Lecture 10: Clicker Bonanza and Dirac Notation

Clicker part

(1) $\frac{d^2}{dx^2}\sin kx = -k^2 \sin kx$ $\quad -k^2$ so

$\frac{d^2}{dx^2} e^{-x} = -\left(-e^{(-x)}\right) = e^{-x}$ (1) (3)

$\frac{d^2}{dx^2} e^{(jkx)} = j^2 k^2 e^{jkx} = -k^2 e^{jkx}$ $-k^2$

(2) I would say (A) $|g\rangle$, because of linearity. $\hat{}$

(3) I would think (A) or (D). A because the finite well has ∞ spatial extension so less energy. But, D, maybe depends on well height? Don't know.

(A): the gradient of the potential is the force, so in right case we have less force confining, so the states are less squished. Since the states are less confined (there are the evanescent tails) at the well boundaries, there is no "discontinuous" change of slope. The curve is less, so energy is lower

(4) Ψ is a wavefunction, NOT NECESSARILY an energy eigenstate. So, (D). This seems an old question =C

$\psi(x) = \sum_n c_n \varphi_n(x)$ $\qquad \hat{E}\varphi_n(x) = E_n \varphi_n(x)$

$\langle \varphi_n | \varphi_m \rangle = \int \varphi_n^* \psi(x)\, dx = \int dx\, \varphi_n^* \sum_m c_m \varphi_m$

$= \sum_m c_m \int \varphi_n^* \varphi_m\, dx = c_n$

(5) I would say C

(6) I know that $\hat{H} u_n$ is an energy eigenstate. So, u_n is another energy eigenstate. I would say C: they're two different energy eigenstates. This, because I expect eigenstates to be orthogonal. Exact =) Perfect.

Note: here he used $\hat{H}$ instead of $\hat{E}$. $\hat{H}$ is the hamiltonian: the generator of time translation. He says $\hat{E}$, and energy operator, that is just energy. The hamiltonian is exactly the same, but it does not evoke, when said, the "taste" of energy.

(7) I would say (A). Not C and D for sure.

(8) B, for sure $\neq 0$

(9) The answer is C, already asked.

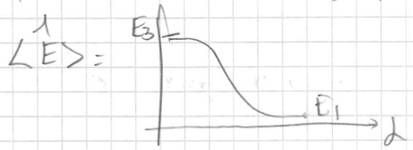
(10) The answer is B

(11) I would say that: you have a $\psi(x)$, generic, and you measure something like
$\langle \hat{E} \rangle = \int \psi^* \hat{E} \psi \, dx$

$\hat{E}\psi$ is an eigenstate, a single one.
Not B, probably
Don't know. Let's wait & then.

If we had
$\psi = c e_n$,
$\langle \hat{E} \rangle = \sum_m E_m |P(E_m)| = \boxed{\sum_m E_m |c_m|^2 = E_n}$

But, if we had $\psi = \alpha e_1 + \sqrt{1-|\alpha|^2}\, e_2$,



when α is 1, $\langle \hat{E} \rangle = E_1$
when α is 0, $\langle \hat{E} \rangle = E_3$
... and then, quadratic interpolation $\sqrt{1-\alpha^2}$

So, to solve this question, you must know

$\langle \hat{E} \rangle = \sum_m E_m |P(E_m)| = \sum_m E_m |c_m|^2$
↳ coefficients of each eigenstate in the expansion of the general wavefunction $\psi(x)$!

(12) I would say, A: ψ_1

(12 bis) State $\psi = \psi_1 = \frac{2}{\sqrt{13}} \phi_1 + \frac{3}{\sqrt{13}} \phi_2$

$\hat{B}\psi_1 = ?$ $\boxed{\phi_1 / \phi_2}$

I would say $\frac{4}{13} \cdot E$

It is the norm square of the coefficient.

(12 tris) I would say (B): 100% possibly, because after the first time the WF collapses to ψ_1

(13) C

Question: does exist an odd linear potential
The problem is not having it odd. The problem is that it is not bounded from below. An odd potential may exist.

The lowering and rising operators cannot be generally used for any potential! We can define an operator that maps e_n to e_{n+1}, $\hat{A}^\dagger$, but, not with a jump law!
Or, with those annoying commutation properties? No! This depends on the energy spectrum!
The point is: this works just with harmonic oscillators (or similar systems), because of the jumps.

The energy eigenfunctions for bound states can be expressed as purely real.

Two ideas: ~~Dirac notation~~, and meaning of commutators

One more clever question

(14) It is A. I don't absolutely know why, but it is (A).
This gives us some intuition about what uncertainty is. And the commutator
Given $\hat{A}, \hat{B}$ two operators, is it possible to have an eigenfunction $\phi_{a,b}$ which is SIMULTANEOUSLY an eigenfunction of $\hat{A}$ and of $\hat{B}$?

Yes!

$\hat{A}\,\phi_a = a\,\phi_a$ $\qquad$ $\hat{B}\,\phi_a = b\,\phi_a$

What can you say from the existence of such state ϕ_a, about the operators $\hat{A}$ and $\hat{B}$?

Let's think about the commutator, $[\hat{A},\hat{B}]$.

$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

This is a new operator. Let us apply to our function.

$\hat{B}\,\phi_a = b\,\phi_a$; $\qquad \hat{A}\hat{B}\,\phi_a = \hat{A}(b\,\phi_a) = ab\,\phi_a$

and $\hat{B}\hat{A}\,\phi_a = ab\,\phi_a$, for the same reason! So,

$[\hat{A},\hat{B}] = 0$ for ϕ_a!

In practice, there is no "collapse" problem: the operator does not make the function collapse!

So, in order for ϕ_a to be eigenfunction of $\hat{A}$ and $\hat{B}$, $\hat{A}$ and $\hat{B}$ must commute.

If $[\hat{A},\hat{B}] = c\hat{I}$, $\hat{A}$ and $\hat{B}$ does not share eigenfunctions!

What does this mean in terms of observables? The eigenstate of a possible operator, as we know, is a possible state with a definite value, of that operator.

This means, if $[\hat{A},\hat{B}] = c\hat{I}$, that there is NO STATE with a definite value of a and of b: it is not possible to measure, simultaneously, these two values: there is NO STATE having definite a and b. Think of position and momentum!

$[\hat{X},\hat{P}] = j\hbar\hat{I}$.

There are NO STATES that are, simultaneously, eigenfunctions of position and momentum operators, meaning that there are no states with both definite position and definite momentum!

This says us that if we have very good knowledge of position, so very low position uncertainty Δx, we have a terribly high Δp!

We will prove this relation:

$\Delta_\psi \hat{A}\;\Delta_\psi \hat{B} \geq \frac{1}{2}\left|\langle[\hat{A},\hat{B}]\rangle\right|$ (*) we will prove this relationship!

(*)

$\geq \frac{1}{2}\left|\langle\psi|[\hat{A},\hat{B}]|\psi\rangle\right|$

In fact, for $\hat{x}$ and $\hat{p}$,

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

$\langle\psi|j\hbar|\psi\rangle = j\hbar$

Δp,

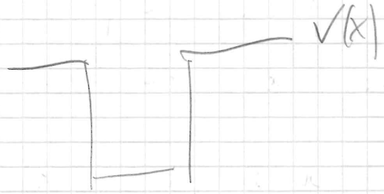
$$\boxed{\Delta x\,\Delta p \geq \frac{1}{2}\hbar}$$

This is the uncertainty relation!

Lecture 11: Dispersion of the Gaussian and the Finite Well

Last part of bound states; from next lecture, we will pass on scattering

So, FINITE POTENTIAL WELL



We are interested in a system, that is a finite well with a finite width: a piece-wise constant potential.

This is a very useful toy model.

For instance, with two opposite walls, field is non-zero inside and zero outside.

We want to find the energy eigenstates for this system, so that we can study easily the time evolution through the Schrödinger equation, by expanding with energy eigenstates.

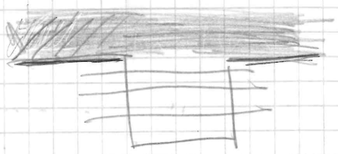
So, the equation we want to solve is

$$E\,\phi_E(x) = -\frac{\hbar^2}{2m}\phi_E''(x) + V(x)\phi_E(x).$$

Then, we use:

$\phi_E''(x) = \frac{2m}{\hbar^2}\left[V(x) - E\right]\phi_E(x)$, where we expect E to be, in general, discrete, constant values. Discrete spectrum.

So, we will have a ground state, some other states and, when energies will be higher than the potential $V(x)$ everywhere, allowed energies will vary continuously: any energy will be allowed above the potential:
we will have a continuous spectrum.



This intuition comes from our qualitative studies of the energy eigenfunctions

What we need to do is to solve (1), subject to some boundary conditions, that are: finite function, to obtain normalizable everywhere, so that the solution should be vanishing far away from the well, and the condition for the wave function to be everywhere smooth, at least continuous. This means: we will solve in each of the 3 regions (1), and then patch together the solution at these boundaries

If a potential is constant, $\psi(x) = e^{\pm kx}$, because $E > V(x)$ (classically allowed region)

So, if we call that

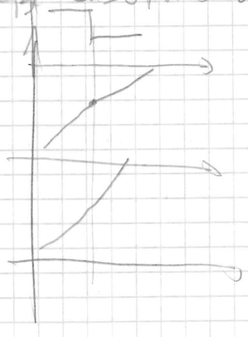
$$E = \frac{\hbar^2 k^2}{2m}.$$

Then ~~and~~ we want to find the solution in the region where energy is lower than the potential, and here, solutions are $e^{+\alpha x}$ and $e^{-\alpha x}$: growing and dying exponentials.

So we know the solutions in both kinds of regions, now we have to patch them, by a continuity condition: continuity of $\phi_E(x)$.

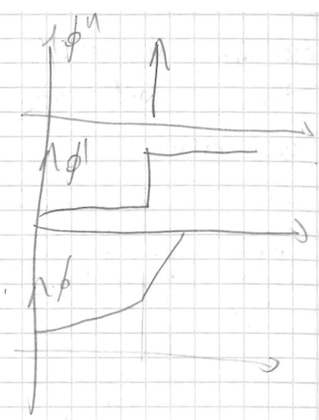
Let's suppose $V(x)$ is continuous. Then, ϕ_E'' does something smooth, as (1) says. Then, ϕ_E' and ϕ are smooth as well. The regularity of ϕ'' is the same as that of the potential.

In fact, if $V(x)$ has a step discontinuity, $\phi_E''(x)$ will have a step discontinuity as well. However, ϕ_E' will have just a steep discontinuous: it would be not smooth, but continuous.



What about $V(x)$ being a δ function?
Well, ϕ'' will be a δ as well, but ϕ' and ϕ will be more regular. In fact,

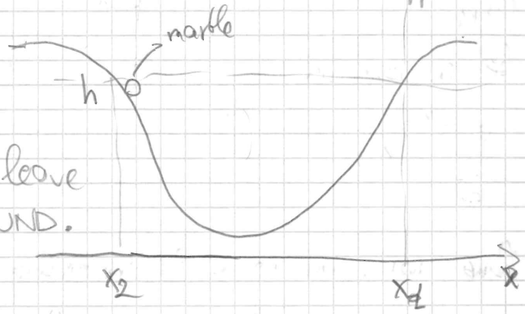
$\phi_E(x)$ will be even continuous.
If $V(x) = \delta(x - x_0)$, which is something funky unphysical, ϕ' will be continuous.



A δ function in the potential results in a kink, a non-derivability point, in $\phi_E(x)$, but still it would be regular.

Now, finite well.

First, quick note. What is a "bound state"? Well, it is the "opposite" of "scattering state".
Why "bound"? Well, let's think of and a domed hole, with some marble.
If it starts at height "h", it will never leave the well: it is stuck inside, it is BOUND.
Bound marble.



But, if instead of just releasing the marble I kick it, it reaches a big velocity, so it can get out, and it is no longer bound. This would be, in quantum mechanics a scattering state.

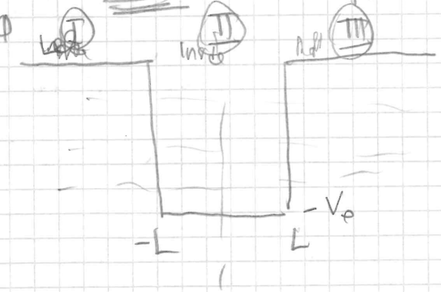
Bound: stuck in the well.
We have a state with some energy, and such energy is lower than the asymptotic value of potential far away from the well. When $E < V_1$ such as $x >> x_2$, the wavefunction will be roughly $e^{-\alpha x}$, and for $x < x_2$ it will be $e^{+\alpha x}$; this for normalizability. So, for $x \to \infty$, $|\psi(x \to \infty)| \to 0$, exponentially.

A quantum bound state is an energy eigenstate such that, probably, falls down exponentially, going far away from the well. It is a state that is exponentially localized.

Consider by contrast a free particle: are those bound states? No!

What about a $\sim \nu(x)$, Gaussian. It is a bound state? Well, it is

certainly localized in space, but NOT expanded: e^{-x^2}! So, at some time, it will spread out, because a Gauss is NOT an energy eigenstate!



Finite well: asymptotically $V(x)=0$.
$V(x)=-V_0$ in the well, x has origin in the center. So,

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

Our bound states, then, will surely have E<0.
Remarks: if the potential is even, then any energy eigenfunction can be written as

ϕ_E^{sym} and/or ϕ_E^{anti} : symmetry affects ϕ_E.
even odd

N.B: We have BOTH odd and even solutions: a bound state can be either odd or even.

Nice fact: we know the solutions in regions I, II, III.

Now: if $E>V(x)$, then $\frac{2m}{\hbar^2}(V(x)-E)$ is some negative number, and

$\phi_E'' = -k^2\phi_E \Rightarrow$ exp if $E>V(x)$

$\phi_E'' = +\alpha^2\phi_E \Rightarrow$ exp if $E<V(x)$

In particular, $k^2=\frac{2m}{\hbar^2}\left|E-V(x)=\right|$,

$\alpha^2=\frac{2m}{\hbar^2}\left(V(x)=E\right|$

Inside, so region II,

$$k=\sqrt{\frac{2m}{\hbar^2}\left(E+V_0\right|} \qquad \left(-\left(-V_0\right)\right),$$

where k controls how rapidly $\phi_E(x)$ changes in the classically allowed region.
In region III, $\alpha=\sqrt{\frac{2m}{\hbar^2}|E|}$ $\left(V(x)=0\ !\right)$

So, the general solution, accounting symmetry, is:

$$\phi_E(x)=\begin{cases}A\cos(kx)+B\sin(kx) & \text{inside (II)}\\ C\exp(\alpha x)+D\exp(-\alpha x) & \text{left (I)}\\ F\exp(\alpha x)+G\exp(-\alpha x) & \text{right (III)}\end{cases}$$

So, solutions are written as superposition of sine/cosine, and exponentials.
We have boundary conditions at ∞, and on the interfaces.
At ∞, $\phi_E(x)\to 0$, so

Normalizability
① $\phi_E(x\to\infty)=0$
② $\phi_E(x\to-\infty)=0$

Left boundary
③ ϕ_E continuous
④ ϕ_E' continuous

Right boundary
⑤ ϕ_E continuous
⑥ ϕ_E' continuous

We have 6 undetermined coefficients and 6 boundary conditions.

For ②, $D=0$, and for ①, $F=0$.

For parity of the potential, the system is even, so $G=C$, and $B=0$ (no sine, so odd contribution).
If it would be only symmetric, we would had $G=-C$, $A=0$. But this is not our case =) Actually it is, but we focus only on even, today. [NOTA: può chiamare le costanti C_1 C_2 C_3, come le B.-C. comportano! =)].

So, our solution reduces to; (focusing, just, for example, on even solutions)

$$\phi_E=\phi_E^{even}=\begin{cases}A\cos(kx) & \text{inside}\\ C\exp(\alpha x) & \text{left}\\ C\exp(-\alpha x) & \text{right}\end{cases}$$

Now, we have to impose the conditions on ϕ_E and ϕ_E'.
Right B.C.: $\boxed{x=+L}$,

$\phi_E = A\cos(kL) \qquad C\exp(-\alpha L)$

inside outside

$$C = A \exp(\alpha L)\cos(KL) \qquad (2)$$

On the other hand, we also have a condition on the derivative:

$$\underbrace{\phi_E' = -AK\sin(KL)}_{\text{inside}} \qquad \underbrace{\phi_E' = -\alpha C e^{-\alpha L}}_{\text{outside}}$$

So, this says that

$$C = +A\frac{K}{\alpha}\sin(KL)\exp(\alpha L) \qquad (3)$$

This is bad, because C cannot satisfy simultaneously two different conditions!

Let us focus on (2): what is K, what is α? Well, it seems that, for any value of energy, we get a solution of (2). But this can't possibly be right, because we are expecting a discrete spectrum!

If we want a correct solution, if we enforce just the continuity of the function, we find a solution, that we don't like.
What could we do? Well, take one condition, e.g. (3), and divide (by the other, i.e. (2)), and we get

$$\alpha = K\tan(KL) \xrightarrow{\text{multiply by } L} \overbrace{\alpha L = KL\tan(KL)}^{\text{this is dimensionless}} \qquad (4)$$

This is the consistency condition such that the wavefunction is continuous with also continuous derivatives. This is a non-linear equation, whose solution is energy E, a trascendental condition, that comes from continuity and normalizability.
At the left wall, we have the very same expression!
Let's write (4) differently:

$$K^2 = \frac{2m}{\hbar^2}(V_0 + E)$$

$$\alpha^2 = \frac{2m}{\hbar^2}(-E)$$

Which are the bound states of the well, as a function of L? For example? Sadly, this equation cannot be solved.

We can also solve qualitatively this equation, and this is useful.

Graphical solution

Let us give, to the nice, pretty dimensionless value αL and KL, names so that

$$\underbrace{KL = z}, \quad \underbrace{\alpha L = y}, \quad \text{so that}$$

$$\overbrace{z^2 + y^2 \equiv \frac{2m}{\hbar^2}L^2 V_0}^{R_0^2} \equiv R_0^2 \qquad (5)$$

Note that (5) is the equation of a circle, with radius R_0.
So we have 2 equations:

$$\begin{cases} z\tan(z) = y \\ z^2 + y^2 = R_0^2 \end{cases}$$

where R_0, V_0 depend on the well parameters L, V_0.

We want to solve these equations.

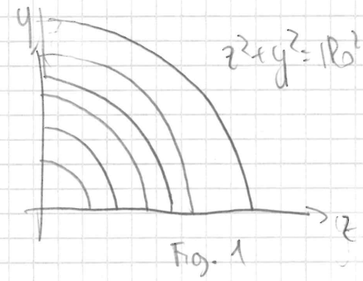
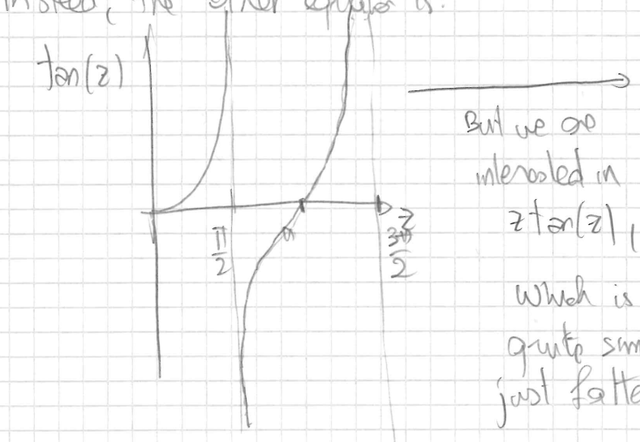


Fig. 1

For fixed value of R_0, solutions lie on circles. Both positive, because we have x^2, y^2, K, L, α positive!

Instead, the other equation is:



But we are interested in $z\tan(z)$, which is quite similar, just flatter

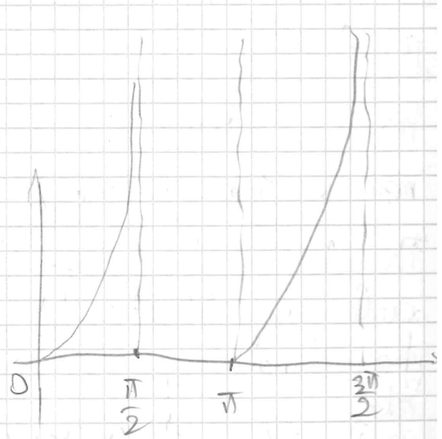


Fig. 2

We want to combine them together, so to put Figs. 1, 2 together.
Then, we draw Fig. 2 "as background", then we draw the arc of circle corresponding to R_0, and the intersections correspond to the solution of our evil equation. This is shown in Fig. 3

In this example, with $|R_0^{(1)}|$, we have 1 solution, that means 1 bound state.

If we make the well deeper, i.e., V_0 larger, the radius gets larger, and we still have a solution, but, as in $|R_0^{(2)}|$, we may also have (2), or (3), or more!
And, we can even see the critical value of depth/width that leads to a new solution! If $|R_0| = \pi$, we have a second solution.

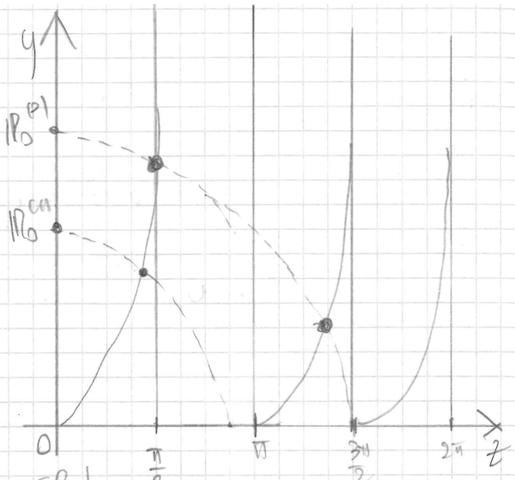


Fig. 3

If we make the well be deeper and deeper, the number of states increases.

Instead, what happens if we make the well be shallower and shallower?
Well, at what width do we lose the ground state? Never! We always have 1 bound state! This is not true in 3 dimensions, but in 1 dimension yes!

Which state is most deeply bound? Well, the ground state! Because it has the biggest value of α, so, since

$$\alpha^2 = \frac{2m}{\hbar^2}(-E),$$

the ground state, which has the maximum absolute value of E, is the more confined.

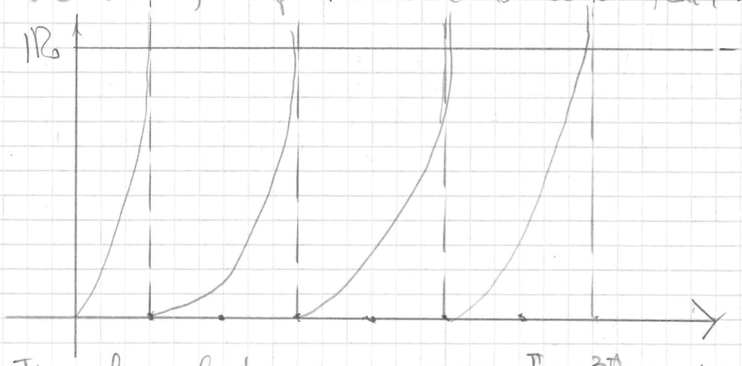
The value of α corresponds to "z", so to the position of the intersection circle - hyperbola(tangent). In other words, the lower is the z of the intersection, the bigger is $|E|$, so α, that is the decaying rate.
↳ the bigger is the y of the intersection that is $|E|$,

Note that, for $|R_0| = \pi$, $E = 0$: zero-energy state! Like, the turning point between continuous and bound state! In such "new" bound state" occurrency, i.e. "at threshold", Energy is 0, and $|R_0| = \pi$.
So, how looks our "new" wavefunction?
Well, in the "non-classical" region, we would have $\psi_E(x) = e^{-\alpha x}$, but, if $E = 0$, $\alpha = 0$! So, it is a constant!

So, it is oscillatory in the classical region, and constant (nonzero) outside. If the well deeper, it becomes bound, with a slowly decaying exponential.
If we make the well shallower, the state is no longer bound, and the exponential tends to explode: the threshold indicates when the state ceases to be normalizable, and then disappears!

A similar problem to this was one of its one limits: the ∞ well, i.e., $V_0 \to -\infty$. Do we recover the infinite well?

If $V_0 \to \infty$, we have a huge circle: $|R_0| \to \infty$. So, the potential becomes very deep. The circle is almost flat, so, $|R_0|$ is gigantically big, if increased, the "valid" targets that are evenly spaced!



=)

The values of the curves are $z = \frac{\pi}{2}, \frac{3\pi}{2}$, and so on: $\frac{(2n+1)\pi}{2}$

So

$$kL = \frac{(2n+1)\pi}{2}, \quad k = \frac{(2n+1)\pi}{2L} \qquad k \text{ even}$$

This... Well, does not seem the full story: it should be

$$k = \frac{(n+1)\pi}{2L}$$

We are missing... the ODD solutions! That are left for exercise!

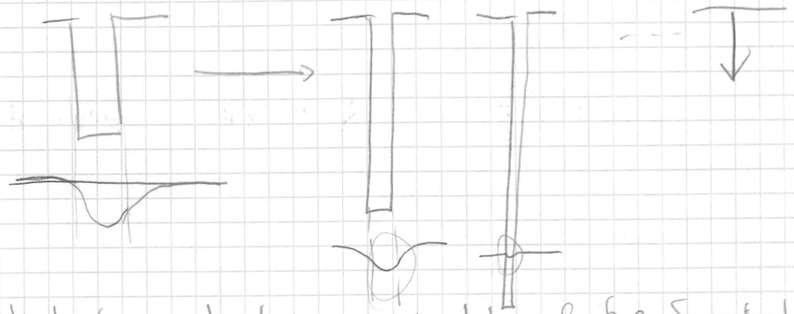
$$k^{odd} = \frac{2n+2}{2L}\pi \qquad \text{(guess)}$$

and curves are co-tangent! Almost.

This means, in other words that, if the well is deep, the first states can be reasonably approximated with those of the ∞ well =)!

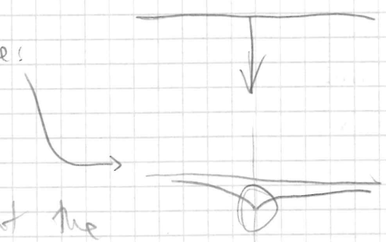
Another funny limit of the system: $V_0 \to \infty$, $L \to 0$.

So, a well deeper and deeper, but also narrower and narrower: as a limit, a δ function: area of $V(x)$, fixed.



$\delta(x)$!

What happens to the ground state of the δ potential?
Well, if we make the potential deeper, the oscillation rate increases, (as the curvature), however, as we make the well narrower the wavefunction has less place to oscillate: oscillates more rapidly, but doesn't oscillate as far!
With the δ function, we have:

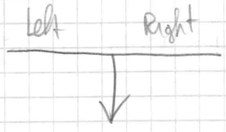


this sort of kink at $x = x_0$, where $\delta(x - x_0)$ lies!
This is what we were expecting at the beginning of the lecture!

This, for the ground state.

What about the first excited state?

Example:



$V = V_0 \delta(x)$

NOTE: $[V_0]$ = Energy x length!

Is there a bound state? We think yes with a kink.
Let us try to write the general solution, in left and right, with appropriate B.C. (normalizability + interfaces).

$$\phi_E(x) = \begin{cases} A \exp(\alpha x) + B \exp(-\alpha x) & x < 0 \\ C \exp(\alpha x) + D \exp(-\alpha x) & x > 0 \end{cases} \qquad (6)$$

So, for normalizability, $B = 0$, $C = 0$. For symmetry, $A = D$.

So, looks like we have our solution!

But, there is another B.C.: continuity! matching!

$$\phi_E'' = -\frac{2m}{\hbar^2}\left(V_0 \delta(x) + E\right)\phi_E$$

Let us integrate this, to understand what happens to ϕ_E' (that we understood have a step discontinuity).

$$\int_{-\varepsilon}^{\varepsilon} \phi_E''(x)\,dx = -\frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}(V_0\,\delta(x) + E)\,\phi\,dx$$

ε, very small number

$$= \phi'(\varepsilon) - \phi'(-\varepsilon)$$

this is the discontinuity in the derivative in 0

$$-\frac{2m}{\hbar^2}\left[V_0 + E\varepsilon - E\varepsilon\right]\phi = -\frac{2m}{\hbar}V_0\,\phi_E(0)$$

So, for $\varepsilon \to 0$,

$$\lim_{\varepsilon \to 0} \phi'(\varepsilon) - \phi'(-\varepsilon) = \underbrace{\Delta\phi'(0)}_{\substack{\text{change of} \\ \text{slope in} \\ \text{the origin} \\ \text{step size.}}} = -\frac{2m}{\hbar^2} V_0\,\phi(0)$$

This is our condition for the proper discontinuity!

By plugging this in (6) (algebra not reported here), we obtain a very specific value of α. This is solvable if

$$\alpha = \frac{m V_0}{\hbar^2} \quad (m > 0), \quad \text{where } [V_0] = \text{Energy} \times \text{length}.$$

So,

$$E = -\frac{\hbar^2 \alpha^2}{2m}$$

$\Rightarrow$ there is a SINGLE BOUND STATE!

This, by assuming even states.
What about odd? We would have $D = -A$, then we would have 1 node for sure. So at the origin, $\phi(0) = 0$, with discontinuity Φ, as if there's no potential: a Φ right corresponds to the δ!
So, there is NO BOUND STATE!

Note: 2 delta function problem: is an awesome model for binding of atoms! (problem set --- =C)

Lecture 12: The Dirac well and Scattering off the Finite Step

Both bound and scattering states are energy eigenstates.
Why do we care about non-bound states, such as scattering states?
Well, as most of world's things, things can "go away", are not strictly localized.
A scattering experiment is where you have some fixed target, through something against it and see what comes back, how the object responses.
For example, LHC: bounding two protons in a ring and making them collide boom to produce something from the collision, and by studying the collision products you can get physical insight.
Scattering is how you interact with the world.
We will study scattering processes: quantum particles sent, from some distance, incident on some potential, and we will try to understand how they are transmitted/reflected.

Easiest case: free particle
Given an object of mass m, $V(x) = \text{constant}$,

$$\phi_E = Ae^{jkx} + Be^{-jkx}, \quad (1)$$

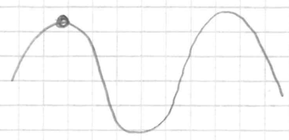
normalization is encoded in A and B; usually, to 1.
In order for (1) to be a solution of Schrödinger's equation (SE), we need the frequency, a.k.a. the energy E (remind de Broglie $E = \hbar\omega$), to be

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

and, knowing that, we can immediately write the solution of the SE by tacking on (1) including the following time dependence:

$$\phi_E(x,t) = \underbrace{Ae^{j(kx-\omega t)}}_{+} + \underbrace{Be^{-j(kx-\omega t)}}_{-} \quad (2)$$

This is not so shocking, since we are working with a free particle.
But -- What do these states mean?
Well, the "+" component is a right-moving wave, because, if we draw the real part of this, at some t_1 and then we draw it on a short bit of time later, how the wave has moved? For example, let's think of a peak in the wave: when $kx - \omega t = 0$, i.e., $x = \frac{\omega}{k} t_1$ as time increases, x increases, so



$\exp(j(kx-\omega t))$ is traveling towards right as t increases! =) Left-moving the other.

So, in general, the solution is given by a superposition of a left-moving and a right-moving wave.

But, problem: $\phi_E(x)$ is not normalizable! In fact, if $B=0$ for example, the norm squared of a pure plane is 1, so the probability density is constant and equal to 1 from $-\infty$ to $+\infty$. The probability to find a particle in any given point is equal!
Usually, our k-th states $\phi_k(x)$ are normalized by $\frac{1}{\sqrt{2\pi}}$, such that

$$\langle \phi_k | \phi_{k'} \rangle = \delta(k-k')$$

Question: can a quantum particle be "placed" on a bound state, i.e., an energy eigenstate that is bound? Sure!
Instead, can we put a particle in the $k=?$ state of a free particle? No! You can never truly put your particle in a scattering state, since it is not normalizable! There will be some approximation, by plane waves (asymptotically scattering states are always plane waves!)
However, we can build a wave packet by using scattering states as

bases functions for states, and those resulting states will be normalizable! And so, reasonably localized. Remember: normalization is important to guarantee one set of localization!
So, we will have to deal with wave packets, rather than just scattering states!
Now, and from now on, we will deal with the evolution of a wave packet! In time!
So, we will study the evolution of a wave packet in a constant potential, and we intuitions obtained on such an example later.

Example
Consider a free particle (FP) in a minimum uncertainty wave packet.
(That is, a Gaussian wavepacket).
Let us assume to have our particle and place it, at $t=0$, in a Gaussian, properly normalized.

$$\psi(x,0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \qquad (3)$$

How does such a system evolve in time? Well we could just plug this in the SE, and, by brute force, find a solution.
Instead, we could: take the known wavefunction, expand it in terms of energy eigenstates, make each eigenstate evolve, and re-sum everything.
So, for the free particle, the energy eigenstates are those progressive and regressive waves. So, since those are also the Fourier harmonics we can represent the wavefunction by means of the Fourier theorem, that is

$$(3) = \psi(x,0) = \int_{-\infty}^{+\infty} \frac{dk}{\sqrt{2\pi}} \left(\exp(jkx)\right) \tilde{\psi}(k) = \int \frac{dk}{\sqrt{2\pi}} \exp(jkx) \left[\frac{\sqrt{\sigma}}{\sqrt[4]{\pi}} \exp\left(-\frac{k^2\sigma^2}{2}\right)\right], \qquad (4)$$

where σ in one domain is at the denominator, in the other it is at the numerator due to uncertainty principle.

But, we know how to time-evolve this wavefunction:

$$\psi(x,t) = \sqrt{\frac{\sigma}{\sqrt{\pi}}} \int \frac{dk}{\sqrt{2\pi}} \exp\left(jkx - \omega_k t\right) \exp\left(-\frac{k^2\sigma^2}{2}\right), \qquad (5)$$

where we just introduced the time evolution in the Fourier harmonics.
We happen to know that $E = \frac{\hbar^2 k^2}{2m}$, that means that $\omega = \frac{\hbar k^2}{2m}$, so

$$(5) = \sqrt{\frac{\sigma}{\sqrt{\pi}}} \int \frac{dk}{\sqrt{2\pi}} \exp\left(j\left(kx - \frac{\hbar k^2}{2m} t\right)\right) \exp\left[-\frac{k^2\sigma^2}{2}\right]$$

this can be written in a more form, by simplifying:

$$= \sqrt{\frac{\sigma}{\sqrt{\pi}}} \int \frac{dk}{\sqrt{2\pi}} \exp(jkx) \exp\left(-\frac{k^2}{2}\left(\sigma^2 + j\frac{\hbar}{m}t\right)\right)$$

(to dimensional analysis: $[\hbar] = [p][x]_r = [m][x][t^{-1}]$, and that's fine!)
So, again, this is a Gaussian! Just with width not equal just to "σ", but with a "complex width"! And this is quite similar, from, to the initial gaussian!
So, this tells about $\psi(x,t)$ that, (by using the inverse transform from (3) with the new width),

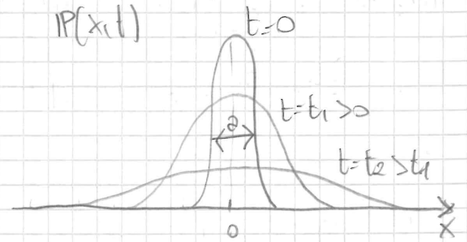
$$\psi(x,t) = \sqrt{\frac{\sigma}{\sqrt{\pi}}} \frac{1}{\sqrt{\sigma^2 + j\frac{\hbar}{m}t}} \exp\left(-\frac{x^2}{2\sigma^2 + j\frac{\hbar}{m}t}\right) \qquad (6)$$

(is this related to the propagation of complex rays of Orta?)

Note that (6) is not so transparent, because there is still a phase term!
Let us understand this by looking at something purely real: $|\psi(x,t)|^2$!
After some algebra, we could find that

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{\sigma^2 + \left(\frac{\hbar}{2m\sigma}\right)^2 t^2}} \exp\left(-\frac{x^2}{2\left[\sigma^2 + \left(\frac{\hbar}{2m\sigma}\right)^2 t^2\right]}\right)$$

Probability is again a Gaussian but at any given moment in time, the width of the Gaussian is changing, and then the amplitude is changing as well!
The time $t=0$ (initial time) is that with the minimum denominator.
Then, for increasing t, both amplitude grows and probability spreads!
The probability at any given point is decreasing.
Graphically, this means that the Gaussian became lower and wider!

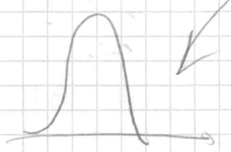


Starting from a well-localized wave packet, it disperses!
Is this reasonable?

Well, if we take $t<0$, negative time, by this analysis it disperses again! =) Firstly it goes back to localized, and then disperse again!
Note also that the sharpest case is $t=0$ (2), the fastest it spreads, because σ is at the denominator: $\frac{\hbar}{2m\sigma}$!

He asks students to generate a Gaussian wavepacket moving, with momentum.
In fact, that we just studied spreads, it stands still: it doesn't move.
THINK ABOUT THIS! 29 min! Well defined momentum expectation value!

Let's imagine that we perform a measurement, and, with some uncertainty, we measure this. Then, the system starts "spreading" (the probability)!



When we measure anything, we leave the system in some state, depending on precision, on accuracy!
By the law of great numbers, it will probably be a Gaussian centered in the "correct", in the most probable position.

Note: how to give a momentum (2 o'clock question)?
Take (3) and multiply times e^{jK_0x}. This gives a momentum K_0!

$$\psi(x,0)=\frac{1}{\sqrt{2\sigma\sqrt{\pi}}}\exp\left(-\frac{x^2}{2\sigma^2}\right)\exp(jK_0x)$$

and the expectation value will be shifted to be $\hbar K_0$ for momentum.
Then, the Fourier transform will shift K to $K-K_0$, and, by repeating the previous analysis, we will come out with new phase terms!
The wave packet will continue move across, breaking the $t \leftrightarrow -t$ invariance.

Now, Allan shows us PhET simulations to see this effect (Colorado)

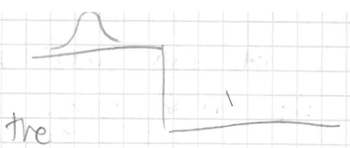
He notes that the wave packet moves quicker than phase in fact,

$v_p = \frac{\omega}{K} = \frac{\hbar K}{2m}$ (phase velocity) $= \frac{v_{classic}}{2}$

$v_g = \frac{\partial\omega}{\partial K} = \frac{\hbar K}{m} = v_c$ (classic velocity!)

→ phase and group velocity.

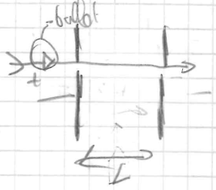
Experiment 2: jump in the potential



What happens is that most of probability overcomes the barrier, but not all of it: part remains in the left region! :o
The wave has scattered off the barrier going downhill, mostly transmitted, but some of it, reflected.

Note: if you have energy lower than the potential, you can't have any wavepacket moving! And, if energy is just above the barrier, most of probability is back "reflected"!

Example of real step potential: a capacitor, with a hole in the middle, and a bullet passing through it! If L is short, it is almost a step potential.



Particle against barrier (52 min): almost no energy (green) is above the barrier, so everything is reflected back!
But still there is a finite, non-zero probability to overcome the barrier! An exponential tail!
This is very different from the classical situation: we hit the wall, we bounce back, period. No! We have strange effects close to the wall!
This is the POSSIBILITY!

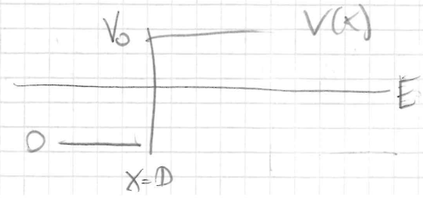
Tunneling: even if classically the barrier would stop everything, a huge amount of energy goes through it! 56 min. AMAZING!

Last example: well!
↳ There are peaks where with total transmission: resonance energies!

A classical particle can NOT reflect back. A quantum, yes!
Such reflection property comes from SE. These reflection effects appear in several systems even classical, but definitely NOT in classical particle physics! Just in wave systems, such as acoustics, optics!

Example: potential step

We want to find the eigenfunctions (?) of this system



We saw that a wavepacket and its time evolution can be studied by expressing it as the sum of energy eigenfunctions. So, let's first find the energy eigenstates for this potential! $\phi_E(x)$

$\phi_E(x)$ is almost known, because we know that, for $x<0$ and $x>0$, potential is constant and the behavior is more or less that of a free particle!

$$\phi_E(x) = \begin{cases} A\exp(jkx) + B\exp(-jkx) & \text{left : classically allowed region} \\ C\exp(+\alpha x) + D\exp(-\alpha x) & \text{right : classically disallowed region} \end{cases}$$

$$E = \frac{\hbar^2 k^2}{2m} \quad \text{(Left)}$$

$$\frac{\hbar^2 \alpha^2}{2m} = V_0 - E \quad \text{(Right)}$$

To have normalizable wavefunctions (ignore left), $C=0$.

For continuity @ $x=0$, ϕ, ϕ' must be continuous. So,

$$A+B=D \quad \text{(continuity of } \phi_E\text{)}$$

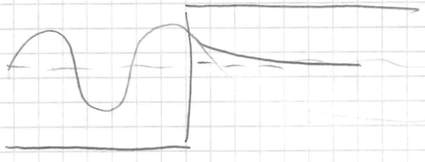
$$jk(A-B) = -\alpha D \quad \text{(continuity of } \phi_E'\text{)}$$

So, by inserting this,

$$D = \frac{2k}{k+j\alpha}$$

$$B = \frac{k-j\alpha}{k+j\alpha}$$

By plugging these back, we obtain the solution. Note that this is not the bound state problem: any energy is fine. There is no constraint on energy at all!



Energy eigenvalues, here, are continuous!

The wave function oscillates for $x<0$, and decays for $x>0$! Smoothly.

How does this system evolve in time? Add $\exp(-j\omega t)$ dependence!

$$\phi_E(x,t) = \begin{cases} A\exp(j(kx-\omega t)) + B\exp(-j(kx+\omega t)) & \text{Left} \\ D\exp(-\alpha x - j\omega t) & \text{Right} \end{cases}$$

$$\omega = \frac{E}{\hbar}$$

So, doing that, comparing to the free particle, we can obtain an easy interpretation. The "A" term is a propagating wave, the "B" a reverse.

On the right, we have an exponentially falling function: NOT a propagating wave: it doesn't have any crest / any peak!

Note that the norm squared of B is

$$|B|^2 = 1$$

If $|B|=1$, the left-moving wave has the same amplitude of the right-moving: it is a standing wave!

So, the probability to go arbitrarily far to the right is 0 (we have exponential suppression). This is a perfect mirror! With just a phase ϕ!

$$B = \frac{k-j\alpha}{k+j\alpha} = \exp(j\phi)$$

B is the reflection.

If potential height is ∞, there is no exponential tail, or strong phase shifts.

If then α is gigantic, $\phi = \pi$: phase inversion

In quantum mechanics, we have a small part inside the mirror. ϕ is called "scattering phase shift" and it creates an enormous amount of the physics. Especially for bonds and solids.

Let us define ρ the probability density, J^x the probability current.

$$\rho = |\psi|^2 \qquad J^x = \frac{\hbar}{2m_i}\left(\psi^* \partial_x \psi - \psi \partial_x \psi^*\right)$$

m_i or m_j?

These guys satisfy the conservation equation

$$\frac{d\rho(x,t)}{dt} = -\frac{\partial}{\partial x} J^x \qquad (J^x : \text{current in } x \text{ direction})$$

Now, unambiguous definition of how much stuff goes to the left and how much to the right.
In general, when we have a wavefunction, at some point it can be approximated if the potential is roughly constant, in that point, in the following way

$\psi = \psi_I + \psi_R$ left

ψ_I: incident divided to right

ψ_R: reflected

ψ_T: transmitted — right

To understand how much goes left or right, reflected or transmitted, is to use the probability current, and to say that to the incident function is associated a current J_I,

$J_I = \frac{\hbar k}{m} |A|^2$, and,

to the reflected term,

$J_R = -\frac{\hbar k}{m} |B|^2$,

and, in this peculiar case of no transmission,

$J_T = 0$

A current is an amount of stuff moving per unit time. The stuff is, for instance, a charge (ρ ...). $|A|^2$ is the probability of the right-moving piece of wavefunction in isolation. $\hbar k$ is the momentum of such wavefunction but divided by m: the classical velocity. Stuff ($|A|^2$) times velocity = current.
Similarly for J_R, with momentum $-\hbar k$.
DEFINITION
Transmission probability

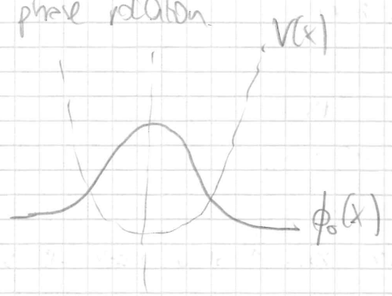
$T = \left|\frac{J_T}{J_I}\right|$ ($= 0$ in this case) (how much current is moving in to the right?)

$R = \left|\frac{J_R}{J_I}\right|$

Lecture 13 - Scattering, Take 2

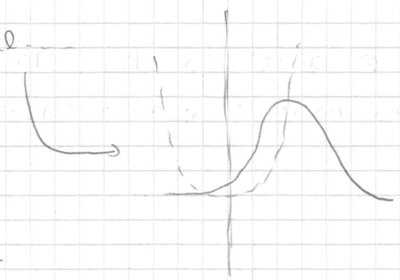
A student asks about coherent states.
Basic idea
The ground state of a harmonic oscillator is a Gaussian, which evolves in time, simply by phase variation: in time, only phase variates.
So, such wavefunction of the ground state, ϕ_0, is:
$\phi_0 \sim N e^{-\frac{x^2}{2\sigma^2}}$ N a normalization factor

So, in time, this thing is just a Gaussian, + phase rotation



But, what if we take our Gaussian, and displace it a little?

Like...



same state, just displaced a little.

How does this state evolve in time? Well, we expand this thing in energy eigenstate, and we know that they can be "evolved" one by one, we put the phase, we re-do the sum, and that's all. But... Is there a nicer solution? The "algorithmic" solution would be...

$\sum_n c_n \phi_n(x) e^{-j\omega_n t}$ (1)

But, this "translated Gaussian", also known as "coherent state", has a nice property: all the interference effects from the phases in (1) "conspire" together, to evolve this state leaving a Gaussian that does NOTHING, except moving back and forth.
In fact, the peak of the resulting Gaussian moves exactly with the frequency of the "step": it behaves just as a damped particle oscillating.
However, its momentum changes in time, in such a way to admit this. This is sort of magical. So, to understand this, let us take a state, ϕ_0, translated in x_0: $\phi_0(x - x_0)$.

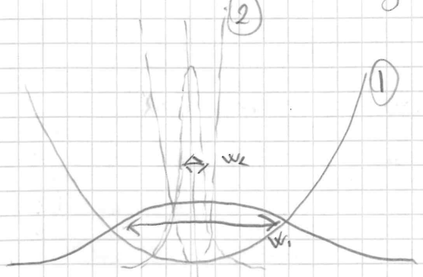
To be in the ground state of the harmonic oscillator, it means that, by applying $\hat{a}$, we annihilate the state:

$$\hat{a}\,\varphi_0(x) = 0$$

So, if $\varphi_0(x-x_0)$ is considered in place of φ_0, this is no longer the ground state, then we will not get 0, but some random schmutz, IN GENERAL. Except for this one: displaced Gaussian. In this case, we obtain

$$\hat{a}\,\varphi_0(x-x_0) = c\,\varphi_0(x-x_0)$$

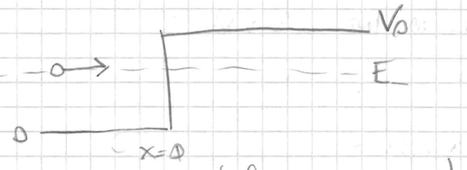
These displaced Gaussians are eigenstates of the annihilation operator!
And you can prove that a coherent state satisfies all these properties, by performing explicitly the deviations from (1).
We can say that a coherent state it's as close to a classical object as we're going to get by building a quantum wavefunction: it's the closest thing in the quantum world, to the classical world. In the harmonic oscillator. this is like the spherical cow of wavefunctions.
A coherent state is a state which is Gaussian.
Note that it does not change its width while moving. This would be true also for a Gaussian with an initial width different from that of the ground state. This is called "squeeze state".
Given an harmonic oscillator, if we put the system in the ground state, at some frequency, we know that potential is created by some laser field. If we for instance double the laser power, but our system is already in a state which is Gaussian, (1), we obtain (2): our squeezed state has too much position uncertainty, and too little momentum uncertainty (2): the (2) is much narrower than before in the position space, so much broader in momentum space.



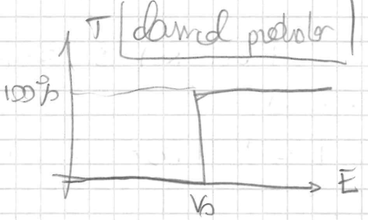
So, with potential ②, the grand state ① has too much position uncertainty (too broad) and too little momentum uncertainty, compared to the ground state of ②: it has been squeezed! This guy, just like coherent states, is periodic, it evolves almost as a classical particle, but they change shape. There are quantum optics with something like coherent states, but like superposition. Hard still ;-)

Scattering

We discussed scattering of a particle against a barrier.



The probability that it transmits across this barrier, T, is basically 0 for low energies, 100% for $E > V_0$



Then, we knew the quantum solution in the left and right regions, which are just plane waves,

$$\varphi_E = A \begin{cases} e^{jkx} + \frac{k-j\lambda}{k+j\lambda} e^{-jkx} & \text{Left} \quad E = \frac{\hbar^2 k^2}{2m} \\ \frac{2k}{k+j\lambda} e^{-\lambda x} & \text{Right} \quad V_0 - E = \frac{\hbar^2 \lambda^2}{2m} \end{cases} \qquad (2)$$

In particular we understood that e^{jkx} is a progressive term, and $\frac{k-j\lambda}{k+j\lambda}$ is a pure phase, and let's call it "r"

$$r = \frac{k-j\lambda}{k+j\lambda} \qquad (3)$$

r is small (not capital) because it is an amplitude, other than a probability.
What is the transmission probability to get for out $x=0$? 0. Because probability is the norm squared of $\frac{2k}{k+j\lambda} e^{jkx}$, and, for $x \to \infty$, it is 0.
We defined a current J_T

$$J_T = \frac{\hbar}{2jm}\left(\psi_R^* \partial_x \psi_R - \psi_R \partial_x \psi_R^*\right) = 0,$$

and such current vanishes when the wave function can be made real, up to a constant phase.
This current is a flux of transmitted particles [Orta, Schrödinger notes]
We define

$$T = \left|\frac{J_I}{J_T}\right| \qquad R = \left|\frac{J_R}{J_I}\right| \qquad (4)$$

Now, let us move on, with a new scenario.

A particle with $E > V_0$!

Which is now the form of the wavefunction?

$$\phi_E = \begin{cases} A\exp(jk_1x) + B\exp(-jk_1x) & \text{Left} \\ C\exp(jk_2x) + D\exp(-jk_2x) & \text{Right} \end{cases}$$

$e^{-j\omega t}$ (5)

$$E = \frac{\hbar^2 k_1^2}{2m} \qquad E - V_0 = \frac{\hbar^2 k_2^2}{2m}$$

Left Right

Interpretation: "A" and "C" are progressive waves. They are energy eigenstates, so they evolve in time by a phase term. "B" and "D" are regressive

We can imagine 2 scattering experiments: one where we send a particle from the left: it can go through, or scatter back.
If we send a particle from the left, $A \neq 0$, $D = 0$.
In the other case, particle from right, $A = 0$, $D \neq 0$
So, A and D are "input" terms, whereas B and C are outgoing terms.
Note that in principle one could have both $A \neq 0$ and $D \neq 0$ if we are sending something from left and right simultaneously, but, it is convenient to study each incidence as stand alone, and obtain the general solution by superposition. Everything is linear, so it is allowed.

Now, results for (5): ($D = 0$)

$$C = \frac{2k_1}{k_1+k_2}A \qquad B = \frac{k_1-k_2}{k_1+k_2}A$$ (by enforcing continuity and so-)

So,

$$R = \left|\frac{k_1-k_2}{k_1+k_2}\right|^2 \qquad T = \frac{4k_1k_2}{|k_1+k_2|^2}$$

But k_1 and k_2 are encoding information of E and V_0. So, by doing some algebra, we can see that

$$R = \left|\frac{k_1-k_2}{k_1+k_2}\right|^2 = \left|\frac{1-\sqrt{1-\frac{V_0}{E}}}{1+\sqrt{1-\frac{V_0}{E}}}\right|^2 \qquad (6a)$$

$$T = \frac{4\sqrt{1-\frac{V_0}{E}}}{\left|1+\sqrt{1-\frac{V_0}{E}}\right|^2} \qquad (6b)$$

Having (6) allows us to plot the "quantum version" of the tunnel, classical prediction of the previous page.
We could see, by plotting, that T tends asymptotically to 1 as E increases.
In other words, if our energy scales are gigantic, compared to the potential height, we recover the classical result.
Moreover, it could be noted that

$$R + T = 1$$

This is necessary to be able to apply our interpretation as probabilities!
Note: there is no such thing as particle reflection in classical world!

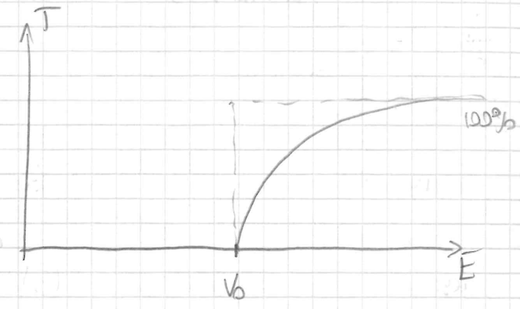


Fig. 1

Question: why is/are the definition in (4) squared?
(Typo) But still, note that J_T, J_I are quadratic in the wavefunction!

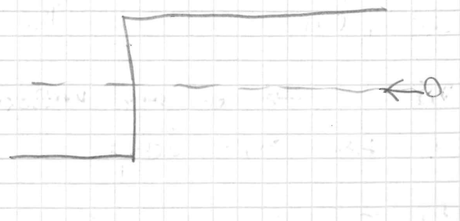
Note that the meaning of R and T are: made and measure far away from the potential jump. Doesn't matter the 'tail' of X slightly greater than 0.

If you do the same calculation/experiment from the right, you find

$$\boxed{A = 0} \qquad C = \frac{k_1-k_2}{k_1+k_2}D$$

$$B = \frac{2k_1}{k_1+k_2}D$$

This means that reflection and transmission are the same uphill as downhill.
This is so weird! If we are in a situation like this, it's the same as



0→

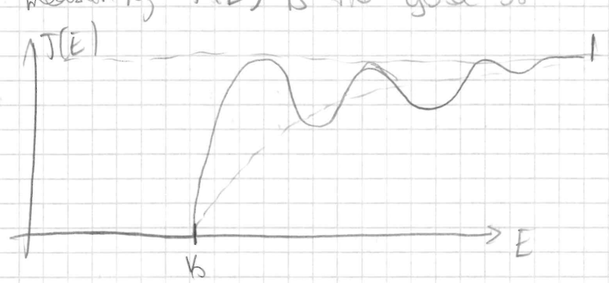
(actually, the particle in this case cannot move.)

There is NO EXPERIMENT in which R and T sum up to 1: NO!
It would mean that the particle could disappear!
Moreover, from (4), it comes from the definition.
Note: the current satisfies a conservation equation, that is,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot j$$

by construction.
It should not surprise us, the fact that incidence from right is the same as from the left. We could just prove it analytically, by flipping our drawing! This, also from (5)! Or (2)!

Note that, from Fig. 1, so just from $T(E)$, we could deduce what the potential is! This is useful because, if we don't have access to the system, we could just send particles with more and more energy, and, from the shape of the curve, deduce $V(x)$.
Deducing potential properties just by measuring $T(E)$ is the goal of scattering!
Let us imagine that our $T(E)$ is something like:



What can we say?
It is kind of like the potential step V_0. But it also has oscillations!
What can we do? What is $V(x)$?
More precisely: we want to understand what our potential is, knowing that it is constant up to $x=0$ something happens inside, and then again constant for $x \geq L$.

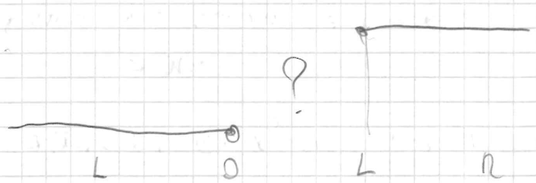


Fig. 2

Example of this is the hydrogen atom: neutral, but inside there are the proton and the electron interacting and so on.
Well. We know that, always, in L, the wave finds
(L) $A\exp(jkx) + B\exp(-jkx)$
(R) $C\exp(jkx) + D\exp(-jkx)$

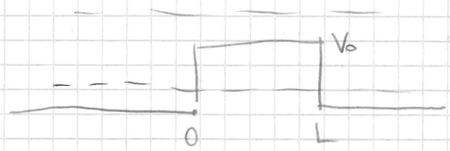
We have, asymptotically for $t \to \infty$:

$$T = \left|\frac{C}{A}\right|^2 \qquad R = \left|\frac{B}{A}\right|^2$$

So, it suffices to compute B, C as functions of A, D.
So, fixed energy E ("I don't know where they are, but I'm sure of what their momentum is"), and we perform the scattering experiment.

We can assume that potential goes to 0 also at $x \to \infty$. We can say that, even if in general it is not the case, L and R go to the same limit.

Simplest example: what we've done before, twice!



$D = 0$ (scattering from left)
We could either study energy from above or from below the potential.

Let us start from $E > V_0$.
We don't know the form of the wavefunction in $0 < x < L$, but it is, actually, just

$$F\exp(jk'x) + G\exp(-jk'x) \qquad k' \neq k$$

So,

$$\frac{\hbar^2 k^2}{2m} = E, \qquad \frac{\hbar^2 k'^2}{2m} = E - V_0$$

We have to apply the matching conditions, plus $D = 0$, and normalize from A.
After a lot of algebra we obtain

$$T = \left|\frac{C}{A}\right|^2 = \frac{4k^2k'^2}{4k^2k'^2\cos^2(k'L) + (k^2 + k'^2)^2 \sin^2(k'L)} =$$

By including the parameters of the system, $m, \hbar, V_0, L, E$, let us define

$$g_0^2 = \frac{2mL^2 V_0}{\hbar^2},$$

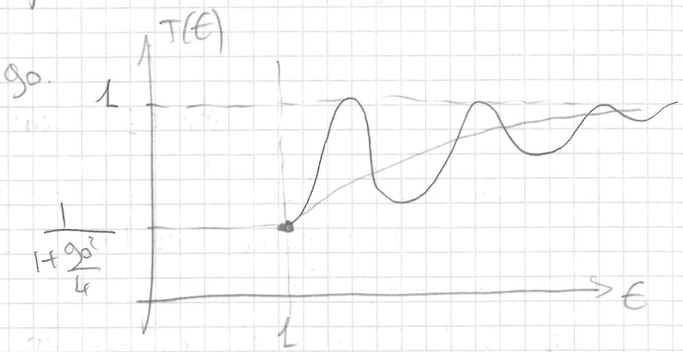
which is a dimensionless measure of the depth of the potential. $\frac{1}{L^2}$ is a k^2, and $\frac{k^2}{2m}$ is an energy.
So this is the ratio of the height of the potential, V_0,

to the characteristic energy corresponding to the lenght scale L.
Then, let ϵ be $\frac{E}{V_0}$ a dimensionless energy.
So after a bit of algebra,

$$T = \frac{1}{1 + \frac{1}{4\epsilon(\epsilon-1)} \sin^2\left(g_0\sqrt{\epsilon-1}\right)}$$

for $\epsilon > 1$, i.e., $E > V_0$. (1)

Let us plot $T(\epsilon)$ for some fixed g_0.



When $\epsilon = 1$, with Taylor limit

$$T \approx \frac{1}{1 + \frac{g_0^2}{4}}$$

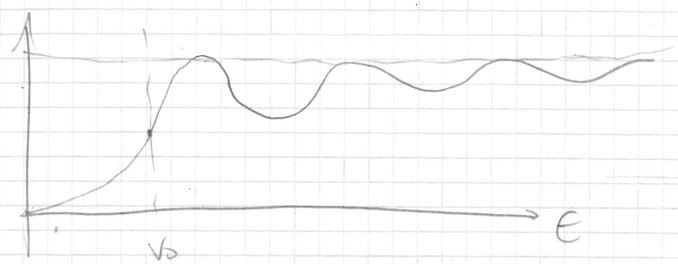
If $g_0 = 0$, $T = 1$: 100% transmission, 'cause no barrier appears!

For $\epsilon \to \infty$, it goes to 1. But there is the sine, with frequency g_0, and it gets wider and wider because of $\sqrt{\quad}$ of ϵ.
Moreover, the minima is higher because $\epsilon(\epsilon-1)$ appears at
At speed does of ϵ, we have perfect transmission!
So, why? Well, because the sine or g_0 to 0 ;-)
But, more physically?
Well. First, at high energies, the particle does not even notice the finite ("in height") barrier. So, 100% transmission, asymptotically.
At low energies we could assume some kind of suppression. Still, we assumed $E > V_0$, so right now we don't know.
But 100% points!
If you know that there is 100% transmission at some ϵ, we know how to approximate our system with a square step barrier!
What about $E < V_0$? Well, we are in a classically disallowed region, so we could just replace "ik" with "$-k$" in the exponential.
You can get, by this way,

$$T_{E<V_0} = \frac{1}{1 + \frac{1}{4\epsilon(1-\epsilon)} \sinh^2\left(g_0\sqrt{1-\epsilon}\right)}$$

and it matches the (1) for $E = V_0$.

But, $\sinh$ is not a step function: it goes smoothly to 0.



So, for $E < V_0$, there is some probability for the particle to pass through the barrier, even if we are in a classically unallowed region.

We do not get resonances for $E < V_0$, but we have $T \neq 0$.
This is the tunnelling effect.

> NOTA che fisicamente anche $\exp(+kx)$!

If E is fixed, and we vary L, i.e. the width of the barrier, which is only contained in g_0, how does $T(L)$ vary?
It goes like $e^{-2\kappa L}$ (κ depends only on E and V_0.
So, the probability of tunnelling through a wall depends on the width of the wall. Exponentially!

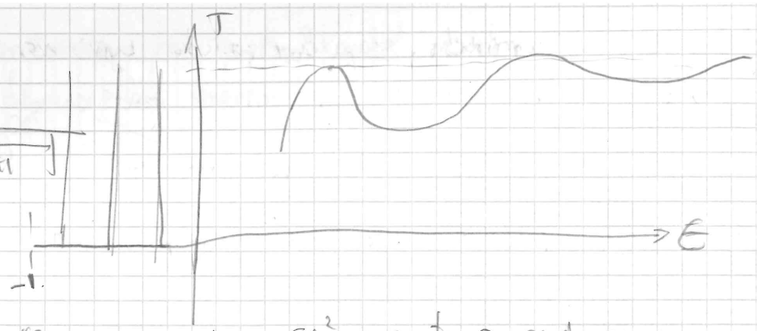
Lecture 14: Resonance and the S-matrix

Last lecture on scattering: phase-shift and S-matrix.
No questions? Sign of knowledge, competence, mastering.
We want to understand what's behind these resonances, i.e., 100% transmission points, and their connection with minima.
Note that we have something much different, from a single step!
Little variation from the problem: square well, instead than square barrier: how behave scattering states?
We could have the very same results from the barrier, and put $V_0 \longleftrightarrow -V_0$: substitute V_0 with $-V_0$, and that would be it!

So, for a square well,

$$T = \frac{1}{1+\frac{1}{4\epsilon(\epsilon+1)}\sin^2\left(\varphi_0\sqrt{\epsilon+1}\right)}$$

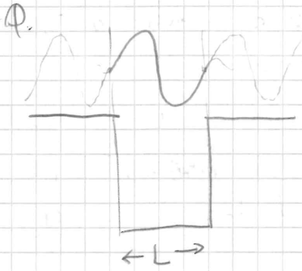
$$\varphi_0 = \frac{2mL^2}{\hbar^2}V_0, \quad \epsilon = \frac{E}{V},$$



Again we can observe resonances, when $\sin^2$ goes to 0 and so on. But for the well, for $\epsilon<0$, we also have bound states! Remind that bound states are always above $-V_0$: $E>-V_0$!

Why are these resonances there? Well, imagine that kL is multiple of 2π, so $\sin(\cdot)=0$.

If $kL=2\pi$,

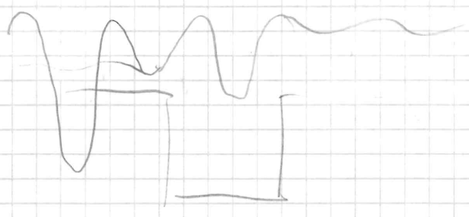


So, a situation in which the wavefunction is periodic, with the same (beginning and ending) slope. So, it would not be ok.

So, the wavefunction inside, matches perfectly in amplitude and period the one outside. This due to matching conditions: if inside the well we have exactly 1 period, and with the outside we have the b.c., we must have constant amplitude inside and outside.

The transmission probability is the norm squared of right to left, but since they are the same as we just assumed, it is ①! 100%! As if there was no interviewing region!

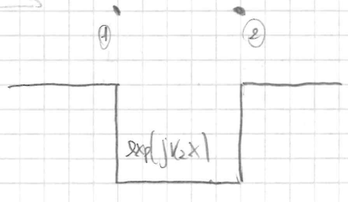
If instead of being perfectly periodic it would be something like same period, different amplitude!



But, this is just showing how different are the solutions of 2nd order differential equations with the proper matching conditions.

We can do something better!

Suppose that we have our square well, with some amplitude, hence some momentum, being in motion towards right.



Which is the probability that our particle overcomes the well, and passes to the other end (2), so that it scatters across?

Well, it can be seen as the probability of the left step, ↘, plus some propagation, and then jump across the second, ↗, step.

Something like the product of the probabilities... Or not?

NO! In fact, neither of the two exhibit a resonating structure so we need something more sophisticated.

This because this misses: ① Reflection

② The propagation distance between the two steps!

(L)

③ But in particular, probabilities do not add in quantum mechanics. What can be combined is the wavefunction, the complex number, NOT the probability! The correct step is: first, combine the wavefunctions. Then take the norm square of it!

The amplitude, the state, comes from transmission, evolution (propagation), reflection, and so on!

This for an ∞ number of times!

$$t_{\lrcorner\lrcorner} = t_{\lrcorner}\, e^{jk_2L}\, t_{\lrcorner} + t_{\lrcorner}\exp(jk_2L)\, r\exp(-jk_2L)\, r\exp(jk_2L)\, t_{\lrcorner} + \dots$$

this recalls a term from a geometric series!

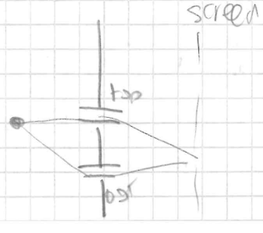
$$= t\exp(jk_2L)\, t\left(\frac{1}{1-|r|^2e^{-2jk_2L}}\right) \quad (1)$$

$(t_{\lrcorner} = t_{\llcorner}$ for hypothesis$)$

This is what we predict (1) from multiple bounces. (Just like in the 2-slits experiment: here, it's like having ∞ slits!) (Dog because of the back-forth reflections o_o)

What happens in the 2-slit experiment?

First I compute the two amplitudes, the two wavefunctions. Then, norm square of the sum. This, to keep to account interference!



To sum up, this is a bad-ass way of exploiting superposition.

If we use the reflection/transmission from the step discontinuity in (1), we obtain

$$t_{TF} = \frac{1}{e^{jk_2 L} - \frac{2j}{T_F}\sin(k_2 L)} \qquad (2)$$

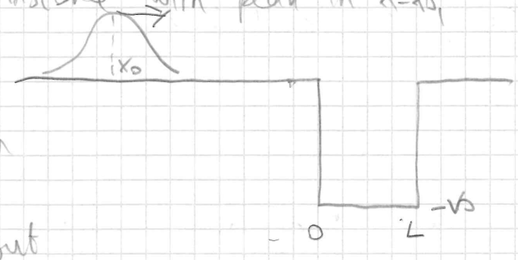
Note that (2) is not the same formula of the previous lecture, i.e., the probability! But this is natural: this is the amplitude, NOT the probability!

If we take the norm square of t_{TF}, we obtain

$$\rightarrow |t_{TF}|^2 = \frac{1}{1 + \frac{1}{4E(E+1)}\sin^2(g_0\sqrt{E+1})} = T$$

But, this "new derivation" says us why we have spread values, where resonance occurs. Well, in this process where multiple interactions, multiple scattering events occur, there are several transmission terms, not just the "fundamental", "direct" one! Each of these terms, either coming from no reflections, 2, 4, 6, whatever number of reflections is carrying a phase. When the phase is the same for all terms, they add constructively! In other cases, they interfer! This interference is what distinguishes quantum and classical mechanics! Classically, one can combine probability! Here, no due to interference!

We always discussed just monochromatic plane waves, even if it is not possible to put a particle, a single particle, in a state which is a plane wave: it is not normalizable. When we talk about single particles is we put them in some well-localized wavepacket. For instance, with peak in $x=x_0$, with no expectation value of its momentum. So, what happens to this beast, to this whole wavepacket, when it meets the potential well?



We studied this for a plane wave, but a plane wave is not localized, so not a realistic model for a particle =C

What can we do with the results we already have?

Well, for a free particle (no potential, constant), we know that

$$\psi(x,0) = \eta \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) e^{jk_0 x}$$

to evolve in time, we expand in energy eigenstates (with constant potential, plane waves),

$$\psi(x,0) = \int dk \frac{e^{jkx}}{\sqrt{2\pi}} \tilde{\psi}(k) = \int dk \frac{e^{jkx}}{\sqrt{2\pi}} \eta \exp\left(-\sigma^2 \frac{(k-k_0)^2}{2}\right) e^{-jkx_0},$$

so information about x_0 is just in the last exponential (property of the Fourier transform).

Since they are energy eigenstate, their time evolution ends themselves less than a phase rotation. So,

$$\psi(x,t) = \int dk \exp(jkx) \frac{1}{\sqrt{2\pi}} \exp(j(kx-\omega t)) \exp(-jkx_0)$$

This, for the free particle. What about the potential hole? (well?)

Well, $\psi(x,0)$ is the same. But energy eigenstates are no longer plane waves! As we know from the system, given $E = \frac{\hbar^2 k^2}{2m}$,

$$\phi_k = \frac{1}{\sqrt{2\pi}}\left(\exp(jkx)\Theta(-x) + r\exp(-jkx)\Theta(-x) + t\exp(+jkx)\Theta(x-L)\right)$$

[QUICK WAY OF WRITING OUR SOLUTION] [NOT INTERESTED INSIDE WELL]

$\Theta(x)$: function equal to 0 when its argument is negative and 1 when its argument is positive!

So now, we want to decompose our wavefunction in terms of energy eigenstates!

First, expand $\psi(x,0)$:

$$\psi(x,0) = \int \frac{dk}{\sqrt{2\pi}} \tilde{\psi}(k)\,\phi_k(x) =$$

($\tilde{\psi}(k)$: different from before)

$$= \int \frac{dk}{\sqrt{2\pi}}\left[\tilde{\psi}(k) e^{jkx}\Theta(-x) + \tilde{\psi}(k) r e^{-jkx}\Theta(-x) + \tilde{\psi} t e^{jkx}\Theta(x-L)\right]$$

(e^{jkx}: exp(jωt); e^{-jkx}: exp(jωt); e^{jkx}: exp(jωt))

Well, this, suppresses exp(jωt). Now, if we account for it, we can

say that the first and third terms are moving to the right (propagating), the central to the left.

So, when $t=0$, what does the first term look like?

$$\int \tilde{f}(k)\, e^{ikx}\, \frac{dk}{\sqrt{2\pi}}\Big]\Theta(-x) = \text{initial Gaussian! } G(x, k_0, 0)\,\Theta(-x)$$

So, putting time dependence:

$$\int \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\, \exp\left[j\left(kx-\omega t\right)\right]\, \Theta(-x)\,,$$

and $\tilde{f}(k)$, the "envelope" of the plane waves, is well-localized in position (Gaussian) and momentum (around k_0). By using the method of stationary phase, or just asking where is the phase constant stationary, we find the peak of the wave function

$$\frac{d}{dk}\left(kx-\omega(k)t\right)\Big|_{k_0} = x - \frac{\hbar k}{m}t$$

in the free particle regime (just with this constraint),

$$\omega = \frac{\hbar k^2}{2m} \rightarrow \frac{d\omega}{dk} = 2\frac{\hbar k}{2m}$$

For the stationary phase $x - \frac{\hbar k}{m}t = 0$, we have that the stationary phase point moves in time,

$$\boxed{x = \frac{\hbar k_0}{m}t} = \frac{p_0}{m}t \rightarrow \boxed{v_0 t}$$ v_0 the classical velocity!

Then, what happens at late times? Still focusing on this first term, $v_0 > 0$, $t > 0$, so it continues moving right. But there is also the $\Theta(-x)$ term, which kills the wavefunction: when the "first term" reaches $x=0$, i.e., the well, it gets killed, and replaced by the remaining 2 terms. One moves to the left, the other right.

Focusing on the third, transmitted term, it looks like

$$\int \frac{dk}{\sqrt{2\pi}}\, \tilde{f}\, t\, \exp\left[j\left(kx-\omega t\right)\right]\, \Theta(x-L)\,, \text{ where } t = \sqrt{T}\, e^{-j\varphi(k)}.$$

t is the square root of T, but it has a phase term. What is this? What information is contained in it? $\varphi(k)$ is a function of k! It depends on E, so k.

$$\hookrightarrow = \Theta(x-L)\int \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\sqrt{T}\, \exp\left[j\left(kx-\omega t-\varphi(k)\right)\right]$$

With what velocity does this wave packet move? Again, let us make an argument by stationary phase: let us look how does the packet move by looking how its stationary phase point moves

$$\frac{d}{dk}\left[-\omega t + kx - \varphi(k)\right]\Big|_{k_0} = 0\,,$$

$$= x - v_0 t - \frac{d\varphi}{dk}\,,$$

$$\frac{d\varphi}{dk} = \frac{d\omega}{dk}\frac{d\varphi}{d\omega} = v_0\frac{d\varphi}{d\omega} = v_0\hbar\frac{d\varphi}{d(\hbar\omega)} = v_0\hbar\frac{d\varphi}{dE}\,.$$

So,

$$\hookrightarrow = x - v_0\left(t + \hbar\frac{\partial\varphi}{\partial E}\right)$$

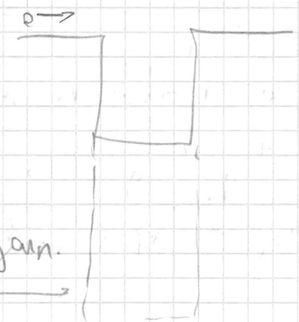
So,

$$x = v_0\left(t + \hbar\frac{\partial\varphi}{\partial E}\right)$$

is the velocity of movement of the stationary point, so the peak.

The point is that, in addition to the $v_0 t$ constant velocity term, which is nice (if not constant it would be accelerated, so it would lose energy), but it has this $\frac{\partial\varphi}{\partial E}$, which is some sort of time shift! A shift in the time of where the wave packet is! What does this mean?

Interpretation



Classically, we have an object with some energy, and when it hits the well, it acquires energy and then it speeds up. Then it reaches the second wall of the well, it leaves it, and slows down again. If we assume the well extraordinary deep, it means that, while "falling", our particle acquires a lot of energy, so of speed, so it stays in the barrier for a very short time, just like if the barrier was not there! So its position before the well would be $x = v_0 t$, but, after the well,

it becomes different: there is a time shift, that is the time we didn't need to cross the gap! $\frac{L}{V_0}$! We did not need $\delta t = \frac{L}{V_0}$, so, the presence of the well allowed to anticipate this time, compared to what would happen for a free particle. For a plain potential!

$$x = V_0\left(t + \frac{L}{V_0}\right)$$

This is a classical picture, because, here, the particle goes faster inside the well.

And, in the quantum computation, we obtained something somehow similar! Let's compare the two results!

$$\delta t_{classical} = \frac{L}{V_0} \quad \overset{?}{=} \quad \hbar \left.\frac{\partial \varphi}{\partial E}\right|_{E=V_0} \quad ?$$

Well, from last time, knowing that $T = \frac{C}{A}$ (coefficients of the global) with Mathematica or whatever,

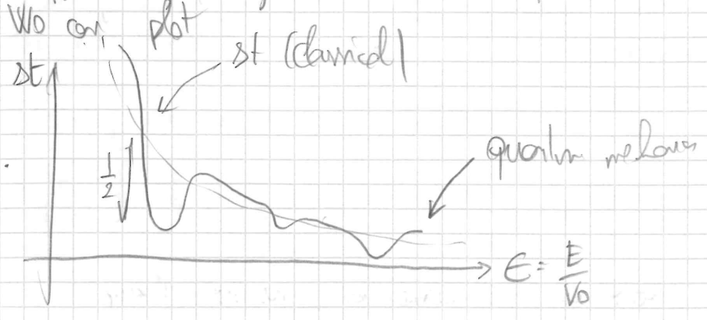
$$\varphi = LT = k_2 L - \operatorname{atan}\left(\frac{k_1^2 + k_2^2}{2k_1 k_2} \tan(k_2 L)\right)$$

Very complicated, not immediately possible to learn something from this. Is this somehow close to the classical result?
Well, first let us study this guy close to resonance! Here $k_2 L \approx N\pi$, so, we can show (after some computation)

$$\hbar \left.\frac{\partial \varphi}{\partial E}\right|_k \approx \frac{L}{2V_0}\left(1 + \frac{E}{V_0}\right)$$

In our "classical" hypothesis we assumed V_0 very large so $\frac{E}{V_0} \approx 0$.
So, the quantum mechanical result is the same, down by a factor of 2.
Apparently, things slow down, compared to classical physics!

We can plot



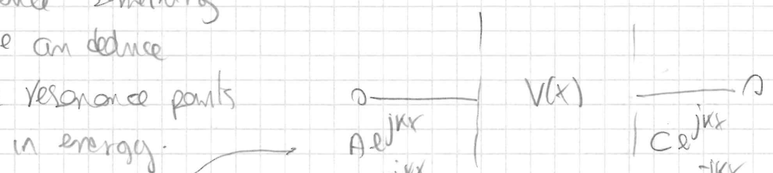
So, it has variations and, on the valleys, this "factor of 2" appears.
So it fits quite well, except in resonance.

Why?! Because the classical particle just "jumps" and walks across, whereas the quantum particle has all this back-forth stuff! This superposition of multiple reflections! And with some effort you can also find this 1/2 factor. Still, it is important to remark how incredible is this constructive interference! This can let us glimpse how much physics we can find in this φ !

S-matrix

One thing which is very useful to organize, to describe scattering in 1D but even in 2D or 3D is the scattering matrix.

Basic idea: given some unknown potential in some bounded region, and we want to deduce something about the $V(x)$, we can deduce something from the resonance points and the phase shift, in energy.



In general, we have

We can ask the following: if we put something to have some A or/and D, what do we have on the respective "other sides", so "B" and "C"?

$$\begin{bmatrix} B \\ C \end{bmatrix} = \underline{\underline{S}} \begin{bmatrix} A \\ D \end{bmatrix} \qquad \underline{\underline{S}} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$$

this matrix $\underline{\underline{S}}$ takes the amplitudes of the "input" signals and provides the amplitudes of the "output" signals.

Note: we know that our physics is linear because if we double A, B must double, or probability is not conserved $\Rightarrow$ so, a matrix approach is allowed.
Basically for scattering problems, if one tells you the scattering matrix and in particular how all the coefficients of $\underline{\underline{S}}$ vary with energy, then you have the solution of the scattering problem.

Properties of the $\underline{\underline{S}}$ matrix

① Stuff doesn't disappear
so, $|A|^2 + |D|^2 = |B|^2 + |C|^2$!
This because we are in energy eigenstates, so probability does not change in time.

We can write this as:

$$|A|^2 + |D|^2 = |B|^2 + |C|^2$$

$$\begin{bmatrix} A^* & D^* \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} = \begin{bmatrix} B^* & C^* \end{bmatrix} \begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} B^* & C^* \end{bmatrix} \underline{\underline{S}} \begin{bmatrix} A \\ D \end{bmatrix} =$$

But, $\begin{bmatrix} B^* & C^* \end{bmatrix} = \begin{bmatrix} B \\ C \end{bmatrix}^{T*} = \left[\underline{\underline{S}} \begin{bmatrix} A \\ D \end{bmatrix} \right]^{T*} = \begin{bmatrix} A^* & D^* \end{bmatrix} \underline{\underline{S}}^{+}$

(adjoint = transpose complex conjugate)

So,

$$\begin{bmatrix} A^* & D^* \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} \begin{bmatrix} A^* & D^* \end{bmatrix} \underline{\underline{S}}^{+} \underline{\underline{S}} \begin{bmatrix} A \\ D \end{bmatrix}$$

So, $\underline{\underline{S}}^{+} \underline{\underline{S}} = \underline{\underline{I}}$

If stuff doesn't disappear, then $\underline{\underline{S}}$ is a unitary matrix.

A consequence of this is that the eigenvalues of $\underline{\underline{S}}$ are pure phases:

$s_1 = \exp(j\varphi_1)$, $s_2 = \exp(j\varphi_2)$

This leads to constraints on the coefficients:

$|S_{11}| = |S_{22}|$ $\quad$ $|S_{12}|^2 + |S_{11}|^2 = 1$

$|S_{12}| = |S_{21}|$ $\quad$ $S_{11} S_{12}^* + S_{21} S_{22}^* = 0$

These conditions are consequences of probability conservation, but they have a meaning: assuming that we send something from the left, and nothing from the right,

$$B = S_{11} A \quad \text{so} \quad \frac{B}{A} = S_{11}$$

and $\frac{C}{A} = S_{21}$

But $\frac{C}{A}$ is what we called "T". And $\frac{B}{A}$ is "V".

This obviously holds when sending stuff from the right.

But, now, this means that reflection from the left equals reflection from the right.

$|\Gamma_{\rightarrow}| = |\Gamma_{\leftarrow}|$, and $|t_{\rightarrow}| = |t_{\leftarrow}|$

And we also saw that $R+T=1$!

Now

Suppose that our system is time-reversal invariant: by substituting "$-t$" to "$+t$", nothing changes. This is not true for electric current for instance, because current would change sign, so the direction of the associated magnetic field.

When time invariance holds Ψ is a scalar, and so is Ψ^*, and we can show that we have, under time inversion,

$$\Psi^* \rightarrow \begin{matrix} A^* e^{-jkx} & C^* e^{-jkx} \\ B^* e^{jkx} & D^* e^{-jkx} \end{matrix}$$

So it must be true that

$$\begin{bmatrix} A^* \\ D^* \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{21} \end{bmatrix} \begin{bmatrix} B^* \\ C^* \end{bmatrix}$$

therefore, $\underline{\underline{S}}^{*} \underline{\underline{S}} = \underline{\underline{1}}$

$\underline{\underline{S}}^*$ is just the complex conjugate of $\underline{\underline{S}}$. Then, $\underline{\underline{S}}^{-1} = \underline{\underline{S}}^{T} = \underline{\underline{S}}^{+}$

So, time reversal invariance implies $\underline{\underline{S}}^{*} = \underline{\underline{S}}^{+} = \underline{\underline{S}}^{T}$

And in particular, that $S_{12} = S_{21}$, not just in magnitude!

Now, some fact about $\underline{\underline{S}}$ matrix.

All the information about scattering is in the $\underline{\underline{S}}$ matrix: by knowing what is input, you know what goes out. And you can measure this! And, with wave packets on average, or on product time delay or acceleration, phase and so on. You can measure also the energy dependence, the S_{11}, S_{22}, and so on. And plot them.

But, if you plot them, and look at negative energies, you can derive the energy of the bound states of the system!!!!

We in Bet now

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} S_{11}(E) & S_{12}(E) \\ S_{21}(E) & S_{22}(E) \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix}$$

what if $E<0$? Well, K is replaced by $j\alpha$, α_1 in place of propagation exponents, we have decaying / growing exponents.
In order for the state to be normalizable, $A=0$ $D=0$.

For a bound state, $A=D=0$! α, B and C? Well, to be non-zero, $\underline{\underline{S}}$ should diverge ($\infty \times 0$ = finite)! α, $\underline{\underline{S}}$ must have a pole!

$$\begin{bmatrix} B \\ C \end{bmatrix} = \underline{\underline{S}} \begin{bmatrix} A \\ \not{0} \end{bmatrix}$$

finite ∞ 0

α, looking at S_{21}, also known as "t",

$$S_{21} = \frac{2K_1K_2\, e^{jk_2L}}{2K_1K_2\cos(k'L) - j\left[K_1^2+K_2^2\right]\sin(k_2L)}$$

You can find that S_{21} has a pole if

$$\frac{K_2L}{2} + \tan\left(\frac{K_2L}{2}\right) = \frac{K_1L}{2}$$

Reminds something? This is what we found studying bound states, but now we computed it just working on bound states!
A-M-A-Z-I-N-G

Lecture 15 : Eigenstates of the Angular Momentum - Part II
Brief review

① $[\hat{E}, \hat{A}] = +\hbar\omega\hat{A}$ → this implies that the spectrum of $\hat{E}$ is a ladder
En evenly spaced by $\hbar\omega$: $\hat{A}\phi_E \propto \phi_{E+\hbar\omega}$
This every time we see this commutation relation

② $[\hat{E}, \hat{B}] = 0$ ⇝ (a) Exist $\phi_{E,b}$ also eigenfunctions of $\hat{E}$ and $\hat{B}$, both $\hat{E}$ and $\hat{B}$

(b) Note that, for $\omega = 0$, $[\hat{E}, \hat{A}] = [\hat{E}, \hat{B}]$. α, $\hat{B}\phi_E \propto \phi_E$, and

In particular, if $[\hat{E}, \hat{B}] \neq 0$, we have:

$\hat{B}\phi_E = \tilde{\phi}_E$: an eigenfunction of $\hat{E}$, but, maybe, a different eigenfunction: same energy E, but possibly a different eigenfunction

Example : free particle

$$\hat{E} = \frac{\hat{p}^2}{2m}$$ α, $[\hat{E}, \hat{p}]$ commute!

So, when an operator commutes to the energy, there are multiple states with the same energy which are different states.
In this example, free particle,

e^{jkx}, $E = \frac{\hbar^2k^2}{2m}$,

But there is also another state, with the same energy, e^{-jkx}!

When an operator commutes to energy, you can have multiple eigenfunctions with the same energy.

If we consider the harmonic oscillator instead than the free particle,

$$\hat{E} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2,$$

But, in this case, $[\hat{E}, \hat{p}] \neq 0$! The potential is not translationally invariant, so, since there is the $\hat{x}$, it don't commute with momentum!

So, if we have a non-trivial potential, momentum will not commute to energy; this is, in general, the case of a system exhibiting some bound states. Then, if you have bound states you can't have degeneracies.

This story is different, in 3D. We will see it very soon! :)

③ If we have an energy operator commuting with a unitary operator,

$[\hat{E}, \hat{U}] = 0$, $\hat{U}^+\hat{U} = \hat{1}$, well:

(a) we can have eigenfunctions simultaneously of $\hat{E}$ and $\hat{U}$ (line (2a))

(b) $\hat{U}\phi_E = \tilde{\phi}_E$, with the same energy eigenvalue E

(c) We can write $\hat{U} \propto e^{j\hat{H}}$, where $\hat{H}$ is a Hermitian operator. We can

write $\hat{U}$ in two ways!

What is two Hermitian operators? Well, unitary operators are somehow related to unitary transformations, and to symmetries. A symmetry is when we take our system and we like rotate or and translate it, and energy does not change. For instance, translations do not change energy.

Like, translate by L

$$\hat{T}_L = e^{-L\partial x} \quad \left[\partial x = \frac{\partial}{\partial x}\right] \quad = e^{-j\frac{L}{\hbar}\hat{P}} \qquad \text{[translate by } L\text{]}$$

Boost operator (boost by q)

$$\hat{B}_q = e^{-q\partial p} = e^{-j\frac{q}{\hbar}\hat{x}} \qquad \partial p = \frac{\partial}{\partial p} \qquad \text{(boost by momentum } q\text{)}$$

Time translation operator,

$$\hat{U}_t = e^{-j\frac{t}{\hbar}\hat{E}} \qquad \text{(evolve in time by } t\text{)}$$

Earlier we understood the role of momentum, having to do with translations, with Noether's theorem: if the system is invariant to translation, then there is a conserved quantity associated to such translation, and this is the momentum. Quantum mechanically, the "generator" of that transformation is, the Hermitian operator, that goes at the "exponent", is the operator associated to that conserved quantity, so to that observable.

The operator that generates the translation, then, is the operator that represents momentum.

Translation: $\frac{\partial}{\partial x}$ (varying space). momentum, $\hat{P}$

Now 3D!

In 3D, in addition to just $\hat{x}$, $\hat{p}_x$, we also have other operators associated to other directions: $\hat{y}$, $\hat{z}$, $\hat{P}_y$, $\hat{P}_z$!

So we know for instance that

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

But,

$$[\hat{x}, \hat{y}] = 0 \; ?$$

Well, $[\hat{x}, \hat{P}_x]$ says us that there is an uncertainty principle among the two,

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

Also, no simultaneous eigenfunctions of x and p_x exist.

But, we expect, reasonably, to be able to know the position in x and in y, simultaneously!

$$[\hat{x}, \hat{y}] = 0 \qquad \text{[this is some sort of obvious!]}$$

Similarly,

$$[\hat{P}_x, \hat{P}_y] = 0$$

$$[\hat{P}_y, \hat{y}] = -j\hbar$$

We will be interested in systems like:

$$\frac{\hat{\vec{P}}^2}{2m} + U(\hat{x}, \hat{y}, \hat{z}) = 0$$

So, in this language, we can directly extend the 1D Schrödinger equation to

$$j\hbar \frac{\partial}{\partial t}\Psi(x,y,z,t) =$$

$$j\hbar \frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right]\Psi(\vec{r},t)$$

Note: in 3D, $[\Psi(\vec{r},t)] = \frac{1}{(\text{Length})^{3/2}}$

In fact, integrated, with a triple integral, and before now squared, we have a probability:

$$P(\vec{x} \to d\vec{r}) = \int\int\int dx\,dy\,dz\,|\Psi(\vec{r},t)|^2$$

Sometimes it's easier to work in cartesian, other times in polar coordinates.

Example 1: free particle, Cartesian coordinates

What is the energy eigenfunctions equation?

$$\hat{E}\,\phi_E = -\frac{\hbar^2}{2m}\left[\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right]\phi_E \qquad (1)$$

Lucky property! separable!

This PDE is the sum of 3 pieces, separated, where we done with respect to different vars! In such cases you can separate, meaning that:

$$\phi_E(x,y,z) = \phi_x(x)\,\phi_y(y)\,\phi_z(z) \qquad (1bis)$$

If we plug in (1):

$$\hat{E}\,\phi_E = -\frac{\hbar^2}{2m}\left(\phi_x''\phi_y\phi_z + \phi_y''\phi_x\phi_z + \phi_z''\phi_x\phi_y\right)$$

$$\hat{E}\,\phi_E = E\,\phi_E$$

If I divide both term times ϕ_E:

$$\frac{E\cancel{\phi_E}}{\cancel{\phi_E}} = -\frac{\hbar^2}{2m}\left[\frac{\phi_x''}{\phi_x} + \frac{\phi_y''}{\phi_y} + \frac{\phi_z''}{\phi_z}\right]$$

$\phi_x''/\phi_x = f(x)$, $\phi_y''/\phi_y = g(y)$, $\phi_z''/\phi_z = h(z)$

So,

$$-\frac{2m}{\hbar^2}E = f(x) + g(y) + h(z)$$

If this equation must be true for any value of x, y, z, they must be constant! The sum is constant! If I fix y, z, x must be constant!

So, $f(x)$ is constant, so $\frac{\phi_x''}{\phi_x} = \epsilon_x$; $-\epsilon_x$ a constant

" $g(y)$ " " " " $-\epsilon_y$

" $h(z)$ " " " " $-\epsilon_z$

So,

$$\boxed{-\frac{2m}{\hbar^2}E = -\epsilon_x - \epsilon_y - \epsilon_z} \qquad (2)$$

Now let's work equation in x:

$\phi_x'' + \epsilon_x\phi_x = 0$, so eigenvalues:

$$\phi_x = A\exp\left(j\sqrt{\epsilon_x}\,x\right) + B\exp\left(-j\sqrt{\epsilon_x}\,x\right)$$

$\boxed{k_x^2 \equiv \epsilon_x}$ Obviously, wavefunctions would be NOT NORMALIZABLE $= C$

So, you can say about ϵ_x that are positive numbers (they are squares of a k_x).

$$\boxed{E = \frac{\hbar^2}{2m}\left[k_x^2 + k_y^2 + k_z^2\right]} = \frac{\hbar^2}{2m}\left\|\vec{k}\right\|^2,$$

and

$$\phi_E = \eta\exp\left(j\left(k_x x + k_y y + k_z z\right)\right) + \ldots$$

$$= \eta\exp\left(j\,\vec{k}\cdot\vec{r}\right)$$

This is (a) solution of free particle in 3D - the other solution is with $\exp\left(-j\,\vec{k}\cdot\vec{r}\right)$

Note: for us, (1bis) was an assumption! However, they form a good basis, so they build, they can represent, a completely general solution. Then, the assumption was also sufficient, according to this last claim, to build ALL solutions!

Please note. Let $\vec{k}_1$ be such that

$$\frac{\vec{k}_1\cdot\vec{k}_1}{2m}\hbar^2 = E$$

There are many vectors $\vec{k}$ with same magnitude, but different directions! This is recalling what we were discussing previously in the lecture about degeneracies! In 1D, $(\vec{k}, -\vec{k})$ (may) have the same energy. Now, here are several degeneracies! There are ∞ directions with the same momentum!

This because OUR SYSTEM IS INVARIANT UNDER ROTATION!

And, where there is symmetry there is a unitary operator which affects that rotation, that it commutes with energy! But when we have an operator commuting to energy, then we have **degeneracies!!!** Different states with same energies!

3D $\Longrightarrow$ **symmetry $\Longleftrightarrow$ degeneracy!** 1D: line segment, with 2 possible directions: 1 dimension sphere!

In 3D we could have bound states but, with symmetries, we could have degeneracies.

This leads us to —

The 3D Harmonic Oscillator

Potential is, for the harmonic oscillator, rotationally symmetric:

$$V = \frac{m\omega^2}{2}\left(\hat{x}^2+\hat{y}^2+\hat{z}^2\right) = \frac{m\omega^2}{2}|\vec{r}|^2$$

We can immediately deduce, for the form of the energy eigenfunctions, that

$$E\phi_E = \left(-\frac{\hbar^2}{2m}\left[\partial_x^2+\partial_y^2+\partial_z^2\right] + \frac{m\omega^2}{2}\left[\hat{x}^2+\hat{y}^2+\hat{z}^2\right]\right)\phi_E =$$

$$= \left[\left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega^2}{2}x^2\right) + \left(-\frac{\hbar^2}{2m}\partial_y^2 + \frac{m\omega^2}{2}y^2\right) + \left(-\frac{\hbar^2}{2m}\partial_z^2 + \frac{m\omega^2}{2}z^2\right)\right]\phi_E$$

3 differential operators, each of them acting on a different direction/component. This, then, is separable, just like before!

So, we could solve separately this equation for each component. Let's do this for x:

$$\phi_x E_x = \left(-\frac{\hbar^2}{2m}\frac{\partial}{\partial x} + \frac{m\omega^2}{2}x^2\right)\phi_x \qquad (3)$$

$$\phi_E = \phi_x(x)\,\phi_y(y)\,\phi_z(z)$$

$$E = E_x + E_y + E_z$$

But (3) is exactly the equation of the 1D oscillator problem! So, the solution for the 3D oscillator can be written as the product of the 3. We can recall the "ladder" of states, the operator $\hat{a}$, and so on.

Let us use a different notation:

$$\phi_E = \phi_{n_x}(x)\,\phi_{n_y}(y)\,\phi_{n_z}(z) \quad , \quad E = E_{n_x} + E_{n_y} + E_{n_z}.$$

(just the same, with a different notation)

Let us change notation (slightly)

$$\phi_E = \phi_\ell(x)\,\phi_m(y)\,\phi_n(z)$$

So, ℓ is the excitation number, the index of the found state, along x, 1D. So,

$$E_{n_x} = E_\ell = \hbar\omega_0\left(\ell+\frac{1}{2}\right) \qquad \left[\text{check results, reference to them!!!}\right]$$

Similarly,

$$E_{n_y} = E_m = \hbar\omega_0\left(m+\frac{1}{2}\right) \qquad E_{n_z} = \hbar\omega_0\left(n+\frac{1}{2}\right),$$

and

$$E_{\ell mn} = E_{n_x} + E_{n_y} + E_{n_z} = \hbar\omega_0\left(\ell+m+n+\frac{3}{2}\right)$$

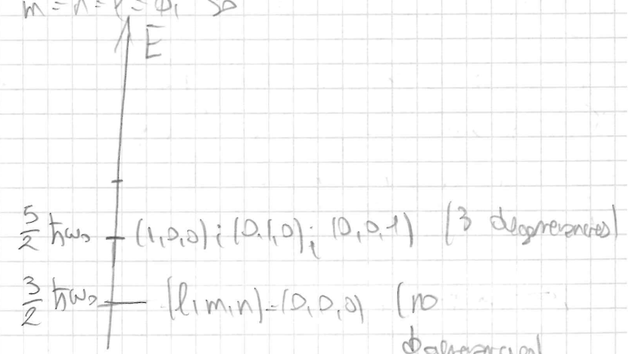
So, this is a 3D found state system, but there are degeneracies!!!

For instance, if $\ell=1$, $m=n=0$, or $m=1$, $\ell=n=0$, we have degenerate states! & plethora of degeneracies!

Let us write a list of degeneracies as a function of energy. Firstly, which is the ground state? Well, $m=n=\ell=0$, so

$$E_0 = \frac{3}{2}\hbar\omega_0 \quad \text{(3 times the 1D ground state)}$$

$$E_{100} = \hbar\omega_0\left(1+\frac{3}{2}\right)$$



What does (1,0,0) mean? Well, you have a node along x, and Gaussian profiles along y and z! Similarly, (0,1,0) has a node in y, Gaussian ("campana") in x and z. And so on.

So, there can be degeneracies among bound states in 3D.
Up to the first excited state, the 3 degenerated states are just rotations one of each other.
But, for the 2nd excited state, things become even more messy!

$$E_{200} = \left(2+\frac{3}{2}\right)\hbar\omega_0 = \frac{7}{2}\hbar\omega_0 ,$$

And, to achieve this, you could have: $(2,0,0)$, $(0,2,0)$, $(0,0,2)$, But also $(1,1,0)$, $(0,1,1)$, $(1,0,1)$!!! So, in addition to the 2-node + rotation, also other possibilities occur.

Well, let d_i be the degeneracy of the i-th state. Then, $d_0 = 1$: for ground state, we have just 1 state exhibiting that energy. For $i=2$, 3 states! $d_1 = 3$. $d_2 = 6$.

The strange thing for $i=2$ is: to degeneracy, a symmetry must be associated, for Noether's theorem. For $(1,0,0)$ and $(0,1,0)$, or $(0,2,0)$ and $(0,0,2)$ (for example), it is clear what is occurring: rotational symmetry !!! Instead, what is conserved between $(1,1,0)$ and $(0,0,2)$ is NOT clear at all! From $(2,0,0)$ to $(1,0,1)$ there is not simply a rotation!

By proceeding, studying higher levels, we could see that $d_3 = 10$, and $d_4 = 15$, $d_5 = 21$. In general,

$$d_n = \frac{(n+1)(n+2)}{2} \qquad n = 0,1,2 \ldots \qquad (L_4)$$

Where does (L_4) come from?!

It is to be remarked that the bond between symmetry and degeneracy is fundamental, is the most important point.
For instance, if we would had, as $\hat{E}$ operator, something with a different z dependence, like

$$\tilde{V} = \frac{m\omega_0^2}{2}(x^2+y^2) + \frac{m\tilde{\omega}^2}{2}z^2 , \qquad \omega_0 \neq \tilde{\omega} ,$$

system still separable!

energy would have a different form, like,

$$E = \hbar\omega_0\left(\underbrace{l+m+1}_{\to\frac{1}{2}}\right) + \hbar\tilde{\omega}\left(n+\tfrac{1}{2}\right) ,$$

and several degeneracies are broken, or symmetries are broken!

If you measure several energies, and they are equal, well, we should have a high suspicious that there is some symmetry protecting, or enforcing, it. This is useful to build models for physical systems!

It's very rare to have accidental degeneracy (not caused by symmetries)!

Well, it seems then wise to study rotations, since they seem to be behind the degeneracies we've discussed (or at least some of them). As we studied before, the "generator" of a translation is momentum. So, the "generator" of a rotation is "angular momentum"!

Quantum mechanics: angular momentum, is the deepest thing.

Angular Momentum

Question: in the same sense as we started out by asking what represents position and "linear" momentum in quantum mechanics, what operator represents angular momentum in quantum mechanics?

Well, to start, let's recall what angular momentum is in classical mechanics, $\vec{L}$.

$$\vec{L} = \vec{r}\times\vec{p}$$

So, what is this thing in quantum mechanics? $\hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}}$, [PUOI USARE $\hat{L}$ per altro!!!]

where these are vectors of operators! Do $\hat{r}$ and $\hat{p}$ commute? Naaaa. However, this is better than first appears! In fact, in coordinates,

$$\hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}} = \begin{bmatrix} \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{bmatrix} \equiv \begin{bmatrix} \hat{L}_x \\ \hat{L}_y \\ \hat{L}_z \end{bmatrix} \qquad (5)$$

And $\hat{y}\hat{p}_z$ or $\hat{p}_z\hat{y}$ commute, as well as all other couples, so we have no problem about operator ordering! So, no ambiguity exists! It is well defined under "ordering" point of view!

So, (5) is the definition of the components of angular momentum! $\hat{L}_x, \hat{L}_y, \hat{L}_z$!

But, we also know that $\hat{p}_x, \hat{p}_y, \hat{p}_z$ can be written as derivatives:

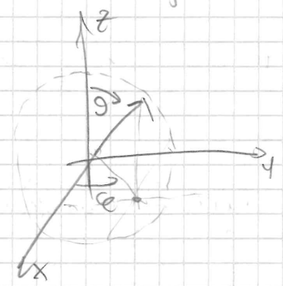
so

$$L_x = y\frac{\hbar}{j}\frac{\partial}{\partial z} - z\frac{\hbar}{j}\frac{\partial}{\partial y},$$

and so on.

But, we can also write $\hat{\vec{L}}$ in spherical coordinates!! Starting how L_z in Cartesian.

$$\hat{L}_z = -j\hbar\frac{\partial}{\partial \varphi}$$



We can also build the operators associated to the square of the momentum, that shows up in the Hamiltonian, in the energy!

$$\hat{\vec{L}}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial}{\partial\varphi}\right) \quad (6) \quad \text{(it could be proven)}$$

What are the dimensions of angular momentum? Length × momentum (from $\vec{r}\times\vec{p}$!). But, also $\hbar$ has the same dimensions!

Now, let's imagine that someone asks us the eigenfunctions of this "angular momentum" operator. We can answer them by looking at them. For instance, for $\hat{L}_z$,

$$\hat{L}_z Y_m = -j\hbar\frac{\partial}{\partial\varphi}Y_m = \hbar n Y_m$$

(some number times $\hbar$, to have the same dimension)

The solution can be obtained simply:

$$\phi_m = C e^{jm\varphi},$$

where φ is the variable, the azimuth: the angle around the equator, periodic of 2π. Our function is "non-stupid", so single-valued. Then, m, to let the function be single valued must be an integer. In fact, otherwise, it would go twice or more on the same points (?, this)

This for $\hat{L}_z$. What for $\hat{\vec{L}}^2$? The same thing, but the eigenvalue eq. will be much more complicated, as (6) suggests $=C$

We could use our brute-force method but ... Let's just NOT.

Let us try some better idea. Like, try to work with the operators method! Thus, we recall, is based on some commutation relations. The following relations can be proved (problem set)

$$\left[\hat{L}_x, \hat{L}_y\right] = \left[\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z\right] = \left[\hat{y}\hat{p}_z, \hat{z}\hat{p}_x\right] - \left[\hat{y}\hat{p}_z, \hat{x}\hat{p}_z\right] +$$
$$- \left[\hat{z}\hat{p}_y, \hat{z}\hat{p}_x\right] + \left[\hat{z}\hat{p}_y, \hat{x}\hat{p}_z\right]$$

First term: $\left[\hat{y}\hat{p}_z, \hat{z}\hat{p}_x\right]$. We can notice that $\hat{y}$ commutes with all other terms!

$$= \hat{y}\hat{p}_z\hat{z}\hat{p}_x - \hat{z}\hat{p}_x\hat{y}\hat{p}_z = \hat{y}\left(\hat{p}_z\hat{z}\hat{p}_x - \hat{z}\hat{p}_x\hat{p}_z\right) = \hat{y}\hat{p}_x\left(\hat{p}_z\hat{z} - \hat{z}\hat{p}_z\right) =$$

$$= \hat{y}\hat{p}_x\left[\hat{p}_z, \hat{z}\right] = \quad \text{(also } \hat{p}_x \text{ commutes with everything!)}$$

$$= -j\hbar\,\hat{p}_x\hat{y}$$

We can do similar things with the other terms!

$$\left[\hat{y}\hat{p}_z, \hat{x}\hat{p}_z\right] = \hat{y}\hat{x}\left[\hat{p}_z, \hat{p}_z\right] = 0$$

Similarly

$$\left[\hat{z}\hat{p}_y, \hat{z}\hat{p}_x\right] = \hat{p}_y\hat{p}_x\left[\hat{z}, \hat{z}\right] = 0$$

And

$$\left[\hat{z}\hat{p}_y, \hat{x}\hat{p}_z\right] = \hat{x}\hat{p}_y\left[\hat{z}, \hat{p}_z\right] = j\hbar\,\hat{p}_y\hat{x},$$

so

$$\left[\hat{L}_x, \hat{L}_y\right] = j\hbar\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right) = j\hbar L_z \quad (7)$$

And, more generally, we can show that

$$\left[\hat{L}_y, \hat{L}_z\right] = j\hbar L_x \qquad \left[\hat{L}_z, \hat{L}_x\right] = j\hbar L_y \quad (8)$$

Now, fancier:

$$\left[\hat{\vec{L}}^2, \hat{L}_x\right] = 0, \quad \left[\hat{\vec{L}}^2, \hat{L}_y\right] = 0, \quad \left[\hat{\vec{L}}^2, \hat{L}_z\right] = 0 \quad \text{[problem set]}$$

where $\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

We are somehow learning a tremendous amount of information on the angular momentum eigenfunctions!
In fact, recalling the introduction of the lecture, you can find, simultaneously, eigenfunctions of $\hat{\vec{L}}^2$ and $\hat{L}_x$ or $\hat{L}_y$ or $\hat{L}_z$!
$\{\hat{\vec{L}}^2, \hat{L}_x\}$, or $\{\hat{\vec{L}}^2, \hat{L}_y\}$, or $\{\hat{\vec{L}}^2, \hat{L}_z\}$!
Idea: complete set of commuting observables.
We can always write down a lot of operators, but, what is needed to define the state of a particle? Step back
Classically, like a classical particle in a room, we need to define its state, $\vec{r}$ and $\vec{p}$: 3+3 components, so 6 numbers. Not 5, 7 either!
In quantum mechanics the state of a system can be spoken as a particular superposition of a certain basis: you pick a basis, and you specify the coefficients of the linear combination! Then, which are the eigenvalues of the operators we've diagonalized, in that basis. Let us consider an example:
In 1D, we have $\hat{x}$ and $\hat{p}$. What is a complete set of commuting operators? Well, the number of operators we need, such that the eigenvalues specify a state. For instance, $\{\hat{x}\}$ is enough: $\hat{x}$ tells us that the particle is in a δ function state, and this specifies the state. The same for $\hat{p}$, with momentum.
But, we cannot specify both x and p, both position and momentum! They don't commute. So in 1D, $\{x\}$ or $\{p\}$ are a complete set, of commuting operators! 1 operator! Not both!
In 3D, $\hat{x}$ is not sufficient: it solves the problem for x, but still nothing is determined for y and z.
In 3D for instance we could have $\{\hat{x}, \hat{y}, \hat{z}\}$, or $\{\hat{p}_x, \hat{p}_y, \hat{p}_z\}$, or also $\{\hat{x}, \hat{p}_y, \hat{z}\}$, and they are complete: they SPECIFY MY STATE in all 3 dimensions! This does not mean to have all determined position & momentum, JUST TO SPECIFY A STATE IN WHICH THE SYSTEM IS!
$\{\hat{x}, \hat{p}_y, \hat{z}\}$ has $\delta(x)\delta(z)e^{-jk_y y}$: it is a STATE.
Two are not explicit: $\{\hat{x}, \hat{p}_y\}$ is NOT complete: nothing is said on z, that is NOT SPECIFIED. And $\{\hat{x}, \hat{p}_y, \hat{y}, \hat{z}\}$ is not commuting!
Complete set of observables: the most operators we can write down that all commute with each other, and the minimum number whose eigenvalues completely specify the state of the system.
So, what is the complete set of commuting operators for angular momentum? For example, using $\hat{L}_z$ (it's the same to use $\hat{L}_x$, $\hat{L}_y$),
$\{\hat{\vec{L}}^2, \hat{L}_z\}$ forms a complete set of commuting observables for the angular momentum system, (CSCO for AM)
Now, what are the eigenfunctions? Of a CSCO $\{\hat{\vec{L}}^2, \hat{L}_z\}$?
We can notice that the way $\hat{L}_x, \hat{L}_y$ commute, is forming $\hat{L}_z$! This gives us some magic, some power!
We can write down operators $\hat{L}_+$ and $\hat{L}_-$, (define)

$$\hat{L}_+ = \hat{L}_x + j\hat{L}_y \qquad \hat{L}_- = \hat{L}_x - j\hat{L}_y \qquad (82)$$

Since $\hat{L}_x, \hat{L}_y$ are observables as operators: they are Hermitian, so

$$\hat{L}_+^\dagger = \hat{L}_x - j\hat{L}_y = \hat{L}_- \quad \text{(adjoint)} \qquad (83)$$

Now. By taking commutators, something magic happens:

$$\left[\hat{\vec{L}}^2, \hat{L}_\pm\right] = 0$$

($\hat{\vec{L}}^2$ commutes with both $\hat{L}_x$ and $\hat{L}_y$!)

$$\left[\hat{L}_z, \hat{L}_+\right] = j\hbar \hat{L}_+$$
$$\left[\hat{L}_z, \hat{L}_-\right] = -j\hbar \hat{L}_- \qquad (85)$$

(is (j) present?)

Wait: $\hat{L}_z$ is Hermitian, $\hat{L}_+, \hat{L}_-$ are NOT. But, from the beginning of this lecture, we recalled that, in a situation like (85), the eigenfunctions of $\hat{L}_z$ are staggered in a ladder space by $\hbar$.
The eigenvalues of $\hat{L}_z$ come in a ladder spaced $\hbar$, we can raise with $\hat{L}_+$, lower with $\hat{L}_-$, just like in the harmonic oscillator!

Lecture 16 : Eigenstates of the Angular Momentum, part 2

From a question: angular momentum is, somehow, related to energy.
Also, the "ladder" thing in both quantities is interesting!
Note: if a system is spherically invariant, there must be constraints about the energy eigenvalues, and their relation with angular momentum. In fact, rotations do not change energy. Slightly different point of view: when we talked about the 1D free particle, we can write the energy eigenfunctions as momentum eigenfunctions, since $\hat{E}$ and $\hat{p}$ commute: the two operators share the same eigenfunctions. Similarly, in a 3D system, it's going to be useful in talking about energy eigenfunctions to know a basis of eigenfunctions of the angular momentum. Or, oppositely, studying the angular momentum will help us writing eigenfunctions of the energy operator, as well as momentum led to energy!

Recall for instance

$$[\hat{\vec{L}}^2, \hat{L}_\pm] = 0, \quad [\hat{L}_z, \hat{L}_\pm] = \pm j\hbar \hat{L}_\pm$$

Goal: build eigenfunctions and eigenvalues of the angular momentum operators and in particular using $\{\hat{\vec{L}}^2, \hat{L}_z\}$ as CSCO. We choose to work with $\hat{L}_z$ because z is a nicer coordinate to work with spherical coordinates ($\vec{z}$ corresponds to $\vartheta = 0$).

Let Y_{lm} be the common eigenfunctions of $\hat{\vec{L}}^2$, $\hat{L}_z$, i.e.

$$\hat{\vec{L}}^2 Y_{lm} = \hbar^2 Y_{lm} \underbrace{l(l+1)}_{\text{eigenvalue}}, \quad (1)$$

we call the eigenvalue of Y_{lm}, eigenstate of $\hat{\vec{L}}^2$, "$l(l+1)$". This will make degree much easier! =)
Similarly,

$$\hat{L}_z Y_{lm} = \hbar m Y_{lm} \qquad m \text{ is the eigenvalue for } \hat{L}_z \quad (2)$$

(1) and (2) are, let's say, the "notation" that we are going to use.

Now: what are the properties of Y_{lm}? What are the allowed values of the eigenvalues?

Note that $\hat{L}_\pm$ leave "l", eigenvalue of $\hat{\vec{L}}^2$, alone:

(1) $\hat{\vec{L}}^2 \hat{L}_\pm Y_{lm} = \hat{L}_\pm \hat{\vec{L}}^2 Y_{lm} = \hbar^2 l(l+1) L_\pm Y_{lm}$ (they commute!),

so we have the same eigenvalue

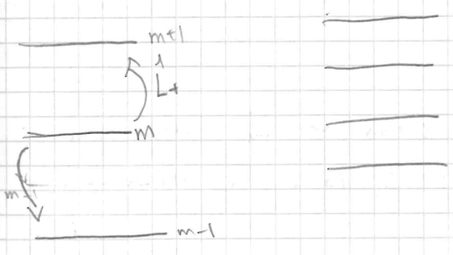
(2) $\hat{L}_\pm$ raise/lower m by 1. In fact,

$$\hat{L}_z \hat{L}_\pm Y_{lm} = \left([\hat{L}_z, \hat{L}_\pm] + \hat{L}_\pm \hat{L}_z \right) Y_{lm} =$$

$$= \left(\hbar \hat{L}_\pm + \hbar m \hat{L}_\pm \right) Y_{lm} = \hbar (m \pm 1) \hat{L}_\pm Y_{lm},$$

so m is increased by 1! The same with $\hat{L}_-$ and -1!

So, we have a ladder of states! And, if we apply raising/lowering, we don't touch l, but just m.
We have several ladders:



Given a l_1 we have a tower, given l_2 another tower, and so on. So, we can separate towers with different values of $\hat{\vec{L}}^2$! And within each ladder we can increase or decrease! But l!

So: is this tower infinite, or does it end? Why?
One could be tempted to state that, by applying infinite times the raising operator, we could have whatever eigenvalue of $\hat{L}_z$. Still, since we also have $\hat{\vec{L}}^2$, whose value is fixed, and it is $l(l+1)\hbar^2$, since $\hat{\vec{L}}^2$ is the sum of $\hat{L}_x^2, \hat{L}_y^2, \hat{L}_z^2$, there is no way to go beyond $\hat{\vec{L}}^2$!!!
So, "probably" for this reason, the tower is not infinite!
Let us make this observation more formal, through the following trick:

Suppose that the tower ends. Just like for lowering and raising operators in 1D for the harmonic oscillator.
In order for the tower to end, when we reach the top and apply the rising operator once more, the state must go to zero:

$$\hat{L}_+ Y_{\ell m^+} = 0 \quad , \quad m^+ \text{ is the "last state"!} \qquad (*)$$

Argument for finiteness

$$\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 .$$

Let us take the expectation value in the state $Y_{\ell m}$ of both sides of this equation:

$$\langle \hat{\vec{L}}^2 \rangle_{Y_{\ell m}} = \langle \hat{L}_x^2 \rangle + \langle \hat{L}_y^2 \rangle + \langle L_z^2 \rangle$$

$$\hbar^2 \ell(\ell+1) = \text{(strictly pos.)} + \text{(strictly pos.)} + \hbar^2 m^2$$

$\langle \hat{L}_x^2 \rangle$ is, in fact, the sum over all possible values of $\hat{L}_x^2$, which is the square of the possible eigenvalues of $\hat{L}_x$, times the probability (unitarity): sum of positive quantities.

So,

$$\hbar^2 \ell(\ell+1) \geq \hbar^2 m^2 !$$

So, for the most, it is possible to have $m^2 = \ell(\ell+1)$, not greater!
So, m is bounded!

So, which is the top value of each tower?

(*) If (*) is true,

$$\Rightarrow (\hat{L}_+ Y_{\ell m^+} | \hat{L}_+ Y_{\ell m^+}) = 0 \quad , \text{ so} \qquad (3)$$

the magnitude of this function, the function times itself, is 0!
But, (3) is equal to (bringing $\hat{L}_+$ right with the adjoint)

$$(3) = (Y_{\ell m} | \hat{L}_+^\dagger \hat{L}_+ Y_{\ell m^+}) = (Y_{\ell m} | \hat{L}_- \hat{L}_+ Y_{\ell m^+}) .$$

But, from the definition of $\hat{L}_-$, $\hat{L}_+$, this equals:

$$= \left(Y_{\ell m^+} \middle| \left[\hat{L}_x^2 + \hat{L}_y^2 + i \underbrace{[\hat{L}_x, \hat{L}_y]}_{\text{Commutator}} \right] Y_{\ell m^+} \right) \qquad (4)$$

But

$$\hat{L}_x^2 + \hat{L}_y^2 = \hat{\vec{L}}^2 - \hat{L}_z^2$$

(we know how these operators act on $Y_{\ell m}$:=)

$$= \left(Y_{\ell m^+} \middle| \left[\hat{\vec{L}}^2 - \hat{L}_z^2 - \hbar \hat{L}_z \right] Y_{\ell m^+} \right) = \left(\hbar^2 \ell(\ell+1) - m_+^2 \hbar^2 - m_+ \hbar^2 \right) = 0$$

(in fact, $(Y_{\ell m} | Y_{\ell m}) = 1$, for proper normalization)

Thus, for $m = m^+$, "last state".

$$\Rightarrow \hbar^2 \left(\ell(\ell+1) - m^+ (m^+ + 1) \right) = 0$$

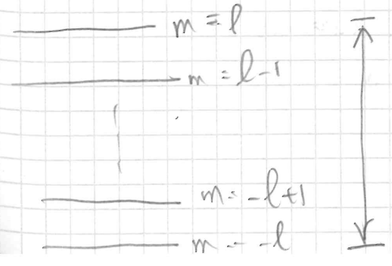
$$\hookrightarrow \boxed{m^+ = \ell}$$

The trick was based on, since we were knowing that something is 0, as a function, we can say that its norm is 0, and then apply tricks on adjoints or so

With similar steps, applying $\hat{L}_-$ to the "minimum" state m^-, the only thing that happens is, in (4), to have $[\hat{L}_y, \hat{L}_x]$ instead, and some minus signs.
The upshot is

$$\boxed{m^- = -\ell}$$

So, there is some symmetry.
But this is providing us with many information about what the possible eigenvalues are. Thinking about our "towers", the $\hat{L}_z$ angular momentum is raised/lowered by $\hat{L}_\pm$, and "ℓ" remains the same. The maximum state is $+\ell$, the minimum is $-\ell$. In other words, how big or how "tall" is our tower, it depends on ℓ! So, what does this tell us for m?
Well, m spans the values from $-\ell$ to ℓ, in unit steps!



so, the difference from the top to the bottom level is 2ℓ; however, given N_ℓ the number of states,

$$2\ell = N_\ell - 1$$

For instance, if $N_\ell = 2$ (2 states),

$$2\ell + 1 = 2 \Rightarrow \ell = \frac{1}{2}$$

More generally, in order for this process to make sense, so the m^- and m^+ to match up with $\mp\ell$, we need ℓ to be of the form of an integer

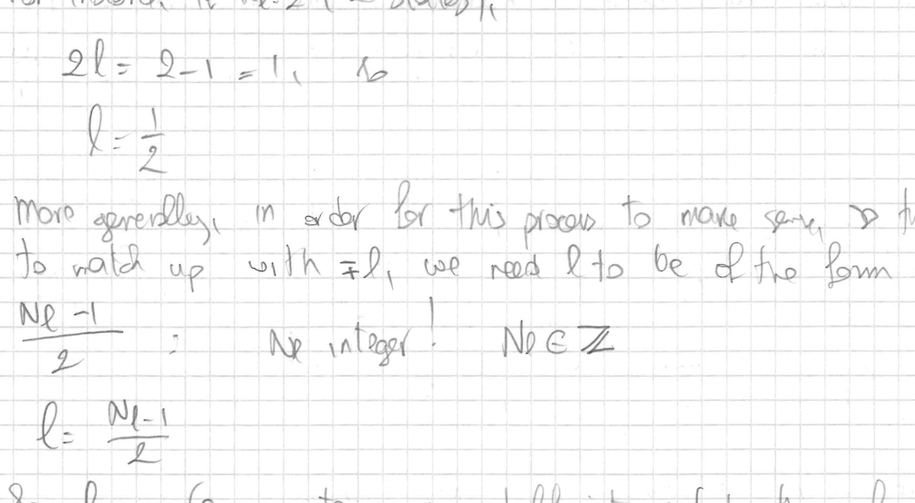
$$\frac{N_\ell - 1}{2} \quad : \quad N_\ell \text{ integer!} \quad N_\ell \in \mathbb{Z}$$

$$\ell = \frac{N_\ell - 1}{2}$$

So, ℓ can be an integer, or a half integer, but nothing else!

In particular for example it can be: $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}$ (half-integer) or $0, 1, 2, \dots$

So, we can plot our system in the following way. For instance, if $\ell = 0$, how many states do we have? Well, which is the largest allowed value of $\hat{L}_z$, if the $\ell(\ell+1)$ has $\ell = 0$? 1! We go from -0 to $+0$. So, we have a single state!



For $\ell = \frac{1}{2}$, we can go from $-\ell$ to $+\ell$ with unit steps! And so on! This for all values of ℓ! (integer or half-integer).

Is there something strange? Well, for the $\ell = 0$ state, what do we have? We have no z angular momentum, so by symmetry neither $\hat{L}_x$ or $\hat{L}_y$ - the thing is not rotating! The particle has no angular momentum!

What about $\ell = 1$? If we have $\ell = 1$, $m = 0$, the particle, the system, is carrying angular momentum, just not in the z direction! But its total angular momentum on average, $\ell(\ell+1)$, is 2 (times $\hbar^2$). So, by measuring $\hat{L}_x^2$ or $\hat{L}_y^2$, we probably expect to measure a non-zero quantity.

Instead, for $\ell = 1$, $m = 1$, we expect to have maximum angular momentum in the z direction. Is, in this case, the whole, the entire, angular momentum? In general, if we have the state ℓ, $m = \ell$, the maximum possible angular momentum in z, is it also the total angular momentum? NO.

Two angulars! If $\hat{L}_x = \hat{L}_y = 0$, can this satisfy the uncertainty principle due to the commutators? No! There must be some angular momentum in L_x and L_y, because L_z has some non-zero expectation value (and $[\hat{L}_x, \hat{L}_y] = i\hbar L_z$)

Moreover, let us recall that

$\langle \hat{\vec{L}}^2 \rangle = \hbar^2 \ell(\ell+1)$, (state $Y_{\ell\ell}$), and

$\langle \hat{L}_z^2 \rangle = \hbar^2 \ell^2$

But $\langle \hat{\vec{L}}^2 \rangle = \langle \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \rangle$

So,

$$\langle \hat{L}_x^2 \rangle + \langle \hat{L}_y^2 \rangle = \langle \hat{\vec{L}}^2 \rangle - \langle \hat{L}_z^2 \rangle = \hbar^2 \ell(\ell+1) - \hbar^2 \ell^2 = \cancel{\hbar^2 \ell^2} + \hbar^2 \ell - \cancel{\hbar^2 \ell^2}$$

And, for symmetry,

$$\langle \hat{L}_x^2 \rangle = \frac{1}{2}\hbar^2 \ell \quad - \langle \hat{L}_y^2 \rangle \quad \text{(not trivial)}$$

↳ this is the amount for what we fail to have all possible angular momentum in $\hat{L}_z$!

Why does the $\ell = m = 0$ case not violate the uncertainty principle? Well:

$$\Delta A_\psi \, \Delta B_\psi \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle_\psi \right|$$

So,

$$\Delta L_{x\,Y_{00}} \, \Delta L_{y\,Y_{00}} \geq \frac{1}{2} \left| \langle [\hat{L}_x, \hat{L}_y] \rangle \right| = \frac{\hbar}{2} \left| \langle \hat{L}_z \rangle \right|$$

So, they can have (L_x and L_y) a uncertainty, since the expectation value of L_z is equal to zero.

BUT, we have 2 more uncertainty relations which are breaking our balls! From all of them we could deduce that all $\hat{L}^2$, $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ must have 0 expectation value! To have 0 uncertainty.

Ok. In addition to this, there is still something quite strange. Focusing on $l=\frac{1}{2}$, well, do we "have to have" some angular momentum along z? Classically no! But this seems in contradiction with the $l=\frac{1}{2}$ case, which allows only $m=-\frac{1}{2}$ and $m=\frac{1}{2}$! o_o
For the half-integer guys we are unescapably spinning! o_o
Something described by these states is perpetually rotating, spinning!

Well, but, in the classical limit, where we have very large angular momentum, the $m=\pm\frac{1}{2}$ states are arbitrarily small compared to angular momentum L! Well, if we build, let's say for instance, a piece of chalk, well, the $\pm\frac{1}{2}$ is preposterously small for a macroscopic object. Why do we notice? Well, if we take an atom, in quantum regime, and we measure its orbital angular momentum in z, or indeed in any direction, well, it will NEVER be 0. And this measure is something we do often, such as when we measure a light spectrum!

Before further proceeding on these considerations, let us say something more about the Y_{lm} and the tower structure.
Firstly, let's drew these wavefunctions! Just like momentum (linear) eigenfunctions were functions of position, these angular momentum eigenfunctions will be functions of the angular position! $Y_{lm}(\vartheta,\varphi)$!
How do we get this? Well, we know what happens by applying $\hat{L}^2$ or $\hat{L}_z$!
But we also have other expressions for these operators: the spherical coordinate ones!
We had:

$$\hat{L}_z = \frac{\hbar}{j}\frac{\partial}{\partial\varphi}$$

$$\hat{L}_\pm = \hbar\, e^{\pm j\varphi}\left[\frac{\partial}{\partial\vartheta} \pm j\cot g\vartheta\,\frac{\partial}{\partial\varphi}\right]$$

It is clearly easier to work on $\hat{L}_z$ (easier expression). So,

$$\hat{L}_z Y_{lm} = \hbar m Y_{lm} = \frac{\hbar}{j}\frac{\partial}{\partial\varphi} Y_{lm}(\vartheta,\varphi)$$

So,

$$jm Y_{lm} = \frac{\partial}{\partial\varphi} Y_{lm}(\vartheta,\varphi)$$ this is the equation for the eigenfunctions of $\hat{L}_z$

$$\hookrightarrow Y_{lm}(\vartheta,\varphi) = e^{jm\varphi} P_{lm}(\vartheta)$$

where this $P_{lm}(\vartheta)$ is some function of ϑ, not yet discussed!

So, we learned that the dependence on φ is just a $e^{jm\varphi}$! (φ is the azimuth!)
This means that

$$Y_{lm}(\vartheta,2\pi) = e^{jm2\pi} P_{lm}(\vartheta), \quad Y_{lm}(\vartheta,2\pi) = e^{j2\pi m} P_{lm}(\vartheta) = \begin{cases} Y_{lm}(\vartheta,0) & m \text{ integer} \\ -Y_{lm}(\vartheta,0) & m \text{ half integer} \end{cases}$$

and if m is integer, $e^{jm2\pi}=1$, always. But, if m is a half-integer,

So, for m integer, it's ok. But, if half-integer, $Y_{lm}(\vartheta,0) = -Y_{lm}(\vartheta,0)$!
This is absurd! This means that $Y_{lm}(\vartheta,0)=0$! Identically equal to 0, if m is half-integer! o_o So, the probability density to be found at any angular momentum... is 0 o_o
So, the $l=\frac{1}{2}, \frac{3}{2}$ and so on, are not even normalizable: they are states indicating not the presence, but the absence of a particle! They cannot be used to label wavefunctions of physical states (depending to wavefunctions on a sphere!
What does this mean? Well, sphere is the keyword! We cannot describe those states on a sphere, with spherical coordinates! We will need a different description!! We cannot use the wavefunction to describe these states: we need something doubly valued! This will be a "spinner", but we will describe this later.

So, we will work with this $m=\frac{1}{2}$ things later, and now focus on the integer ones.
Now we need to find the ϑ dependence, $P_{lm}(\vartheta)$!

Idea! solve the ground state equation (just like with the harmonic oscillator), that says that a ground state is annihilated by $\hat{a}$!

Here, we have the following annihilation condition:

$$\hat{L}_+ Y_{ll} = 0$$

$$= \hbar e^{j\varphi}\left[\frac{\partial}{\partial\vartheta} + j\,\mathrm{cotg}(\vartheta)\frac{\partial}{\partial\varphi}\right] e^{jl\varphi} P_{lm}(\vartheta)$$

$$= \hbar e^{j\varphi}\left[\frac{\partial}{\partial\vartheta} - l\,\mathrm{cotg}(\vartheta)\right] e^{jl\varphi} P_{lm}(\vartheta).$$

Since this has to equal 0, it means:

$$\left[\frac{\partial}{\partial\vartheta} - l\,\mathrm{cotg}(\vartheta)\right] P_{lm}(\vartheta) = 0$$

$$\Rightarrow P_{ll} \propto \sin^l(\vartheta)$$

Why? Well, $\mathrm{cotg}(\vartheta) = \frac{\cos(\vartheta)}{\sin(\vartheta)}$, and thus can be seen as lots of derivatives of sine

$$\frac{\partial}{\partial\vartheta} P_{ll}(\vartheta) = l\,\frac{\cos\vartheta}{\sin\vartheta} P_{ll}(\vartheta)$$

this l comes from a derivation of $\sin^l(\vartheta)$: $\frac{\partial}{\partial\vartheta}\sin^l\vartheta = l\sin^{l-1}\vartheta\cos\vartheta$

$$l\sin^{l-1}\cos\vartheta = l\,\sin^l\vartheta\,\frac{\cos\vartheta}{\sin\vartheta} = l\,\frac{\cos\varphi}{\sin\vartheta} P_{ll}(\vartheta)$$

Well, knowing already the solution, this is a way of proving it =c

In other words, with some normalization coefficient N_{ll},

$$Y_{ll} = N_{ll}\, e^{jl\varphi}\sin^l(\vartheta)$$

Note aside: $\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = \frac{\hbar}{j}\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)$, and, since we know that $\frac{\partial}{\partial z} = \frac{\partial}{\partial\varphi}\frac{\partial\varphi}{\partial z} + \frac{\partial}{\partial\vartheta}\frac{\partial\vartheta}{\partial z}$ and so on, we can transform these operators in spherical coordinates.
From these we can find $\hat{L}_\pm$ easily! =)

Now! We know the top state of the tower. How can we obtain the other states? Well, with the lowering operator!

$$Y_{l,l-1} \propto \hat{L}_- Y_{ll}$$

These functions, $Y_{lm}(\vartheta,\varphi)$, are referred to as "spherical harmonics". This, because they solve the Laplacian equation on the sphere (the eigenvalue eq.).

Examples

For $l=0$ $\quad Y_{ll} = Y_{00} = \frac{1}{\sqrt{4\pi}}$.

$l=1$, Y_{10}, Y_{11}, $Y_{1,-1}$.

$Y_{11} = N_{11} e^{j\varphi}\sin\vartheta$ → top state

$Y_{10} = N\cos\vartheta$ → well, by lowering

$Y_{1,-1} = N e^{-j\varphi}\sin\vartheta$ → lowering again

$l=2$

$Y_{22} = N e^{j2\varphi}\sin^2\vartheta$

$Y_{20} = N\left(3\cos^2\vartheta - 1\right)$

$Y_{2,-2} = N\, e^{-j2\varphi}\sin^2\vartheta$

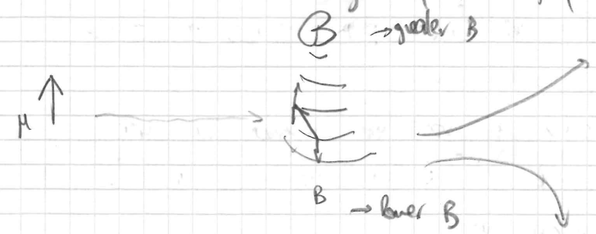
Normalize: we have to integrate them over a spheroid surface, not a volume!

Y_{10}: no probability to have in the xy plane, the particle, because $m=0$ (no angular momentum).

Note: phase is contained in $e^{j\varphi}$! Not in ϑ!

Lecture 17: Central Potentials, Take 2

Question: what about the "half-ℓ" states? Well, details in few lectures but -- When we studied the commutation relations, so like the angular momentum, just with commutations relations, we found that states go in towers. $\ell=0$ tower 1 state, $\ell=\frac{1}{2}$ two states, and so on
We understood that it is impossible to represent the half-integer states with a wave function which represents a probability distribution on a sphere. In fact, if we take the hypothetical wavefunction that should do it, if we rotate it by 2π in any direction, it equals itself... Just with a "-" sign! And this is absurd: it should exactly replicate itself!
Because we are moving on a sphere, and after 2π we have the same point as before! So, it must be 0!
So, what we will discover is... Let's explain with some Bods, analogies!
If we have a magnet, the "↑", with magnetization μ,



and we send it in a region with a magnetic field gradient.

One end of our dipole will be affected by a stronger torque than the other, and we will have a net force, F, that will be proportional to $|\mu|$ and $|B|$

$$F \propto |\mu|\,|B|$$

Depending on force, the field can deflect the magnet in one region (upper) or the other (lower). A "bigger" magnet (μ) is more deflected

Fact 2: imagine to have a sphere of uniform charge distribution, and make it rotate. Motion generates current, current generates magnetic field, along the axis of rotation. Such magnetic sphere, thus, is related to the angular momentum. So, $\mu \propto \vec{L}$

Since in "Fact 1" deflection depends on μ, by measuring deflection, we can measure the angular momentum!

Now, take an electron: if we send it through the magnetic field in order to measure its angular momentum with this trick, well, what happens? Well, if electrons were not rotating, they would just go through straight! Not deflected!
From experiments, what is observed is that electrons deflect up or down, by a fixed amount. Never more, never less, never 0.

This tells us that angular momentum can have only 2 values!
Stein-Gerlach experiment!
So, L_z (for instance) takes one of 2 values: $+\hbar/2$, or $-\hbar/2$!
Which set of states describe an electron in this apparatus? What tower?
Well... $\ell=\frac{1}{2}$!!! But we just said that these states cannot be described as rotations on a sphere.
Well, we will discover that electrons carry a form of angular momentum, some other form: $\vec{\mu} = \mu_s \vec{S}$, where $\vec{S}$ is the spin: it is this "alternative" form of angular momentum!
Spin is a vector, S_x, S_y, S_z, that satisfies the same commutation relations, but it cannot be represented this as:

$$S_z = \text{[illegible]}\, \partial_\varphi$$

This internal form of angular momentum exists only in quantum mechanics, no classically.

Real, physical systems, in 3D
Let us write the Laplacian in 3D in spherical coordinates.

$$\vec{\nabla}^2 = \underbrace{\partial_r^2 + \frac{2}{r}\partial_r}_{\left(\frac{1}{r}\frac{\partial}{\partial r}r\right)^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r} + \frac{1}{r^2}\underbrace{\left[\frac{\partial^2}{\partial\vartheta^2} + \operatorname{ctg}\vartheta\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right]}_{-\frac{1}{\hbar^2}\hat{L}^2\ :\ \text{this horrible thing is just } L^2!} \qquad (1)$$

$$\left(\frac{1}{r}\frac{\partial}{\partial r}r\right)^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r$$

$$= \frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\frac{1}{r}+\frac{\partial}{\partial r}\right)\right]$$

So, such Laplacian has this simpler form!

Central potentials: Systems in 3D which are spherically symmetric. This is the isotropic harmonic oscillator, but also hydrogen! Where the system is rotationally independent! The force of the potential depends only on the radial distance!
For this, the energy operator is:

$$\hat{E} = \frac{\vec{p}^2}{2m} + U(r),$$

But $\vec{p}^2 = -\hbar \vec{\nabla}^2$, in 3D (just like $\frac{\partial}{\partial x}$ in 1D),

and this, has the expression of (1)

$$\vec{p}^2 = -\hbar^2 \vec{\nabla}^2 = -\hbar^2 \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{\hat{L}^2}{r^2} \qquad (2)$$

So,

$$\hat{E} = -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2mr^2} \vec{L}^2 + U(r) \qquad (3)$$

this is always true for a spherically invariant potential!
The first and last pieces of $\hat{E}$ depend just on r, while the second part depends on ϑ and φ but just through $\vec{L}^2$!
So, if we want to find the eigenfunctions of $\hat{E}$, our life will be much easier if we work in eigenfunctions of $\hat{L}$! So, question: can we do it?
Can we find eigenfunctions of $\hat{E}$ and $\hat{L}^2$, simultaneously? That means, what is the commutator

$$[\hat{E}, \hat{L}^2] = ?$$

[per alleggerire la notazione potrei anche SEMPRE $\hat{L}^2$ $\hat{=}$ $\hat{L}$!]

Well, $=0$! $\hat{L}$ commutes with the derivative w.r.t. r (all depends on r), commutes with itself, and also with the last term! Yay! We can find a common eigenbasis!

So, to solve the eigenproblem

$$\hat{E} \phi_E = E \phi_E,$$

we can use the eigenfunctions of $\hat{L}$:

$$\phi_E(\vec{r}) = \varrho(r)\, Y_{lm}(\vartheta, \varphi),$$

that means, use separation and exploit the solution known from the computations on the angular momentum!

And the (ϑ, φ) dependence is just in the Y_{lm} !!! =)

Of course, l is an integer: we are working on angular momentum, NOT talking about spin, right now!
From now on, "L" refers to the "rotational" angular momentum. "S" will be spin. "L" will accept only integer values.

So, now that we have this separation of variables,

$$\hat{E} \phi_E = \left(-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial}{\partial r} r + \frac{\hbar^2 l(l+1)}{2mr^2} + U(r) \right) \phi_E$$

in fact, $\hat{L} \phi_E = l(l+1) \phi_E$! We just eliminated the (ϑ, φ) dependence from this equation with this trick! So, we could simplify the Y_{lm} from both sides, to obtain

$$\hat{E} \varrho(r) = \left[-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial}{\partial r} r + \frac{\hbar^2 l(l+1)}{2mr^2} + U(r) \right] \varrho(r) = \underbrace{E}_{\text{energy eigenvalue}} \varrho(r)$$

Even if this is just a 1D equation, it could be, let's say, simpler $=C$ (typical U BIG). Let us reduce it with some trick! If we have $V_{eff} \equiv \frac{\hbar^2 (l+1) l}{2mr^2} + U(r)$ (typical U BIG)

$$E \varrho(r) = \left[-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + V_{eff}(r) \right] \varrho(r) =$$

$=$ potential + ang. momentum

Let $\varrho(r)$ equal

$$\varrho(r) = \frac{1}{r} u(r), \text{ then}$$

$$\frac{1}{r} \frac{\partial^2}{\partial r^2} r \varrho(r) = \frac{1}{r} \frac{\partial^2}{\partial r^2} u(r),$$

$$V_{eff} \varrho = \frac{1}{r} V_{eff} u$$

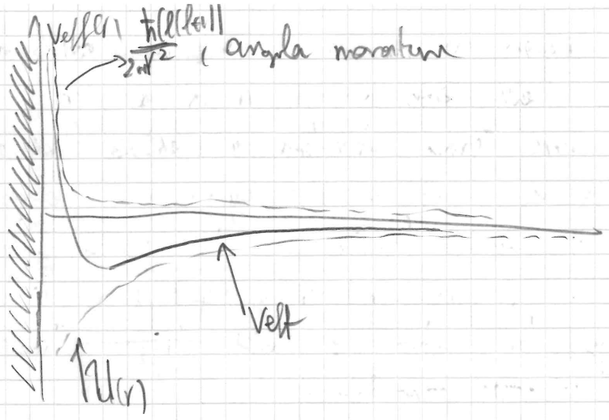
BE CAREFUL, u vs U or as r instead of U

So

$$E u = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + V_{eff}(r) \right] \overbrace{u(r)}^{\text{small } u},$$

and this is exactly the eigenvalue equation for a 1D problem, with $V_{eff}(r)$ having this possible behaviour.

This potential does the following things:
Suppose that we have the Coloumb potential, $U = -\frac{e^2}{r}$: (example)
In addition to it, V_{eff} has another term, which is the angular momentum term: $\frac{\ell(\ell+1)\hbar}{2mr^2}$:
constant divided by r^2, which goes to 0 more rapidly.



Of course, $r \geq 0$: for definition! So, it's like having ∞ potential, for $r < 0$.
The V_{eff} solid curve is the sum of the two contributes

35 min for NOTATION

Now, let's go further and think more in detail about this problem, involving Coulomb potential.

First, brief life lecture
If we have a differential equation like

$$\left(\frac{\partial}{\partial r} + \frac{c}{r} + \dots\right)\phi = 0,$$

if the "..." was 0 the equation would be

$$\left(\frac{\partial}{\partial r} + \frac{c}{r}\right)\phi = 0,$$

with solution

$$\phi \sim r^{-c}$$

So, for the full equation, we can assume

$$\phi = r^{-c}\, u,$$

leading to the following eq:

$$\left(\frac{\partial}{\partial r} + \dots\right) u = 0, \quad \text{easier!}$$

We applied the 2nd order version of this ☺

The term coming from the angular momentum originally came from the kinetic energy, so it is a kinetic energy term. Why? Well, if we have some angular momentum (in other words, $\ell \neq 0$!), as we get closer and closer to the origin ($r \to 0$), potential energy gets large. This makes sense, because, if we spin, rotate around ourselves (like ice skaters), when we have open arms our velocity (i.e., kinetic energy) is lower than when we retire them. This is a consequence of conservation of angular momentum
So, let us call

$$\frac{\hbar^2\ell(\ell+1)}{2mr^2}$$ the "angular momentum barrier".

due to radiation (and so on...)

Question: from a classical standpoint, rotation makes the atom decay? No! Is the angular momentum barrier the reason why atoms don't decay? No! Conservation of angular momentum, is not what is saving the universe!

"Why do things exist"? Well, we will understand it. First, let us study some...

General facts for central potentials

(1)- What are the boundary conditions at the origin? What must be true for $u(r)$ near the origin? Well, for $r \to 0$ thinking about not $u(r)$, but $\phi_E(r)$, which is the actual wavefunction, we know that it goes like

$$\phi_E(r) \approx \frac{u(r)}{r}, \quad r \to 0$$

So, what for $u(r)$? Well, if it would tend to a constant, near the origin, then the $\phi_E(r)$ would diverge! This would mean that... ϕ_E is not normalizable! :o
Let's think about the laplacian of $\frac{1}{r}$:

$$\vec{\nabla}^2 \frac{1}{r} = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left[r\left(\frac{1}{r}\right)\right] = \frac{1}{r}\frac{\partial^2}{\partial r^2}[1] = 0$$ NO stress!

Can this be possibly true, at $r \to 0$? no! As we approach the origin, $\frac{1}{r}$ is growing, in any direction! So, it should tend to ∞, not to 0! If r is an ill-defined problem!
In fact,

$$\vec{\nabla}^2 \frac{1}{r} = \delta(r)$$ it can be proved! =) A δ function!

So if we have a wavefunction that goes like $\frac{1}{r}$, then the energy contribution gives a δ function at the origin, which makes the eigenvalue equation impossible to be solved: nothing can simplify this δ!

So, $u(r)$ must go to 0, as $r \to 0$! Otherwise, we would have a bad divergence on energy! this means that ϕ_E must tend to a constant: it does not vanish, so, still, it is ok for our beloved interpretation as a probability density. Lucatau's rule

2- The energy depends on l, but NOT on m !!!
In both, in the eigenvalue equation, it does not appear!
So, for each m, in the range $\{l, l-1, \dots, -l+1, -l\}$, ($2l+1$ values) the energy is the same!!! :o This energy is related to as E_l.
In other words, the degeneracy of E_l is $(2l+1)$. $d(E_l) = 2l+1$
Why? Always remember: we have degeneracies, when we have symmetries! These come from rotational invariance: when we have some angular momentum, energy does not depend on the fact that it is in x, y, or z direction: energy does not depend on this, this is a central potential! And m is telling us precisely how much energy is in one direction or another! :o
There is a nice way to phrase this: rotational symmetry is the statement that the energy does not care about rotations. So, it must commute with $\hat{L}_x, \hat{L}_y, \hat{L}_z$:

$$\left[\hat{E}, \hat{L}_x\right] = \left[\hat{E}, \hat{L}_y\right] = \left[\hat{E}, \hat{L}_z\right] = 0 \qquad \text{this is rotational symmetry!}$$

This guy tells us we can find common eigenfunctions, and more in detail a full common eigenbasis of $\hat{E}$ and $\hat{L}_z$ (focusing as usual on $\hat{L}_z$). Fixed $\hat{L}_z$, $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$, we know that

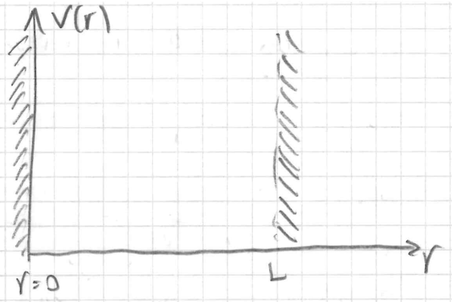
$$\left[\hat{E}, \hat{L}_\pm\right] = 0,$$

where $\hat{L}_\pm$ acts as raising/lowering operator. This gives our $(2l+1)$ degeneracy, because we can climb or descend the stair, the ladder.
This is a nice example of the symmetry - degeneracy connection

|Examples| of using central potentials

Spherical well

What is the potential in a spherical well? Well, let's say it is ∞ after some distance "L", 0 inside.



We have to perform the separation, reside with the function "u" by $\frac{1}{r}$, and get the following equation:

$$E_l u_l = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \hbar^2 \frac{l(l+1)}{2mr^2}\right) u_l =$$

$$= \frac{\hbar^2}{2m}\left(-\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2}\right) u_l, \qquad V(0) = \infty, \; V(L) = \infty, \; V = 0 \text{ inside}$$

This is not a terrible differential equation, but here we will not spend time to solve it.

Let us study a simple case for now: $l = 0$ (0 angular momentum) =

$$E_0 u_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} u_0$$

This is very very easy! In fact,

$u_0(r) = A\cos(kr) + B\sin(kr)$, and

$$E_0 = \frac{\hbar^2 k^2}{2m}$$

With boundary conditions, $u_0(0) = 0 \Rightarrow A = 0$,

$$u_0(L) = 0 \Rightarrow kL = n\pi$$

Just exactly like the 1D system!

Therefore, the wavefunctions $\phi_{E_0}(r, \theta, \varphi) = Y_{00}(\theta, \varphi)\frac{1}{r}u(r) =$

$= Y_{00}\frac{1}{r}\sin\left(\frac{n\pi}{L}r\right)$; Y_{00} is a constant (from previous lectures),

$\hookrightarrow = N\frac{1}{r}\sin\left(\frac{n\pi}{L}r\right)$ — N: normalization constant

Note that $\frac{1}{r}$ of the solution is compensated by the sine!

So, we has a ψ_0 but ψ_{E_0} doesn't!

This has a very nice more general story, for larger l, not explored here :D

However, two notes: the origin is a special point, since there are central potentials, and the origin is the center of symmetry of the system.
Moreover, we could think about the fact that we have two zeros.
So go against our principles on the nodes of the eigenfunction, or say that nothing occurs (no probability) @ the origin. WRONG! ψ_{E_0} that is the object exhibiting properties like being associated with probability density has NO zeros at all!
"the origin is where the proton is! =D"

Hydrogen

Now we are going to construct a nice toy model, which turns out to be useful as first pass to understand the properties in hydrogen gases, their emission spectra, and so on. This is a bad model: doesn't fit data! But we will improve it later!
So, we are going to study the solution of the Coulomb potential!

Coulomb potential

$$V(r) = -\frac{e^2}{r} \qquad \text{where } e \text{ is the elementary charge!}$$

This is what we get if we have a charged particle with ∞ mass and charge $+e$, and another particle with charge $-e$ and mass m.
And let's say that we don't care about things like spin, relativity et similia. Point particles.
The equation for our u becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u(r) + \left(\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{e^2}{r}\right)u = E_e\, u$$

(1) Firstly, let's do dimensional analysis: $[e^2]$ = energy × length $= \left[\frac{p^2}{2m}L\right]$

$[\hbar] = p \cdot L$, $[m]$ is a mass, so, we can build the following quantities:

$$r_0 = \frac{\hbar^2}{2me^2} \qquad \text{(a radius)}$$

From here we can build a characteristic energy, E_0,

$$E_0 = \frac{e^2}{r_0} = \frac{2me^4}{\hbar^2}$$

This is a 1D quantum mechanical problem, so our ground state will have some finite energy.
Roughly, the ground state energy of this system could be $\simeq -E_0$! It is the "only" dimensionally sensible quantity! maybe with some factor, but something close to it!

This is (E_0) different, by a factor of 4, to the Rydberg energy. That is, 13.6 eV. This is the <u>observed</u> binding energy of hydrogen.

Before doing any calculation, just from dimensional analysis, we almost got hydrogen binding energy!
Instead, r_0 will be something like the expectation value of the radius of the atom!

When studying the 1D harmonic oscillator with the brute force method, firstly we performed asymptotic analysis and extracted the overall asymptotic form, in order to obtain another differential equation free of singularities, then we performed a series approximation. In this case, we have, by miracle, an closed-form solution! :D

(2) Let's make everything dimensionless! let's use

$$r = r_0\,\rho, \qquad \rho \text{ dimensionless,}$$

$$E = -E_0\,\varepsilon, \qquad \varepsilon \text{ dim'less!}$$

So, we obtain:

$$\left(\frac{\partial^2}{\partial\rho^2} + \frac{l(l+1)}{\rho^2} - \frac{1}{\rho} + \varepsilon\right)u = 0$$

(3) Asymptotic analysis!
This is just the result (steps not reported)
When $\rho \to \infty$ the equation becomes $\simeq \left(-\frac{\partial^2}{\partial\rho^2} + \varepsilon\right)u = 0$, that is the usual exponential! $u \simeq e^{-\sqrt{\varepsilon}\rho}$

* as $\rho \to 0$, $u \approx \rho^{(\ell+1)} + \cancel{\rho^{\ell}}$ → this is badly diverging, so no!

→ the second derivative is $\frac{\ell(\ell+1)}{\rho^2}$ times function u!

So, given this asymptotic analysis, we could write

$$u = \rho^{\ell+1} e^{-\sqrt{\varepsilon}\rho} v(\rho),$$

where this $v(\rho)$ must go to a constant at the origin ($u \to 0$), and vanish slower than an exponential at ∞.

(4) We plug the asymptotic analysis result, perform a change of variables, and get:

$$\rho v'' + 2\left(1+\ell - \sqrt{\varepsilon}\rho\right)v' + \left[1 - 2\sqrt{\varepsilon}(\ell+1)\right]v = 0$$

(5) We perform a series expansion,

$$v = \sum_{j=0}^{\infty} a_j \rho^j$$

and plug it in the differential equation, just like for the harmonic oscillator!

This series expansion has a solution, that is

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

In order for this series to terminate, we must have some $a_{j_{max}}$ such that $a_{j_{max}+1} = 0$. So, for some j, we have

$$2\sqrt{\varepsilon}(j+\ell+1) - 1 = 0$$

When we go through it, we discover that

$$\varepsilon = \frac{1}{4n^2}, \qquad n = j_{max} + \ell + 1$$

This tells us that energy is labeled by an integer n, an ℓ, an m, and n comes from this series expansion approach, and

$$E_{n,\ell,m} = -\frac{E_0}{4n^2}$$, independently of ℓ, m.

So, we discover that the energy eigenvalues are evenly $\frac{1}{4}$ of E_0! And spaced by $\frac{1}{n^2}$! Which does two things

This does not just explain the R, the 13.6 eV we discussed/introduced, but also more! Remembering the first lecture, we said that the spectrum of hydrogen is something like

$$\approx \frac{E_0}{4n^2}$$ (Rydberg relation)

We discovered that this energy is not just independent of m, but also on ℓ, and this was unexpected! °_° What symmetry is explaining this extra degeneracy? I mean, the degeneracy in m comes from the fact that we are dealing with central potentials, but, for ℓ? °_°

Next time!