Lecture 18: Hydrogen and its discontents

Remind of what we did last time; today we will include also some steps promised for recitation (yay!)

Review: we talked about central potentials,

$$\hat{E} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2} r}_{\text{radial derivative term}} \quad \underbrace{+\frac{\hat{L}^2}{2mr^2}}_{\text{angular momentum term}} \quad \underbrace{+V(r)}_{\text{potential term}}$$

3 contributions! radial + angular + potential

Then we can apply separation of variable, and our eigenstate will have form

$$\phi_{E,l,m} = \frac{1}{r}\underbrace{R_{El}(r)}_{\text{radial part}}\underbrace{Y_{l,m}(\vartheta,\varphi)}_{\text{spherical harmonic}}$$

2 contributions!

By using spherical harmonics, which are eigenfunctions of the angular momentum operator, it is equal just to a constant times the eigenfunction, so we simplify the problem under the angular standpoint!

By separating in this form, so also extracting the sneaky $\frac{1}{r}$ factor, the energy eigenvalue equation reduces to a single 1-D effective energy eigenvalue equation!

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V_{eff}(r)\right) R = E R,$$

much simpler than the previous, where

$$V_{eff} = \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r)$$

is the effective potential! Here, $\frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}$ is referred to as the "angular momentum barrier"!

This energy eigenvalue equation exhibits no dependence on m, so energy can not consequently depend on m! Although it depends on l.

In other words, for different values of m, I will get the same energy: we have a degeneracy, i.e., symmetry (and, then, a conserved quantity!)

For a fixed l, we have $(2l+1)$ possible values of m! This is the entity of our degeneracy in m! This is a general property for any central potential, so it arises just from spherical symmetry!

Then, we started a discussion about Coloumb potential,

$$V(r) = -\frac{e^2}{r},$$

and we quickly reviewed the solution of the corresponding energy eigenvalue equation. We discovered that

$$R_{n,l} = \underbrace{e^{-\frac{r}{2r_0 n}}}_{\substack{\text{asymptotic}\\ r\to\infty}} \underbrace{\left(\frac{r}{r_0}\right)^{l+1}}_{\substack{\text{asymptotic}\\ r\to 0}} \nu_{nl}\left(\frac{r}{r_0}\right), \qquad E_{nlm} = -\frac{E_{Ry}}{n^2} \rightsquigarrow \text{Rydberg energy} \quad (1)$$

Discussion: the fact that we have an exponential decay, e^{-r^2}, came from the asymptotic analysis for $r\to\infty$, more or less as in bound states!

The $(r/r_0)^{l+1}$ arises from asymptotic analysis for $r\to 0$, in order to ensure to have a regular solution (see previous lecture). We studied this with $\rho = \frac{r}{r_0}$, now we just replaced. The function $\nu_{nl}(\rho)$ satisfies the energy eigenvalue equation, such that, asymptotically, it is regular. So, $\nu_{nl}\left(\frac{r}{r_0}\right)$ must be smooth, with no poles, and for $r\to\infty$ should not be crazy. We "solved" this for series expansion and found that, for series termination, we got a relationship between energy, l, and n, (1)!

We have an additional condition! $n > l$, integer! And, of course $l \geq 0$.
How does this condition arise? It comes from the series expansion:

$$\nu = \sum_j a_j \left(\frac{r}{r_0}\right)^j \qquad \text{(power series)}$$

after some steps we could derive the recursion relation

$$a_{j+1} = a_j \frac{2\sqrt{\varepsilon}\,(j+l+1) - 1}{(j+1)(j+2l+2)}.$$

So, if we know a_0, so, a constant, $\neq 0$ (otherwise $a_j = 0$, always since $a_{j+1} \propto a_j$),

we can obtain a_1 from a_0, and so on. However, note that, as j gets large, so as we consider higher order terms in the series, j gets larger than 2, than l, so this relation asymptotically tends to

$$a_{j+1} \simeq \frac{2\sqrt{\varepsilon}\,j}{j(j+1)} \simeq \frac{2\sqrt{\varepsilon}}{j+1}$$

What does this imply? Well, every time I increase j by 1, I multiply times $2\sqrt{\varepsilon}$ and divide by j, so, taking a_0,

$$a_j \cong a_0 \frac{(2\sqrt{\varepsilon})^j}{j!} \qquad \text{Since } \forall j \text{ we multiply times } j \text{ itself...}$$

And... These are the Taylor expansion coefficient of an exponential!
This is bad! If the series goes like an exponential, then, this series tends to $e^{2\sqrt{\varepsilon}\frac{r}{r_0}}$, that is swamping the exponential derived at the very beginning, from the asymptotic analysis! If ν is growing twice as rapidly as $r\to\infty$, then we are screwed! The product diverges at ∞!

So, it must be true that j does not go large enough to allow the exponential in ν to dominate, to overwhelm that from the asymptotic analysis.
So, the series has to terminate! So, at some j, j_{max} (j_{max})

$$2\sqrt{\varepsilon}\,(j_{max} + l + 1) - 1 = 0,$$

or,

$$\varepsilon = \frac{1}{4(j_{max} + l + 1)^2}$$

This means that our solutions, or states, ψ, are labeled by 3 indexes:

$\psi = \psi_{l,m,j_{max}}$, where j_{max} could be any number, from 0 on!

Technically, not 0, not ∞ but hey, almost any number! Integer!

Then,

$$E_{l,m,j_{max}} = -\frac{E_0}{4(j_{max} + l + 1)^2}$$

We can call $n = j_{max} + l + 1$, and n can be any number (except l):
$n > l$, but with this, any integer is fine. So,

$E_{l,m,n}$.

By subtracting $l+1$ from n $(n-(l+1))$ we have the j such that the series terminates.

This power series for ν, if $n = l+1$, has only the 0 term: just 1! In fact, if $n = l+1$, then $j_{max} = n-(l+1) = 0$, so only a_0 is not null! Then, being this the coefficient of a power series, if we have only a_0, then ν is a constant function!

If $n = l+2$, we have just 2 terms, so it is a straight line.
We also obtained the form of the energy.

However, even if we obtained the solution, this brute force approach didn't provide us with much of an insight.
For example, we have no clue about the reason behind this huge degeneracy: the one of m $(2l+1)$, but also in l! We have dependence just on "n"!
For any given E_n, we have, fixing n, that l can go from 0 to $n-1$; in fact, the limit is $n = l+1$, so l can span from 0 to

$n = l+1 \Leftrightarrow \boxed{n-1 = l}$ (otherwise we would have also $a_0 = 0$!)

Moreover, for each l, we have m, spanning from $-l$ to $+l$: $2l+1$, for each l!

$$d(E_n) = \sum_{l=0}^{n-1} \sum_{m=-l}^{+l} 1 = \sum_{l=0}^{n-1} (2l+1) = n^2$$ (from series arithmetics)

This is a huge degeneracy! Why?! Why do we have this?

Always remember: from degeneracy, we know that we have some symmetry:
When we have symmetry, we have energy (we are talking about energy) commuting with some operator. So, we can construct new states, given a single energy eigenstate, by acting with that operator (the one commuting with energy).
So, there must be some new symmetry which currently we haven't noticed.
What is different from a stupid central potential? This is hydrogen. Why is it so different from the 3D harmonic oscillator?
Well, when we have degeneracy, we have symmetry. But Noether's theorem tells us that when we have symmetry, we have a conserved quantity!
And, in quantum mechanics, having a conserved quantity means that energy commutes with some quantity! $[\hat{E}, ?] = 0$: that controls the time evolution of the expected value!

What is commuting, in this case? Well, for the Coulomb problem, or the Kepler problem, in classical mechanics, there is a vector that is conserved, that is

$$\vec{A} = \vec{p} \times \vec{L} - \overset{\text{mass of the electron}}{m_e} e^2 \vec{r}$$ [this is often referred to as Runge-Lenz vector]

Born from Kepler, because orbits close, form ellipses, and have a bunch of nice properties that beg for an exploration in terms of symmetry.
$\vec{A}$ can be transformed to an operator, and it could be proved that

$$[\hat{E}, \hat{\vec{A}}] = 0$$

This, really, is NON-OBVIOUS.
Note that

$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$, now we have $\hat{\vec{p}} \times \hat{\vec{r}} \times \hat{\vec{p}}$! There is an ordering ambiguity! For instance, for $\hat{\vec{L}}$, we can write $\hat{p}_x \hat{l}_y$, $\hat{l}_x \hat{p}_y$, but there is also the second $\hat{p}$, so there is some ambiguity!

Now, OK! We have a conserved quantity! VICTORY!. But no, calm down! we still haven't found any symmetry! :-o What's the symmetry behind this?! Which symmetry is ensuring us that this is a conserved quantity?
Well, there are many answers to this question.

- One, involves an explicit expression in phase space, a nonlinear change of variables $\delta x = \vec{f}(\vec{x}, \vec{p})$
  and this change of coordinates depends both on position and momentum.

- Something much more interesting was proposed by Fock, one of the fathers of quantum field theory in 1935; Fock observed that when you take the Kepler problem, and work in momentum space (so you write everything in terms of momentum), it turns out that the Kepler/Coulomb problem, in 3D, is exactly equivalent, through an almost complicated change of variables, to the problem of a free particle in four dimensions, constrained to the surface of a sphere (in 3D): S^3.
The sphere is invariant under rotations in 4 dimensions: which is the symmetry group of this system? A system with a marble constrained on a sphere, that we can kick, and then can move forming circles (24 min)? SO(4): orthogonal rotations in 4 dimensions!
Angular momentum group in 3D is SO(3)! The rotations, which don't change length, in 3 dimensions (4 for Kepler problem).
With angular momentum we have 3 conserved quantities (L_x, L_y, L_z), here we have (we can do the computation) 6! When remapping how the sphere in 4D to the Kepler problem in 3D, we can understand

that 3 of these quantities are L_x, L_y, L_z, and the other 3 are the components of the vector $\vec{A}$!

So, the spectrum of hydrogen or, at least, of its simplified Coulomb model, has an enhanced symmetry: the symmetry group of rotations in 4 dimensions, SO(4)!
Why? Boh! But it's awesome!

What does it mean in quantum mechanics to have a conserved quantity? Well, given $\hat{A}$ an operator, that its expectation value is conserved!

$$j\hbar \frac{d}{dt} \langle \hat{A} \rangle_{\psi(t)} , = \ldots$$

and this depends on time, thanks to $\psi(t)$. But we proved that this equals

$$\ldots = \langle [\hat{E}, \hat{A}] \rangle_{\psi(t)},$$

So, if this commutator vanishes, $\frac{d}{dt} = 0$, and that means conservation!

Even if we can't know simultaneously L_x, L_y, L_z, we know that all of them commute with $\hat{E}$, so they are all conserved!

Now that we understood (more or less...) from where this degeneracy come, well, can we break it? Or lift it?
What does "lift" a degeneracy mean? Well, if we have a system with two degenerate states, can we somehow kick the system in such a way that one energy level gets lifted from the other? Eliminating the degeneracy?
Lift, break, split: all synonyms!
Sure we can! We can do it, by breaking symmetry!
One symmetry is related to the fact that we are dealing with a central potential, the $2l+1$, so to the conservation of angular momentum. The other is related to the Runge-Lenz vector, which is a consequence of dealing exactly with a Coulomb potential, $-\frac{e^2}{r}$!

Let's change the system! With some small correction! We want to model hydrogen, so, what should we do to get closer to it?
For example, since we know that the electron may move quite fast, should we add some relativistic correction? Well, for sure, relativistic corrections don't break spherical symmetry! They do not privilege any direction!
So we will correct kinetic energy, then $\hat{E}$, but preserve rotational symmetry!

Which correction should we introduce? Well,

$$\text{Kinetic } E = \sqrt{m^2c^4 + p^2c^2} - mc^2 = mc^2 \left(\sqrt{1 + \frac{p^2}{m^2c^2}} - 1 \right),$$

and if we Taylor expand this guy, with p^2 small with respect to $(mc)^2$,

$$\simeq mc^2 \left(\cancel{1} + \frac{1}{2} \frac{p^2}{m^2c^2} - \cancel{1} \right) = \frac{p^2}{2m} \quad ! \Rightarrow \text{Rock on!}$$

The first-order relativistic correction is the second-order expansion of the square root,

$$\sqrt{1+x} \simeq 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3, \quad \text{so}$$

$$\simeq mc^2 \left(\cancel{1} + \frac{1}{2} \frac{p^2}{m^2c^2} - \frac{1}{8} \frac{p^4}{m^4c^4} \cancel{-1} \right) = \frac{p}{2m} - \underbrace{\frac{1}{8} \frac{p^4}{m^3c^2}}_{\text{relativistic correction}}$$

Therefore, a better model of hydrogen, $E_{\tilde{H}_y}$, is:

$$\hat{E}_{\tilde{H}_y} = \underset{\substack{\uparrow \\ E_{\text{Coulomb}}}}{\hat{E}_C} - \frac{\hat{\vec{p}}^4}{8m^3c^2}$$

↳ relativistic. This should be quite a small term.

We know that

$$E_{nlm} = -\frac{E_0}{4n^2},$$

then, for the "new" operator, with relativistic corrections,

$$E_{nlm}^{\tilde{H}_y},$$

we should re-solve from scratch the problem, but, since we have that $\vec{p}^4$ term and so on, this is much, much more complicated! 4 derivatives!
Well, a "rigorous" way might be perturbation analysis, but, can

Can we try something easier? Just to grab an idea on what happens? Well... Dimensional analysis! Well, good idea, but, from dimensional analysis we can grab just the order of magnitude of what we are studying. In this case, we want something more! We want to appreciate, to see that degeneracy gets splitted! See different energies! See that different values of l lead to different energies! Emphasize the l dependence!

Second proposal: study the expectation value of $\vec{p}^4$!

$$E_{\tilde{H}_y} = E_C - \frac{\langle \vec{p}^4 \rangle}{8m^3c^2}$$

in 8.05 we will discover that this approach was exact, by reaching it rigorously!

So, by doing calculations of $\langle \vec{p}^4 \rangle$, we discover

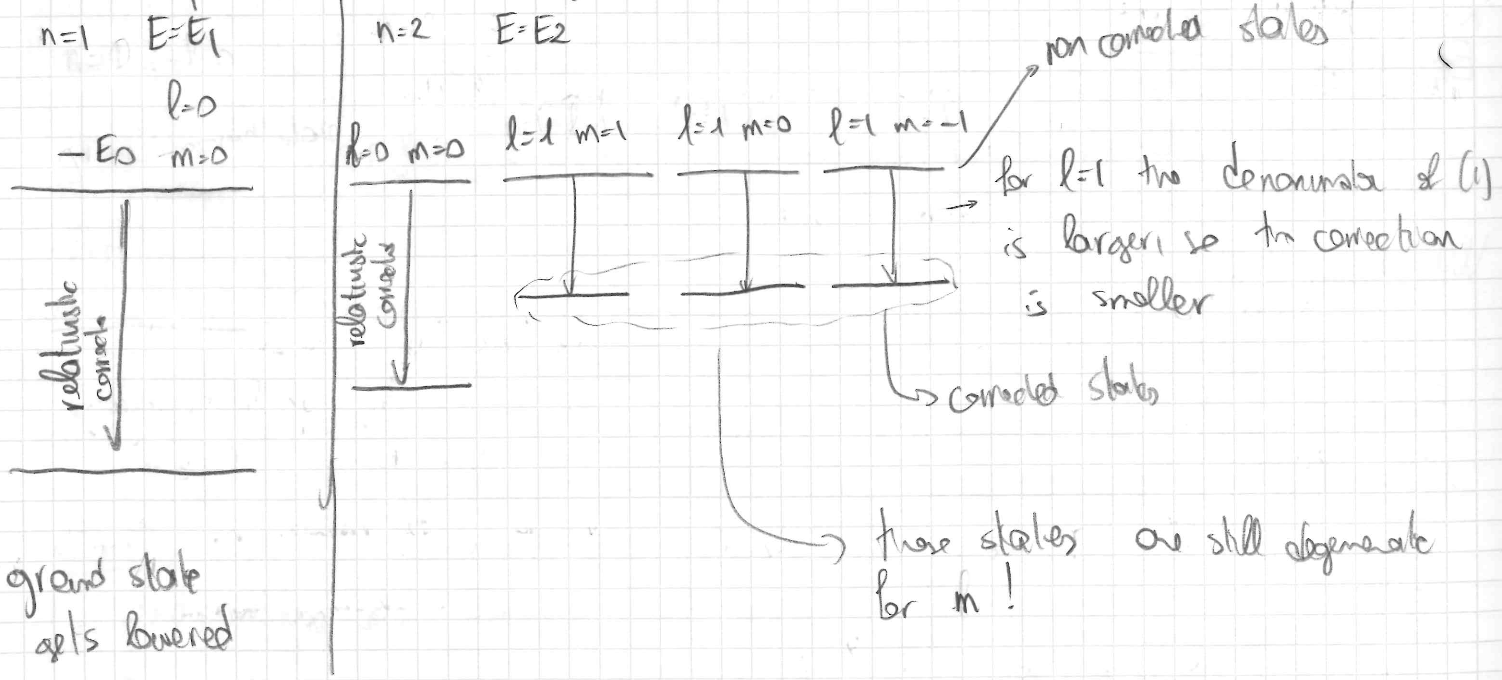
$$E_{\tilde{H}_y} = \underbrace{-\frac{E_0}{n^2}}_{\text{original}} - \frac{E_0^2}{n^4 mc^2}\left(\frac{4n}{l+\frac{1}{2}} - 3\right) \qquad (1)$$

AND HERE, WE HAVE l! Different values of l give different energies! So in particular, now it must be true that the energy operator for this improved model of hydrogen does not commute with $\hat{\vec{A}}$!

$$\left[\hat{E}^{\tilde{H}_y}, \hat{\vec{A}}\right] \neq 0$$

this, we can prove, is true!

Let us plot / draw something.

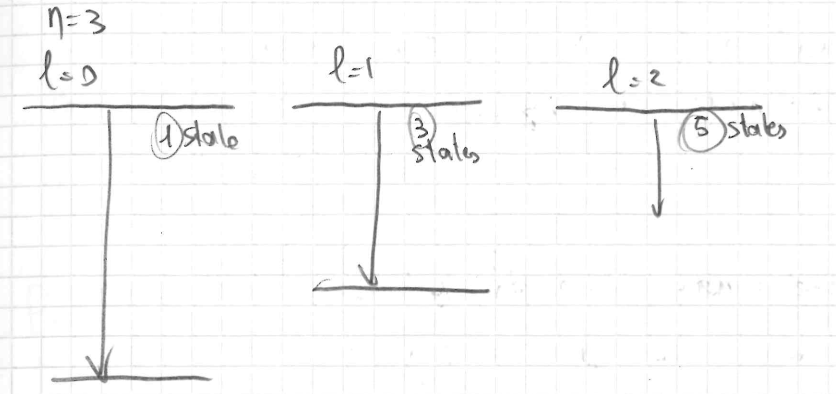


for l=1 the denominator of (1) is larger, so the correction is smaller

these states are still degenerate for m!

grand state gets lowered

We could proceed with n=3. We would have:



Now let us perform something different, introduce something else! For instance... Let us add a magnetic field! This can break both the $\vec{A}$ degeneracy and the spherical symmetry. In fact, $\vec{B}$ introduces some preferred direction.

Zeeman effect: turn on a magnetic field (uniform) next to a hot, glowing gas, look the spectrum, and you can see that...

$$E = E_C \underbrace{-\vec{\mu}\cdot\vec{B}}$$

$\vec{\mu}$ → magnetic moment

$\vec{B}$ → background magnetic field

→ if the atom is like an electron, that carries some angular momentum in presence of a proton, and it also have a charge, charge × ang. mom is a magnetic moment, μ:

$$\mu = \frac{IA}{c}$$

I: current caused by motion of the elec

A: area

c: speed of light

So, we can say that

$$\mu = -\frac{e}{2m_e c}\vec{L}$$

$\vec{L}$ → angular momentum:

we have that current is charge with velocity, so by combining you find this $\hat{L}$. $I = e\vec{v}$, $\vec{v} = \frac{\vec{p}}{m_e}$, A = radius r, and that's it!

m_e: electron mass

If we assume $\vec{B} = B_z\hat{z}$, we have

$$E = E_C - \mu_z B_z = E_C + \frac{eB_z}{2m_e c}L_z$$

Now, we have that $\hat{L}_z$ appears, instead of $\hat{L}$, in our equation, so "m" (eigenvalue of $\hat{L}_z$) will surely appear in the energy!

$\left(\hat{L}_z R = \hbar m R \ ! \right)$ something like this

So, with Zeeman effect, E^Z,

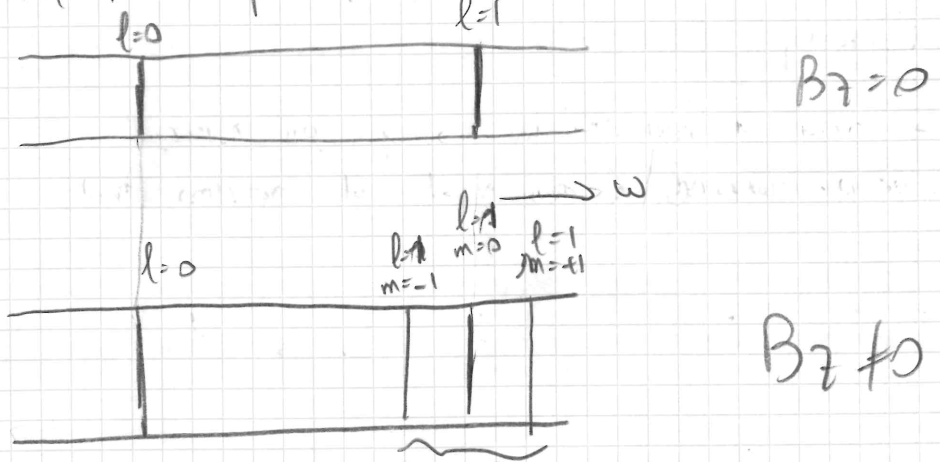
$$E^Z_{nlm} = -\frac{E_0}{n^2} + \frac{e\hbar}{2m_e c} B_z \boxed{m} \rightarrow \text{eigenvalue of } \hat{L}_z \ !$$

Moreover, now we just mentioned the magnetic field, but we could also do some computations including relativistic corrections!

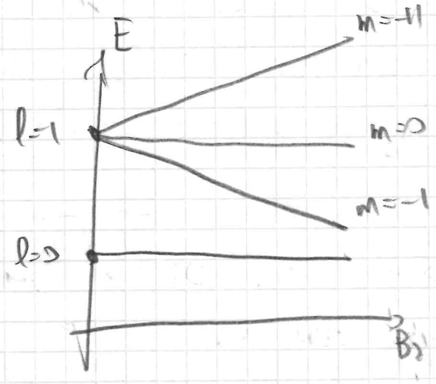
$$E^Z_{nlm} = E^{\tilde{H}_H}_{nlm} + \frac{e\hbar}{2m_e c} B_z m$$

So, what does this second correction introduce? Well, a splitting of levels with the same "l"!

So, for a prism, where we separate spectral lines,

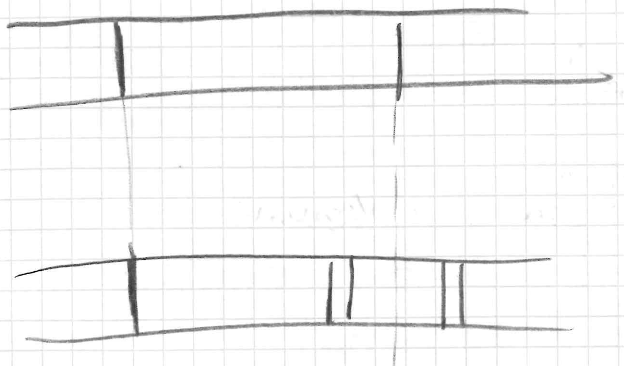


these lines get splitted, by Bz!



As a function of B_z, the $m \neq 0$ levels split!

This, for what concerns hydrogen. Fully quantum effect: impossible to explain classically!
Then, Zeeman performed the same experiments with sodium, but something strange happened



Some lines remained equal, but other got splitted in 4 levels, with no common level from the $B_z = 0$ one! o_o

In order to have 4 states in the lower, it means that l is a half integer number! o_o $l = \frac{3}{2}$! o_o
But then, all the formalism based on $Y_{lm}(\theta, \phi)$ fails! We are screwed!

The second effect, on sodium, is called "anomalous Zeeman effect"!

Before studying other, new things or go deeper into these, let us perform the following observation.
On one hand, we studied the Coulomb potential, and we discovered that the degeneracy of energy states $d(E)$ is something like n^2.

Meanwhile, chemists people observed that the number of states of the n-th level in the periodic table is: 2 for the first, 8 for the second, 18 for the third, well, like $2n^2$ $(2 \times 1^2, 2 \times 2^2, 2 \times 3^2 \ldots)$,
So, similar, but, with a factor of 2!
Maybe, there is some relationship!

Well, let us imagine that only 1 electron can occupy an energy state. Then, atoms could be discriminated by the number of electrons that could carry!

Pauli noticed the factor "2" of difference, and did a conjecture for 2 things:

① no 2 electrons can inhabit the same energy state

② there exist twice as many states as we think, in hydrogen.

This is the Pauli's exclusion principle, that postulates another quantum number, so that identifies twice as the expected (at least, compared to our present knowledge) states.

THIS GIVES US THE FULL PERIODIC TABLE!

Uhlenbeck, Goudsmit project $\boxed{\text{Alsos}}$

1h14 history of spin, follow the lecture (just history!)

Lecture 19: Identical Particles

Next 6 lectures: understand why solids exist. Why there is conductivity, why diamond is transparent.

Question: spin-orbit coupling.

For/In the Zeeman effect, there are other terms to be accounted, such as a second term, which is an induced magnetic moment: even with the angular momentum is zero, there's still a contribution to energy from the externally imposed magnetic field.
What is spin-orbit coupling? We know that the "full" energy operator for hydrogen has: Coloumb, the relativistic term (with some coeff β), the angular momentum part,

$$\hat{E}_{Hy} = \hat{E}_{Coulomb} + \beta \hat{p}^4 + \vec{B} \cdot \mu_B \vec{L} + K \vec{S} \cdot \vec{L} \qquad (1)$$

↳Bohr magneton

But there are additional contributions. One of them is: a constant K, times spin $\vec{S}$ dotted by the electron angular momentum $\vec{L}$.
The existence of this term can be derived by studying the relativistic version of the hydrogen system, we're not doing it, but the idea is: when you have some orbital angular momentum, and some spin angular momentum, both of them correspond to an angular momentum of an object that carries some charge. It is not unreasonable to have some interaction between the two, where the two magnetic moments either want to be aligned or anti-aligned depending on the sign of K. So, spin-orbit coupling is this: a coupling between spin ang. momentum and orbital ang. momentum (orbital: related to $\vec{L}$).
Note: for $\langle \hat{p}^4 \rangle$, you do not want to perform explicitly the computation

$$\langle \hat{p}^4 \rangle = \int \psi^* \frac{\partial^4}{\partial x^4} \psi \, dx$$

this is crazy, insane. But, with some (not specified here) trick, we can get to reduce the calculation of $\langle \hat{p}^4 \rangle$ to the calculation of $\langle \frac{1}{r} \rangle, \langle \frac{1}{r^2} \rangle$. Knowing these two expectation values suffices to compute $\langle \hat{p}^4 \rangle$, if we account that the eigenfunctions satisfy the original energy eigenvalue equation.

NOTE: if the operators were not Hermitian and then Energy E complex, then time evolution would lead to losing probability conservation: like in waveguides we would have an e^{-Et}, with $E \in \mathbb{C}$, and this means losing probability: this is nonphysical. This is why physicists care so much about working with selfadjoint operators!!!

Let us focus on the term from (1),

$$\vec{B} \cdot \mu_B \vec{L}$$

We said: we turn on an external magnetic field, and the electron system, if it carries some angular momentum, having also a charge, has a magnetic moment, $\mu_B \vec{L}$. Since we have "+" sign, this wants to align to the magnetic field (anti-align with "−" sign).
Now let's imagine to take an electron in a purely Coloumb system, put it in the ground state, we ask: is it moving? No! It's a stationary state! The expectation value of position does not change in time! Nothing changes in time!!!
Ok, fine, ground state carries 0 angular momentum: not so upsetting!
Then, let's consider the first excited state, with angular momentum: $n=2$, $l=1$, $m=1$: the state with as much angular momentum L_z as possible. This electron DOES NOT MOVE, yet we say that there's a current associated with it, that this current induces a magnetic moment, Biot-Savart like, and that magnetic moment, let's say that infinitesimal loop, causes the Zeeman interaction. This is true, this fits the data, but how can it generate current ?!?!

Let us assume to have our electron in a stationary state of the Coulomb potential. Such states are labeled by 3 indices: ψ_{nlm}, and we wrote these wavefunctions:

$$\psi_{nlm} = \underset{\substack{\downarrow \\ \text{normal.}}}{\eta} \frac{1}{r} R_{nl}(r) Y_{lm}(\theta, \varphi) = \eta \frac{1}{r} R_{nl} \, \underbrace{P_l(\cos\theta)}_{} e^{im\varphi}$$

We just wrote the spherical harmonic as a polynomial in cosine of θ, times an exponential in φ.

Now: does the electron move? Well, no, not in the conventional sense!
If we compute the expectation value of position and take its time derivative it goes to zero. And even without all those computations, this is a stationary state! THIS GUY IS NOT MOVING! So why, current?
But this is quantum mechanics! We don't know position: we have a probability density for it!

$$\rho(\vec{r}) = |\psi_{n\ell m}(\vec{r})|^2 \quad !$$

and probability in quantum mechanics must be conserved! So,

$$\frac{\partial}{\partial t}\rho(\vec{r}) = -\vec{\nabla}\cdot\vec{J} \qquad (2)$$

↑

this conservation equation holds: the time derivative of the probability density $\rho(\vec{r})$ equals the divergence of the probability current $\vec{J}$, which equals:

$$\vec{J} = \underset{\substack{\downarrow\\ \text{mass of the electron}}}{\frac{\hbar}{m_e}}\,\mathrm{Im}\,(\underbrace{\psi^*\vec{\nabla}\psi}_{\text{gradient of }\psi}) \qquad (3)$$

and (2) holds if $\vec{J}$ has form (3) (proved in a problem set), by virtue of Schrödinger's equation.
Let's focus on the fact that we are dealing with this imaginary part!

In the stationary state, $\psi_{n\ell m}$, the time rate of change of probability density is 0, then, by the conservation equation,

$$\vec{\nabla}\cdot\vec{J} = 0$$

This <u>does</u> <u>not</u> <u>tell</u> <u>us</u> that current is 0! So, what's the current? Well, now we are dealing with spherical coordinates, and current is given in terms of a gradient operator, that is, in spherical coordinates,

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\vartheta}\frac{1}{r}\frac{\partial}{\partial\vartheta} + \hat{\varphi}\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}$$

So, what is $\vec{J}$? Well, intuitively, the component along the radial direction r will be 0: mathematically, because it is the derivative of something that is real, so its imaginary part will be 0 (the $e^{+jm\varphi}$ will be compensated when computing $\psi^*\psi$!). $J_r = 0$!

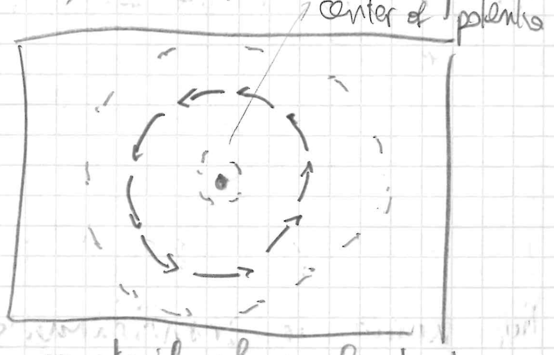
Similarly, for J_ϑ!
Instead, for what concerns J_φ, it will be obtained by deriving the exponential, so... Not so easy!

$$J_\varphi = \frac{\hbar}{m_e}\,\mathrm{Im}\left\{\psi^*\frac{1}{r\sin\vartheta}\,jm\,\psi\right\} = \frac{\hbar}{m_e}|\psi|^2\frac{1}{r\sin\vartheta}\,m,$$

So, this is proportional to $\hbar m$, i.e., the eigenvalue of L_z!
Current, or better, the probability current, for an electron in the stationary state $\psi_{n\ell m}$ of the Coulomb potential, is:

$$\vec{J} = \frac{|\psi_{n\ell m}|^2}{m_e r\sin\vartheta}\,\hbar m\,\hat{\varphi} \quad !$$

Nothing is moving but still we have a probability current!
What is the thing of this is the current? Probability density! Probability density is, then, rotating!
Looking at the equatorial plane, it means that vectors of $\vec{J}$ are oriented parallely to $\hat{\varphi}$!



equatorial plane of hydrogen atom

We know (previous lectures) that $|m| \le \ell$, so $\ell \neq 0$ to have $m \neq 0$; for what concerns the "r" dependence, we have r power to something greater than m, +1, so r cancels out at the denominator, and then $\vec{J}$ vanishes at the origin. So, the $\vec{J}$ vanishes at the origin, it's small close to the origin, it's maximum at some r, and decays again. The length of the arrows indicate the magnitude of the $\vec{J}$.

Notice that <u>electric</u> current, $\vec{I}$ let's say, is:

$$\vec{I} = \underset{\substack{\downarrow\\ \text{charge}}}{-e}\,\vec{J} \hookrightarrow \text{prob. density!}$$

The fact that we are in a stationary state causes the divergence to be zero, and that's fine! But current is not 0!

By applying Biot-Savart on this $\vec{I}$, we get the magnetic moment

$$\vec{\mu} = \mu_B \; m \; \hat{z}$$

$\hookrightarrow$ z ang. momentum!

Notice that it was crucial to have a complex valued eigenfunction. Is it possible to have real eigenfunctions for the Coloumb potential? Well, we could take $\Psi_{n\ell m}$, $\Psi^*_{n\ell m}$, and sum them! Canceling the imaginary part!
We would have:

$$\Psi_{n\ell m} + \Psi_{n\ell -m},$$

which are a new state, $\Psi_{n\ell}$, where m does not appear, is undefined!
It is not an eigenfunction of $\hat{L}_z$, but it is an energy eigenfunction!
And if we put the system in this state, $\vec{J} = 0$!
However, this would be a state with not definite angular momentum, so, it would be not a great surprise! to have 0 current!
The point is: if we want to work with states with definite angular momentum, we have current!

Identical particles, or "multiple particles"

We found that the electron is in bound states in the Coloumb potential, but in the real, actual, hydrogen atom, we have 2 actors: the electron, and the proton. So, is the proton free and the electron bound?
Now we will discuss this!

Question (from Allan): Let us assume to have a system with multiple particles.
In classical two-particle systems, in order to specify the state I have to specify position of the first particle x_1, its momentum p_1, and x_2, p_2.

In quantum mechanics, the state of the system is specified by the wavefunction $\Psi(x_1, x_2)$, and $\hat{x}_1$, $\hat{x}_2$, $\hat{p}_1$, $\hat{p}_2$ are operators that can represent those observables.

What does this notation mean? Well, $\Psi(x_1, x_2)$! $\rightarrow$ x_1 means that the first particle is in $x = x_1$, and the second particle is at x_2. So, now, $|\Psi|^2$ is the probability to find the first particle in x_1 and the second particle at x_2!
x_1 and x_2 are two points, the positions (the slots of first and second argument of Ψ) indicate the first and the second particle positions!
So, with this notation, or in particular with $|\Psi(x_1, x_2)|^2$, we indicate the probability to have the first particle in x_1 and the second particle in x_2!
Probability density:

$$\mathbb{P}(1^{st} @ x_1, 2^{nd} @ x_2) = |\Psi(x_1, x_2)|^2.$$

What is the value of the commutator $[\hat{x}_1, \hat{x}_2]$? 0: we can know simultaneously the position of the first and of the second particles!
Instead, just like in 1 particle system,

$$[\hat{x}_1, \hat{p}_1] = j\hbar \; . \quad \text{Also,}$$
$$[\hat{x}_1, \hat{p}_2] = 0 \quad \text{(independent quantities! =))}$$

Example: two free particles!

Which is the energy operator for the two free particles?

$$\hat{E} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} \quad (4)$$

m_1, m_2 masses of the two electrons.

Notice that even if we introduce (question from the audience) a force between the particles, it would just contribute to the potentials, not to $\hat{x}_1$, $\hat{x}_2$ or whatever: changing the potentials does not change what quantity is or is not simultaneously observable!

Always remember that commutator relations are relations among operators, NOT involving states: they are independent on states! Always!

Free particles: no interactions whatsoever: $V(x_1, x_2) = 0$!

The problem (4) can be solved by means of the separation ansatz!

$\Psi(A, B) = \chi(A)\,\phi(B)$

From now on, let A, B be the positions of the first and second particles, respectively.
Separation:

$$\frac{\hat{p}_A^2}{2m_A}\chi(A) = \varepsilon_A \chi(A) \implies \chi(A) = \text{coeff} \times e^{jk_A A}$$

remark once again! $A \equiv x_1$ of the previous page.

Similarly, for $\phi(B) = \text{coeff}_B \times e^{jk_B B}$

So,

$$\Psi_E(A, B) = e^{j(k_A A + k_B B)}, \quad \text{where}$$

$$E = \frac{\hbar^2}{2m}\left(k_A^2 + k_B^2\right). \qquad (5)$$

Is it always true, for every system of 2 particles, to have a form like $\chi(A)\phi(B)$? No: we can have arbitrary superpositions of forms of this "separated" type; so, this holds true as long as the energies of the plane wave are equal to the same E of (5), with the same k_A, k_B. Just when we superimpose wavefunctions of the same energy we still find another energy eigenfunction!

What about the proton? Well, let's say now that we have a system which is NOT a free particle, which is (looking at its energy operator)

$$\hat{E} = \frac{\hat{p}_A^2}{2m_A} + \frac{\hat{p}_B^2}{2m_B} + V(|A-B|),$$

so with a potential that depends only on the distance $|A-B|$. This is, for example, what happens in the Coulomb potential when we include the proton mass.

What we can do, in analogy to classical mechanics, is to reorganize the degrees of freedom into the center of mass position:

$$R = \frac{1}{m_A + m_B}\left(m_A A + m_B B\right) \qquad \text{center of mass,}$$

and, the relative distance is equal to:

$$r = A - B, \qquad M = m_A + m_B \text{ (total mass)}$$

so that we can rewrite the energy operator as

$$\hat{E} = \underbrace{-\frac{\hbar^2}{2M}\nabla_R^2}_{\text{center of mass}} \underbrace{-\frac{\hbar^2}{2\mu}\nabla_r \overbrace{+V(r)}^{\text{central potential}}}_{\text{relative coordinate}},$$

where the contribution from the relative coordinate r becomes an independent degree of freedom, with a potential, which is a central potential, and the center of mass coordinate contribution is a free particle! The mass μ in the relative coordinate contribution is:

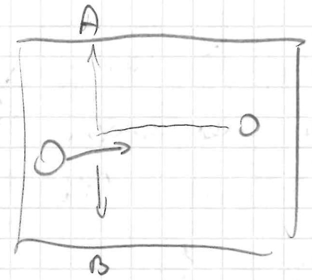
$$\mu = \frac{m_A m_B}{m_A + m_B}. \qquad \text{(reduced mass)}$$

In the case of a proton and an electron, $m_A \gg m_B$, and $\mu \simeq m_B$, mass of the electron.

So, neither the proton nor the electron are described by a Coulomb potential but, their relative radial distance is!

In 1D (question from the audience), $\nabla_R^2 \equiv \frac{\partial^2}{\partial R^2}$, $\nabla_r^2 = \frac{\partial^2}{\partial r^2}$!

Cool things with multiple particles.
Assume that we have identical particles!



Like, classically, two billiard balls: we shoot one from one side, hit the other, then they collide, start to bounce and something chaotic happens. Then, they reach two final positions, A and B (55 mink

Question! which ball goes in A and which in B? The shooted one, or the other? Well, with a high-speed film of the experiment we could trace the motions of the two particles!

Quantum mechanically THIS IS NOT DOABLE! Observing, changes the results! Like putting slits or whatever.

And, electrons can't be labeled: identical means IDENTICAL! Cannot be distinguished, whatsoever!

So, what are the consequences of this? Well,

$\mathbb{P}(A,B) = \mathbb{P}(B,A)$ ⟹ this is what it means to have identical particles!

We can't tell which is which, so these two probabilities must be the same!! If we can't tell this, these probabilities are equal! You cannot tell the difference!

What are the consequences of this?
Let us define the following operator: let $\wp$ be the Weierstraß "P",

$\hat{\wp}_{12}$ is the operator which takes the first particle, the second one, and swaps them:

$$\hat{\wp} : 1 \longleftrightarrow 2$$

So, it takes, from $\mathbb{P}(A,B)$, the $\mathbb{P}(B,A)$!
More importantly,

$$\hat{\wp}\,\Psi(A,B) = \Psi(B,A),$$

swaps the arguments!

Of course, the swapping operator does nothing on the probability, as we just have mentioned; however, if the probability is the same, it does NOT mean that the $\Psi(A,B)$ is equal to $\Psi(B,A)$! Not at all! =)
The important thing is that $|\Psi(A,B)|^2 = |\Psi(B,A)|^2$! So,

$\Psi(B,A) = e^{j\vartheta_{AB}}\,\Psi(A,B)$! the absolute value is preserved, so there could be some phase ϑ_{AB}!

On the other hand, if we swap twice,

$$\hat{\wp}\,\hat{\wp}\,\Psi(A,B) = \Psi(A,B),$$

which is also equal to

$$\hat{\wp}\left(\hat{\wp}\,\Psi(A,B)\right) = \hat{\wp}\left(e^{j\vartheta_{AB}}\,\Psi(A,B)\right) = e^{j\vartheta_{AB}}\,\hat{\wp}\,\Psi(A,B) = e^{j\vartheta_{AB}}\,e^{j\vartheta_{AB}}\,\wp(A,B) =$$

$$= e^{j2\vartheta_{AB}}\,\Psi(A,B),$$

so,

$$e^{j2\vartheta_{AB}} = 1, \text{ so}$$

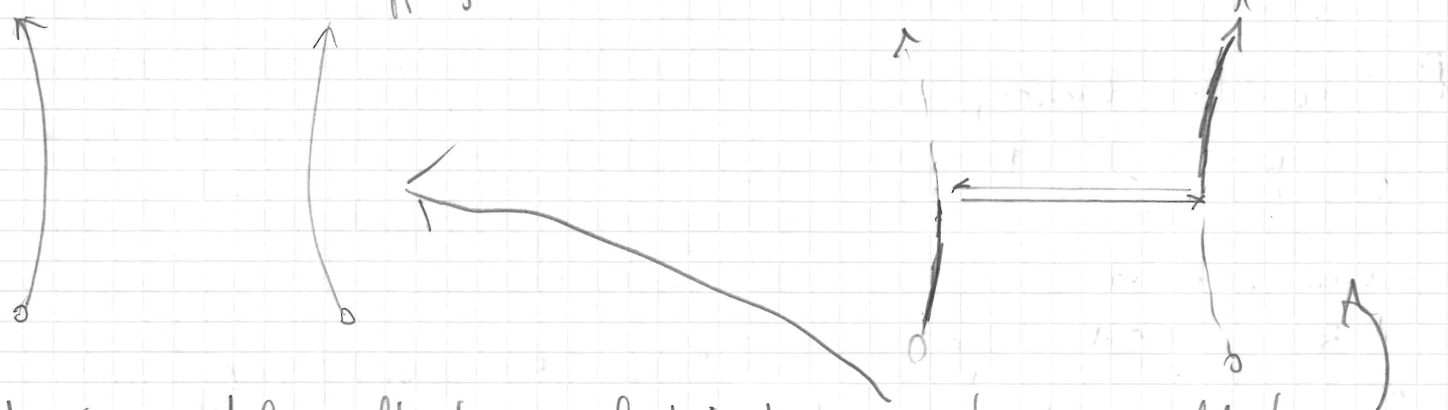
$$\boxed{\vartheta_{AB} = 0 \text{ or } \pi}$$

So,

$$\wp\,\Psi(A,B) = \pm\Psi(A,B) \; ! \; =)$$

Another way to see this is: $\hat{\wp}^2\Psi = \Psi$, so the eigenvalues of $\wp$ must be equal to ± 1!

Observation from the audience: imagine we take 2 electrons, or however 2 identical particles, one on the left hand, one in the right hand.
A while later, is it the same electron in my right hand? They're identical! I can't tell!
If we have a system with weak interactions, and the wavefunction is invariant under swapping (let's ASSUME this for the moment), then



The two particles could have walked in their own path, or could have swapped!

There are 2-3 kinds of particles in the world. First kind: distinguishable particles! Like, one with mass m, one with mass $2000\,m$. We can weight them, so they are distinguishable! One is heavier than the other! Let Ψ_D be the wavefunction of these distinguishable particles. Then,

$$\Psi_D(A,B) = \chi(A)\,\phi(B).$$

This is not invariant for swapping, since $\chi(B)\,\phi(A) \neq \chi(A)\,\phi(B)$.
Moreover, $\mathbb{P}(A,B) \neq \mathbb{P}(B,A)$!

On the other hand, if they are indistinguishable,

$$|\Psi(A,B)|^2 = |\Psi(B,A)|^2,$$

and this is not of form $\chi(A)\,\phi(B)$!

We have two possibilities: $\Psi_\pm$. If we want to express them with the separable form, we do it with a superposition,

$$\Psi_\pm = \frac{1}{\sqrt{2}}\left(\chi(A)\,\phi(B) \pm \chi(B)\,\phi(A)\right) \qquad (6)$$

if we swap A and B, this conserves probability!

The "+" solution is called symmetric, the "−" is "antisymmetric. In fact,

$$P\Psi_\pm = \pm\Psi_\pm \; ! \; = 1 \qquad (7)$$

So, distinguishable particles can just be in some random state, but there are constraints for indistinguishable particles: they must have a form like (7)!

This gives us a couple of nice facts.

① If we have identical particles, energy can't depend on the order: you swap them, then the energy must be the same. If they weren't identical, then they can be distinguished by figuring out what their energy is! So,

$$\hat{E}\hat{P} = \hat{P}\hat{E}$$

: if we first swap them and compute their energy by applying the operator $\hat{E}$, it is the same as first compute their energy, then swap them!

In other words,

$$[\hat{E}, \hat{P}] = 0$$

This tells us that the expectation value of $\hat{P}$ does not change in time! $\frac{d\langle\hat{P}\rangle}{dt} = 0$

In particular, if initially $\hat{P}\Psi = +\Psi$ at $t=0$, then $\hat{P}\Psi = +\Psi$ for all future times!

So, if the wave function is invariant after swapping, this invariance is a persistent property.

In more complex systems, such as an atom of hydrogen and one of deuterium, is it ok to swap the atoms? Hell no! They are different, distinguishable! But, their electrons, are indistinguishable, so can be swapped: just the indistinguishable parts of the whole many-body wavefunction can be swapped!

3 kinds of particles:

ⓐ distinguishable particles

ⓑ identical particles, with the property $P\Psi = +\Psi$] BOSONS

ⓒ identical particles, with the property $P\Psi = -\Psi$] FERMIONS

What are the consequences to have 2/3 kinds of particles in the universe? Fermions and Bosons?

Suppose that we have two fermions, e.g., 2 electrons. Let $\Psi(A,B)$ their wavefunction. So, for a fermion,

$$\Psi(A,B) = -\Psi(B,A),$$

for everything we have said.

So, the probability

$$\Psi(A,A),$$

must be equal to $-\Psi(A,A)$, since we "swap" the two arguments, which are the same, and we have a − sign. So,

$$\Psi(A,A) = -\Psi(A,A) \Rightarrow \boxed{0}$$

The probability amplitude to find two fermions on the same place is 0! Two fermions cannot occupy the same state!

This was the Pauli exclusion principle!

$P\psi_A = -\psi_A$

$P\psi_B = \psi_B$, so, from (6)

$$\psi_{\substack{B+\\F-}} = \frac{1}{\sqrt{2}}\left(\chi(A)\phi(B) \pm \chi(B)\phi(A)\right),$$

Notice that with $A=B$, $\psi_F(A,A) = 0$ immediately!

Bosonic identical particle case,

$$\psi_B(A,A) = \frac{1}{\sqrt{2}}\, 2\, \chi(A)\phi(A) = \sqrt{2}\,\chi(A)\phi(A)!$$

Bosons really like being next to each other!

Moreover, this "sum", this "+" character, is persistent in time, we get lasers (?).

<u>Next</u> lecture: periodic potentials! → Begin 20

The persistence property holds for fermions as well: if a system is fermionic it stays fermionic all the time! This is the consequence of $[\hat{P}, \hat{H}] = 0$!

$\chi(A)$, $\phi(B)$: taken singularly, mean: the <u>first</u> particle (state χ) is in $x=A$, the 2nd particle (state ϕ) is in $x=B$.
<u>This</u> is the meaning of this notation: looking @ single particles! – compound probability of having the 2 particles in A and B!

It turns out that every particle having half-integer angular momentum, so SPIN, turns out to be a fermion.
When you swap them, you take − sign, Fermion!

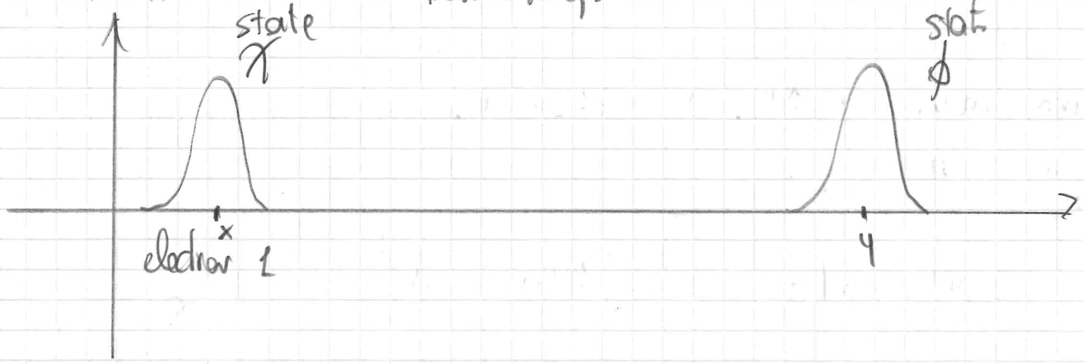
Photons integer angular momentum, are bosons!

Understanding how spin or angular momentum are connected to the fermionic or bosonic character of the particle, requires quantum field theory. Quantum field theory: relativistic version of Schrödinger equation. SPIN STATISTICS THEOREM!

Lecture 20: Periodic Potentials

Now, we start studying solids and in particular conductivity in solids and periodic potentials

Remark: when fermions are separated spatially, and localized, we can treat them independently.



$\chi(x) \neq 0$, $\phi(y) \neq 0$, but $\chi(y) \approx 0$, $\phi(x) \approx 0$,
so, if our fermion has

$$\psi(x,y) = \frac{1}{\sqrt{2}}\left[\chi(x)\phi(y) - \chi(y)\phi(x)\right],$$

$$\mathbb{P}(x,y) = \frac{1}{2}\Big[|\chi(x)|^2|\phi(y)|^2 + \underbrace{\cancel{|\chi(y)|^2}}_{\approx 0}\underbrace{\cancel{|\phi(x)|^2}}_{\approx 0} - 2\,\mathrm{Re}\{\chi^*(x)\phi^*(y)\underbrace{\cancel{\chi(y)}}_{\approx 0}\underbrace{\cancel{\phi(x)}}_{\approx 0}\}\Big]$$

$$\approx \frac{1}{2}|\chi(x)|^2|\phi(y)|^2$$! This is the proof!

Just because our 2 fermions are separated and their wavefunctions χ, ϕ localized in x and y!

Let's move on the study of solids!

PhET: simulation, with N wells.

Allan plots: the state index (abscissa) vs energy. States (20 mn) seem bunch together.

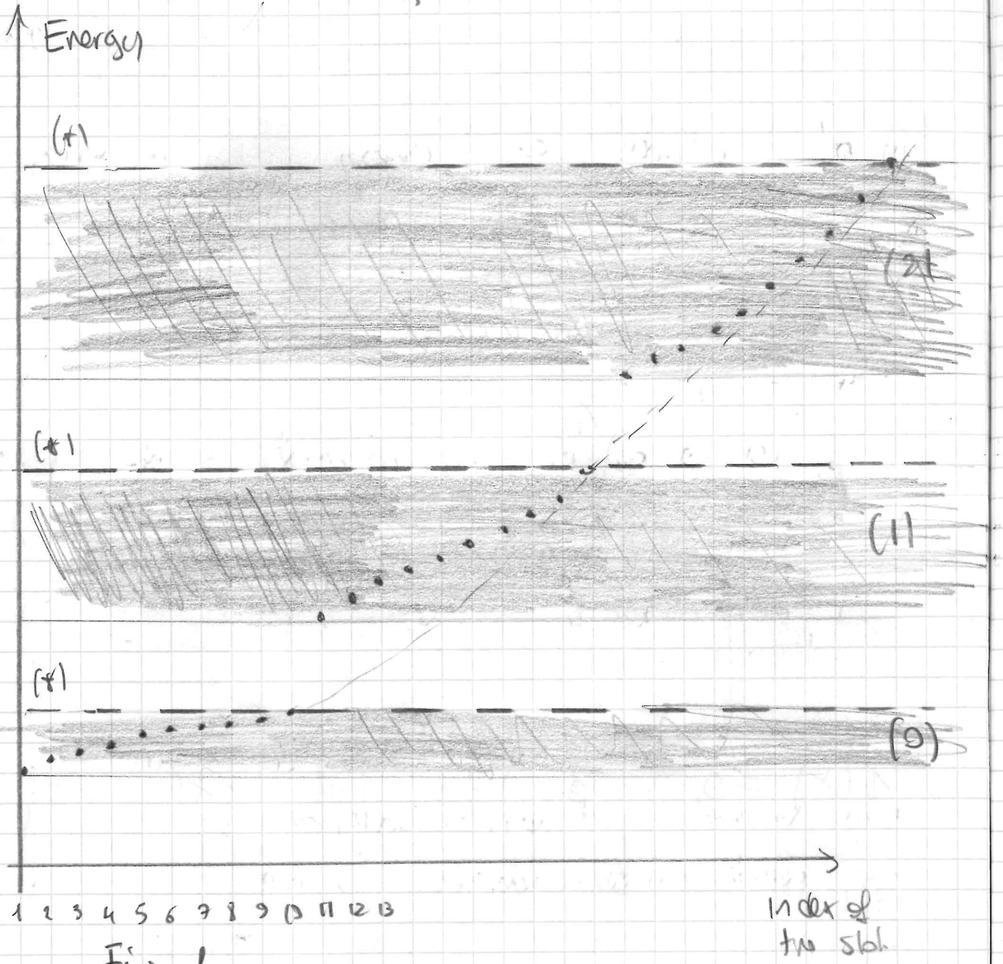


Fig. 1

10 wells.
Curious! these states are sort of grouped, in groups of 10, just like the number of wells.

Recall that if the ground state is the one with better defined position (the most confined one), then the uppermost state is that with most defined momentum, since position is badly defined (not well confined state).

For each group, let's join the topmost states, and we obtain some sort of parabola!

Note: the dashed lines(*) are the energies of the ground state, in absence of our "almost periodic" potential! Free particles!
The curve we obtained, this "parabola", describes a free particle which agrees with the free particle energies at the 3 energy points

The shadow lines identify the bands of states, which are the intervals containing the groups of 10 states.

The abscissa of this plot, which represents the state index $\overset{n}{\vee}$, is also corresponding to a momentum, since each state wiggles, and especially the top state have reasonably well-defined momenta, as already explained. So, the horizontal direction is something like a momentum. The plot has been obtained with 3 defined momenta, with 3 free particles, and we obtained these 30 states

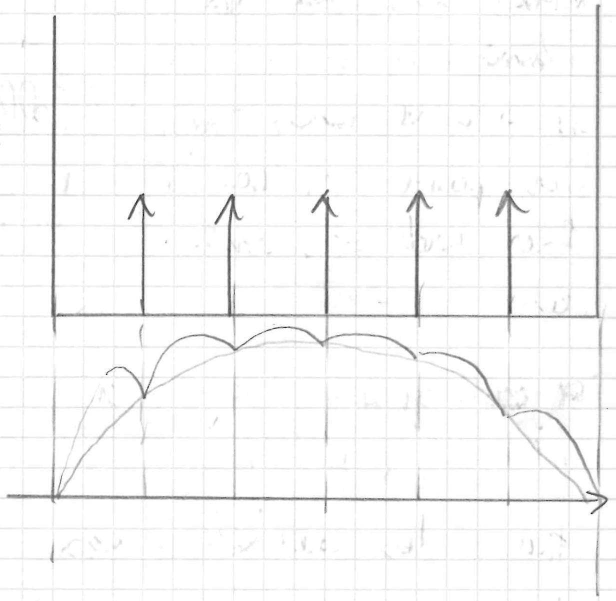
So, near the top state, the energy is a function of the level, then of the momentum, through this parabola

However, the allowed energies are found.
The shadowed part contains the allowed energies, whereas the "white" ones are not allowed. The shaded regions are those containing in other words, some energy eigenstates.

Notice from the PhET simulation that, for the 10 wells simulation, the bottom states in each well have no zeros, and the top of the group is quite similar to it!

States do not exhibit, in general, simple symmetry properties! They are quite ugly! Except the top and bottom ones, which are nicer.

If barriers become stronger, the wavefunctions become ever more messy! o_o



We can also see it as a large well, with several δ function interactions.
From several lectures ago, δ function scattering causes a kink in the wavefunction

So, instead of having a nice, "clean" band state it will exhibit several kinks. This is what Allan shows in the simulation! ☺

The stronger the δ (or wells!) are, the stronger are the interactions, and the corresponding deformations on the potential!

Same thing on the other states! NICE!!!
Envelope + Kinks!!!

There are 2 states: the envelope states, "the states of the big well", which are very close one to each other, and the states between two δ functions, which constitute narrow wells, with very widely separated states. This "band" effect occurs from these two worlds combined!

So in band (0), the states are all ground states within each miniwell, modulated by the ground state of the big well.

Band (1): all states with 1 zero within each mini well, following the envelope of the 1st state

The box controls the "modulation", the envelope, whereas the "mini well", the "individual" well, corresponds to the band we are considering.

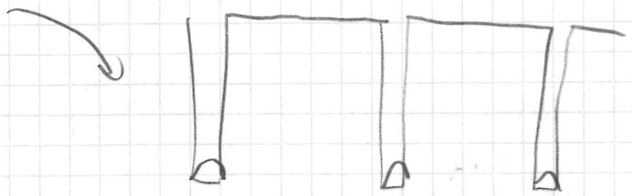
Again

- Which band, which of the shaded regions, corresponds to a state of the individual, "mini" well. Different bands so wide energy splittings!
- Which envelope, corresponds to a state of the box; this corresponds to the tiny splittings in energy between states of the different band.

[to understand this, recall that $E_n \approx \frac{n^2}{L^2}$! $\Rightarrow$ L big, E_{n+1} is close to E_n!

Depending on how strong, how large the barriers are, the more effective they will be, and the effect of the box will become less influent, less apparent.

Notice that for very far separated wells, energy states tend to be degenerate, because the effect of the box will disappear, and the states will simply become those of the individual wells!



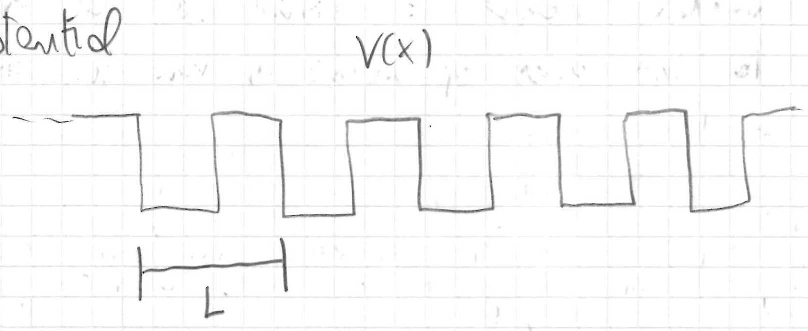
This, because the tails of the individual wells wavefunctions are so attenuated that they have basically no overlap, so no mutual interaction, and no level splitting: levels are degenerate!

Why did we discussed this?
Well, real materials such as metal, can be described in terms of a periodic potential, a crystal of metal atoms bound together, and each atom is some positively charged beast, to which a nucleus exist, to which is bound an electron.
In order to explain things like metal conducting energy, and plastic no, we have to study the physics of electrons, in periodic potentials.

These simulations were a first start: not periodic, but 10 wells, instead of ∞!

What do we expect to happen with ∞ instead of 10?
My guess? Instead of having 10 points, 10 allowed energy levels, we will have the full band ;-) Instead of dots, in Fig. 1, continuous lines!
In facts, more wells, same bands, but more states!
There has to be a continuum of states, and NOT free particle states: the system is clearly subject to our periodic potential!

Electron in a periodic potential



Let us consider a system with an ∞ number of identical wells.
Let L be the period of the lattice. Then,

$$V(x+L) = V(x)$$

There is a nice way to state this: by applying a translation of L, T_L, of $V(x)$, we obtain the same potential back.

$$T_L V(x) = V(x)$$

If we think of these as operator expressions,

$$\hat{T}_L \hat{V}(\hat{x}) f(x) = \hat{V}(\hat{x}) \hat{T}_L f(x),$$

$$\text{in fact, } \hat{T}_L [\hat{V}(x) f(x)] = \hat{V}(x+L) \overbrace{f(x+L)} = \hat{V}(x) \overbrace{\hat{T}_L f(x)}$$

$$=$$

In other words, seen as operators, commute! (just proved! =P)

$$[\hat{T}_L, \hat{V}(x)] = 0$$

Remember that the translation by L is not something new!

$\hat{T}_L = e^{j \frac{\hat{p} L}{\hbar}}$, is the expression of the operator, and then

$[\hat{T}_L, \hat{p}^2] = 0$ $\quad \hat{p}$ or $\hat{p}^2$!

So this tells us that if we take a system with a periodic potential, then

$[\hat{E}, \hat{T}_L] = 0$!!!

So, question from Allen: in this system, with periodic potential, is momentum conserved? Hell yes! We have translation invariance!
Well, not exactly... Let's say, just on a finite set of translations, the finite shifts by L! This, even if $[\hat{E}, \hat{p}] \neq 0$

This translation by L is, well, less than the very strong conditions imposed by having situations such as a free particle, but more than knowing nothing at all!
So, we can find wavefunctions which are simultaneously energy eigenfunctions and eigenfunctions of the translation by $\hat{T}_L$!

$\hat{E} \phi_{E,\alpha} = E \phi_{E,\alpha}$

$\hat{T}_L \phi_{E\alpha} \; (\;) \; \phi_{E\alpha}$, α provisional name.

Remind that $\hat{T}_L$ is unitary (proved on a problem set), so $\hat{T}_L \hat{T}_L^\dagger = \hat{I}$,

so

$\hat{T}_L^\dagger = \exp\left(-j \frac{L}{\hbar} \hat{p}\right)$, so this could also be seen as

$\hat{T}_L^\dagger = \exp\left(j \frac{(-L)}{\hbar} \hat{p}\right) \equiv \hat{T}_{-L}$, translation by $-L$!

When you translate something by L, then by −L, it's like doing nothing: identity! =>
The eigenvalues of a unitary operator are of the form of pure phases!
This, because $\hat{p}$ returns real eigenvalues!

Let α be the phase of the eigenvalue of $\hat{T}_L$.

Notice that this is a property of the Fourier transform $\left(\frac{\partial}{\partial x} \to -jx\right)$

proof

If we have

$\hat{T}_L \phi_\alpha(x) = e^{j\alpha} \phi_\alpha(x)$,

what can we say about $\phi_\alpha(x)$? Which is the form of this function?

Let us define a function $u(x) = e^{-jqx} \phi_\alpha$ (definition), then

$\hat{T}_L u(x) = e^{-jq(x+L)} \phi_\alpha(x+L) = e^{-jqL} e^{-jqx} \underbrace{e^{j\alpha} \phi_\alpha(x)}_{\hat{T}_L \phi_\alpha(x) = \phi_\alpha(x+L) = e^{j\alpha} \phi_\alpha(x)}$

$= e^{j(\alpha - qL)} u(x)$

So, we defined the function u just by using this q at that exponent, and we observed that if we translate this function by L, it takes an overall phase times its original value, and the phase depends on α and q. So,

if $\boxed{q = \frac{\alpha}{L}}$,

$\hat{T}_L u(x) = u(x) \quad =)$

So, u is periodic!
As a result, we can write our wavefunction $\phi_{E,q}$ (q instead of α in the subscript) as

$\phi_{E,q} = \exp(jqx) u(x)$, where $\boxed{\begin{array}{l} e^{j\alpha} = e^{jqL}, \\ u(x) \text{ periodic.} \end{array}}$

We haven't determined yet the explicit expression of the energy eigenfunctions, but just a formulation, a way of writing it.

So the function is periodic up to an overall phase, not a constant phase! Position dependent phase!

Notice that, in our eigenvalue of $\hat{T}_L$, $e^{j\alpha} \equiv e^{jqL}$, if we take q to $q + \frac{2\pi}{L}$, nothing changes!
Different values of q correspond to different eigenvalues of $\hat{T}_L$! This, unless they differ by $\frac{2\pi}{L}$: in this latter case, they are equal! Eigenvalues with q and $q+\frac{2\pi}{L}$ are equal!

$$\underset{\substack{\uparrow \\ \text{equivalent}}}{=}\; q \;\; q + \frac{2\pi}{L}$$

Remark! we specified NOTHING on the potential, except for periodicity!
From just this hypothesis, we can deduce lots of things.

Facts

(1) The eigenfunction $\psi_{E,q}(x)$ is NOT periodic by L!
In fact, $u(x)$ is periodic, NOT $\psi_{E,q}$. This unless $\boxed{q=0}$
(the phase term goes to 1!)
$\psi_{Eq}(x) = e^{jqx} u(x)$, $u(x+L) = u(x)$! =)
This is not surprising: the energy eigenstates that we observed with PhET are NOT periodic at all! Except the top state of the band!

(2) The probability to have $\mathbb{P}(x+L)$ is equal to $\mathbb{P}(x)$. This is clear, since
$\phi_{Eq}(x) = e^{jqx} u(x) \Rightarrow |\phi_{Eq}(x)|^2 = |u(x)|^2$.

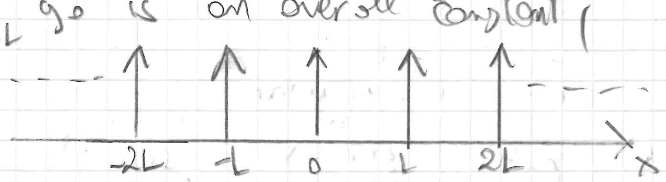
so, the probability distribution is periodic! =)
This is nice! since the potential is periodic, it would be weird to lose periodicity!
This still is weird: we have quantum wells which, taken singularly, provide confinement, but, put together in a lattice, do not provide localization! Just like in the free particle case!

Moreover, for the same reason for which the free particle wave function is not normalizable, these functions will not be normalizable either!

So, in order to be able to provide probability with some meaning we will need to study it with wavepackets!
But, just as in the free particle, wavepackets will NOT be energy eigenstates =C
Understanding how and why $\phi_{E,q}(x)$ are extended, not spatially localized, allows to understand conductivity or not conductivity in solids with different elements.

(3) ϕ_{Eq} (recall, ϕ are en. eigenstates) has q, which, dimensionally, is a momentum. We have seen that $\phi_{Eq} = e^{jqx} \overset{u(x)}{\cancel{\phi_{Eq}}}$. So, it would appear that ϕ has a momentum, q. Now, question: is ϕ_{Eq} a momentum eigenfunction? Absolutely NO! Energy and momentum do not commute! This because of $u(x)$, which is NOT localized in momentum space!
So ϕ_{Eq} is NOT a momentum eigenspace, and q is NOT the momentum! It's NOT the eigenvalue of the momentum operator! Even if it has units of momentum! This is useful, because it suggests us how the state evolves under translation by L!
So, q is called "crystal momentum", we will understand what it is in the following lectures.

These 3 facts follow just from periodicity, without anything else! Periodic systems in general!
Let us now focus on a specific example.
Example! $V(x) = \sum_{n=-\infty}^{+\infty} \frac{\hbar^2}{2mL} g_0 \delta(x - nL)$
train of δ functions! ∞ sequence of δ functions!
L is the spacing between δ barriers; $\frac{\hbar^2}{2mL} g_0$ is an overall constant; this is V_0 usually.



Problem: which are the energy eigenfunctions for a single particle in this potential? =)

Again, g_0 is the dimensionless strength of the potential.

How to solve this? Well, between two δ functions, potential is null, so the particle is free, and then we have as solution

$$e^{jKx} + e^{-jKx} \qquad E = \frac{\hbar^2 K^2}{2m}$$

At the barriers we must satisfy appropriate matching conditions. Apparently, the domain is ∞, we have ∞ boundaries, so ∞ boundary conditions, but, we already know that the wavefunction is "almost" periodic! So, we assume that, for $0 < x < L$,

$$\phi_{E,q} = e^{jqx}\left(Ae^{jKx} + Be^{-jKx}\right), \quad \frac{\hbar^2 K^2}{2m} = E \qquad (1)$$

Then, for $L < x < 2L$, we have:

$$\phi_{E,q} = \underbrace{e^{jqL}}_{\substack{\text{phase}\\ \text{shift}\\ \text{since we go}\\ \text{in } L<x<2L}} \underbrace{\left(Ae^{jKx} + Be^{-jKx}\right)}_{\substack{\text{with the}\\ \text{same coefficients of (1)!}}}$$

At the δ function the boundary conditions require that the slope at right equals the slope on the left, with some proportionality with the amplitude of the δ: the δ enforces a slope discontinuity, proportional to the δ amplitude (see old lectures).
But, except for this, the slope in 0^+ and in L^+ are the same, for periodicity! Less than the phase translation term!
So A and B are the only coefficients thanks to this!

So, let us do it, and impose these conditions in 0

$$\phi(0^+) = \phi(0^-) \qquad \text{continuous wavefunction} \qquad (a)$$

$$= \phi(L^-)e^{-jqL} \qquad (\text{back-propagated from } L \text{ to } 0 = P)$$

$$\Rightarrow \phi(0^+) = A+B = Ae^{j(K-q)L} + Be^{-j(K+q)L}$$

(b)

Derivative condition

$$\phi'(0^+) - \phi'(0^-) = \frac{g_0}{L}\phi(0) \Rightarrow jK(A-B) - jK\left(Ae^{j(K-q)L} - Be^{-j(K+q)L}\right) = \frac{g_0}{L}(A+B)$$

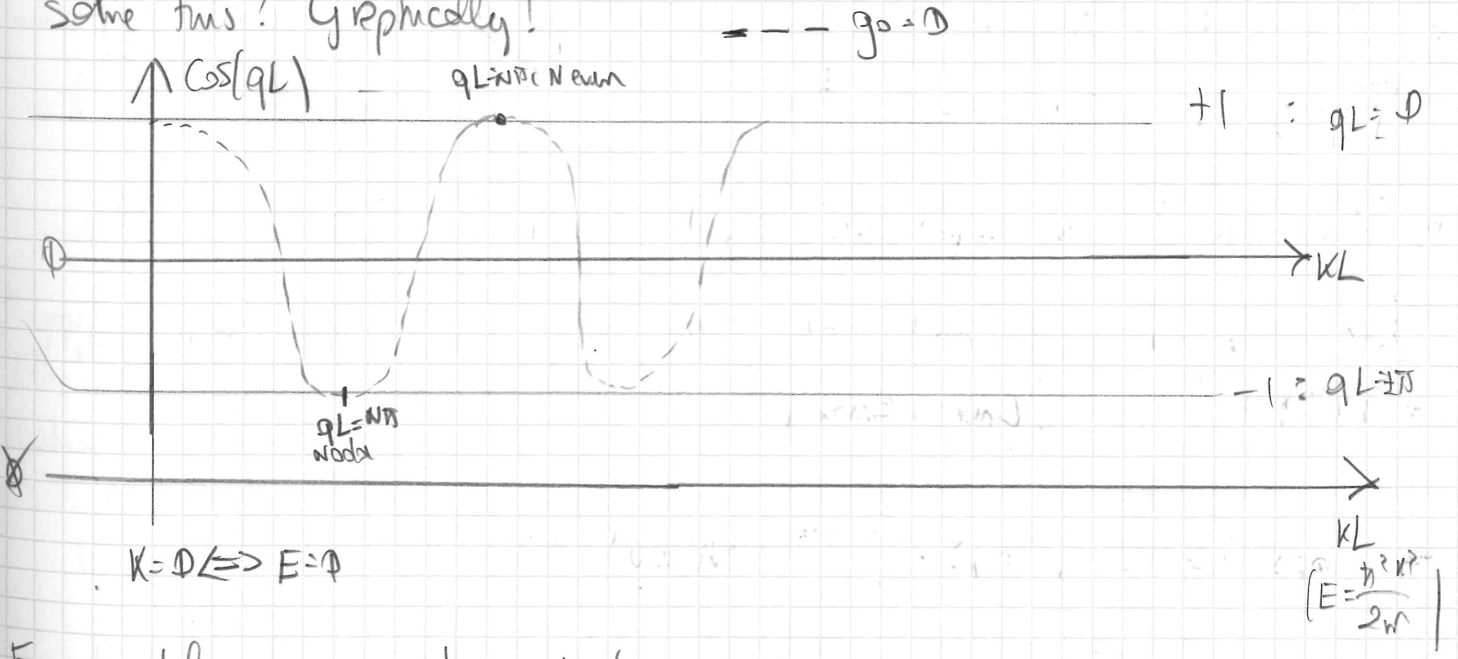
Condition (a) implies that A = B × something.
Condition (b) is another expression between A and B, it is horrible too.

If we set (a) = (b), and do some trigonometry, we find:

$$\cos(qL) = \cos(KL) + \frac{g_0}{2KL}\sin(KL) \qquad (2)$$

So K is related to energy, q is not fixed yet, it is the crystal momentum.

What values of q are allowed by this expression?! Well, so far, before (2), we never set any limit! For any q we could find an eigenfunction! So, as of this moment, q is a free parameter!
Now that we have (2), there exist a wavefunction for any couple (q, E) which satisfies (2). There exist a state for any (q, E) satisfying (2)! Just like in the finite well!
In the finite well, we did not have the cos(qL), LHS term, but just something somehow close to the RHS (more or less...).
Here we have this LHS. What to do with the extra parameter q?
q can vary from $-\frac{\pi}{L}$ and $\frac{\pi}{L}$. So cos(qL) varies from +1 to −1: any value of cos(qL) ∈ [−1, 1] is ok. On the other hand, how can we solve this? Graphically!

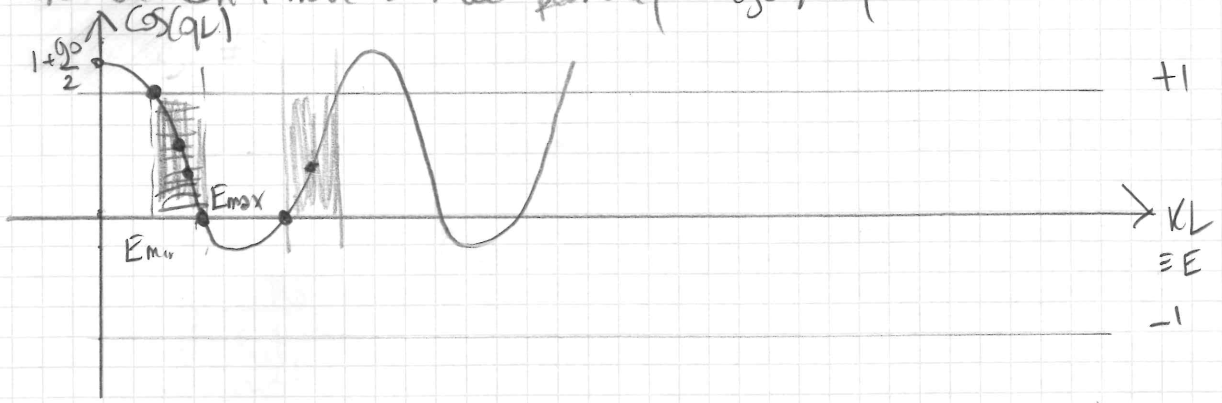


Free particle: $g_0 = 0$, the 2nd term vanishes, ⇒ cos(KL)

Obvious solution! q = K

So, for the free particle, $E = \frac{\hbar^2 q^2}{2m}$

If we don't have a free particle, $g_0 \neq 0$,



If g_0 is a small, positive number, $\frac{\sin(KL)}{KL} \approx 1$, and we got

$$\approx \underset{\downarrow\\ 1}{\cos(KL)} + \frac{g_0}{2}$$

So, @ $KL = 0$, the value of the RHS is greater than 1! ŏ.ŏ

Is there then any eigenstate with $E = 0$? No! We have to wait until the RHS enters in the $[-1, +1]$ interval!

Again, the RHS is periodic, but the deviation from the free particle situation, i.e. g_0, pushes RHS out of the $[-1, +1]$ interval. What does this mean? Well, let's recall that RHS is still to be equal to a cosine!

So, it is not always true that there is an eigenstate for each (q, E) satisfying (2): around $KL = 0$ there is NOT! (q is real!)

For Emin there is a q, specifically, $q = 0$, such that an energy eigenstate exist! $(q, E) = (0, E_{min})$

There is a state for each value of energy such that $RHS \in [-1, 1]$, NOT OUT! $E \in [E_{min}, E_{max}]$!

So in place of discrete levels we have continuous bands, separated by gaps where $|RHS| > 1$. The shaded regions!

When we have a periodic potential, every energy eigenfunction is extended through the entire material, no state is localized.

However, NOT every energy is allowed, only some of them are!

This structure of continuous bands and continuous gaps is going to give us the structure of conductivity in metals or not conducting in plastic. Next time!

Lecture 21: periodical lattice, part 2

Review, where we study a free particle but with the conditions of the previous lecture.

Free particle: $\hat{E} = \frac{\hat{p}^2}{2m}$, which means that

$[\hat{E}, \hat{p}] = 0$: energy, in this case, commutes with momentum. So we can find a basis of eigenfunctions common to $\hat{E}$ and $\hat{p}$.

$$\hat{E}\,\phi_{EK} = E\,\phi_{EK}$$

$$\hat{p}\,\phi_{EK} = \hbar K\,\phi_{EK}$$

Question: can we allow E and K to assume any possible value, independently? Like, $E = 3$, $K = 42$? Well, no! There is a consistency relation, between K and E!

$$E_K = \frac{\hbar^2 K^2}{2m} \qquad \omega_K = \frac{\hbar K^2}{2m}$$

If we know K we know E, the opposite is less trivial since 2 values of K occur for each E. (The eigenfunction could be $e^{\pm iKx}$!)

$$\phi_{EK} = \frac{1}{\sqrt{2\pi}} e^{jKx}$$

So, known the energy, we have 2 possibilities for the momentum! There is a little degeneracy, which arises from the parity symmetry of the system.

Note that $\sin(Kx)$, $\cos(Kx)$ would be energy eigenstates as well, since born from a linear combination of e^{jKx} and e^{-jKx}, but, they would no longer be momentum eigenfunctions. Exponentials are common eigenfunctions for the two operators.

All $\phi_E = e^{j(Kx-\omega t)}$ are extended! not spatially well defined.

So, we have to build wavepackets, to have normalizable states.

$$\Psi = \int dK \, f(K) \, e^{j(Kx-\omega t)}$$

↳ peaked at some $K = K_0$.

One of the properties of these wavepackets concerns the group velocity v_g, which is

$$v_g = \left.\frac{\partial \omega}{\partial K}\right|_{K=K_0} \qquad K_0\text{: peak value of the wavepacket}$$

For the free particle, this equals

$$v_g = \frac{\partial}{\partial K}\left[\frac{\hbar K^2}{2m}\right] = \frac{\hbar K}{m}$$

which, remarkably, equals the expectation value of the momentum over the mass.

By the way, this could be also used to evaluate mass: by measuring momentum, mass is obtained as

$$m = \frac{\langle p \rangle}{v_g}$$

This, is an effective mass which, for a free particle, coincides with the real mass. This is just a consequence of working with these wave packets!

This, was concerning the free particle. What about the periodic potential? Well, how can we do the same analysis?

Let our potential be a periodic step function, period L.

$V(x) =$ 

Our energy operator will be:

$$\hat{E}_{g_0} = \frac{\hat{p}^2}{2m} + g_0 V(x),$$

with g_0 a coefficient. Notice that for $g_0 = 0$ we have the free particle (no potential).

What happens, starting from the $g_0 = 0$ case, and increasing it slowly? The wavefunctions, as well as energy levels, will change!

This procedure can "connect" the free particle concept, with the solution of periodic potentials!

Remind that it is no longer true that energy commutes with momentum due to $V(x)$, so it is impossible to obtain eigenfunctions simultaneously of $\hat{E}_{g_0}$ and $\hat{p}$!

Why? Because our "interaction", our potential, is not translationally invariant! So that momentum is not conserved for an arbitrary translation! Unless the translation is by L

So, energy operator commutes with the translation-by-L operator, $\hat{T}_L$

$$[\hat{E}_{g_0}, \hat{T}_L] = 0 \implies \exists \text{ common eigenbasis.}$$

The eigenfunctions of $\hat{T}_L$ are:

$$\phi_q(x) = e^{jqx} u(x), \qquad u \text{ is a (real) periodic function.}$$

So,

$$\hat{T}_L \phi_q(x) = \phi_q(x+L) = e^{jq(x+L)} u(x+L) = e^{jqL} \phi_q(x)$$

So the energy eigenfunctions can be organized as

$$\left.\begin{aligned} \hat{E}\phi_{Eq} &= E\,\phi_{Eq} \\ \hat{T}_L \phi_{Eq} &= e^{jqL}\,\phi_{Eq} \end{aligned}\right| \text{ common eigenbasis}$$

Now, question, just as that about the free particle: are E and q independent? No!

When solving the eigenvalue equation we get a relation between E and q!

In particular, for $g_0 = 0$ (free particle), we find

$$E = \frac{\hbar^2 q^2}{2m} \qquad \phi_{qE} = \frac{1}{\sqrt{2\pi}} e^{jqx}$$

Just like with the free particle. Here q is the crystal momentum.

Now, thinking about wavepackets, they will be

$$\Psi = \int dq \; e^{j(qx-\omega t)} u_q(x) f(q),$$

So, $u_q(x)$ is periodic, $f(q)$ is a sharply peaked function, around some q_0, then we will find that group velocity is

$$v_g = \left.\frac{\partial \omega}{\partial q}\right|_{q=q_0}$$

And we can again define a nice expression of a mass, the effective mass, as:

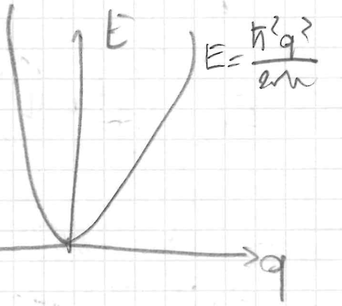
$$m^* = \frac{\langle p \rangle}{v_g}$$

What about $g_0 \neq 0$? An actual periodic potential? Well, analysis of last lecture!

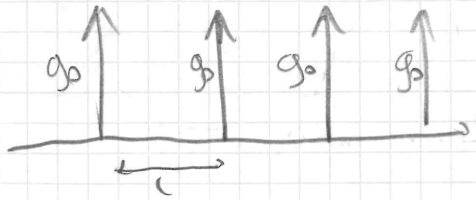
$$\phi_{E,q} = e^{jqx} u(x)$$

Can E and q assume, independently, any values?

Well, $E(q)$ is again a parabola, $g_0 = 0$, but, what happens with $g_0 \neq 0$?



We worked last time with periodic δ function potentials, strenght g_0, spaced by L.



We found that

$$E = \frac{\hbar^2 \mathcal{K}^2}{2m}$$

$\mathcal{K}$ is not k, it's something somehow similar!

$$\mathcal{K} = \sqrt{\frac{2mE}{\hbar^2}} \;!$$

We found that there is a relation like

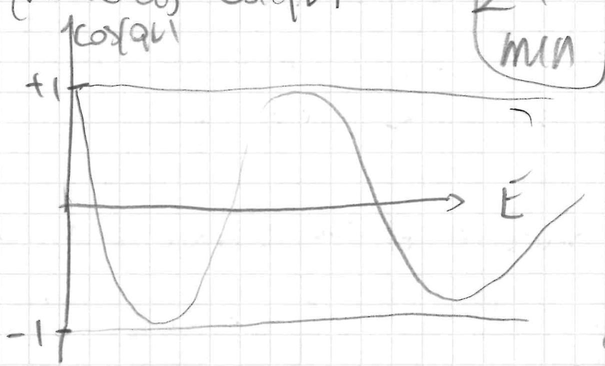
$$\cos(qL) = \cos(\mathcal{K}L) + \frac{g_0}{2\mathcal{K}L}\sin(\mathcal{K}L)$$

If $g_0 = 0$, $\cos(qL) = \cos(\mathcal{K}L) \Rightarrow \mathcal{K} = q$! Free particle result!

Computer: horizontally there is energy, vertically $\cos(qL)$

24 min

The curve is the right-hand side!



What pairs of E and q correspond to allowed energy eigenfunctions?

Well, $\cos(qL)$ = RHS, which is the curve, well, is allowed! And gives sensible eigenfunctions!

Notice that for a value of q, we have a horizontal line, in that plot. So multiple intersections with the curve. So, lots of energies?!

Well, let's remember that q comes from

$$\hat{T}_L \phi_{E,q} = e^{jqL} \phi_{E,q}$$

If we add $\frac{2\pi}{L}$ to q, we have the same eigenvalue e^{jqL}!

So $q + \frac{2\pi}{L}$ is equivalent to q!

If plotting $E(q)$ instead of $E(\cos(qL))$, what do we get? Well, for the free particle we know the solution! a parabola!

As we turn on g_0, the curve starts exceeding the $[-1,1]$ interval, as we described. The procedure to find the (E,q) pairs is the same: find intersections of horizontal lines with the curve. But, there are regions with NO ALLOWED ENERGIES!

Because there are regions with no allowed q, so, with no allowed energies (q should be complex but, in this case, we would have non-normalizable eigenfunctions).

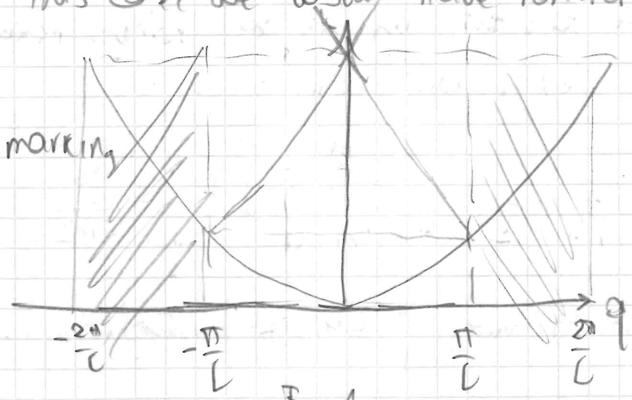


Fig. 1

One more thing about periodicity: marking the $\pm\frac{\pi}{L}$ points in the (q,E) plot,

since q is periodic after $\frac{\pi}{L}$, we could bring the part of curve between $\frac{\pi}{L}$ and $\frac{2\pi}{L}$, and repeat it in the left. So, the parabola can be folded into 1 region, using the periodicity of q as $2\pi/L$. Then, forget what happens for higher or lower values of q. This has a real advantage: when we plot things like in this way, the structure of the energy band and gaps become much more simple!

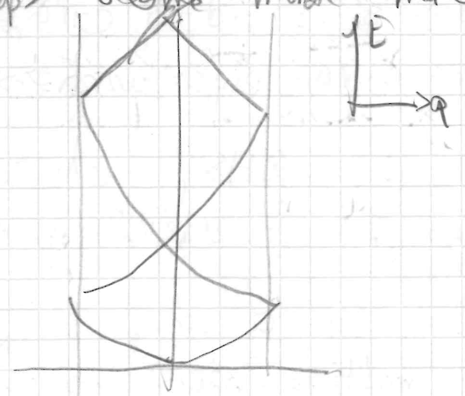
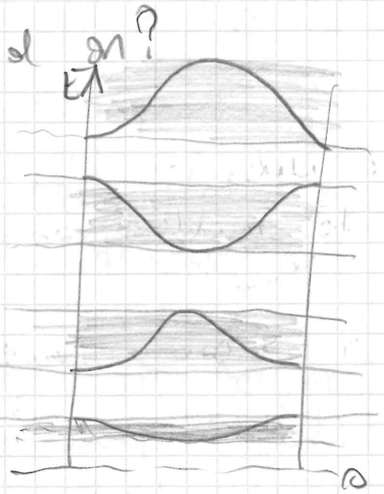


Fig. 2

Notice that, as E increases, the "bands" become broader (1h15 min)
This is a consequence of $\sqrt{E}$ in the sine/cosine: small variations of q correspond to quadratic variations in E (the parabola!)

Physically, having high energies means, if we imagine to stay in a well, being "close to the end, to the top", so the thickness of the band at high energies, grows, as a measure of the fact that we're less tightly constrained by the structure.

What happens to Fig. 2 if we turn potential on?
It happens this: regions with no allowed energy eigenstates appear. There are these gaps! And, increasing g_0, we fall again in the "well" intuition, with the well becoming higher: particles are binded thightly into the wells! Shaded regions are allowed!



But, remind! as g_0 increases, bands don't disappear, and don't overlap!
Notice that, with $g_0 \neq 0$, we have no $E=0$ ground state!

Remind that the ground state has always no nodes, and that states with different numbers of nodes never switch order: states are "sorted" by their number of nodes!

Increasing g_0 will cause the generation of kinks @ the locations of the δ functions, but NO NODES!

Bands don't disappear, because states don't disappear, thanks to the node theorem!

Notice that (problem set), just by knowing the reflection from 1 barrier, we can compute the properties of the whole periodic structure, and its bands!

If $g_0 \to \infty$, we are erecting infinitely high barriers between two periods, the bands shrink, and the allowed energies tend to the levels of the energy eigenvalues of the ∞ well! States tend to become degenerate!

So, why do we have this gap/band structure?
Why do we have gaps? Well, let's think about the Davis and Germer experiment, wave against lattice of atoms: depending on the angle of incidence, scattering changes! This, due to interference effects. So, we can study the reflected wave. By changing the point of view, we can ask to ourselves, "how deep does the wave go, on average?" Does the wave propagate through the crystal? Does it decay?

What we find is that whether the wave propagates in, or decays exponentially, depends on the energy and the lattice spacing of the crystal, and this is the same thing that happens in the scenario we are discussing!

All these wells, these δ, are scattering centers; if we send a wave packet, the probability of propagating contains [50 min] the probability to scatter through these centers, with the relative interference effects.
This is why the band structure is encoded in the reflection amplitude from a single well, a single scattering center.

So, lessons, for $g_0 \neq 0$

① Energy eigenvalues are restricted to lie within a band, and bands are separated by gaps.

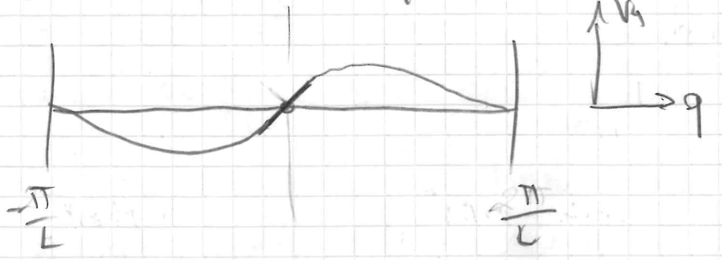
② The energy eigenstates are all extended, meaning that they do not have a well defined position. This because e.eigenstates are also eigenfunctions of the "translation by L" operator.
As a consequence, we have to build wavepackets, with form

$$\psi = \int dq\, f_{q_0}(q)\, e^{j(qx-\omega t)}\, u_q(x) \qquad [\text{sharply peaked in } q=q_0]$$

③ These wavepackets move with group velocity

$$v_g = \left.\frac{\partial\omega}{\partial q}\right|_{q=q_0}$$

With $q_0 \neq 0$, which is the velocity? Let us see: the group velocity v_g as a function of q



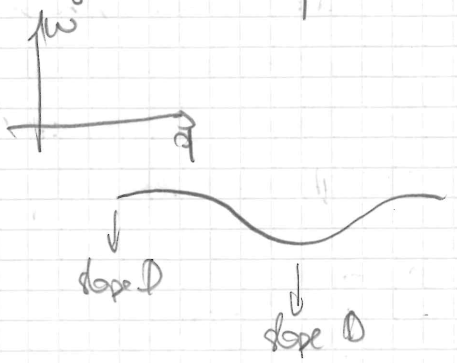


Fig. 1

We can't obtain an analytic solution, but we can see what happens by looking at the first band: bands terminate at $q = \pm\frac{\pi}{L}$, with 0 derivative, since they must be periodic.
The group velocity is the slope of the band, in each point! So in $q=0$ slope is 0, and $\frac{\partial\omega}{\partial q} = 0$!
0 in $q=0$, positive slope after, reaches a maximum and then 0 at the boundaries. As we increase q, velocity increases for a while, just like with k and momentum, but then velocity dies! This is rather different from what we learned about the momentum!
But indeed, in this system, there is no momentum conservation! Momentum can be exchanged between particles and potential!

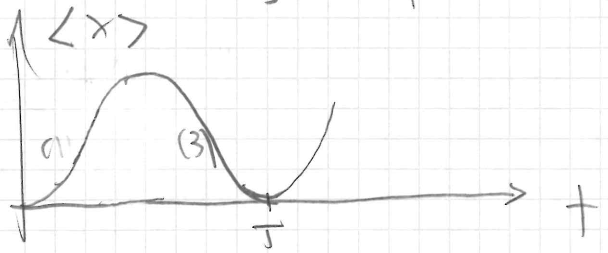
④ (problem set): if we induce a constant force, for example the particle in the periodic potential has a charge and we turn on a constant electric field, then the particle experiences a driving force, like a linearly increasing potential, then the force, or better its expectation value is equal, for a wave packet, sharply localized around some $q=q_0$, ~~given~~ to

$$\langle F \rangle = \frac{d}{dt}\langle \hbar q \rangle$$

So, q increases linearly, constantly! This is quite funny! In fact, if we start from a wavepacket with well localized crystal momentum around $q=0$, how does that wavepacket move? Which is, in other words its group velocity? 0.
If we apply a force, what happens? q increases, so, at first, velocity increases:

this is what we understood from this sine-like shape, Fig. 1

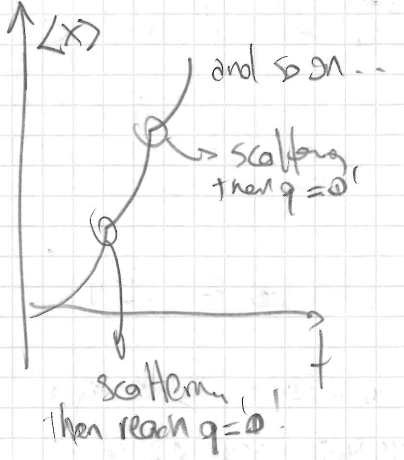
So, if we study the position or, better, its expectation value,



since velocity increases linearly in the first times, position increases quadratically: $\frac{1}{2}at^2$!

When velocity reaches its maximum, it becomes almost constant, and then $\langle x \rangle$ grows just linearly.
But then, once that the maximum has been overcome, what happens? If we further increase the driving force, the velocity starts to decrease, and the velocity starts to decrease, until becoming negative!
And we have this periodic $\langle x \rangle$!
This oscillation in position is called "Bloch oscillation". This is something very weird: normally, if you take a particle, let's say a free particle, and put a driving force, then it continues to increase its velocity. But this is not free: in this scenario it is in a periodic lattice, like "copper", at first the particle starts to behave as an electron in free space, but, then, it senses the presence of the lattice, and it goes backwards! Then, continues to oscillate, back and forth!
Still, even if the electron cannot do anything but go back and forth, copper conducts! Electrons move!

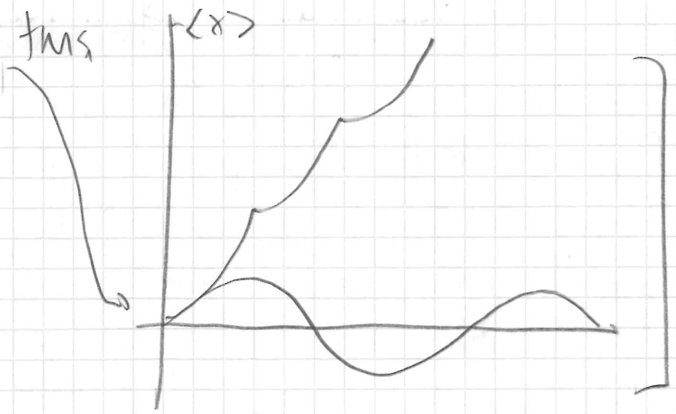
In fact, electrons don't do this back and forth!
Well, there is a bunch of reasons behind this. Ions, for instance, don't have ∞ mass, so, when electrons move, or the driving force acts, ions wiggle! So, the lattice is not perfectly periodic, and then the wavefunctions are not perfectly Bloch functions.
The fact that electrons, bouncing, move the ions, can be described as a scattering phenomenon for which some momentum is exchanged from the electron to the ion, changing the structure of the lattice.
This is what causes conduction.
(*) Instead of having the sine velocity of Fig. 1, the electron starts



moving (as a parabola), scattering occurs, loses momentum, and then re-starts from $q=0$.
Then, new parabolic ⟨x⟩ variation, and another scattering event, and so on.
This effect, understood by Drude, is behind conductivity.
{This disorder, these scattering effects, are essential to conduction.}
Both for these scattering effects, and for the impurities present in the lattice, such as some atoms of carbon in copper or so.

Let's go back to a critical point of the, let's say, perfectly periodic lattice: the fact that we keep increasing force, and get a velocity drop:

[So, the actual picture, instead than this, is this "series" of parabolas (*)]



So we have an "almost" periodic potential: in fact, a periodic potential, with defects. Then, "initially" motion is that of a particle in a periodic potential. But then, scattering from impurities occurs, and then momentum gets lost, and "we start from 0".

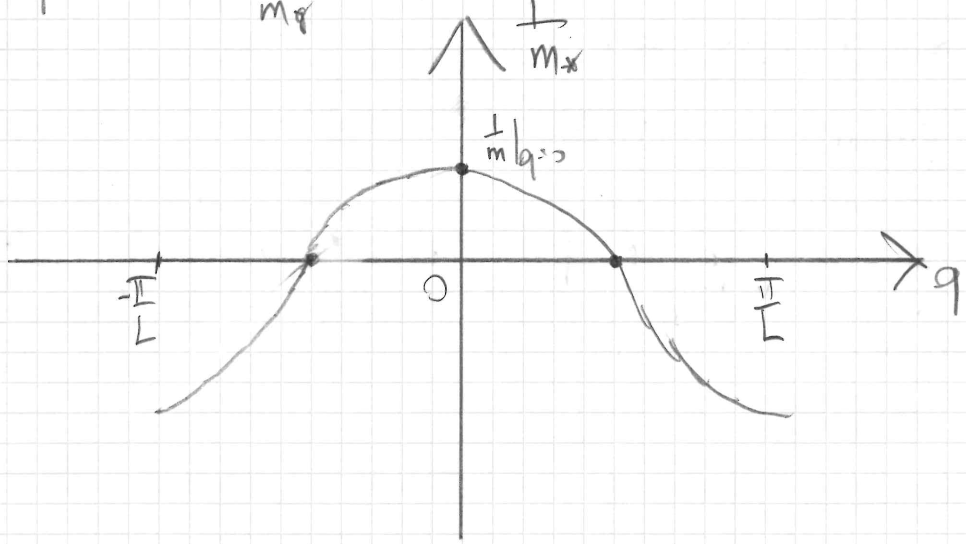
However. There is still some point that we need to discuss: the fact that, for a purely periodical lattice, if we increase force, then, after reaching a maximum, velocity DECREASES! o_o
Well, what happens usually? Positive force, $\underline{F} = m\underline{a}$, then, mass is positive, so why should I have an acceleration (change of velocity!) opposite to the force $\underline{F}$? (at least, classically!)
We have a rule, which allow us to compute mass:

$$m_* = \frac{\langle p \rangle}{v_g} \qquad (*)$$

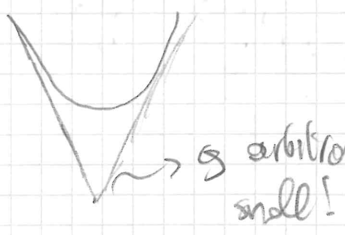
So, what happens here? From problem set, we can prove that the following expression holds:

$$\frac{1}{m_*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial q^2}$$

this, comes just from the application of the chain rule to (*).
So, given this, what is the effective mass of our particle? That means, what is the mass of the object moving in this periodic potential?
Well, let's plot this $\frac{1}{m_*}$:



At the bottom of the band, that means, $\boxed{q=0}$ (let's remember the picture of the band!), the band has some curvature: it's like a parabola! The 2nd derivative is $\neq 0$.
Notice that, by changing q, this curvature changes!



However, by looking at the $V_g(q)$ curve, there is some point for which the velocity becomes maximum, so $\frac{\partial v}{\partial q} = 0$!
Then, intuitively, it reaches some other value, negative, and it is periodic.
But, if $\frac{1}{m_*} = 0$, it means that $m \rightarrow \infty$! o_o
So there is some q for which our object becomes infinitely massive, so, even pushing it with a force, then it does not move!
So, velocity stays constant! This is what we observe!

There is another point: @ $q = 0$, the m_* is NOT equal to the mass of our particle, of the electron!
The mass depends on the bands, depends on the potential! It is an effective mass! What's going on?!

Experiment

Let's say that we measure the mass of a ping pong ball: 2.7 g.
How do we measure it? On a scale, by comparison with some standard. Let's say that the radius of the ping pong ball is 2 cm.
So, the density of this ball is

$$\rho = \frac{1}{12.4}\rho_{water} \qquad [m/vol?]$$

So, let's assume now that we put this ball in water, with some scale (spring scale, "dinamometro"), what is the force?

$\rightarrow \rho_{water} = 12\,\rho_{ball}$

From Archimedes, force is:

$$F = (\overset{\downarrow}{-V\rho_{ball}} + \overset{\uparrow}{V\rho_{water}})g = (-V(\rho_w - \rho_{ball}))g \simeq -11\, m_{ball}\, g$$

the ball gives a force directed to the bottom

water gives a force directed to the top

So, the ball, when released, should accelerate at 11g, like 110 m/s?.

Does this sound possible?
So, the ping pong ball should go from the water @ 11g, and, if we let it fall, just @ g! o_o g vs 11g!

Instead, g wins on 11g! o_o Why?

Because the ping pong ball is interacting with the fluid, with water! So, its mass is not important! When the ball moves in the fluid, it drags and drags more fluid! So the effective mass increases! And acceleration falls off!

Effective mass! Changes with the state of motion!
The idea of the effective mass to change with motion is called "renormalization", and it plays a major role in modern physics!

Lecture 22: Metals, Insulators, Semiconductors

Which is the physical meaning of "crystal momentum"?
On a problem set, it has been shown that, given a wavefunction $\psi(x)$, the expectation value in the state $\psi(x)$ of x

$$\langle x \rangle_\psi = x_0$$

$$\langle p \rangle_\psi = p_0,$$

If we want to increase momentum of $\hbar k$, we need to define a $\tilde{\psi}$

$$\tilde{\psi} = e^{jkx}\psi(x),$$

and then,

$$\langle x \rangle_{\tilde{\psi}} = x_0,$$

$$\langle p \rangle_{\tilde{\psi}} = p_0 + \hbar k.$$

Variations of momentum can be described in terms of phase variations of the wavefunction.

From a different standpoint, momentum is a thing that commutes with position by $j\hbar$:

$$[\hat{x}, \hat{p}] = j\hbar$$

Another definition, momentum is contained in the translation by L, T_L, as

$$T_L = e^{-\frac{j}{\hbar} pL}$$

Another way is: the momentum p governs the spatial variation, the x dependence, of the phase of the wavefunction.
Another defining property: the time variation of momentum, or of its expectation value, is

$$\frac{d}{dt}\langle \hat{p} \rangle = \langle -\frac{\partial V(x)}{\partial x} \rangle$$

↳ that is the force.

This is the Ehrenfest Theorem statement that the classical equation of motion, $\dot{p}$, is equal to $-\frac{dV}{dx}$

Ehrenfest theorem states that this is the quantum version of the classical equation: in quantum physics, it holds, for expectation values!
So, if potential is constant, the momentum expectation value is time independent.
These are properties of momentum.
What about CRYSTAL momentum?
We defined it, given a potential $V(x)$, which is invariant under shifting by one lattice spacing, by some L,

$$V(x+L) = V(x),$$

that

$$[\hat{E}, \hat{T}_L] = 0$$

so that the energy operator commutes by a translation of L.
From this we deduced that the energy eigenfunctions can be written in the form

$$\phi_{E,q} = e^{jqx} u(x),$$

$u(x)$ periodic function

So, q governs the spatial variation of the phase of the wavefunction.
Another fact: if we impose an external force, [problem set]

$$\frac{d}{dt}\langle \hbar q \rangle = \langle F \rangle$$

So, for a wavepacket sharply peaked @ $q = q_0$, so, just like momentum, unless we apply some external force, q has expectation value time independent.

However, it is different from momentum in a crucial way: it is not the eigenvalue of:

$$\hat{p}\,\phi_{E,q} \neq p_0\,\phi_{E,q}$$

because, when we apply $\hat{p}$ to $\phi_{E,q}$, we have e^{jqx}, but we also have $u(x)$ the periodic part! And its spatial variation is generally $\neq 0$.

So $\hbar q$ is NOT the eigenvalue of p.

Moreover, another fundamental difference comes from

$$[E, T_L] = 0,$$

that says that the expectation value of $\hat{T}_L$ is conserved, and in particular this says that the eigenvalue of $\hat{T}_L$ can be found simultaneously to the energy. However, the eigenvalue of $\hat{T}_L$ is e^{jqL},

so q is defined just up to $\frac{2\pi}{L}$! !!! So q is not strictly conserved, but just "mod $\frac{2\pi}{L}$" (mod = %!)

Instead, momentum is <u>strictly</u> conserved!
There is the periodicity!

Question: is $u(x)$ a real function?
Well, we showed, just that

$$\hat{T}_L \phi_q = e^{j\alpha} \phi_q(x)$$

that gives

$$\phi_q e^{-jqx} = u_q(x)$$

If we choose $qL = \alpha$, $\Rightarrow T_L u_q(x) = u_q(x)$! (we proved it)

So,

$$u_q(x) = u_q(x+L)$$

$\Rightarrow$ So, $\phi_q = e^{jqx} u_q(x)$, $u_q(x)$ periodic!

But, since the eigenvalue of T_L is periodic under shift of q by $\frac{2\pi}{L}$ (eig. $= e^{jqL}$), we can choose to define q, mod $\frac{2\pi}{L}$: the eigenvalue remains the same!

Now, there is a subtlety. Does the free particle respect translation by L? Yes! Is constant! So also periodic!
So, which are the common eigenfunctions between $\hat{E}$ and $\hat{T}_L$ for the free particle? They are the

$$\phi_{q,E} = e^{jqx} u(x) = e^{jKx},$$

so, just with $u(x) =$ constant! (for the free particle!)

But then q is NOT periodic by $2\pi/L$: every q is fine, for a free particle! So, u cannot be real!

$$u = e^{j(K-q)x}!$$

By this way,

$$\phi_{q,E} = e^{jqx} e^{j(K-q)x}, \qquad q \in \left[-\frac{\pi}{L}, \frac{\pi}{L}\right]$$

so by this way u is periodic, $-\frac{\pi}{L} < q < \frac{\pi}{L}$, but, u is not real!

So, u is not real, due to the constraint on q to be periodic!
But, if we want u real, well, we should not introduce periodicity!
Periodicity comes from folding all bands in the first Brillouin zone!
This fact is not straightforward.

However, to answer the question, let us assume that u is real, so that q is unconstrained, real (not periodic).
So,

$$\phi_q = e^{jqx} \underset{\mathbb{R}}{\underset{\uparrow}{u(x)}}$$

So, when we construct J, the current,

$$J = \frac{\hbar}{m} \mathrm{Im}\left\{ \underbrace{\phi_q^* \partial_x \phi_q}_{?} \right\}$$

and, if it is not imaginary, we have no current!
So, if the derivative does not introduce an imaginary part, $J = 0$! The only term contributing is $\frac{\partial}{\partial x} e^{jqx}$!

$$\hookrightarrow J_x = \frac{\hbar}{m} q u^2(x)!$$

This computation is so easy because u is real. Then, if we assume that

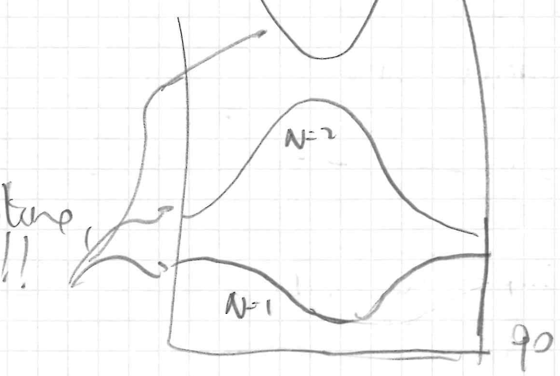
$$q = q_0 + \frac{N\pi}{L},$$

$$\hookrightarrow \phi_{q_0 N} = e^{jq_0x} e^{j\frac{N\pi}{L}x} u(x)$$

So we label ϕ by q_0 and N! Then, q_0 is periodic, N is what we obtain is

$$J_x = \frac{\hbar}{m}\left(q_0 + \frac{N\pi}{L}\right) u^2(x)!$$

Thinking back to our band structure, N is the band that we consider!!!



My comment: consider periodic q means folding the band graph. Unfolding: not constrained q!

[SKIPPED UNFOLDING, UNTIL 31 min]

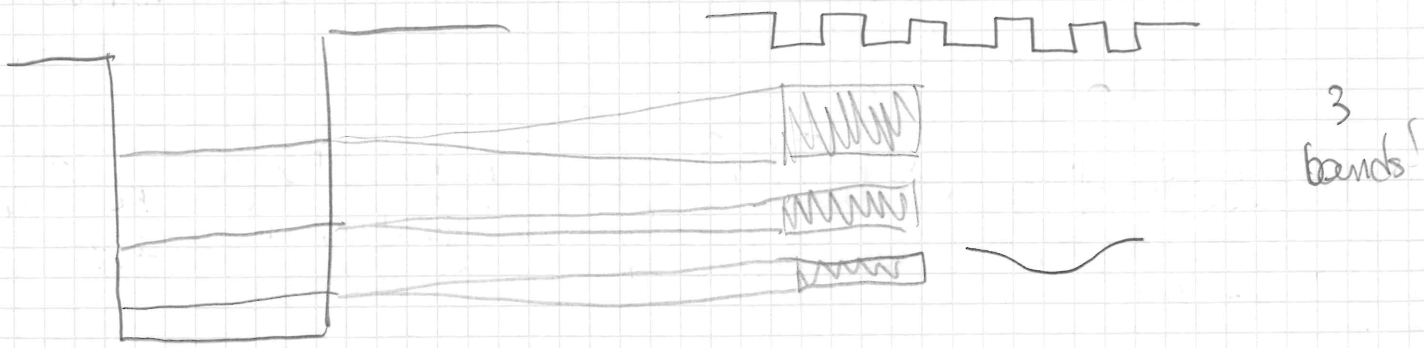
Now

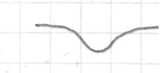
How imperfections in a lattice lead to conduction? =)

Within a perfect lattice, there is actually no conduction: no flow of current due to the presence of an electromagnetic field, generated for example by a capacitor across our "perfect lattice": our particle in our lattice just oscillates back and forth.
Well, so, our model seems to fail, and we could try to improve it, introducing some additional features, and see if its prediction improves.
OR, we could try to study, with experiments, a PERFECT CRYSTAL and see what happens.
What we could do is notice that the equations governing the propagation of light through different dielectrics are exactly equal to Schrödinger's!
The refractive index of the dielectric turns to be analogue to the potential in Schrödinger's equation!
So, doing experiments with LIGHT, instead than electrons! Much easier from an experimental standpoint!
And, it perfectly works! So the model is not wrong: it's not suited to study these systems!

So, let's move to three materials, and discuss their properties: let's imagine to have a quantum well, with some energy eigenstates, and make this system periodic.

What happens to the states?
Each state turns into a band of allowed energies,

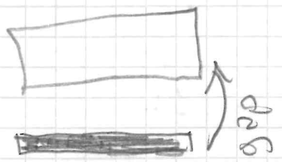


If we put an electron and throw it in this system, what happens?
Eventually, it's going to fall into the ground state.
And we know that the band for the ground state looks like 
Energy eigenstate: it is stationary! So $\frac{d}{dt}\langle x\rangle = 0$!

So, how can we make the electron move? It cannot stay in a single energy eigenstate, but in a superposition!

So, in order to induce a current, so to make this electron move, we have to put the electron in the superposition of 2 states. It must be in a superposition of the ground state and of some excited state!

Now, let's imagine that this lattice is hydrogen: in order for it to be neutral, we must have 1 electron for each well!
As proved in the last lecture, for N wells we have N states within each band! So, N electrons! So, if the system is stuck, the N electrons will fill the first band, and the other bands will be empty!
If we want to make the system move, we have to put an electron in the next available level: IN THE NEXT BAND!
But, in order to make an electron go from the first band to the second one, we must provide a minimum energy: the gap! So, if we excite the system with some light, its energy $E = \hbar\omega$ must be greater then δE, the bandgap!



So, crystals are transparent, unless we look @ sufficiently high frequency: light is not absorbed, because its energy is lower than gap! So it just walks through it!

Let us focus on 2 examples: diamond and copper!
They are both crystals, so given by regular arrays, but... which one has the larger gap? Diamond! Because, it is TRANSPARENT!
So, $\Delta E_{Diamond} > \Delta E_{copper}$

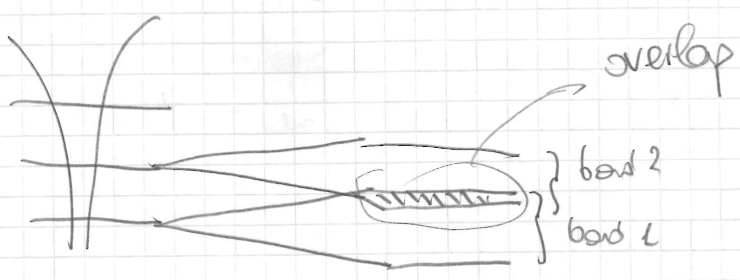
Actually, copper does NOT EVEN have a bandgap!
If an object is transparent, it surely have a bandgap! But, we found just on 1D crystals, where bands cannot overlap! But... What about 3D?!

When we studied the rigid rotor we discovered the $2l+1$ degeneracy,

the states can <u>cross</u>: there is no node theorem in 3D!

$$E = \frac{L^2}{2I} + eL_z$$

And, in 3D, just like for the rigid rotor bands can overlap!



So, in this case, with very small energy we get immediately conductor (transition to a "higher band"!

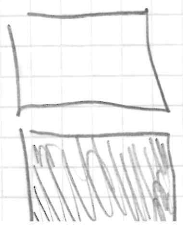
This is like a classical conductor!
Conductor: has an UNFILLED BAND! Two bands, overlapping, so become just like 1!

Insulator: filled bands, separated by gap! (BAND insulator)

What discriminates copper from diamond?
Let's think of 1D: — period of the lattice
\ height of the well (shape of potential)

In 3D, it is more complicated: a lattice can be cubic, hexagonal, complicated... Have different crystallographic structure! And then, different band structure!

There is a 3rd cathegory of systems: the ones with "accidentally small gaps". The gap exists, but it is NOT so big. In this case, the system is not a conductor, but neither considered a "real insulator"! These materials are called "semiconductors".
So, 2 bands, but a TINY gap. What does it mean, "small"?



Small with respect to what? Well, thermal energy, for instance!
And, due to temperature, the probability to have an electron in the upper state is something like

$$\mathbb{P} \sim e^{-\frac{\Delta E}{k_B T}} \qquad k_B\text{: Boltzmann constant!}$$

So,
@ high temperature, such materials are basically conductors and,
@ low temperature, they are basically insulators!

↳ SEMICONDUCTORS!

Butterfly: they don't have pigments, but photonic crystals!

Entanglement
We discussed the problem of identical particles. This for funny states, such as

$$\Psi_D(A,B) = \chi(A)\,\phi(B)$$

$\boxed{\text{Distinguishable}}$

first particle, in state A

2nd particle in state B

But we also studied the symmetric configuration, Ψ_S,

$$\Psi_S = \frac{1}{\sqrt{2}}\left(\chi(A)\,\phi(B) + \chi(B)\,\phi(A)\right)$$

Let's imagine that I measure the first particle and it is in state χ. Then, I know that the 2nd particle is in state ϕ!
So, measuring the first particle reveals something also about the 2nd particle! So, if we had a particle on Mars, one in Torino, we measure that in Torino, and then... We discover also something about the particle on Mars? It's strange!

Lecture 23: More on Spin

When we looked at angular momentum, we found that there are half-integer spin. We discovered that, writing a wavefunction on a sphere that interpret the states as states with definite probability to be at a particular position make the wavefunction double valued.

What are, then, these half-spin states?

The commutation relations for spin are

$$[\hat{S}_x, \hat{S}_y] = j\hbar \hat{S}_z \qquad [\hat{S}_y, \hat{S}_z] = j\hbar \hat{S}_x$$

Moreover, we've seen that we can construct towers of states, defining

$$\hat{S}_\pm = \hat{S}_x \pm j\hat{S}_y$$

these are raising and lowering operators. Then, we've found that the state S^2 has

$$S^2 = \underbrace{s(s+1)}_{\text{number of states}}\hbar^2$$

where "s" (usually l) is integer for orbital angular momentum, half for spin

and

$$S_z = \hbar m_s$$

Then,

m_s go from $-s$ to s. "s" is labeling the tower, m_s is "choosing" the state of the tower "s"!

How do we describe spin?

Let's focus for simplicity on $s = \frac{1}{2}$, so spin equal to $\frac{\hbar}{2}$

Then, we have two states: we call them the $\uparrow$ and $\downarrow$:

"up" $(\uparrow_z)$ in z direction, and "down" $(\downarrow_z)$ in z direction

$\uparrow_z$, $\downarrow_z$

The wavefunction tells us about the state of the system. <u>But</u>, we need to know if spin is $\frac{1}{2}$ up, or $\frac{1}{2}$ down! So, we can write $\Psi(x)$ as:

$$\Psi(x) = \Psi_{+\frac{1}{2}}(x) + \Psi_{-\frac{1}{2}}(x)$$

The probability to be in x, with spin $\pm\frac{\hbar}{2}$, is

$$\mathbb{P}\left(x, \pm\frac{\hbar}{2}\right) = \left|\Psi_{\pm\frac{1}{2}}(x)\right|^2$$

This is a way of describing spin, but it is somehow cumbersome. We will use a formalism based on matrices, presaging the study of "matrix mechanics" to be explored by Barton

Since we need to use 2 functions, $\Psi_{\pm\frac{1}{2}}(x)$, we can organize them in the following way. $\Psi(x)$ can be written as

$$\Psi(x) = \begin{pmatrix} \Psi_\uparrow(x) \\ \Psi_\downarrow(x) \end{pmatrix}$$

a 2 component object, vector, called "spinor";

its adjoint is:

$$\Psi^\dagger = \left(\Psi_\uparrow^*, \Psi_\downarrow^*\right)$$

For normalization, we need that total probability is 1, i.e.,

$$\text{Norm} = (\Psi|\Psi) = 1 = \int dx \left[(\Psi_\uparrow)^2 + (\Psi_\downarrow)^2\right]$$

In other words, with "x" I know where our particle is in space, but we have another information: spin can be either up or down.
In other words, spin is pointing in a vector space that is 2 dimensional: up, or down, as for $+\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$

If we measure spin along some axis, it can take one of 2 values.

There is another notation for this, probably the most common one, consisting of writing $\Psi(x)$ as

$$\Psi(x) = \Psi_\uparrow(x)\begin{pmatrix}1\\0\end{pmatrix} + \Psi_\downarrow(x)\begin{pmatrix}0\\1\end{pmatrix} \qquad (*)$$

this introduces the $\uparrow_z$ and $\downarrow_z$ vectors, aforementioned, as:

"up" vector in z direction! $\uparrow_z = \begin{pmatrix}1\\0\end{pmatrix}$; $\downarrow_z = \begin{pmatrix}0\\1\end{pmatrix}$.

So, we can write all operations about spin as 2x2 matrix operations!

[REMARK! 2 dimensional space because we have $\begin{pmatrix}1\\0\end{pmatrix}$ or $\begin{pmatrix}0\\1\end{pmatrix}$ weighted by the $\psi_\uparrow(x)$ or $\psi_\downarrow(x)$!]

A common notation used by people in Dirac notation is:

$$|\Psi(x)\rangle = |\psi_\uparrow(x)\rangle|\uparrow\rangle + |\psi_\downarrow(x)\rangle|\downarrow\rangle$$

this is the SAME AS last equation (*), last page

We want to develop a theory of spin. With angular momentum, we know the operator $\hat{L}_z$, we act with it on a wavefunction, and we have orbital angular momentum. So we can construct eigenfunctions, and find probabilities! We know that

$$L_z = \frac{\hbar}{j}\frac{\partial}{\partial \phi}$$

With spin we can't do this, because S_z can not be expressed in terms of derivatives along a sphere! That's the problem!

So, what are doing spin operators? Well, $\hat{S}_z$, applied to the state $|\uparrow\rangle$, returns

$$\hat{S}_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle,$$

and

$$\hat{S}_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$$

Similarly for $\hat{S}^2$ operator,

$$\hat{S}^2|\uparrow\rangle = \hbar^2 s(s+1) = \hbar^2\frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{3}{4}\hbar^2 = \hat{S}|\downarrow\rangle$$

In fact, $\hat{S}^2$ does not change angular momentum! it acts the same for all states (spins!) of a tower

Notice that spatial dependence, that is $\psi_\uparrow(x)$ or $\psi_\downarrow(x)$ is treated as some constant: we are focused on $|\uparrow\rangle$, $|\downarrow\rangle$! On spin!

Replacing $|\uparrow\rangle$ and $|\downarrow\rangle$ with their matrix counterparts, we get

$$\hat{S}_z\begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1\\0\end{pmatrix}, \qquad \hat{S}_z\begin{pmatrix}0\\1\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix}$$

$$\hat{S}^2\begin{pmatrix}1\\0\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}1\\0\end{pmatrix}, \qquad \hat{S}^2\begin{pmatrix}0\\1\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}0\\1\end{pmatrix}$$

we have to understand, from these relations, how $\hat{S}_z$ works! We have also to build raising and lowering operators!

[Notice that $\frac{3}{2}$, $\frac{5}{2}$ states can be treated working from $\frac{1}{2}$ states, somehow! Notice! "up" and "down" have nothing to do about pointing towards $+z$ or $-z$: it is just a <u>name</u>!]

Well, these relations state that $\hat{S}_z$ has eigenvectors $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$. Let's try with:

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$: does it work? Well, yes, for the first two!

$$\hat{S}^2 = \frac{3}{4}\hbar^2\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$! Works as well!

We have something more: raising operators! If we apply $\hat{S}_+$ on $\begin{pmatrix}0\\1\end{pmatrix}$, we would like to get $\begin{pmatrix}1\\0\end{pmatrix}$!

$$\hat{S}_+\begin{pmatrix}0\\1\end{pmatrix} = \hbar\begin{pmatrix}1\\0\end{pmatrix}$$

Moreover, we have:

$$\hat{S}_-\begin{pmatrix}0\\1\end{pmatrix} = 0$$ (low tower end: annihilation)

$$\hat{S}_+\begin{pmatrix}1\\0\end{pmatrix} = 0 \quad ; \quad \hat{S}_-\begin{pmatrix}1\\0\end{pmatrix} = \hbar\begin{pmatrix}0\\1\end{pmatrix}$$

So, we get

$\hat{S}_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$! In [illegible],

$\hat{S}_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$

and similarly. Instead,

$S_- = \hbar = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

Now. Since

$\hat{S}_+ = \hat{S}_x + j\hat{S}_y$, $\hat{S}_- = \hat{S}_x - j\hat{S}_y$,

we can say that

$\hat{S}_x = \frac{1}{2}\left(\hat{S}_+ + \hat{S}_-\right)$ $\hat{S}_y = \frac{1}{2j}\left(\hat{S}_+ - \hat{S}_-\right)$,

So

$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -j \\ j & 0 \end{pmatrix}$ (put the j in the matrix!)

This is a nice representation of our spin operators!

$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -j \\ j & 0 \end{pmatrix}$ $\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Why is $\hat{S}_z$ the only one that's diagonal? Because, we chose z as the axis along which we project $\hat{S}^2$!

We decided, at the beginning of the day, to work in a basis of $\uparrow_z$, $\downarrow_z$! Basis of eigenstates of $\hat{S}_z$! That's why $\hat{S}_z$ is diagonal!

The matrices σ_x, σ_y, σ_z can be defined as

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -j \\ j & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and these

are called Pauli matrices.

So! We wanted to build a representation of spin operators! Now: does it satisfy commutation relations? Better hope so!

$[\hat{S}_x, \hat{S}_y] \overset{?}{=} j\hbar\hat{S}_z$?

$$\hookrightarrow = \left(\frac{\hbar}{2}\right)^2 \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -j \\ j & 0 \end{pmatrix}\right] = \frac{\hbar^2}{4}\left[\begin{pmatrix} j & 0 \\ 0 & -j \end{pmatrix} - \begin{pmatrix} -j & 0 \\ 0 & j \end{pmatrix}\right] =$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 2j & 0 \\ 0 & -2j \end{pmatrix} = \frac{\hbar^2}{2}\begin{pmatrix} j & 0 \\ 0 & -j \end{pmatrix} = j\hbar \underbrace{\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\hat{S}_z \;!}$$

So, they work! They represent spin!

So, what do we obtain if we measure spin in z direction?
Well, $+\frac{\hbar}{2}$, or $-\frac{\hbar}{2}$!
What about the eigenvectors? Well, $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$!
What about $\hat{S}_x$? Which are the eigenvalues of $\hat{S}_x$?
Well! we could start working with x: diagonalize $\hat{S}_x$ instead than $\hat{S}_z$. Or, work with our matrix. What are the eigenvalues?
$+\frac{\hbar}{2}$, $-\frac{\hbar}{2}$!
What about the eigenvectors? Well, try with $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$:

$\hat{S}_x \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0+1 \\ 1+0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$! Yay!

$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$!

So,

$\uparrow_x = \frac{1}{\sqrt{2}}\left(\uparrow_z + \downarrow_z\right)$!

$\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$

$\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right) = \frac{1}{\sqrt{2}}\left(\uparrow_z - \downarrow_z\right)$

So, what is this saying? Well, if we know that the system has $+\frac{\hbar}{2}$ spin along the x direction, then we have 50 % probability to measure $\uparrow_z$ (up in z direction) or $\downarrow_z$ (down in z direction)!

In other words,

$\mathbb{P}(\uparrow_z, \downarrow_x)$,

that means "the probability to measure $+\frac{\hbar}{2}$ spin in z direction, known that we have $-\frac{\hbar}{2}$ in x direction" (conditional probability),

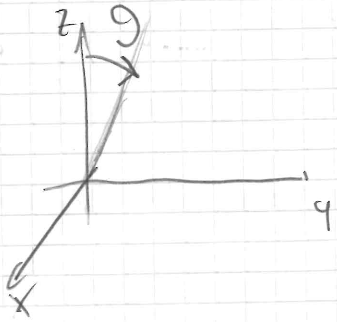
is:

$= \left(\frac{1}{\sqrt{2}}\right)^2 = (50\%)$!

For $\hat{S}_y$ we can do the same;

$$\hat{S}_y : \uparrow_y = \frac{1}{\sqrt{2}} (\uparrow_z + j \downarrow_z)$$

$$\downarrow_y = \frac{1}{\sqrt{2}} (\uparrow_z - j \downarrow_z)!$$



Now, consider the operator $\hat{S}_\theta$ as: spin operator along θ!

$\hat{S}_\theta \Rightarrow \pm \frac{\hbar}{2}$

because, no matter which direction we take, spin can only be $\pm\frac{\hbar}{2}$!

You can find:

$$\uparrow_\theta = \cos\left(\frac{\theta}{2}\right) \uparrow_z + \sin\left(\frac{\theta}{2}\right) \downarrow,$$

$$\downarrow_\theta = \sin\left(\frac{\theta}{2}\right) \uparrow_z - \cos\left(\frac{\theta}{2}\right) \downarrow_z$$

Now. Suppose that I measure $\hat{S}_z$, and find that $s_z = +\frac{\hbar}{2}$.

① What's the state of the system subsequent to this? $\uparrow_z$! (just after measurement)

Then

② If I measure $\hat{S}_x$, what do I get? $\pm\frac{\hbar}{2}$, with 50 % probability!

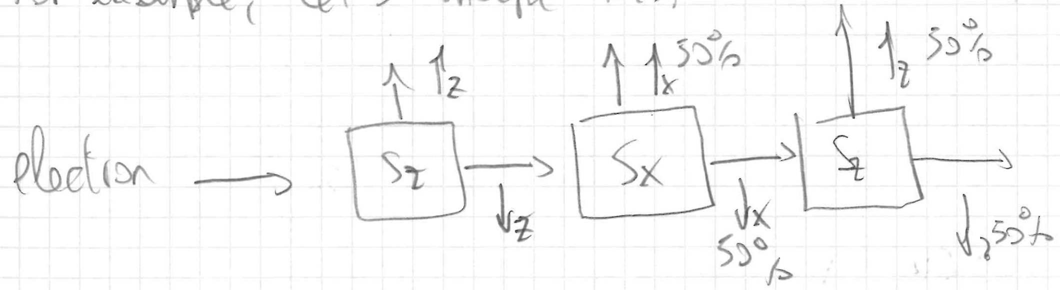
In fact, we can see that

$$\uparrow_z = \frac{1}{\sqrt{2}} (\uparrow_x + \downarrow_x)$$

③ what about $\hat{S}_y$? $\pm\frac{\hbar}{2}$, 50 % probability.

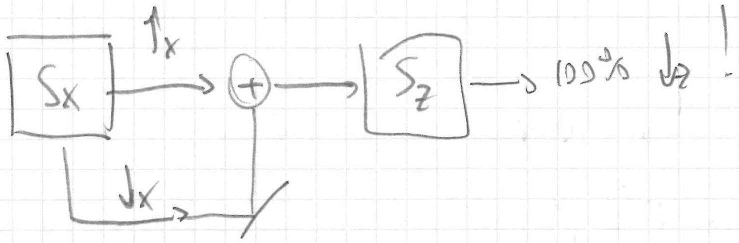
This is exactly what we learned the first lesson with boxes: there we called $\hat{S}_z$ as "hardness", $\hat{S}_x$ as "color", $\hat{S}_y$ as "whimsy"! That was Stein-Gerlach experiment!

For example, let's image this;



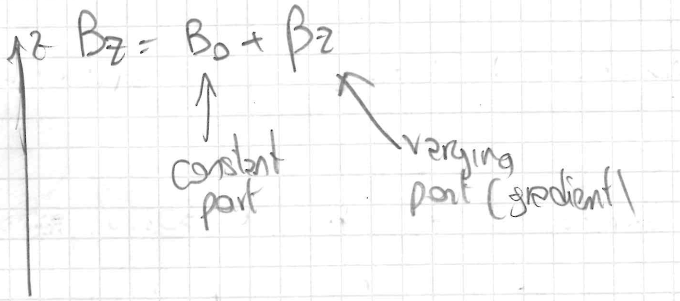
This is what we meant!

But, if we take the $\uparrow_x$, we add by a beam splitter to $\downarrow_x$, we get 100% $\downarrow_z$!



Let's go back to Stein-Gerlach experiment in spin language

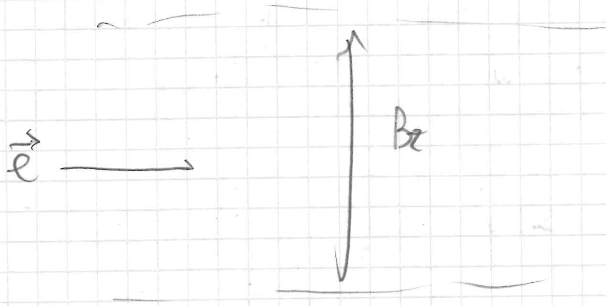
We have a gradient in magnetic field:



$$B_z = B_0 + \beta z$$

this just in some region; out of it, we assume to have no magnetic field.

we send our electron e with wavefunction $\psi_e = a \uparrow_z + b \downarrow_z$



what happens? Well,

the energy of an electron is:

$$E = -\mu_0 \vec{S} \cdot \vec{B} = -\mu_0 S_z (B_0 + \beta z) =$$

spin

magnetic field

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

So; let's focus on phase! What does the matrix look like?

$$-\frac{\hbar}{2}\mu_0 \beta z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} C(z) & 0 \\ 0 & -C(z) \end{pmatrix}$$

: C is some constant depending on z!

$$E \uparrow_z = C(z) \uparrow_z$$

$$E \downarrow_z = -C(z) \downarrow_z$$

So we already had, luckily, the eigenfunctions of energy! Our potential was diagonal!

So, for the $\uparrow_z$ state, energy equals $+C(z)$, and for $\downarrow_z$, it equals $-C(z)$!

The magnetic field splits the degeneracy of energy!

How does wavefunction evolve in time? From Schrödinger we know that

$$\Psi(t) = a e^{-j\frac{E_\uparrow t}{\hbar}} \uparrow_z + b e^{-j\frac{E_\downarrow t}{\hbar}} \downarrow_z = a e^{+j\frac{\mu_0 B_0 t}{2} + j\frac{\mu_0 \beta z t}{2}} \uparrow_z + b e^{-j\frac{\mu_0 B_0 t}{2}} e^{-j \mu_0 \beta z t} \downarrow_z$$

So, the amount of phase rotation depends on z! Since a state with form $e^{jk_z z}$ is, as known (same form as here!), a momentum eigenstate, momentum is NON ZERO! Positive one time ($\uparrow_z$), negative for $\downarrow_z$!

So, $\uparrow_z$ gets a KICK in the +z direction, and $\downarrow_z$ in −z direction!

Stein-Gerlach correlated POSITION of an electron with its SPIN!!!

Depending on the amplitude of the measured electron wavefunction we have $\uparrow_z$ or $\downarrow_z$! this is how our box works!

Entanglement: Suppose we know the property of a particle. Like, we are in a state ψ

$$\psi = U \uparrow_z + D \downarrow_z$$

If we measure spin in z, we could get $\uparrow_z$ or $\downarrow_z$ with 50% probability

But, if I measure U, like, with Stein-Gerlach positive position, I ~~Know~~ that spin is $\uparrow_z$: entanglement spin-position!

this is it!

Se serve risenti gli ultimi 3 minuti, su EPR

Lecture 24 : Entanglement

Review:

$[\hat{S}_x, \hat{S}_y] = \hat{S}_z$ $\qquad \downarrow_\theta = \cos\left(\frac{\theta}{2}\right) + j\sin\left(\frac{\theta}{2}\right)$

$\psi(0) = \frac{1}{\sqrt{2}}\left(\uparrow_z + \downarrow_z\right)\left(= \uparrow_x\right)$ $E = -\mu_0 B_z S_z \Rightarrow E_\pm = \pm\hbar\omega, \quad \omega = \frac{\mu_0 B_z}{2}$

$\psi(t) = \frac{1}{\sqrt{2}}\left(e^{j\omega t}\uparrow_z + e^{-j\omega t}\downarrow_z\right)$ $\qquad$ └→ energy splitting!

Notice that ω depends on μ, which is related to spin, but also on B_z, which I can control! Tune!
Let's say that I keep B_z on for a time T such that $\omega T = \frac{\pi}{2}$. Then, what happens?

$\psi(T) = \frac{j}{\sqrt{2}}\left(\uparrow_z - \downarrow_z\right) = j\downarrow_x$ (we saw it last time).

So. At $t=0$, we had $\psi(0) = \uparrow_x$. At $t=T$, $\psi(T) = \downarrow_x$! This a precession at z axis.
So. When I have a spin state, and I want to obtain another spin state, I have to build a machine that does it by using an appropriate magnetic field for a certain time.
So, it is possible to transform a spinor into another spinor, and this can be done by a series of magnetic field devices!
So, what we have, is :

① A system which can be put in states $\uparrow_z$, $\downarrow_z$

② The ability to rotate states, by evolving them! This, by suitably choosing magnetic fields.

This is the entry point to quantum computing

Classical Computing: we have bits which are binary objects, either 0 or 1, and we realize them by a little magnet (hard disk), and when it points north it equals 0 when points south it's 1 (for example).
Classical computers are machines that, based on classical mechanics, take this initial configuration (like 0, 1) and replaces with a new one, $f([0,0])$.

For example, swap numbers: 1 1 0 0 ⟶ 0 0 1 1
we build some machinery that realizes this operation (for example)
If we have N classical bits, $\{0,1\}^N$, how many numbers should we specify for defining a configuration of N bits? $\textcircled{N}$! ⇒ N binary numbers!

Quantum computing: instead of having bits, we have "Qbits"! A system that has two possible states, named $|0\rangle$ and $|1\rangle$ $\quad \{|0\rangle, |1\rangle\}$
To specify a general configuration, ψ is equal to a linear combination,

$\psi = \alpha|0\rangle + \beta|1\rangle$

If we measure the state, it will be either in $|0\rangle$ or $|1\rangle$, but, at some time, due to time evolution, it will reach a general superposition.
So, how many numbers do we need to specify the state of a single Qbit? Two complex numbers: α and β!

With N Qbits, we have much more: for instance, $N=2$, we have, as states: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. So, $2^2 = 4$ coefficients

$N=3$, $2^3 = 8$, and then 2^N! 2^N complex numbers!

So, facing reality: if we want to simulate a quantum computer with N bits with a classical computer, we need 2^N variables! So, for 10 bits, $N=10$, we need 2^{10} complex numbers!
Instead, we could imagine that the opposite, i.e., simulate a classical computer with a quantum computer, is easier.
So, the idea is: build a computer that uses quantum mechanical bits, whose variables involve all quantum effects (time evolution, superposition, interference) maybe they can be exponentially faster and with exponentially less memory.
Use quantum mechanics as a calculation tool. Do we get speedup?

Let us assume to have N Qbits, where each bit may be ↑, so 1, or ↓, so 0. (interchangeably)

So our input is going to be a wavefunction $\psi_{in}^{(N)}$, for N Qbits, and then it will evolve with some energy operator that implements an algorithm, and time evolution is what "performs the computation". The time evolution would then replace the role, in classical computers, of currents, electric fields etc. used to feed the registers, memories, do computations.

As an output, we would have a wavefunction $\Psi_{out}^{(N)}$.
So, inputs and outputs are not strings of numbers, but wavefunctions!
Outputs are as well superpositions of values we measure.
Measuring causes interference effects in the outputs. So, we will have probabilistic outcomes!
So, we want to orchestrate interference to obtain well definite outcomes: the ones we aim for.
We have to focus on checkable problems! If our output is probably right, it's not enough: we have to be sure that it is correct, so we must be able to check the solution! Like, check with a classical computer, if check is easy!
For example, factorization: if we factorize a number, like, $21 = 7 \times 3$, we can immediately check, by re-multiplying, if it is correct!
The key thing is that, when we have N Qbits, we have interference effects, in particular, entanglement effects. The "secret" of designing a proper quantum algorithm is to attune, to harmonize, entanglement.

Now, let's end with phylosophy!

$\boxed{\text{A Qbit } |0\rangle, |1\rangle}$ is a 2 state system (doesn't matter if implemented with spin or other things! =P)

The general wavefunction is $\Psi = \alpha|0\rangle + \beta|1\rangle$. Then $\mathbb{P}(0) = |\alpha|^2$, $\mathbb{P}(1) = |\beta|^2$.
What are, instead, 2 Qbits?

$$\Psi = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle \qquad (1)$$

Qbits are distinguishable because placed in different locations: they are distinguishable. Then, normalized: $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$.

Then, using as order of Qbits $|A, B\rangle$,

$$\mathbb{P}(A=0) = |\alpha|^2 + |\beta|^2$$

$$\mathbb{P}(A=0, B=1) = |\beta|^2, \qquad \text{and so on.}$$

So. There are 2 kinds of states where a pair of Qbits could be put in.
A very special kind of states is: SEPARABLE states.
This correspond to the full system, $|\Psi\rangle$, where 1 particle is in 1 state, the other in another state:

$$|\Psi\rangle = |\Psi_1\rangle|\Psi_2\rangle$$

e.g., $\underbrace{\frac{1}{\sqrt{2}}(a|0\rangle + b|1\rangle)}_{\text{first particle}}\underbrace{\frac{1}{\sqrt{2}}(c|0\rangle - d|1\rangle)}_{\text{second particle}}$

$$= ac|00\rangle - ad|01\rangle + bc|10\rangle + bd|11\rangle$$

This is a special condition because implies relationships among the coefficients $\alpha, \beta, \gamma, \delta$ in (1)!

This, physically, means that if we are in a state like this, and we ask which is the probability of the first particle to be 0, we don't need information about the second particle! It's just $|a|^2$!

But then, let's say that we measure that the first particle is in $|0\rangle$.

Then, $|\Psi\rangle = |0\rangle \times (c|0\rangle - d|1\rangle)$

We learned NOTHING about the state of 2nd particle!
In a separable system, measuring 1 Qbit tells nothing about the other Qbit!

In a Generic state, NOT separable, example

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$\boxed{\text{33 min}}$

Non-separable states are called entangled. In fact, both ac and bd must be non-zero. But then we would have all crossterms to have a separable state. Here, we have to express with $\alpha, \beta, \gamma, \delta$, and set $\beta = \gamma = 0$!

So, all non-separable states are called entangled. Why? Well.

Let's assume that I measure the first particle state, to be 1. Then, I ALSO know that 2nd particle will be 1, with 100% probability!
Knowing about a particle gives info about the OTHER! o_o
The guys are not independent: they are correlated, "entangled".

Entanglement is a quantum effect, so it should be exploited in a quantum computer!

How do we compute with Qbits?
Computation, as already said, is performed by Schrödinger evolution with an energy operator implementing our algorithm.

Example 1: NOT gate

$|0\rangle \longrightarrow |1\rangle$, and $|1\rangle \longrightarrow |0\rangle$: NOT gate

If $|0\rangle$ is $\begin{pmatrix}1\\0\end{pmatrix}$ and $|1\rangle$ is $\begin{pmatrix}0\\1\end{pmatrix}$, we need time evolution to effect multiplication by an operator! The unitary operation U_{NOT} must be

$$U_{NOT} = \begin{pmatrix}0&1\\1&0\end{pmatrix} \longrightarrow = -j\, e^{j\frac{\pi}{2}}\begin{pmatrix}0&1\\1&0\end{pmatrix} = -j\left(\cos\left(\tfrac{\pi}{2}\right)\underline{\underline{I}} + j\sin\left(\tfrac{\pi}{2}\right)\begin{pmatrix}0&1\\1&0\end{pmatrix}\right)$$

This can be written as:

identity matrix

But, $e^{j\frac{\pi}{2}}$ is Schrödinger evolution by a magnetic field, as last lecture, so $\hat{S}_x$! So, with an x-directed magnetic field!
Unitary translation for field B_x for time T such that $\omega T = \frac{\pi}{2}$.
This is a physical system that allows to use spin for the implementation of a NOT gate for qbits! $|In\rangle \longrightarrow \boxed{U_N} \longrightarrow |Out\rangle$

Example 2: if we turn on a y-directed magnetic field for a time T,

$$|0\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \quad (\uparrow_x \text{ state})$$

$$|1\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \quad (\downarrow_x \text{ state})$$

This is a definite superposition: we know what happens!

This operation is called U_H: Hadamard. Transforms z directed states in x directed states! Superpositions! (another quantum effect)
As a matrix,

$$U_H = \frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$

We gain certainty to measure up or down in the x direction!

$|In\rangle \longrightarrow \boxed{U_H} \longrightarrow |Out\rangle$

Starting from a state that's for sure $|0\rangle$, it puts it in a superposition of $|0\rangle$ and $|1\rangle$. Superposition is a quantum concept! something that classical computers can't do! We lose certainty to measure $\uparrow_z$ (since we have $|0\rangle$ and $|1\rangle$), but we gain certainty to measure $\uparrow_x$ or $\downarrow_x$

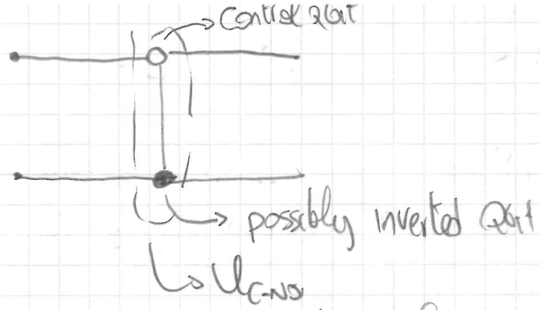
Example 3: C-Not (controlled not)
This operation accepts/requires 2 QBit in input. So,

00
01
10
11

it applies NOT to the 2nd bit if and only if the first Qbit is 1.

input	output
0 0	0 0
0 1	0 1
1 0	1 1
1 1	1 0

For the CNOT, the "graphical" representation is different: first bit "controls", 2nd bit "may" be inverted



Now, even if it is always possible to find some physical representation of particular unitary transformations, what we really need at the end of the day is a table of truth.

Now, another point. We just said what we can do. But, what can't we do?
Let's recall that the basic principle is evolving some "designed" energy operator.
Schrödinger evolution is: linear (allows superposition)
unitary (preserves probability)

These tools introduce strong constraints on what we can do.
For instance, there is a theorem stating that "there's no cloning":
No cloning theorem

Given $|x\rangle|y\rangle$, as input, if we want another system that "copy" the first state into the second, like

In $|x\rangle|y\rangle \longrightarrow$ Out $|x\rangle|x\rangle$

is this possible? No! It would violate both linearity and unitarity!

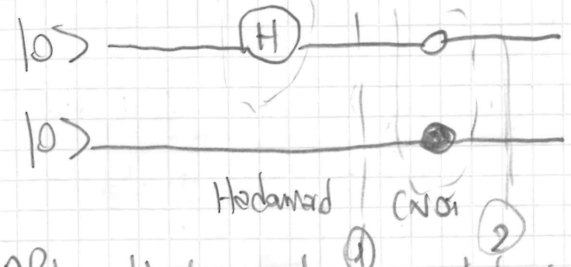
Linearity: if we have as input state something like

$$\alpha|x\rangle|z\rangle + \beta|x\rangle|y\rangle \longrightarrow (\alpha+\beta)\,|x\rangle|x\rangle$$

Left, normalization is $\alpha^2+\beta^2=1$, right is $(\alpha+\beta)^2=1$, that's not generally true! Probability is not conserved!
So, not possible to "copy", to "clone", your system.

No forgetting: quantum evolution never forgets, everything is always "remembered".

Instead, you CAN entangle! So, given two disentangled states we can entangle them! The idea is, for example: take two disentangled states $|0\rangle$, $|0\rangle$, send one of them in Hadamard, then to CNOT:



After Hadamard, our state become: $|0\rangle \longrightarrow \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$

Putting together the two states, at ① we would have

① $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle) \times |0\rangle = \frac{1}{\sqrt{2}}(|00\rangle+|10\rangle)$

this is a separable state, so not good for us. Now, let's apply CNOT on this state, obtain ②:

② $\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle)$

that is <u>NOT</u> a separable state! So, IT IS ENTANGLED!
The prototypical entangled state we wrote before!

These operations were just applications of magnetic fields on purely $|0\rangle$ states (that can be obtained with Stern-Gerlach boxes!)

As an example of quantum algorithm, let's study the

Deutsch-Josza algorithm

This is a set of rules for a quantum computer to evolve in order to perform the calculation we aim for.
Problem to be solved: given a function $f(x)$, that takes a single bit and produces another single bit:

$$f : \{0,1\} \longrightarrow \{0,1\}$$

Is $f(0)$ equal to $f(1)$, or not?
Ok, this doesn't sound like a complicated problem, but, let's consider this as a test bench
Classically, how do we solve it? Well, just by evaluating $f(0)$ and $f(1)$!
Deutsch started studying this problem.

Setup
It is required for the function to work respecting quantum mechanics:
the function should be evaluated with a superposition of more states.

So, we must have a unitary transformation U_f such that

$$U_f : |x\rangle|y\rangle \longrightarrow |x\rangle|f(x) \oplus y\rangle ,$$ where $\oplus$ adds, mod 2

x	y	$\oplus$
0	0	0
0	1	1
1	0	1
1	1	0

Algorithm

Input: let's consider as input a state Ψ such that

$$\Psi = |0\rangle|1\rangle$$

we can implement with our "Stein-Gerlach" boxes.

① Hadamard both qbits

$$\hookrightarrow \Psi \rightarrow \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle) = \frac{1}{2}\left(|0\rangle(|0\rangle+|1\rangle)+|1\rangle(|0\rangle-|1\rangle)\right)$$

② Apply f to this (so U_f):

$$\frac{1}{2}\left[|0\rangle \times (|f(0)\oplus 0\rangle - |f(0)\oplus 1\rangle) + |1\rangle(|f(1)\oplus 0\rangle - |f(1)\oplus 1\rangle)\right]$$

Notice that, for the first term,

$$|f(0)\oplus 0\rangle - |f(0)\oplus 1\rangle = \begin{cases} \boxed{\text{if } f(0)=1} \longrightarrow \begin{matrix} 1\oplus 0 = 1 \\ - \\ 1\oplus 1 = 0 \end{matrix} = (0-1) \\ \text{if } f(0)=0 \longrightarrow \begin{matrix} 0\oplus 0 = 0 \\ - \\ 0\oplus 1 = 1 \end{matrix} = -(0-1) \end{cases}$$

So, this equals, synthetically

$$|f(0)\oplus 0\rangle - |f(0)\oplus 1\rangle = \boxed{(-1)^{f(0)}(|0\rangle-|1\rangle)}$$

With exactly the same logic we have, for the second part:

$$|f(1)\oplus 0\rangle - |f(1)\oplus 1\rangle = (-1)^{f(1)}(|0\rangle-|1\rangle)$$

So that the whole expression becomes:

$$\rightarrow \frac{1}{2}\left[(-1)^{f(0)}|0\rangle \times (|0\rangle-|1\rangle) + (-1)^{f(1)}(|0\rangle-|1\rangle)\right]$$

Now, let's observe that, <u>if</u> $f(0)=f(1)$, then $f(0)\oplus f(1)=0$! $\begin{cases} 1+1=0 \\ 0+0=0 \end{cases}$

So,

$$f(0) \oplus f(1) = \begin{cases} 0, & \text{if } f(0) = f(1) \\ 1, & \text{if } f(0) \neq f(1) \end{cases} \quad !$$

So, instead of measuring both f(0) and f(1), we could measure the sum $f(0) \oplus f(1)$! In this view, let's work again on our expression:

$$= \frac{1}{2}(-1)^{f(0)} \underbrace{\left[|0\rangle + (-1)^{f(0)\oplus f(1)} |1\rangle\right]}\left(|0\rangle - |1\rangle\right)$$

③ Forget about the 2nd Qbit! And then focus just on this guy. Depending on $f(0) \oplus f(1)$, we measure $|0\rangle + |1\rangle$ or $|0\rangle - |1\rangle$, which are $\uparrow_x$ or $\downarrow_x$! But, to work with base states, we could turn these states into the inverse Hadamard application, which is Hadamard itself, so

④ Hadamard the first Qbit, so that

$$\text{out} = \frac{1}{2}\left(1 + (-1)^{f(0)\oplus f(1)}\right)|0\rangle + \frac{1}{2}\left(1 - (-1)^{f(0)\oplus f(1)}\right)|1\rangle$$

So, if $f(0) \oplus f(1) = 0$, we measure $|1\rangle$, and the opposite! NICE!

⑤ Measure the first Qbit : $\Rightarrow |0\rangle$ implies the same, $f(0) = f(1)$
$|1\rangle$ implies $f(1) \neq f(0)$.

With 1 evaluation we have the answer: $f(0) \overset{?}{=} f(1)$!

This was Deutsch, and for N=1 Qbit. By this way, we halved the computational cost of the algorithm.
There is an analogous N-Qbit problem, the Deutsch - Josza problem. (DJ).
Now, there are, for N Qbits 2^N possible states. To verify if f is the same, you should evaluate it for ALL 2^N possible combinations! This, classically.
With quantum algorithm 1 evaluation solves the problem for N Qbits. This is exponentially more efficient than the classical algorithm.
The crucial move is the possibility for quantum algorithm to exploit entanglement: entangle degrees of freedom. This, with the consequent interference.

Now: what's so troubling about entanglement?
EPR : Einstein, Podolsky, Rosen
Let's suppose to consider two Qbits, and put them in a state $(\underset{11}{\uparrow\uparrow}\ \underset{00}{\downarrow\downarrow})\frac{1}{\sqrt{2}}$.
Let's take the first Qbit, and send it far away, to Alice. Send the 2nd Qbit to Bob. Then, Alice measures the spin of her Qbit, and discovers that it is up. But then, also, that Bob's state has spin up.
What upsetted EPR is: either there was an answer to the question all the way along, or there's some deep nonlocality in the universe! Some causally disconnected, distant measurement can influence another part! Alice's measurement influences Bob's spin! Nothing could have traveled that distance to influence!

The 3 responses are:

1) Quantum mechanics is insufficient
There is some hidden variable, a variable we haven't measured, observed, like a property of the electron that determines whether it's ↑ or ↓, that looks probabilistic but actually is not (like a particle in a fluid: its motion seems random, but it's not!). Like there's a classical mechanism "randomizing", "controlling" the probability distribution

2) Focus on the fact that quantum mechanics works and just apply it!
Forget about phylosophical doubts about locality or so.

Bell told that stating that there's an underlying probabilistic classical description tells enough to make this an empirical question: this says that the random statistics for Alice and Bob are correlated by a classical dynamics, other than independent. So, Bell's version:
Let's consider 3 binary properties, A, B, C.
The number of some set

$$N(A, \bar{B}) + N(B, \bar{C}) \geq N(A, \bar{C})$$

If they're deterministic binary properties, then we proved this relationship.

$\rightarrow N(A, \bar{B}, C) + N(\bar{A}, B, \bar{C}) \geq 0$ } you can't have a negative number of elements.

Now, lets apply this to the EPR experiment!

1. Alice measures up or down at 0
2. Bob measures up or down at θ
3. Alice then measures up or down at θ
4. Bob then measures up and down at 2θ

So:

- A is the measurement of spin up at 0
- B " " " " spin up at θ
- $\bar{B}$ " " " " " down " θ

$$\underset{\uparrow_0\ \downarrow_\theta}{N(A, \bar{B})} + \underset{\uparrow_\theta\ \downarrow_{2\theta}}{N(B, \bar{C})} \geq \underset{\uparrow_0\ \downarrow_{2\theta}}{N(A, \bar{C})}$$

Let us rephrase this as the probability that

$$\underbrace{\mathbb{P}(\uparrow_0, \downarrow_\theta)}_{\text{probability that we are up at } 0 \text{ and subsequently down at } \theta} + \underbrace{\mathbb{P}(\uparrow_\theta, \downarrow_{2\theta})}_{\text{we are up at } \theta\text{, down at } 2\theta} \qquad \mathbb{P}(\uparrow_0, \downarrow_{2\theta})$$

Let's recall that

$$\downarrow_\theta = \cos\left(\frac{\theta}{2}\right)\downarrow_0 + j\sin\left(\frac{\theta}{2}\right)\uparrow_0$$

So

$$\mathbb{P}(\uparrow_0, \downarrow_\theta) = \sin^2\left(\frac{\theta}{2}\right)$$

$$\mathbb{P}(\uparrow_0, \downarrow_{2\theta}) = \sin^2(\theta)$$

The LHS is NOT always greater than RHS!
Bell's inequality is <u>NOT</u> always satisfied! In fact, for small θ,

$$\rightarrow \simeq \left(\frac{\theta}{2}\right)^2 + \left(\frac{\theta}{2}\right)^2 = \frac{\theta^2}{2} \geq \theta \ ?$$

NO!

The fact that if we build up statistics using these observables repeatedly, we find explicit violations of Bell's inequality, which we know being correct for classical, deterministic properties. If we observe this with this experiment, we prove that there are no hidden variables, no classically definite configurations underlying the probabilistic nature of quantum mechanics. In other words it is impossible to produce a classical theory with hidden variables randomly distributed and producing the predictions of QM.

Alain Aspect reproduced this experimentally proving this! QM is probabilistic!