$$\frac{\partial^2\psi_{cm}}{\partial x^2} = k^2\psi_{cm}$$

Define $\quad k = \sqrt{\frac{-2M E_{x\,cm}}{\hbar^2}}$

and $\quad ik = i\sqrt{\frac{2M E_{x\,cm}}{\hbar^2}}$

$$k = \sqrt{\frac{2M E_{x,cm}}{\hbar^2}}$$

$\psi_{cm} = Ae^{kx} + Be^{-kx}$

$E_{x\,cm} < 0$ solutions
- growing & shrinking exponential solutions.
- can't be normalized

now included in a normalizable

5-80

wave packet.

$E = 0$ gives linear solution

$$\chi_{dm_x} = A + Bx$$

- also not normalizable nor includable in a normalizable wave packet.

So $\chi_{cm} = \frac{e^{ikx}}{\sqrt{2\pi}}$

where we allow k to run positive and negative over all values.

and $\frac{1}{\sqrt{2\pi}}$ is a conventional coefficient.

Now $x \in [-\infty, \infty]$

so there is no imposed quantization and the eigenstates can't be normalized.

These are also the wave number or momentum eigenstates

$\frac{\hbar}{i}\frac{\partial}{\partial x}\chi = k\chi$

$\frac{1}{i}\frac{\partial}{\partial x}$ wave number observable

$\frac{\hbar}{i}\frac{\partial}{\partial x}$ is the momentum observable

Gv-17

which means

no particle can be
in a pure free
particle energy/wavenumber/
momentum eigenstate.

But as you have seen
before they can be in
an integral linear combination
of such states
which we call a wave packet

$$\psi_{x\,cen}(x) = \int_{-\infty}^{\infty} \psi_{cm}(k)\, \frac{e^{ikx}}{\sqrt{2\pi}}\, dk$$

One has to actually prove these integrals exist and investigate the Dirac delta function of p. 5-61
See Gr-61

The wave number representation of the wave packet at time $t=0$

(CT-23)

$$\psi_{x\,cm}(x,t) = \int_{-\infty}^{\infty} \psi_{cm}(k)\, \frac{e^{i(kx-\omega t)}}{\sqrt{2\pi}}\, dk$$

where $w = \frac{E_{cm}}{\hbar}$

and $E_{cm} = \frac{\hbar^2 k^2}{2m}$

$\psi_{cm_x}(X, 0)$ is the inverse Fourier transform of $\psi_{cm}(k)$

and $\psi_{cm}(k)$ is the Fourier transform of $\psi_{cm}(X, 0)$

(CT-23)

We've done (I hope) free particles before. So we won't go further with them now.

[One curious fact about wave packets is that they tend to spread out with time. However, at least Gaussian packets do. (6v-6r).

This curious

5-83

Digression Wave packets

— There are some obvious questions about wave packets that elementary textbooks (at least) never raise.

1.) What actually are their shapes?

2.) Wave packets in free space spread out forever (ER-79 Gr-67).

So is this real or, as I suspect, do they collapse from time to time or even frequently

In the old days, I suspect no one knew very well.

5-84

Nowadays, I suspect, there has been a lot study → But there seems to be a code of silence on the issues

b) The ~~internet~~ Relativistic Schrodinger

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right)\psi = E\psi$$

(from p. 5-78)

No spin of electron or nucleus,
No relativistic effects,
No magnetic effects,
Point nucleus.

But this is just the ideal H-atom Sch. eqn. again

Except mass m → reduced mass μ

e^2 → Ze^2

So the solutions and ancillary results can be

just written down.

Solution

$$E = -\frac{E_{Ryd}}{n^2}\left(\frac{\mu}{m}\right)Z^2$$

{ energy for the ideal case doesn't depend on angular momentum.

where

$$E_{Ryd} = \frac{1}{2}mc^2\alpha^2 \cong 13{,}6\,eV \qquad (Gr-149)$$

E_{Ryd} ↑ Rydberg energy

mc^2 ↑ electron mass

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \cong \frac{1}{137}$$

is the dimensionless fine structure constant.

Clue that our non-rel. approach is adequate: $E_{Ryd} << E_{rest} = mc^2$ energy of electron

The Bohr radius is

$$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = \frac{\hbar}{\alpha mc} \qquad (Gr-(-1)$$

The generalized Bohr radius must be

$$a_g = \frac{a}{Z}\left(\frac{m}{\mu}\right)$$

Note

$$E_{Ryd} = \frac{1}{2}mc^2\alpha^2 = \frac{1}{2}mc^2\left(\frac{e^2}{4\pi\varepsilon_0\hbar c}\right)\frac{\hbar}{amc}$$

$$= \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 a}$$

Gr-152
5-86

The relative wave function itself is

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-1-l)!}{2n[(n+l)!]^3}}\; e^{-\frac{r}{na_0}} \left(\frac{2r}{na_0}\right)^l$$

(Gr-152)

$$* \, L^{2l+1}_{(n-1)-l}\left(\frac{2r}{na_0}\right) Y_{lm}(\theta,\phi)$$

r is relative. Usually $r = r_2 - r_1$ (r_2 electron, r_1 is nucleus)

associated Laguerre polynomials — Note only odd ones occur

spherical harmonics

magnetic quantum number or (z-component on ang. mom) quantum number (Gr-139):

$m = -l, -l+1, \ldots, l$ for $2l+1$ values

z-component values $L_z = m\hbar$

ang. mom quantum number:

$l = 0, 1, 2, \ldots, n-1$

ang. mom. squared values $L^2 = l(l+1)\hbar^2$

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

principal quantum number

Question:

Do the spherical harmonic angular solutions depend on the potential being the Coulomb potential.

Ans: No, they depend only on the force being a central force.

Actually, they are often useful approximations even when the force has some angular dependence. They are used for all atoms even though magnetic & other (?) effects add some angular dependence.

5-88

Question What is Y_{00}?

Ans $Y_{00} = \frac{1}{\sqrt{4\pi}}$ (Gr-139)

the spherical harmonic everyone should know.

Unlike the central force problem in classical physics, there is a spherically symmetric angular momentum zero solution in the QM central force problem.

$$Y_{10} = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_{1\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{\pm i\phi} \quad \text{(Gr-139)}$$

The ψ_{nlm} states

are called orbitals

rather than orbits as in classical physics. (Gr-214)

The term orbital is extended to all atoms where the quantum numbers n, l, m turn up

— the force is no longer a the Coulomb force of the nucleus because the electron Coulomb force is also present and magnetic contribution but one can still define a principal quantum number

— l and m are also still useful even though the actual states are a bit mixed.

5-90

There also is the electron spin quantum number m_s

Usually ~~Sometimes~~ folks classify the orbitals by $n\ l\ m\ m_s$ ($m_s = \pm \frac{1}{2}$)

This is how I usually think of orbitals

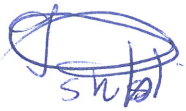
— two spin states double the number of orbitals.

All orbitals of one n, ~~[illegible]~~ constitute a shell (Gr-2A ER-329)

all orbitals of n, l ~~[illegible]~~ constitute a subshell. (ER-329)

Question How many orbitals are there in a subshell of quantum number l counting the spin states as giving different orbitals.

ANS. $m = -\ell, -\ell+1, \ldots, \ell$

$\therefore$ 

$\therefore$ $q_{subshell} = 2(2\ell+1)$

spin states double the number.

Question How many orbitals are there in a shell of quantum number n?

Recall $\ell = 0, 1, 2, \ldots, n-1$

ANS. $q_{shell} = \sum_{\ell=0}^{n-1} 2(2\ell+1)$

$= \frac{(n-1)n}{2} + 2n$

$= 2n^2 - 2n + 2n$

$q_{shell} = 2n^2$

5-92

Question How many ~~orbitals~~ orbitals are there in shells up to $1, 2, \ldots, n$?

Ans $g_N = \sum_{n=1}^{N} 2n^2$

$$= 2\sum_{n=1}^{N} n^2$$

$$= 2\,\frac{N(N+1)(2N+1)}{6}$$

(Wik: list of mathematical series)

	g_n	g_N
$n=1$	2	2
$n=2$	8	$2\cdot\frac{2(2+1)(4+1)}{6} = 10$
$n=3$	18	$2\cdot\frac{3(3+1)(7)}{6} = 28$
$n=4$	32	60
$n=5$	50	110

Important values for atoms.

A bit of jargon

$l = 0$ orbitals are called s orbital

s is for sharp and
meant something in
old spectroscopy

$l = 1$ ~~obit~~ orbitals are p orbitals

p been principal

$l = 2$ orbitals are d orbits

d for diffuse

$l = 3$ orbitals are f orbital

f for fundamental

$l = 3$ are g
4 are h
5 are i

} alphabetic
~~after~~
after f.

5-94

Many Body Problem

Just a few considerations.

— For the 2 body

And another thing

(as Colombo used to say)

$$\psi(\underset{\sim}{r}) = \psi_{nem}(r, \theta, \phi)$$

is a wave function for

$$\underset{\sim}{r} = \underset{\sim}{r}_2 - \underset{\sim}{r}_1$$

i.e., for particle 2 relating to particle 1.

sort of a wave function for a fictitious particle. or relative particle.

Usually one thinks of particle 2 as a lighter particle (usually an electron) and particle 1 as the heavier particle (usually a nucleus)

But what are the actual wave functions for the particles and how do they relate $\psi(\underset{\sim}{r})$?

Well recall what we did

$$\psi_{\text{total}}(\underset{\sim}{r}_1, \underset{\sim}{r}_2) = \psi(\underset{\sim}{r}_2 - \underset{\sim}{r}_1)\,\psi_{CM}(\underset{\sim}{R})$$

$$= \psi(\underset{\sim}{r}_2 - \underset{\sim}{r}_1)\,\psi_{CM}\left(\frac{m_1 \underset{\sim}{r}_1 + m_2 \underset{\sim}{r}_2}{m}\right).$$

We can't exactly separate the wave function ~~the particles~~ into single particle wave functions (quelle dommage)

5-96

But let's consider some special cases for insight.

Say $\psi_{CM}(\underset{\sim}{R})$

Let's write in terms of $\underset{\sim}{r}_2$ and $\underset{\sim}{R}$

$$\underset{\sim}{r}_1 = \underset{\sim}{R} - \frac{m_2}{m_1}\underset{\sim}{r}_2$$

$$\psi_{total}(\underset{\sim}{r}_2, \underset{\sim}{R}) = \psi\left(\underset{\sim}{r}_2\left(1 + \frac{m_2}{m_1}\right) - \frac{m}{m_1}\underset{\sim}{R}\right)\psi_{CM}(\underset{\sim}{R})$$

You could think of this as the wave function for $\underset{\sim}{r}_2$ for a fixed $\underset{\sim}{R}$.

Say $\underset{\sim}{R} = 0$

Then $\psi\left(\underset{\sim}{r}_2\left(1 + \frac{m_2}{m_1}\right)\right)$

If $m_2/m_1 << 1$ and so $\underset{\sim}{r}_1 \cong \underset{\sim}{R} = 0$

Let's write the joint wave function in terms of $\underset{\sim}{r}_1$ and $\underset{\sim}{R}$ and $\underset{\sim}{r}_2$ and $\underset{\sim}{R}_{cm}$.

Note $\underset{\sim}{r}_1 = \dfrac{m\underset{\sim}{R} - m_2 \underset{\sim}{r}_2}{m_1}$

and $\underset{\sim}{r}_2 = \dfrac{m\underset{\sim}{R} - m_1 \underset{\sim}{r}_1}{m_2}$

$\therefore$ $\underset{\sim}{r}_2 - \underset{\sim}{r}_1 = \dfrac{m}{m_2}\underset{\sim}{R} - \dfrac{m_1}{m_2}\underset{\sim}{r}_1 - \underset{\sim}{r}_1$

$= \dfrac{m}{m_2}\underset{\sim}{R} - \dfrac{m}{m_2}\underset{\sim}{r}_1$

$= \dfrac{m}{m_2}(\underset{\sim}{R} - \underset{\sim}{r}_1)$

and $\underset{\sim}{r}_2 - \underset{\sim}{r}_1 = \underset{\sim}{r}_2 - \dfrac{m}{m_1}\underset{\sim}{R} - \dfrac{m_2}{m_1}\underset{\sim}{r}_2$

$= \dfrac{m}{m_1}\underset{\sim}{r}_2 - \dfrac{m}{m_1}\underset{\sim}{R}$

$= \dfrac{m}{m_1}(\underset{\sim}{r}_2 - \underset{\sim}{R})$

$\therefore$ $\psi_{total}(\underset{\sim}{r}_2, \underset{\sim}{r}_1) = \psi\left(\dfrac{m}{m_2}(\underset{\sim}{R} - \underset{\sim}{r}_1)\right)\psi_{cm}(\underset{\sim}{R})$

$= \psi_1(\underset{\sim}{r}_1 - \underset{\sim}{R})\psi_{cm}(\underset{\sim}{R})$

$= \psi_2\left(\dfrac{m}{m_1}(\underset{\sim}{r}_2 - \underset{\sim}{R})\right)\psi_{cm}(\underset{\sim}{R})$

$\psi_1(\underset{\sim}{r}) = \psi\left(-\dfrac{m}{m_2}\underset{\sim}{r}\right)$

$\psi_2(\underset{\sim}{r}) = \psi\left(\dfrac{m}{m_1}\underset{\sim}{r}\right)$

So we get relative to CM wave functions for the two particles.

$$\psi_1(\underset{\sim}{r}_1 - \underset{\sim}{R}) = \psi\left(\frac{m}{m_2}(\underset{\sim}{R} - \underset{\sim}{r}_1)\right)$$
$$= \psi(\underset{\sim}{r}_2 - \underset{\sim}{r}_1)$$

$$\psi_2(\underset{\sim}{r}_2 - \underset{\sim}{R}) = \psi\left(\frac{m}{m_1}(\underset{\sim}{r}_2 - \underset{\sim}{R})\right)$$
$$= \psi(\underset{\sim}{r}_2 - \underset{\sim}{r}_1)$$

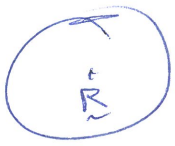
$P_1(\underset{\sim}{r}_1 - \underset{\sim}{R}) = |\psi_1|^2$ for fixed $\underset{\sim}{R}$

$P_2(\underset{\sim}{r}_2 - \underset{\sim}{R}) = |\psi_2|^2$ for fixed $\underset{\sim}{R}$

The particles are in superpositions of positions for fixed $\underset{\sim}{R}$.

But from $\psi_{cm}(\underset{\sim}{R})$ there is a "superposition of superposition".

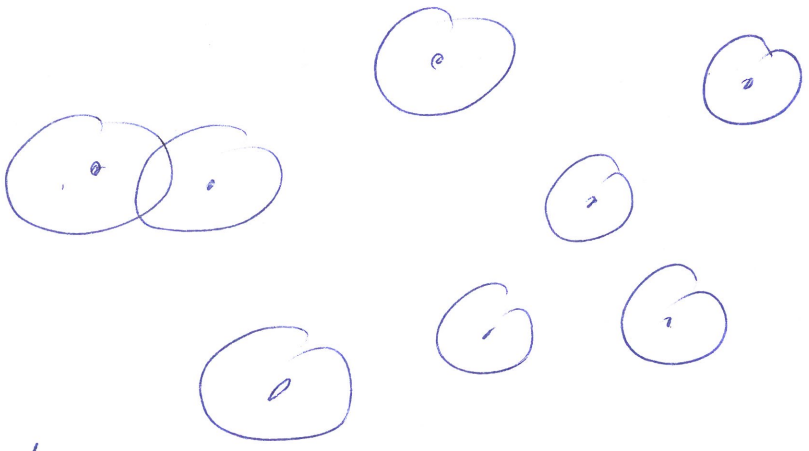
Schematically



~~stands~~ stands for the ψ_1 and ψ_2 structures for fixed $\underset{\sim}{R}$.

i.e. At every $\underset{\sim}{R}$ in space one has

e.g.,



We can only draw a finite number but they are everywhere and totally overlap. — A continuum of ψ_1 & ψ_2 structures.

If you wanted to find total probability density for particle 1 at ~~a position~~ $\underset{\sim}{r}_1$.

$$P(\underset{\sim}{r}_1) = \int |\psi_1(\underset{\sim}{r}_1 - \underset{\sim}{R})|^2 \left| \psi_{cm}(\underset{\sim}{R}) \right|^2 d\underset{\sim}{R}$$

5-98c)

which can probably be best described as a convolution of $|\psi_{cm}|^2$ and $|\psi_1|^2$. (Wiki: convolution)

I'd describe $P_1(\underset{\sim}{r}_1)$ as a modified version of $|\psi_{cm}|^2$.

if ψ_{cm} was very broad compared to ψ_1 and a modified version of $|\psi_1|^2$ if ψ_{cm} is very narrow compared to ψ_1 - extreme examples illustrate.

Special cases

a) Say $|\psi_1|^2 = \delta(\underset{\sim}{r}_1 - \underset{\sim}{R})$

$$P_1(\underset{\sim}{r}_1) = |\psi_{cm}(\underset{\sim}{r}_1)|^2$$

b) Say $\psi_{cm}(\underset{\sim}{R}) = \delta(\underset{\sim}{R} - \underset{\sim}{R}_a)$

$$P_1(\underset{\sim}{r}_1) = |\psi_1(\underset{\sim}{r}_1 - \underset{\sim}{R}_a)|^2$$

c) Say $|\psi_1(\underset{\sim}{r}_1 - \underset{\sim}{R})|^2 = A e^{-|\underset{\sim}{r}_1 - \underset{\sim}{R}|/a}$ { hydrogenic like

$$|\psi_{cm}(\underset{\sim}{R})|^2 = B e^{-(R-R_a)^2/(2\sigma)}$$ { Gaussian wave packet like

or 1-d for simplicity

$$|\psi_1(x_1 - X)|^2 = A e^{-(x_1 - X)/a}$$

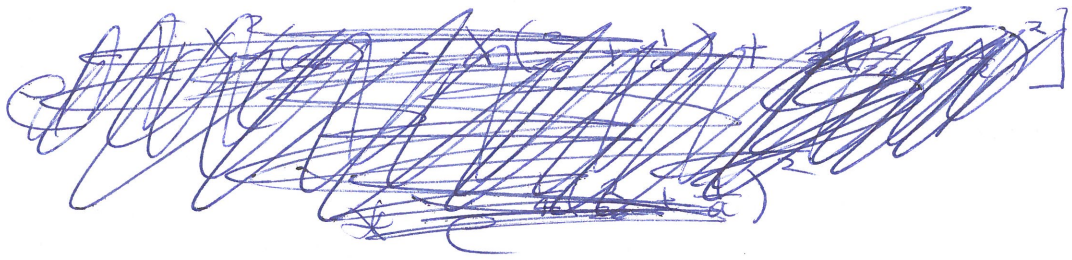
$$|\psi_{cm}(X)|^2 = B e^{-(X - X_a)^2/(2\sigma)}$$

A & B are normalizations

$$P_1(x_1) = \int_{-\infty}^{\infty} AB e^{-(x_1 - X)/a} * e^{-(X - X_a)^2/(2\sigma^2)} dX$$

$$= AB e^{-x_1/a} \int_{-\infty}^{\infty} e^{-X^2/(2\sigma^2) - X_a^2/(2\sigma^2)} * e^{+X\left(\frac{2}{2\sigma^2} + \frac{1}{a}\right)} dX$$

One needs to complete the square



$$= e^{-\frac{1}{2\sigma^2}\left[X^2 - X\left(2 + \frac{2\sigma^2}{a}\right) + \frac{1}{4}\left(2 + \frac{2\sigma^2}{a}\right)^2\right]} * e^{\frac{1}{4}\left(2 + \frac{2\sigma^2}{a}\right)^2} e^{-X_a^2/(2\sigma^2)}$$

$$P_1(x_1) = A e^{\frac{1}{4}\left(2 + \frac{2\sigma^2}{a}\right)^2} e^{-X_a^2/(2\sigma^2)} e^{-x_1/a}$$

— well not a very interesting result actually.

5-98e

d) — two convolved Gaussians is cute since you get another Gaussian. Will not quite in this case.

$$|\psi|^2 = A e^{-(x-X)^2/(2\sigma_1^2)}$$

$$|\psi_{cm}|^2 = B e^{-(X-X_a)^2/(2\sigma_2^2)}$$

$$P_1(x) = AB \int_{-\infty}^{\infty} e^{-X^2\left[\frac{1}{2\sigma_1^2}+\frac{1}{2\sigma_2^2}\right]} * e^{X\left[\frac{2x}{2\sigma_1^2}+\frac{2X_a}{2\sigma_2^2}\right]} * e^{-\frac{x^2}{2\sigma_1^2}} e^{-X_a^2/2\sigma_2^2} dX$$

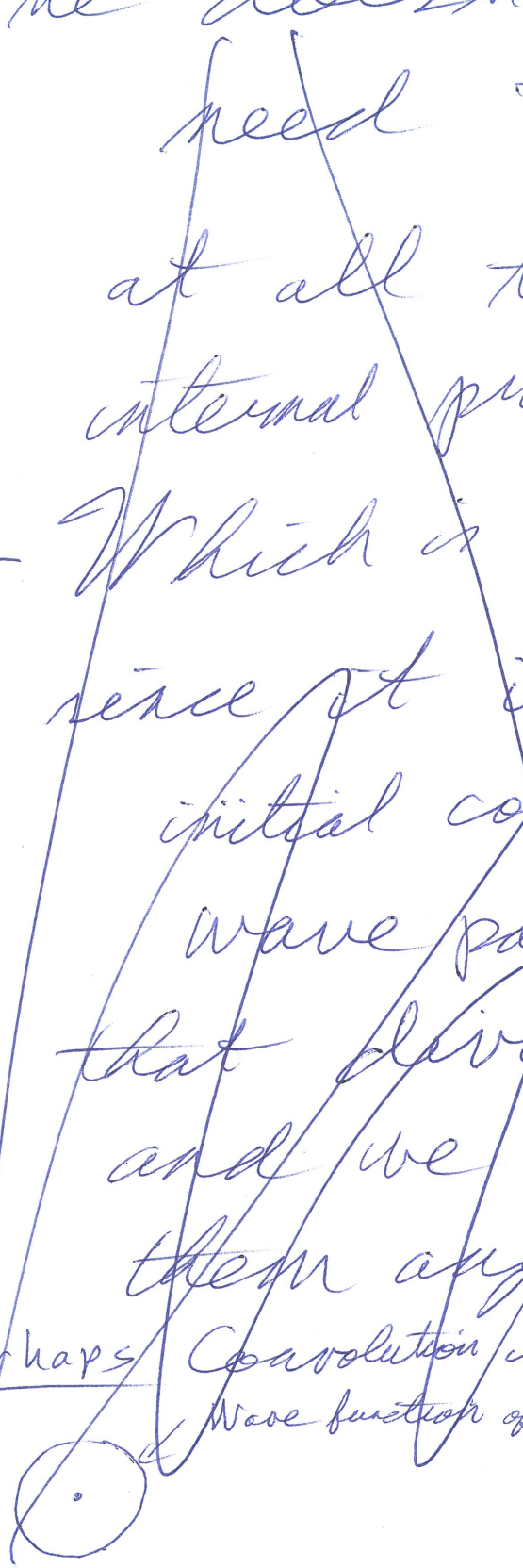
— I give up, too tedious.

5-99

One doesn't need $\psi_{CM}(\vec{R})$ at all to study the internal properties.

— Which is a good thing since it is set by initial conditions and wave packet spreading that diverge and we don't know them anyway.

Perhaps Convolution is best suggested diagramatically.



4) Many Body - Problem & Inertial Frames & Center-of-Mass Wave function

Just a few considerations.

For the 2-body problem, we can as we've seen separate the internal relative part and the CM of mass parts exactly.

This takes care of non-inertial frame effects exactly.

But can this be done for the Many-Body problem?

And should it be done?

The answers apparently are Yes and No.

I'll show below in a digression, how I think one can separate the relative and CM parts.

The CM part is again a free particle wave function if there are no external forces.

I think in principle, it is good to know this can be done.

However a great expert (my friend Lindmilla in Idaho)

tells me that one should just take the origin ~~at the~~ to be some symmetry point of the body that must be close to ~~the~~ CM expectation value.

The error in this approximation is usually much smaller than all the other approximation errors and so is negligible.

But that's usually. There might

be special cases where one does need to separate the CM wave function exactly.

Consideration of CM wave functions leads to an interesting point about the wavelength of macroscopic objects.

Recall the de Broglie formula $p = \frac{h}{\lambda}$

$= \hbar k$

where k is wavenumber

$k = \frac{2\pi}{\lambda}$.

de Broglie proposed this as a postulate ~1924 or so

But in the Sch. eqn free-particle picture — a free particle is a wave function is

5-104

wave packet

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k) \frac{e^{i(kx-\omega t)}}{\sqrt{2\pi}} dk$$

(Gr-65)

If the packet can be viewed as narrow then

$$v_{group} = 2 v_{phase_0} = 2 \frac{\omega_0}{k_0}$$

(Gr-65)

corresponds to classical velocity

$\omega_0 = \frac{\hbar k_0^2}{2m}$ where k_0 is at peak of packet which declines rapidly away from the peak

$$\therefore \quad p_{classical} \cong 2 m v_{phase_0}$$

$$= 2m \frac{\omega_0}{k_0}$$

$$= 2m \frac{\frac{\hbar k_0^2}{2m}}{k_0}$$

$$p_{classical} = \hbar k_0 = h/\lambda_0$$

Which is sort of the ~~de~~ Broglie formula applicable to macroscopic objects.

So say you had a macro-object, then it's mean wavelength is

$$\lambda_0 = \frac{h}{p_{cm}}$$

But what is this the wavelength of exactly.

The center of mass I'd say.

What else are putting into the formula.

Nothing about structure of the object.

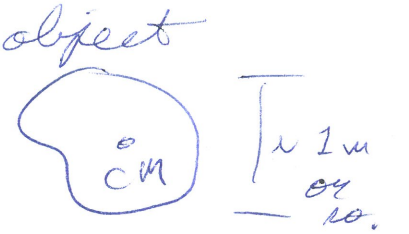
— same formula for a point mass.

— ergo it is the formula for a point mass. — the CM of the object.

4-106) Example

$m = 1\,kg$

$\lambda_0 \cong \dfrac{7\times10^{-34}\,kg\,m^2/s}{1\,kg\cdot v_{class}}$



If you could make v_{class} really small in some direction,

$\lambda_0 \cong 10^{-7}\,m$

say $v_{class} = 10^{-28}\,m/s$,

then could you diffract the object with a slit of $s \lesssim 10^{-7}\,m$?

Which is probably much smaller than the thermal fluctuations of the CM

Ideal gas

$v \sim \sqrt{\dfrac{3kT}{m}}$

$\simeq \sqrt{\dfrac{4\times10^{-23}}{2\cdot1.7\times10^{-27}}\sqrt{T}}$

$\cong 10^2\sqrt{T}\,m/s$

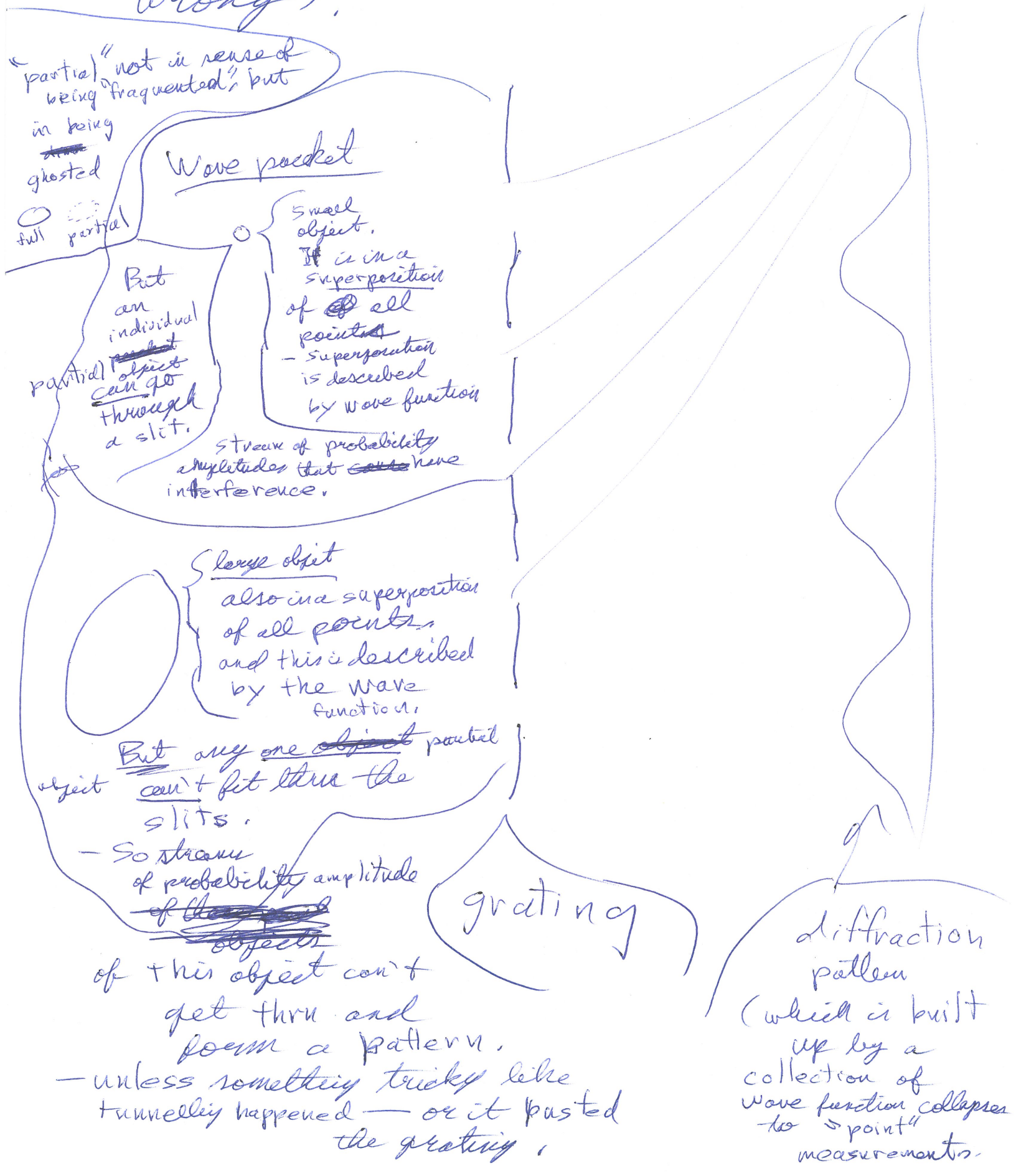
Say for a balloon of H_2 gas.

~~This is one of those (but obvious) which textbooks~~

This is one of those obvious questions on which textbook authors grow coy.

But I think the answer is NO.

The following figure illustrates my argument (which may be wrong).



5-108

So yes in principal a macro-object can be diffracted but the slits have to be big enough.

The situation is so different from classical physics.

You CANNOT completely separate the CM motion from the object structure.

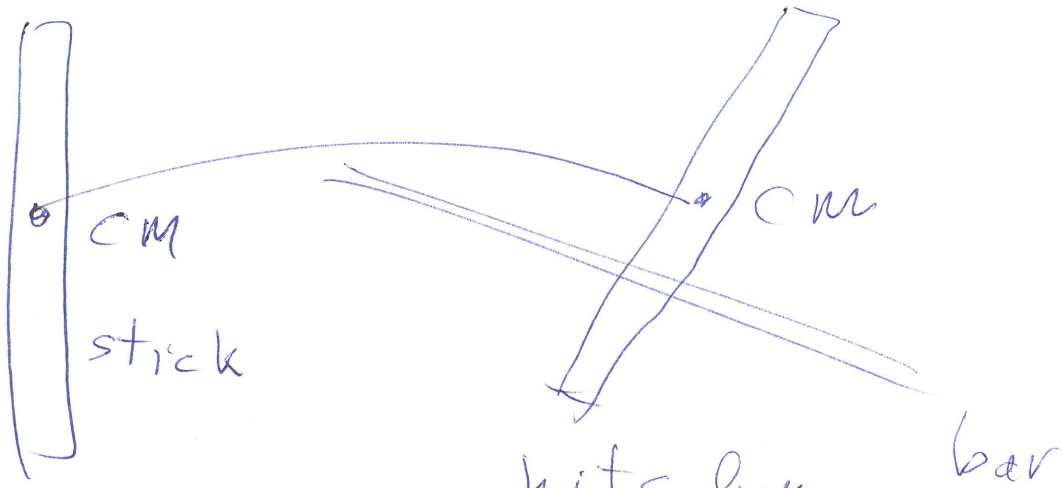
Recall $\underset{\text{net external}}{\vec{F}} = m\vec{a}_{CM}$

— Superficially it looks like you could describe the CM motion without reference to the object structure.

But which external forces act on the object or that structure.

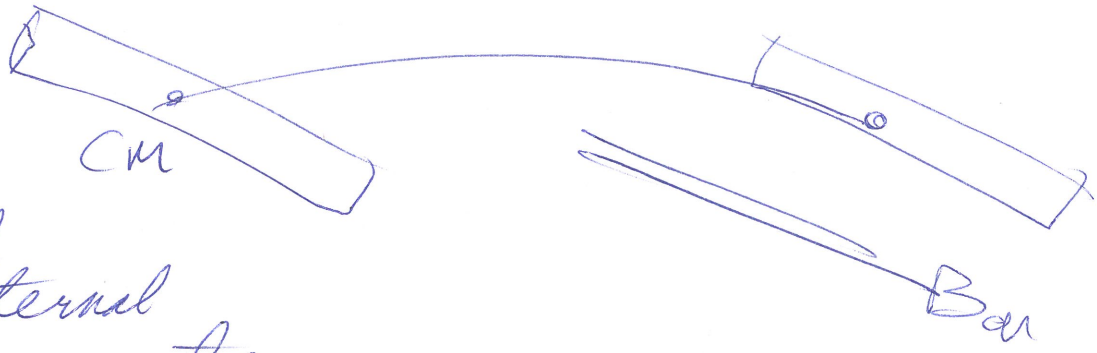
Ex. Throw a meterstick at a bar

Case 1



Case 2

- stick misses bar and no external force acts.



There is, in fact, no upper limit on the size of an object that can be diffracted — no limit on

F-110

wave-particle duality of QM.

But our experimental technique has limits.

→ You have to prevent premature wave function collapse or decoherence as one can call it.

→ If one found a limit that could bust the QM paradigm.

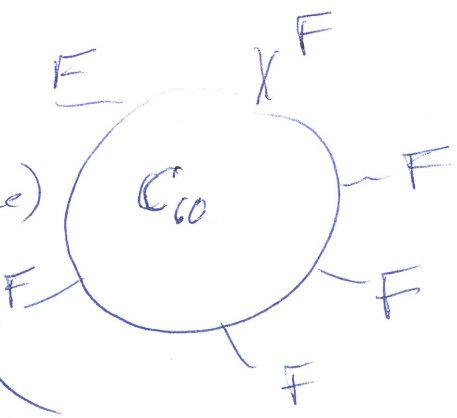
The current record largest diffracted object is a $C_{60}F_{48}$ (fluorofullerene) molecule (according to Wik: Wave-particle duality)

by Hackermüller, Hornberger, Brezger, Zeilinger, & Arndt, 2003
- they are Austrians
- Zeilinger's group in Vienna

$M = 1632$ amu

$P_{diameter} \cong 1$ nm

(Wik: buckminsterfullerene)



They used

$v_{mean} = 105\ m/s$

$\lambda_{de\ Broglie} \cong \dfrac{7 \times 10^{-34}}{1600 \cdot 1.7 \times 10^{-27} \cdot 100}$

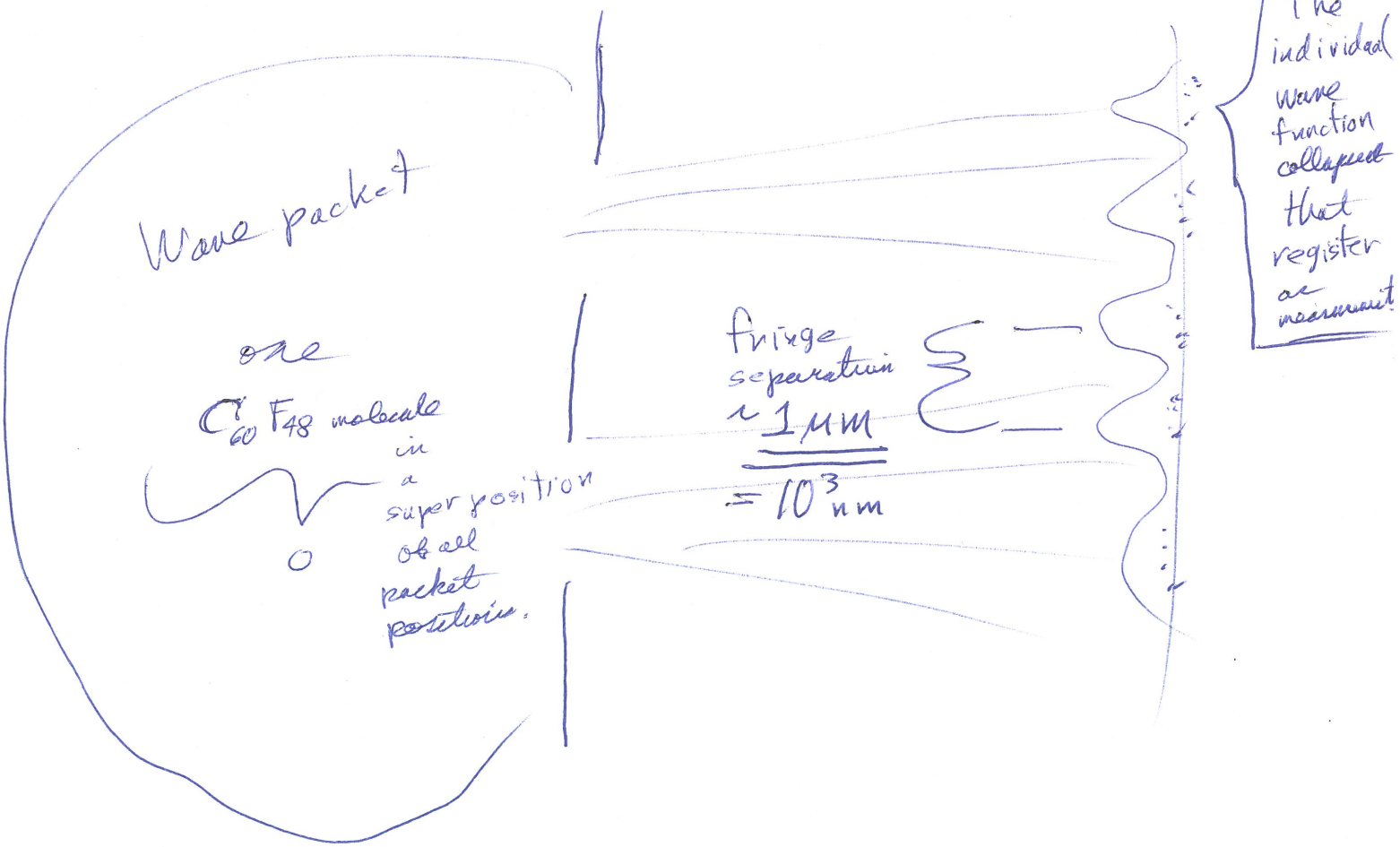
$\cong 2 \times 10^{-12}\ m$

$= .002\ nm$

$S_{slit\ width\ on\ grating} = 500\ nm$

{ Actually not a simple on grating setup. These used multi-grating device. So a bit complex.

So $\lambda_{deB} << D_{diameter} << S$



5-112

Digression

- separately the CM wave function from the relative wave function.
- maybe not so useful in practice, but a proof in principle that the CM wave function can be separated in some cases and that can talk of CM motion in isolation sometimes —— e.g., the $C_{60}F_{48}$ diffraction experiment of Hackermüller et al. (2003)

Consider a system of particles. There are n of them.

Wave function is

$$\Psi(\underset{\sim}{r}_1, \underset{\sim}{r}_2, \ldots, \underset{\sim}{r}_i, \ldots, \underset{\sim}{r}_n)$$

and Sch. eqn is

$$H\Psi = E\Psi$$

Coordinates relative to a fixed inertial frame

where

$$H = \left(\sum_i -\frac{\hbar^2}{2m_i}\nabla_i^2\right) + V(\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_n)$$

Could include internal and external potentials in general.

Let's use Cartesian coordinates.

We will only explicitly work with the x-coordinates. The y and z coordinates are treated the same way.

We want to replace the inertial frame coordinates $\{x_i\}$ by relative coordinates x_i' and Center-of-mass coordinate X.

4-114

Define $n-1$ relative coordinates

$$x_i' = x_i - x_n$$

It seems we must treat one particle as a special case.
- The particle to which all the others are referenced.
- maybe some way around this, but I couldn't find it.

and $$X = \frac{\sum_i m_i x_i}{m}$$

where $$m = \sum_i m_i$$

The x_i' and X are n independent coordinates, but we've got to eliminate x_n

$$m_n x_n = mX - \sum_j m_j x_j$$

$$x_n = \frac{m}{m_n} X - \sum_j \frac{m_j}{m_n} x_j$$

$$\therefore x_i' = x_i + \sum_j \frac{m_j}{m_n} x_j - \frac{m}{m_n} X$$

primed here means sum of all particles except n.

$$m_n x_n = m X - \sum_j{}' m_j x_j$$

Prime means exclude $j=n$ from the sum

$$x_n = \frac{m}{m_n} X - \sum_j{}' \frac{m_j}{m_n} x_j$$

Note $\frac{\partial x_n}{\partial x_i} = \frac{m}{m_n}\frac{m_i}{m_n} - \frac{m_i}{m_n} = 0$ for $i \neq n$ as it should since x_n is independent of x_i for $i \neq n$

$$Y(\xi x_i \xi) = Y(\xi x_i' \xi, X)$$

which is easy but we have to convert the partial derivative

$$\frac{\partial^2 Y}{\partial x_i^2}$$ into terms which are only derivatives of x_i' and X.

One uses the chain rule.

A priori, one might expect a mess. It turns out not so bad, but not so good.

5-116

For $i \neq n$ terms

$$\frac{\partial^2 \chi}{\partial x_i^2} = \sum_j \frac{\partial^2 \chi}{\partial x_j' \partial x_i} \frac{\partial x_j'}{\partial x_i} + \frac{\partial \chi}{\partial X} \frac{\partial X}{\partial x_i}$$

$$\frac{\partial x_j'}{\partial x_i} = \frac{\partial}{\partial x_i}(x_j - x_n)$$

$$= \delta_{ij}$$

$$\frac{\partial X}{\partial x_i} = \frac{m_i}{m}$$

$$\frac{\partial \gamma}{\partial x_i} = \frac{\partial \gamma}{\partial x_i'} + \frac{\partial \gamma}{\partial X} \frac{m_i}{m}$$

$$\frac{\partial^2 \gamma}{\partial x_i^2} = \frac{\partial}{\partial x_i'}\left(\frac{\partial \chi}{\partial x_i}\right) + \frac{\partial}{\partial X}\left(\frac{\partial \chi}{\partial x_i}\right)\frac{m_i}{m}$$

$$= \frac{\partial^2 \gamma}{\partial x_i'^2} + \frac{\partial^2 \gamma}{\partial x_i' \partial X} \frac{m_i}{m} + \frac{\partial^2 \chi}{\partial X \partial x_i'} \frac{m_i}{m} + \frac{\partial^2 \gamma}{\partial X^2}\left(\frac{m_i}{m}\right)^2$$

$$= \frac{\partial^2 \chi}{\partial x_i'^2} + 2\frac{\partial^2 \chi}{\partial x_i' \partial X} \frac{m_i}{m} + \frac{\partial^2 \gamma}{\partial X^2}\left(\frac{m_i}{m}\right)^2$$

If we add up all the terms

$$\sum_i{}' \frac{1}{m_i} \frac{\partial^2 \chi}{\partial x_i'^2}$$

$$= \sum_i{}' \frac{1}{m_i} \frac{\partial^2 \chi}{\partial x_i'^2} + 2 \sum_i{}' \frac{\partial^2 \chi}{\partial x_i' \partial X} \frac{1}{m}$$

$$+ \sum_i{}' \frac{\partial^2 \chi}{\partial X} \frac{m_i}{m^2}$$

$$= \sum_i{}' \frac{1}{m_i} \frac{\partial^2 \chi}{\partial x_i'^2} + 2 \sum_i{}' \frac{\partial^2 \chi}{\partial x_i' \partial X} \frac{1}{m}$$

$$+ \frac{\partial^2 \chi}{\partial X} \left(\frac{m - m_n}{m^2} \right)$$

Now for n term

$$\frac{\partial \chi}{\partial x_n} = \sum_j{}' \frac{\partial \chi}{\partial x_j'}(-1) + \frac{\partial \chi}{\partial X} \frac{m_n}{m}$$

since $\frac{\partial}{\partial x_n}(x_i' - x_n) = -1$

and $\frac{\partial X}{\partial x_n} = \frac{m_n}{m}$

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$$\frac{\partial^2\psi}{\partial x_n^2} = \sum_{jk}{}' \frac{\partial^2\psi}{\partial x_j' \partial x_k'}(-1)^2$$) This term doesn't cancel.

$$+ \sum_j \frac{\partial^2\psi}{\partial X \partial x_j'}(-1)\frac{m_n}{m}$$

$$+ \sum_j \frac{\partial^2\psi}{\partial x_j' \partial X}(-1)\frac{m_n}{m}$$) fortunately these two terms cancel

$$+ \frac{\partial^2\psi}{\partial X^2}\left(\frac{m_n}{m}\right)^2$$

$$\text{So} \quad \sum_i{}' \frac{1}{m_i}\frac{\partial^2\psi}{\partial x_i^2} + \frac{1}{m_n}\frac{\partial^2\psi}{\partial x_n^2}$$

$$= \sum_i{}' \frac{1}{m_i}\frac{\partial^2\psi}{\partial x_i'^2} + \sum_{jk}{}' \frac{\partial^2\psi}{\partial x_j' \partial x_k'}\frac{1}{m_n}$$

$$+ \frac{\partial^2\psi}{\partial X^2}\left(\frac{m}{m} - \frac{m_n}{m} + \frac{m_n}{m}\right)$$

$$= \sum_i{}' \frac{1}{m_i}\frac{\partial^2\psi}{\partial x_i'^2} + \sum_{jk}{}' \frac{\partial^2\psi}{\partial x_j' \partial x_k'}\frac{1}{m_n} + \frac{\partial^2\psi}{\partial X^2}\frac{1}{m}$$

The middle term is the ruin of our hopes.

It prevents the relative part from being a Sch. eqn itself.

There is no way to get rid of the mixed derivatives in $\sum_{\substack{j,k \\ j \neq k}} \frac{\partial^2 \psi}{\partial x_j' \partial x_k'} \frac{1}{m_n}$

unless there were only two particles in which there are no mixed terms.

Or unless some symmetry dictates $\frac{\partial^2 \psi}{\partial x_i' \partial x_k'}$

dictates $\sum_{\substack{j,k \\ j \neq k}} \frac{\partial^2 \psi}{\partial x_j' \partial x_k'} \frac{1}{m_n} = 0$

Possible but seems unlikely.

Remember $\frac{\partial^2 \psi}{\partial x_j' \partial x_k'} = \frac{\partial^2 \psi}{\partial x_k' \partial x_j'}$

Any way now we have

$$\sum_i{}' -\frac{\hbar^2}{2m_i}\frac{\partial^2\chi}{\partial x_i'^2} + \sum_{jk}{}' \frac{-\hbar^2}{2m_n}\frac{\partial^2\chi}{\partial x_j' \partial x_k'}$$

$$+ \frac{\hbar^2}{2m}\frac{\partial^2\chi}{\partial X^2} + V_{Rel}(\{x_i'\},\xi)\chi$$

$$+ V_{ext}(\{x_i\},\xi)\chi$$

original particle coordinates

$$= E\chi$$

We still cannot effect a separation unless

$$V_{ext} = 0$$

or $V_{ext}(\{x_i\},\xi) \cong V_{ext}(X)$

The external potentials vary sufficiently slowly with position that x_i can.

Anyway the Sch. eqn for 3-d is now

$$\left[\sum_i{}' -\frac{\hbar^2}{2m_i}\nabla'^2 + \sum_{jk}{}' -\frac{\hbar^2}{2m_n}\left(\frac{\partial^2}{\partial x_j' \partial x_k'} + \frac{\partial^2}{\partial y_j' \partial y_k'} + \frac{\partial^2}{\partial z_j' \partial z_k'} \right) \right.$$

$$- \frac{\hbar^2}{2M}\nabla_{CM}^2$$

$$\left. + V_{int}(\{\vec{r}_{ni}\}) + V_{ext}(\{\vec{r}_{ni}\}) \right] \psi = E\psi$$

There are the original coordinates still.

In general, we can't effect a separation of variables it seems to me unless $V_{ext}(\{\vec{r}_{ni}\}) = 0$

or $V_{ext}(\{\vec{r}_{ni}\}) = V_{ext}(\vec{R}_n)$

i.e., the external forces

on the particles vary sufficiently slowly with position that $\underset{\sim}{r}_i$ can be approximated by $\underset{\sim}{R}$ for V_{ext}.

This does seem a distinction from classical physics where one can separate off a CM equation of motion

$$\underset{\sim}{F}_{\substack{net \\ ext}} = M \underset{\sim}{a}_{CM}$$

but ~~maybe~~ it is not so different after all.
As we discussed on p. 5-108-109,

$\underset{\sim}{F}_{\substack{net \\ ext}}$ depends on the structure of system, and so CM motion is coupled to the ~~not~~ internal structure of the system really unless $\underset{\sim}{F}_{\substack{net \\ ext}} = 0$

or $\underset{\sim}{F}_{\substack{net \\ ext}}$ is independent of the internal structure by its particular nature.

Separation if we can

$$\psi_{total}(\{\underline{r}_i\}, \underline{R}) = \psi(\{\underline{r}_i\}) \psi_{CM}(\underline{R})$$

Given

$$\frac{\left[\ldots \right] \psi(\{\underline{r}_i\})}{\psi(\{\underline{r}_i\})} + \frac{\left(-\frac{\hbar^2}{2M} \nabla_{cm}^2 + V_{ext}(\underline{R}) \right) \psi_{CM}}{\psi_{CM}} = E_{total}$$

$$\underbrace{\qquad\qquad}_{E} \qquad \underbrace{\qquad\qquad}_{E_{CM}}$$

$$\therefore \left(-\frac{\hbar^2}{2M} \nabla_{cm} + V_{ext}(\underline{R}) \right) \psi_{CM}(\underline{R}) = E_{CM} \psi_{CM}(\underline{R})$$

is the CM Sch. eqn.

If $V_{ext} = 0$, the CM is a free particle.

The relative equation

$$\left[\sum_i{}' -\frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{jk}{}' -\frac{\hbar^2}{2m_n} \left(\frac{\partial^2}{\partial x_j \partial x_k} + \frac{\partial^2}{\partial y_j \partial y_k} + \frac{\partial^2}{\partial z_j \partial z_k} \right) + V_{int}(\{\underline{r}_{ij}\}) \right] \psi = E \psi$$

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The messy mixed term is a real pain.
It spoils us from getting a Sch. eqn for the internal motions.
If $m_n >> m_i$, then we could drop the mixed term.

If there are only two particles, then the mixed term becomes

$$\sum_i \frac{-\hbar^2}{2m_n} \nabla_i'^2 ,$$

then we can combine the first and second term as

$$\frac{-\hbar^2}{2\mu} \nabla'^2$$

where $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$

↑ only i term is 1

↑ n is 2, or vice versa.

In this case, we are back to the relative Sch. eqn. for the 2-body problem (5-§4).

I say we managed to solve the relative equation of p5-123, and got

$$\psi_{\text{total}}(\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_n) = \psi(\underset{\sim}{r}_1 - \underset{\sim}{r}_n, \ldots, \underset{\sim}{r}_{n-1} - \underset{\sim}{r}_n)\, \psi_{CM}(\underset{\sim}{R})$$

Can we eliminate $\underset{\sim}{r}_n$ in favor of a coordinate relative to $\underset{\sim}{R}$ as we did in the 2-body case of p. 5-97?

$$\underset{\sim}{r}_i - \underset{\sim}{r}_n = \underset{\sim}{r}_i - \left(\underset{\sim}{R} - \frac{\sum_j{}' m_j \underset{\sim}{r}_j}{m_n} \right)$$

remember this omits $\underset{\sim}{r}_n$

$$= \underset{\sim}{r}_i \left(1 + \frac{m_i}{m_n}\right) \underset{\sim}{R} + \sum_j{}' \frac{m_j}{m_n} \underset{\sim}{r}_j$$

omits $\underset{\sim}{r}_i$ & $\underset{\sim}{r}_n$

$$= \underset{\sim}{r}_i - \frac{m}{m_n} \underset{\sim}{R} + \sum_j{}' \frac{m_j}{m_n} \underset{\sim}{r}_j$$

Well no.

Perhaps we should have explicitly written in terms of

$$\underset{\sim}{v}_i' = \underset{\sim}{v}_i - \underset{\sim}{R} = \underset{\sim}{v}_i - \frac{\sum_j m_j \underset{\sim}{v}_j}{M},$$

But there is always the problem that $\underset{\sim}{R}$ is NOT an independent coordinate unless one drops one of the particle coordinates — but that creates an asymmetric treatment.

There must be some treatment analogous to Lagrange multipliers for treating all coordinates on an equal footing.

But I'm at the end of my tricks.

In this case we are back to the relativ Sch. equ. for the 2 body problem.

(See p. 5-84)

Our relativ equation is probably not really useful.

There must be better ways of doing things.

My old friend Lindmilla told me one usually first takes a point of ~~system~~ expected symmetry of a system, defines that as the origin, and hopes it's close enough to CM to define an inertial frame.

The real ~~point~~ good thing about the derivation is that the CM part can be separated off — in some important cases — and we know how the CM motion sometimes.

Anything we can imagine doing with the relative equation on p. 5-123.

i) Try to see if the mixed term vanishes with certain symmetries

ii) Try making particle N an artificial particle at center of symmetry with no force acting on it.

↳ nothing I could think of led to any great formal improvements. The gurus must know better ways.

5) Identical Particles

~~The Symmetr~~

Classically we assume we can always tell two interacting objects apart. — and unobstrusively.

→ We could put labels on them that were too small to perturb the motion significantly or follow their motion with a camera — assuming the light scattering did not perturb the motions significantly.

But if the objects were truly identical (which for macro-objects is an ideal limit)

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— and we didn't ~~what~~ want to perturb them at all.

— We ~~go~~ could still ~~know~~ know which was which.

Given their initial conditions, all ~~their~~ motions are strictly determined and at an later time we'd know which was which.

But when go the QM micro-world, the situation is different.

First of all truly identical particles exist
— at least that is as far as we know.

Actually, there are identical particles in two senses.

~~a) Indistinguishable~~

a) Indivisible or non-composite identical particles
e.g., electrons, quarks, neutrinos.

— each of these are truly identical
↳ except for dynamic properties
i.e., position and spin orientation.

- their intrinsic ~~properties~~ characteristics are always the same.

Two electrons are exactly alike and you cannot put labels or scratches on them to distinguish them.

All you can do to an electron is destroy it.

e.g., $e^- + e^+ \rightarrow 2\gamma$

↳ pair annihilation with a positron.

b) Composite identical Particles.

- these particles are exactly alike in their properties but they can be in different states.

~~Statistics~~ For example two hydrogen atoms have identical properties but they can be in different states: e.g., One in $n=1$ state (ground state)

one in $n=2$ ~~state~~ first excited state.

— actually even if the Hydrogen atoms were in the same state for most descriptive purposes, their states can't be exactly the same — the environment always causes fluctuating perturbations.

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— protons & neutrons are sort of a special case

— we often think of them as fundamental and non-composite

But in the modern view they are composites of quarks

↳ and at high temperature and density can be broken into a quark-gluon plasma (QGP)

~~Maybe~~

My guess is this is not all or nothing, there must be stages of perturbed protons & neutrons before unbinding (I'm not sure)

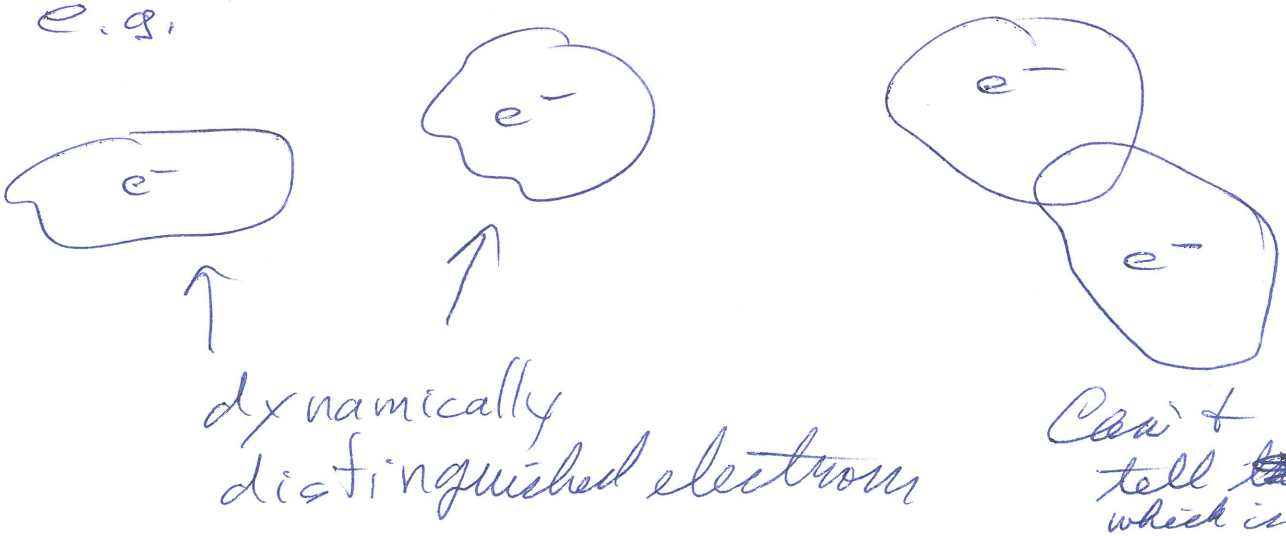
But certainly in most environments protons & neutrons act like non-composite particles.

Wave function Overlap

Now even ~~though~~ you can mark the composite particles (say put two into two different states) both they and the fundamental particles

CANNOT be separately tracked when their Wave functions overlap

e.g.



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Now why can't we tell them apart with wave function overlap?

Well the real reason is the symmetrization principle

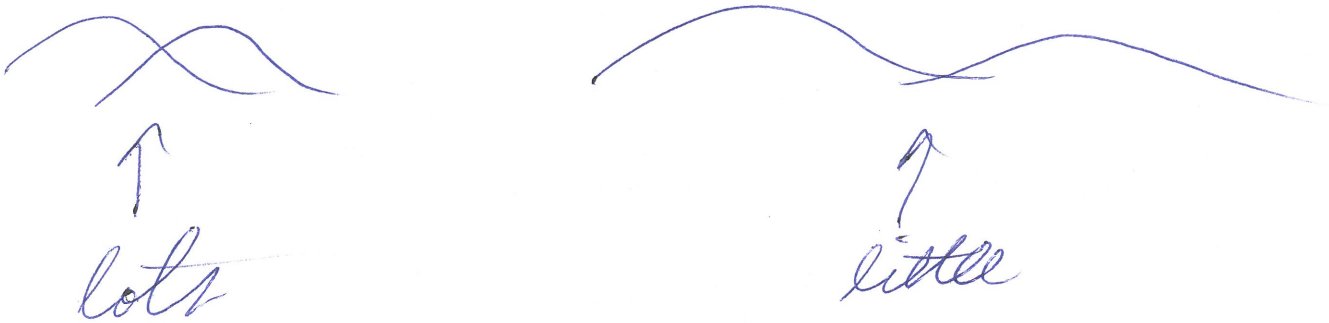
Applies to both fundamental particles and, by derivation, composite particles.

rules that out as we'll see.

The symmetrization principle dictates that all identical particles wave functions must be symmetrized when the wave functions overlap

— we'll get to what that means in a bit. (patience).

But how much overlap does there have to be to require symmetrization?



Well - it's not all or nothing.

Doing without symmetrization is an approximation.

— the less overlap, the better the approximation.

— We'll look at this quantitatively in a bit too.

The more you can think of the identical particles as dynamically distinguished.

Actually there are other cases where full ~~where~~ symmetrization can be neglected as an approximation.

Thank goodness — like would be tough without this.

6) Particle Exchange and Permutation Operators

Say you have two particles.
— Let's say they are distinct.
but they have the same spin. and individual state spaces are isomorphic → same sets of eigenstates of spin

Apparently (CT-1378 implies without bluntly stating)
that a joint eigenstate. state of the two particles can always be formed as a tensor product

sums of product states can be formed too, of course

$$|1;2\rangle = |1,u_i;2,u_j\rangle$$

abstractly written so