MIT - Quantum Physics I (2013), 8.04

Allan Adams

Lecture 1: Introduction to Superposition

This is a course in quantum mechanics.

"Stellar" website, all material. Also, ocw 1-.

Objective: learn some intuition for quantum mechanics. It requires some concerted effort, not trivial.

Problem sets, very important.

Will use clickers. (?!)

Textbooks: no specific textbook - 4 books

Wave mechanics: based on PDE

Matrix mechanics: linear algebra.

This lecture has a standalone subject.

Book: David Albert: Quantum mechanics and Experience (for philosophers).

First few chapters.

Experiments involving electrons

2 properties:

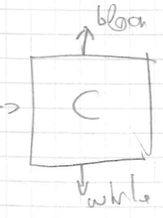
- color
- hardness

} not the technical names [Artificial properties, just not to put hard names in 1st lecture]

Empirical fact: every electron is "either black or white": no other color. No blue electron: black or white! Binary property

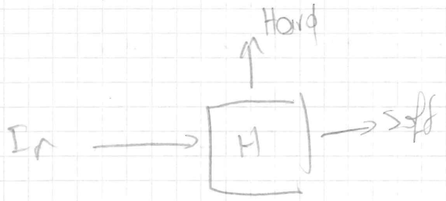
Moreover, they can be either hard or soft.

It is possible to build a device, a box, which measures color.



a box can identify if the electron is "C" is "white" or "black", and sends them to different outputs.

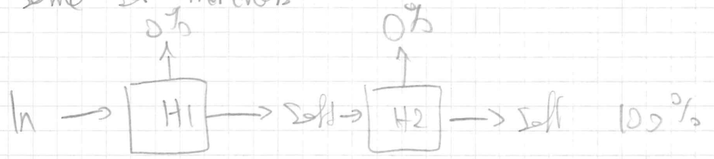
Similarly we can build a hardness box:



We can imagine that these box contain something which can discriminate this. It does NOT matter what it is inside.

A key property of these boxes is that they are repeatable: we put out of a color box, and then in another and the result is the same, 100% of time! Repeatability!

The same for hardness!



Question: might color and hardness be related, correlated? Does color affect hardness? Like, you have a red shirt and you are not going back to the Enterprise

Suppose that we know that the electron is white. Does it affect its hardness?



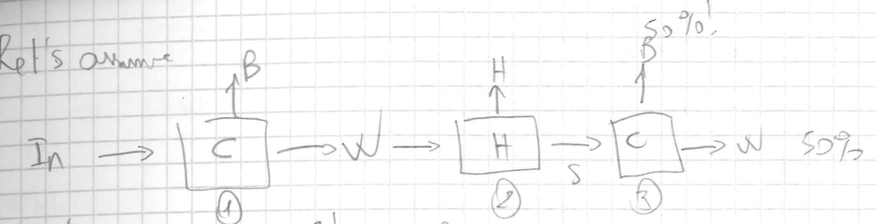
50% is hard, 50% gives out soft.
Obviously also if we switch H and C boxes.

Which means knowing color does NOT affect hardness, and viceversa! Independent properties (color & hardness)

Measuring color gives 0 predicting power for hardness and viceversa! Hardness and color are uncorrelated.

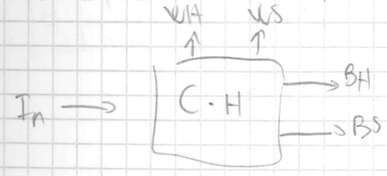
More experiments

Let's assume



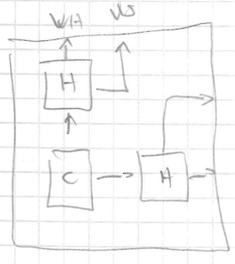
what does happen?! 50% is H, 50% Soft. And then, what happens is that 100% electrons are white, 0% black (in ③)
The point is that, out of here, 50% of electrons are white, 50% black! NOT PERSISTENT in this sense.
Something else comes out here.
No property determines whether an electron goes B or W in ③: it is completely random!
There is something indeterminable, a priori!
This property does NOT change with technology: it is NOT a problem of our boxes!
This property of indeterminism is true.

We cannot:
-build a color & hardness box: only color, only hardness NOT both!



NOT POSSIBLE

Like:

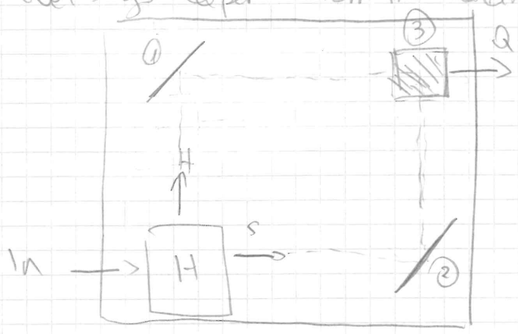


color is NOT persistent after the H box!

This is the uncertainty principle. Something cannot be hard and white, simultaneously. It has NO SENSE to say this!
And, this is true for each object in the world, not just electrons!

This uncertainty rules everything.
The "miracle" is not that electrons have uncertainty. The miracle is that 10^{27} electrons behave as "cheese"! (they are ORGANIZED!)

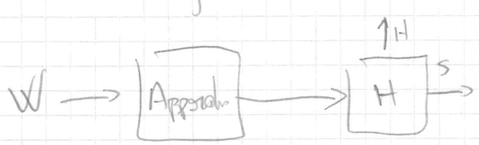
Let's go deeper. From the hardware box, let's add mirrors



these mirrors ①, ② change the direction of motion, nothing else. They just change direction, NOT the property. What was hard, remains hard
③ is a 2nd mirror, which joins the two beams.

This apparatus, with output Q, is:

(I) Let's send in just white electrons, and measure out the hardness.

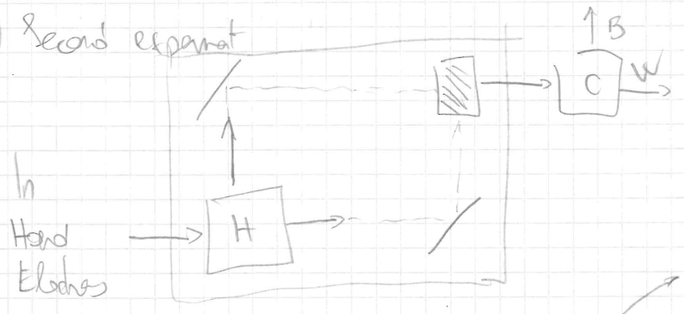


H 50% ?
S 50%

How many electrons are H, how many S?

This is what seem reasonable, since color does not affect.
Well, this is OK.

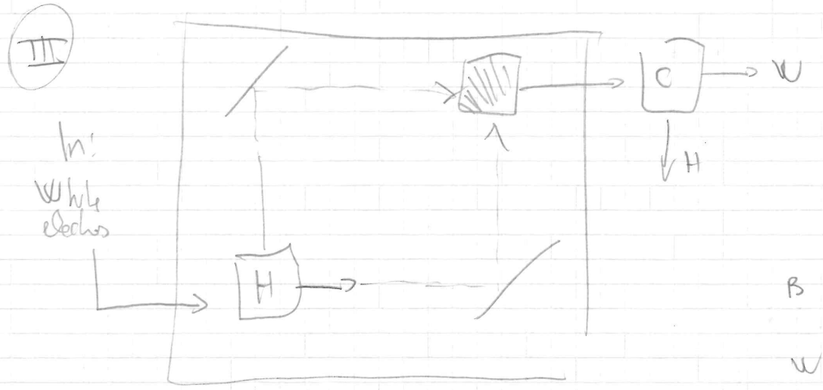
(II) Second experiment



measure color
out of it

B 50% ?
W 50%

It is the same as before. This is correct



B 50
W 50

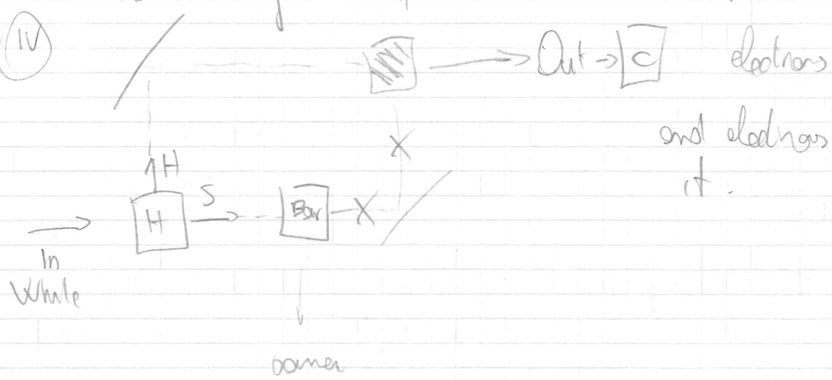
How many W, how many B?

50%, 50%: this, because we already did this!

And, wrong! 0% black, 100% white!

What does change with respect to before?
Which difference is there from the two experiments?

Let us modify the experiment.



This time absorbs all electrons from the soft path and electrons do not go through it.

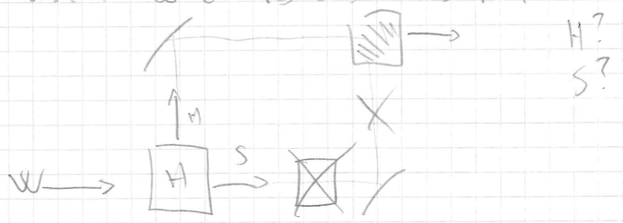
So, (IV): we stop the electrons in (S) branch, what does come out?

1) the Out is down by 50%.
2) But, 100% of electrons appear to be white. By intuition!
This is what we could expect. Well, if electrons do not know the position of the barrier!

The output is, oddly, down by 50%, but 50% wide!

The presence of 2 paths changed what the electrons see, changed the experiment!

Consider a single electron inside the apparatus. We know that everyone will go out from the W output.
Question: which route has it taken?



H? Well, if it goes out 50% W, 50% B, it is different from the situation without the beam, and there is the beam, so NO H.

But, not possible for single path, there is the beam!

Both? NO

And neither "neither of the paths".

These electrons are doing something which we are not considering with our logic.

This is SUPERPOSITION. Up to this moment, it is a way of calling "what the hell?"

They are a superposition of being hard and soft.

Knowing the color means having a superposition of being hard and soft. A superposition!

Not every electron is either hard or soft: it can also be a superposition!

Quantum mechanics is the language which allows to define better superposition.

This is what we are going to study.

These effects are involved with low energies and scales. Single electrons work like two. Many electrons work like cheese, or chalk!

Lecture 2: experimental facts of life

Allan Adams

This lecture is an outline of experiments to be understood and modeled.

Physics doesn't tell you some abstract truth about "why the Universe is what it is"; Physics gives you models to understand how things work and predict what happens next.

Outline

1) Atoms exist
2) Randomness exists in the world
3) Atomic spectra are discrete and structured
4) We have a photoelectric effect
5) Electrons diffract
6) Bell's poor inequality

Atoms are made of electrons and nuclei. This was used in CRT televisions: the cathode ray tube was a gun shooting electrons towards a phosphorescent screen. If you can spray electrons, they exist.

We can see electrons individually. This has been done in CERN, in the experiment Gargamelle: a 30 cubic meter tank full of freon, pulsing just as its vapor pressure 60 times a second. The de-pressurizing freon wants to create bubbles, but you have to nucleate them. You can see a single electron nailed by a neutrino incident from a beam at CERN. This revealed that we can see single electrons, and study their properties. It also reveals that electrons can be hit by neutrinos: this is the so-called "weak neutral current".

Nuclei exist because you can shoot α particles to them, as done by Rutherford and Geiger. Once in a while, α particles deflect back. Just like throwing a bowling ball against a sheet of paper and having it bounce. Atoms are almost 0 density, but have high density cores, so that α particles hit them only sometimes.
This would suggest that nuclei and electrons are charged through Coulomb rule (we have $\oplus$ nuclei, $\ominus$ atoms)

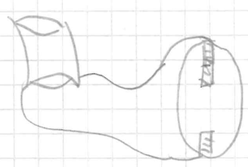
But then, in classical physics, atoms could not exist, and yet they do! In fact, when accelerated, charges radiate. But then the atom should collapse (the electron hit nuclei).

Geiger counter (7 min).
Geiger decay: we know that in a Geiger counter there is a decay, we know a statistic prediction, not exactly how it works.
Geiger was a postdoc of Rutherford, and wanted to count α particles. He took a capacitor, with good voltage (not high enough to break the dielectric). Every time a α particle is passing through the capacitor, it interacts and a spark occurs.
This occurs randomly. This is an example of randomness.

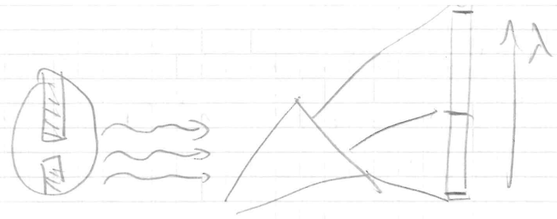
By shooting just like Rutherford did with α particles and atoms' electrons on protons, it was discovered that (60s) protons are not self-consistent, not elementary! They are made of "3" "quarks" (fractional charge) (Kendall, Friedman).

Now, people is working on colliding protons at ultra high energies.

Back to atoms, spectra. Let's start from a power plant, connect through electrodes, through a spark gap (two pieces of metal), putting some gas, like H_2 or Ne, inside a container.



We want to excite the H_2. Exciting hydrogen will produce light.



By putting a prism collecting light, you discover that light is not continuous, but has a very discrete set of lines.
Around 1000 angstroms you have a set of lines, around 3000 another set, 7000 another.

1000: ~~Balmer~~ Lyman
3000: Balmer
10^4: Paschen

Different elements, different sets of lines.
Ballmer discovered that these lines can be written as

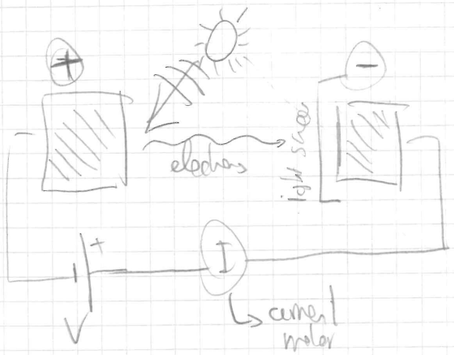
$$\lambda_n = 3646\ \text{Å}\left[\frac{n^2}{n^2-4}\right], \quad n = 3,4,\dots$$

this, for H_2.
So, Rydberg & Ritz found another expression:

$$\frac{1}{\lambda} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right), \quad n > m, \quad \forall n, m$$

But, why?
Spectra are discrete, with a structure. This holds for hydrogen.
Other holds for other elements.

Other experiment
Given a piece of metal, illuminate it, electrons come off.
Experiment: change intensity or frequency.
This electron has a kinetic energy and we want to measure it.



The sun illuminates the left piece of metal, not the right one. It emits electrons. These go towards the right metal, and current is measured.
A voltage V sets the voltage across the two plates.

Potential energy: qV = we want to measure the kinetic energy of an electron excited by photoelectric effect

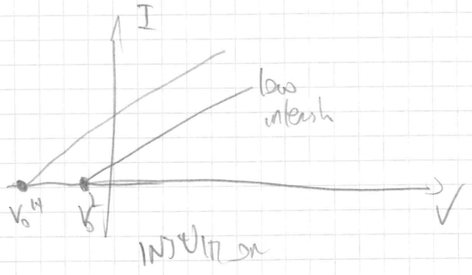
So, if V < V_{stop}, no electron can go in the circuit.



$I \approx E^2 + B^2$

If the kinetic energy is not strong enough to overcome voltage V_{stop}, current = 0.

With a more intense beam, electrons should be more energetic: V_0 should be greater, to stop the beam.

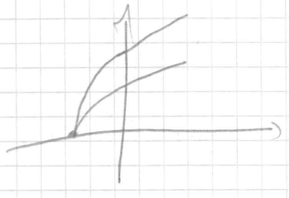


For a high intensity beam, V should be stronger in magnitude.

This is at least what we would expect from Maxwell's electrodynamics.

Moreover, we would expect that energy is independent from frequency!

ACTUALLY, what occurs is:



V_0 is always (V_{stop}) the same, independently on the beam intensity!

Instead, V_0 varies linearly in frequency!

V_0 does not change with intensity, but frequency!

1905, Einstein: light comes in chunks with definite energy.

$E = h\nu$

Intensity is related not to energy, but to the number of packets, or chunks!

So, the kinetic energy KE is

$KE = h\nu - W$

↳ energy required to suck electrons off metal!

If $h\nu$ is too small, KE would be kinetic, so go to 0.

NO MATTER HOW INTENSE IS BEAM, ν does!

It is known that

$E = cP$ P: momentum, c = 3×10^8 m/s

$\nu\lambda = c$

Now,

$E = h\nu$

So,

$P = \frac{h}{\lambda}$ momentum = $\frac{h}{\lambda}$

h is the Planck's constant. This is related to Black-Body radiation. He (Planck) was studying the Black Body. Just doing curve fitting. Einstein found a simple relation.

This was amazing because we always said that light is a wave, Einstein said that it is particle

Double-slit experiment.



this is an experiment on light, performed by Young. (1803)

The wave is a distributed object, not point-wise, so some amplitude exists everywhere in the screen.
Of course, if they were balls shooting two



would occur:

NO INTERFERENCE.

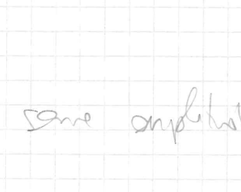
Waves interfere. Packets, no.
This, is the basic picture.

Light is creamy on smoothy like a wave.

But actually, light is both chunky and soft.

Both experiments are true.

What about electrons? Which of these worlds is better to describe electrons?
Sent 1 at time, electron appear localized.
Sent fast, they exhibit interference fringes.



When you send single electrons they firstly appear localized, but a bunch of electrons, waves interfere.
An electron is neither a wave or a ball: it is neither a particle nor a wave. It is an electron!

"

053 run: The mental images - - -
Heisenberg. READ IT

56 run

The "box" experiment of lecture 1 can be repeated with a modification of the 2-slit experiment. We can block one or the other slit, but, when we open both, we can not say if an electron goes through the top, the bottom, or no one. It goes through a superposition of the two.

This is the 2-box experiment.

We could try to build a detector, such that it sends very low-intensity light,
to detect if electrons go through the top or bottom slit.

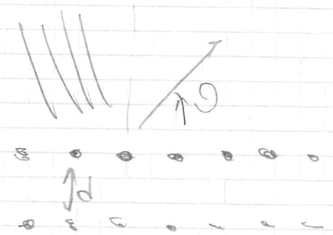


The point is that with light does not matter INTENSITY, but λ.

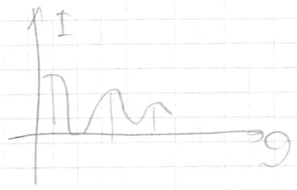
So, if λ is such that perturbation to electron energy is small, means that λ is so large that the slits cannot be distinguished, by diffraction. If λ is short to distinguish the slits, the energy perturbation is so strong to destroy the electron interference fringes.

Instead of light, I could use... Gravitational waves.

Davisson & Germer: they took a crystal, which is a lattice. They sent a beam of electrons.



They discovered that intensity vs θ has



If distance between crystal planes is d,

$$\frac{1}{\lambda} = \frac{n}{2d\sin\theta}$$

electrons behave exactly as waves! And then, to p, momentum, which is

$p = \frac{h}{\lambda}$ just like light!

So electrons DIFFRACT.

Bell's inequality

Question: the number of people of the room who are Undergraduates (U) and NOT BLONDE ($\bar{B}$), plus people of room who are Blond, but NOT Harvardians ($\bar{H}$) are $\geq$ # undergraduates, not from Harvard:

$$N(U, \bar{B}) + N(B, \bar{H}) \geq N(U, \bar{H})$$

$$N(U, \bar{B}) = N(U, \bar{B}, H) + N(U, \bar{B}, \bar{H})$$

$$N(B, \bar{H}) = N(B, \bar{H}, U) + N(B, \bar{H}, \bar{U})$$

$$N(U, \bar{H}, B) + N(U, \bar{H}, \bar{B}) = N(U, \bar{H}, B) + N(U, \bar{H}, \bar{B})$$

$$N(U, \bar{B}, H) + N(U, \bar{B}, \bar{H}) + N(U, B, \bar{H}) + N(\bar{U}, B, \bar{H}) =$$

$$= N(U, B, \bar{H}) + N(U, \bar{B}, H)$$

So LHS is ≥ 0 ($N \geq 0$)

This is Bell's inequality!

Given objects satisfying these binary properties, this is always true.

BUT, electrons have a 3rd property "whimsy", in addition to color and handness.

$N(H, \bar{B}) + N(B, \bar{W}) \not\geq N(H, \bar{W})$

H: angular momentum along x axis

C: angular momentum along y axis

W: angular momentum on z axis

and Bell's is UNSATISFIED. Bell's inequality is VIOLATED.

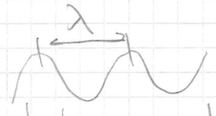
Lecture 3: the wave function

First part of the lecture: polarizers to describe the hyper-intelligent monkey thing: turning polarizers 90°, or 45°. Colors are equated to the amount of non-filtered light.

This is a polarization analogy to the Stein-Gerlach experiment.

This is a crowded analogy interfaces.

Last lecture: he adds something to last lecture. Given a ray of light, it is an EM wave, with some wavelength λ.



The photoelectric effect suggests that energy is proportional to frequency, $\hbar\omega$ ($\omega = 2\pi\nu$, $\hbar = h/(2\pi)$)

Instead, momentum p is $p = \hbar k$, $= \frac{h}{\lambda}$, so $k = \frac{2\pi}{\lambda}$. k is called "wavenumber". There are some relations for electromagnetic waves

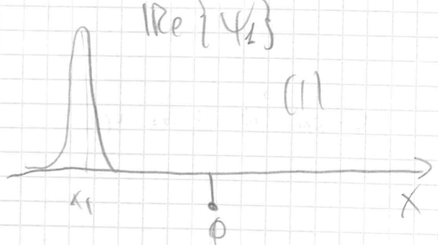
the basis of the photoelectric effect is that energy and momentum of the light are quantized, so that light comes in chunks. So, it has both a wave aspect and properties familiar from particles.
de Broglie understood something like that: he conjectured that every object with momentum p has associated a wavelength λ. The same for energy. So, also electrons. Davisson-Germer proved that electrons satisfy both wave and particle "requirements". De Broglie relations.

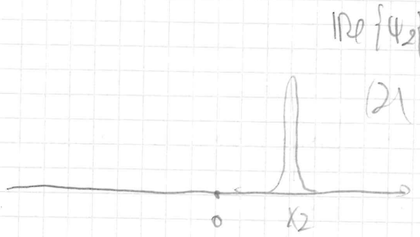
In next lectures we will study rules and postulates: the rules of quantum mechanics. QM is a set of rules to perform predictions about the world. Start from scratch

Definition of a system
In classical mechanics, how did we specify the configuration, the state of, for instance, a single particle, which is the simplest system?
We specify position and momentum: $\vec{x}$ and $\vec{p}$. Then, energy is a function of $\vec{x}$ and $\vec{p}$, as well as the angular momentum $\vec{x}$ and $\vec{p}$ give complete characterization of the system. Every information which can be obtain from a meaningful experiment can be obtained from $\vec{x}$ and $\vec{p}$.
But, this, can't be done in quantum mechanics, since there is an uncertainty: $\Delta x \Delta p \geq \hbar$
we can't be arbitrarily confident of both position and momentum.
We need to specify the configuration of the system, its state. First postulate:

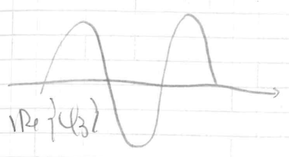
(I) The configuration of a quantum object is completely specified by a wavefunction $\psi(x)$ which is a complex function (in $\mathbb{C}$).

Example: these are wavefunctions

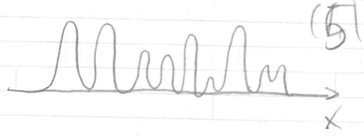


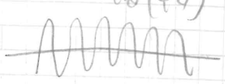


Or,



this is another possible wavefunction, as well as





ψ is a complex function, and "not stupid". We have to define what "stupid" means.

Postulate (II): the meaning of the wavefunction is that the probability for the quantum object to be in position x equals the norm squared of ψ:

$$\mathbb{P}(x) = |\psi(x)|^2$$

this means that $\mathbb{P}$ determines the probability density that the object in state $\psi(x)$ will be found at x.
This means that

$$\mathbb{P}(x, x+dx) = \mathbb{P}(x)\,dx = |\psi(x)|^2\,dx$$

the probability that the object is found in this infinitesimal interval is this density times dx.
the wavefunction must be normalized: the sum of all probabilities must be 1. So,

$$\int_{\text{all } x \text{ values}} \mathbb{P}(x)\,dx = 1 = \int_{\text{all } x \text{ values}} |\psi(x)|^2\,dx$$

Note: $\mathbb{P}(x)$ has 1 argument because it is a probability density. $\mathbb{P}(x, x+dx)$ has 2 arguments, therefore it is a total probability.
What are the dimensions of the wavefunction? $1/m$! $1/speed$! Indeed,

$$[\psi] = \frac{1}{\sqrt{L}},$$

because the integral must be 1, and dx has dimension of length, L^n.
Always do dimensional analysis!

Well, back to the previous examples, such as (1), we can see that $|\psi(x)|^2$ is almost equal to $\psi(x)$ ($\Pi_m = 0$ in this example),

so this means that $|P(x)$ is non-zero only around x_1, and then this means that, in this system, $x \approx x_1$, with small Δx : it is probably there, the electron! (the quantum object).

Similarly in (2).

Instead, in (3), we have:

$$\psi = e^{jk_1 x}$$

so that this was the IPE part. In (4) we have $e^{jk_2 x}$.

What is $|P(x)$? Well,

$$|e^{jk_1 x}|^2 = 1$$

In fact, given a complex number β,

$$|\beta|^2 = \beta \beta^*$$

So, for (3), $|P(x)$ is constant; moreover, now it is not properly normalized. $|P(x)$ is INDEPENDENT of x!

Such we measure the position of the particle in state $\psi_3(x)$, it could be everywhere! x could be everywhere, so very large Δx!

In (4), we don't know where x is, but Δx is not infinite, it's just not "gigantic"!

A multiply defined function cannot be a ψ: the wave functions should be single-valued! We will also see that it has to be continuous.

Well, to know position of the objects (1) and (2) seem ok, (and (3) and (4) no.

Except, let's recall de-Broglie relations, which states that

$$p = \hbar k = \frac{h}{\lambda}, \quad E = \hbar \omega$$

ψ_3 and ψ_4 have not defined x, but very well-defined wavelengths! They are PERIODIC functions with well-defined wavelength, so frequency, so p!

In particular, ψ_3 has $\lambda_3 = \frac{2\pi}{k_1}$, $p = \hbar k_1 = \frac{h}{\lambda_3}$

So the estimation of the momentum in ψ_3 is very good: $p = \hbar k_3$, with very small Δp! Similarly for 4

Note: in ψ_3, we don't have a definite wavelength.

What de Broglie missed is that to every object it is associated a plane wave (PW)

$$e^{j(\vec{k}\cdot\vec{x} - \omega t)} \quad \text{or even} \quad \boxed{e^{j(kx - \omega t)}}$$

we will do almost everytime 1-D quantum mechanics.

Somehow associated, there is a PW with k and ω.

Some wave packets are well localized, some are just more complicated waves.

Back to our postulates,

(III) This is the most important thing in quantum mechanics: it has EVERYTHING, the two-slit experiment, everything

Given two possible wavefunctions (or states, or configurations) of a quantum system, $\psi_1(x)$, $\psi_2(x)$, the system can also be in a superposition of ψ_1 and ψ_2:

$$\psi(x) = \alpha \psi_1(x) + \beta \psi_2(x), \quad \alpha, \beta \in \mathbb{C} \text{ (complex numbers)}.$$

Given any two possible configurations of the system, there is also an allowed configuration corresponding to be an arbitrary superposition of them.

If an electron can be hard and it can be soft, it can also be in an arbitrary superposition of being hard and soft. Superposition: linear combination.

α, β are subject to the normalization condition!

Remark: normalization,

$$|P(x) = \frac{|\psi(x)|^2}{\int_{-\infty}^{\infty} |\psi(x)|^2 dx}$$

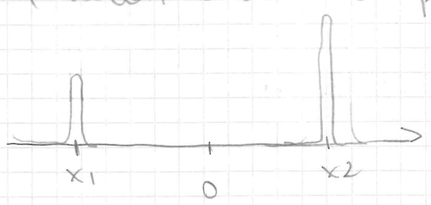
we can also forget about normalizing and just define $|P(x)$ in this way!

This is the beating soul of QM: everything of QM is in postulate III

This also means that wavefunctions ψ_1 and ψ_2 may interfere.

EXAMPLE

The two wave packets ① and ② indicate the state of the system and that the particle is in x_1 and x_2. (momentum is not known, the spectrum is ok) Suppose we want to build a superposition of them. Similarly, ③ + ④.



① + ②



③ + ④

↓

This is a particle that is either in x_1 or x_2, more probably in x_2 but still possibly in x_0. The uncertainty in position is much bigger: $\approx |x_1 - x_2|$.

What about ③ + ①, what is? Well, it does not have just a wavelength!

$\psi_{3+4} = e^{jk_1 x} + e^{jk_2 x}$: 2 wavelengths. The norm squared is no longer constant, but it has some interference!



$$P(x) = |\alpha\psi_3 + \beta\psi_4|^2 = |\alpha|^2 |\psi_1|^2 + |\beta|^2 |\psi_2|^2 + \alpha^* \psi_3^* \beta \psi_4 + \alpha \psi_3 \beta^* \psi_4^* =$$

$$= |\beta|^2 P_3 + |\beta|^2 P_4 + \text{interference terms}$$

These interference terms are a correction to the classical addition of probabilities! Notice that $\alpha, \beta, \psi_3, \psi_4$ are not necessarily real or positive, so they can also be negative! The probability to add these two configurations has a positive, plus a negative (possibly) term.

This is related to what we said about Bell's inequality, because, there, we assumed that the probability of the sum was just the sum of the probabilities. In QM, probabilities don't add that simply!

ψ_{3+4} now contains some more information, with regard to 3 and 4, about the position of the object. Some more info. Δx is still gigantic.

What happens if we superimpose 3 or 4 wavelengths? He shows something with Mathematica @ Personal Computer. Superposition of wave packets, so of plane waves. By adding several plane waves, the probability distribution becomes more and more localized



so that particle is very probably here.

Adding several PWs means losing information on momentum. Superimposing several momenta means increasing Δp!
This is the uncertainty relation.

Example ① and ② are far from being periodic, so there is no defined λ. By this way, momentum is NOT well defined.
This could be also observed by performing the Fourier analysis of this ψ! No definite λ, BY de Broglie means no definite momentum!

Fourier transform

Theorem: any function $f(x)$ sufficiently well behaving (not singular, not discontinuous) can be built by superimposing enough plane waves e^{jkx}. Enough means infinite. So,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{f}(k)\, e^{jkx}\, dk$$

we sum over plane waves e^{jkx}, $\lambda = \frac{2\pi}{k}$. $\tilde{f}(k)$ tell us the amplitude of each k plane wave. This, also for non-periodic functions.
Similarly,

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-jkx}\, dx$$

inverse Fourier transform

Knowing ψ means knowing $\tilde{\psi}$ and viceversa.

The "physical" version of this is that any wave function $\psi(x)$ can be expressed as the superposition in the form

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{\psi}(k)\, e^{jkx}\, dk$$

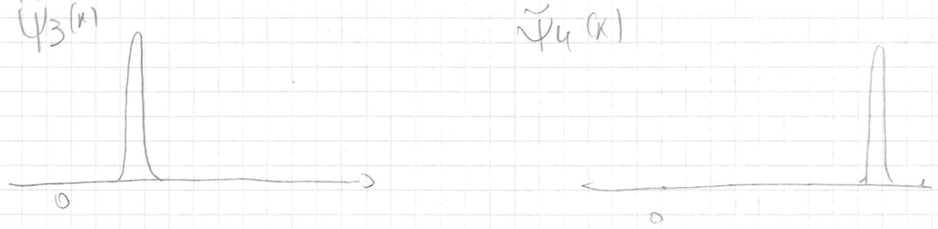
of states (or, wavefunctions), with a definite momentum $p = \hbar k$.

It is useful to sketch the Fourier transform of our examples ① ÷ ④

① $\tilde{\psi}_1$ $\qquad$ $\tilde{\psi}_2$



$\tilde{\psi}_3(x)$ $\qquad$ $\tilde{\psi}_4(x)$



Similarly for the ② and ③-④, they are basically one the transform of the other!

There is some sort of pleasing symetry here!

Fourier transforms are continuous in k: NOT discrete, because otherwise $\psi(x)$ would be always periodic!

Note: just like for position, we can say that, in k,

$$\mathbb{P}(k) = |\tilde{\psi}(k)|^2 \quad : \text{the Fourier transform!}$$

(probably, this is related to Parseval - Plancherel!)

Lecture 4: Expectations, momentum, and uncertainty

We discussed the 3 postulates

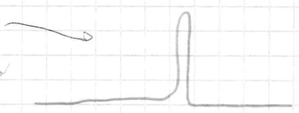
Ⅰ Configuration of a particle is described by $\psi(x)$: wavefunction.
if we had 2 particles, we would have $\psi(x_1, x_2)$: position of the 2 particles x_1, x_2

Ⅱ $|\psi(x)|^2\, dx = \mathbb{P}(x, x+dx)$: probability of finding the particle in $[x, x+dx]$.

Ⅲ Superposition principle: if we have two possible configurations of the system, $\psi_1(x)$, $\psi_2(x)$, it is also possible to have the system in $\psi(x) = \alpha\psi_1 + \beta\psi_2$.

Note: • Normalize : $\int |\psi(x)|^2 dx = 1$

- All reasonable $\psi(x)$ are equally reasonable wavefunctions! For instance, multivalued or discontinuous functions are NOT ok!
- Some wavefunctions are more equal than others; i.e., they have simpler interpretations, such as this, which lend itself to an interpretation as: the particle is in the room.



Any reasonable $\psi(x)$ can be expressed as the superposition of "more equal wavefunctions" (easily interpretable):

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{\psi}(k)\, e^{jkx}\, dk$$

superposition of plane waves! :)

Recall: $e^{jkx} = \cos(kx) + j\sin(kx)$

Similarly, any $\psi(x)$ could be expressed not in terms of plane waves, but of Dirac delta functions: combination of states in all possible positions i.e.,

$$\psi(x) = \int \psi(x_0)\, \delta(x - x_0)\, dx_0$$

δ functions are our friends! They are maps from integrals to numbers or functions! So, we replace x by x_0, and so on. This is correct: this is a superposition of definite positions!

Let's imagine to have a vector in 2D, it is a superposition of 2 other vectors! For instance, of $\hat{x}$ and $\hat{y}$!



This is a convenient choice of basis!

This is true in vectors, this is also for wavefunctions! Here, we take them as those with well-defined position and/or momentum.

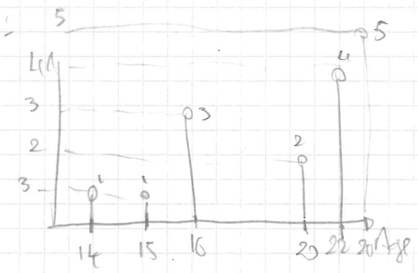
Question: how are λ in this $\Psi(x)$?



Due to these discontinuities of derivatives we need a lot of plane waves to represent those kinky points: large momentum. Small x-scale discontinuity (very wide p range! (or k)

Uncertainty principle. To study it, we need to define Δx, and Δp.

Let's recall something from probability. Let's assume that we have a room with some people, and they are divided by age:



what's the probability to have a person of age "a"?

$$\mathbb{P}(a) = \frac{N(a)}{N_{tot}} \qquad N_{tot} = 1+1+3+2+4+5$$

Of course,

$$\sum_a \mathbb{P}(a) = 1$$

Which is the most likely age? 24. And the average? 19.2. But, there is no 19?! NO ONE! 19 is not an observable value!

Average: average age "a" is

$$\langle a \rangle = \frac{\sum_a N(a)\, a}{N_{tot}} = \sum_a a\, \mathbb{P}(a)$$

Does have the average to be measurable? Observable? NO, it doesn't!

What about the square of ages?

$$\langle a^2 \rangle = \sum_a a^2\, \mathbb{P}(a)$$

More generally,

$$\langle f(a) \rangle = \sum_a f(a)\, \mathbb{P}(a) \qquad \text{with the same logic.}$$

Question: is $\langle a^2 \rangle$ equal to $\langle a \rangle^2$? NO. Not necessarily.

The width of a distribution is defined from: the deviation, $(a - \langle a \rangle)$.

Note that:

$$\langle (a - \langle a \rangle) \rangle = \langle a \rangle - \langle \langle a \rangle \rangle = \langle a \rangle - \langle a \rangle = 0.$$

(the average value of a number is the number itself).

Deviation is not good on average: it is always 0. So, it is more convenient to take another measure: the deviation squared! (and its mean)

$$\langle (dev)^2 \rangle = \langle (a - \langle a \rangle)^2 \rangle \qquad \text{(standard deviation)}$$

If the standard deviation is 0, it means that the distribution has no width, because any ~~contribution~~ part out of the average would give a non-zero contribution, strictly positive. So std dev

So standard deviation is a good measure for width. Or uncertainty! =)

So:

$$\langle (a - \langle a \rangle)^2 \rangle = \langle a^2 - 2a\langle a \rangle + \langle a \rangle^2 \rangle = \langle a^2 \rangle - 2\langle a \rangle\langle a \rangle + \langle a \rangle^2 =$$

$$= \langle a^2 \rangle - \langle a \rangle^2 \qquad \text{[alternative formula]}$$

The notation is:

$$\langle (a - \langle a \rangle)^2 \rangle \equiv \Delta a^2$$

The uncertainty will be Δa: the square root of standard deviation.

For continuous variables, given x a probability distribution, we have

$$\langle x \rangle = \int_{-\infty}^{+\infty} |P(x)|\, x\, dx \qquad \langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\, |P(x)|\, dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2\, |P(x)|\, dx$$

The uncertainty in x is:

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

In the notation of quantum mechanics,

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\, |\psi(x)|^2\, dx$$

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\, |\psi(x)|^2\, dx$$

The expected value depends on what the state of the system is. For this reason, this notation is dangerous, and it should be improved. One way is to specify in the subscript the state ψ of the system,

$$\langle x \rangle_\psi = \langle \psi | x | \psi \rangle \qquad \text{[expectation value of } x\text{]}$$

This notation is very useful and it will be used, and it means the very same thing, just with a "different flavour". The two ψ somehow recall the $|\psi|^2$ in the integral.

How do we do the same thing for momentum? Well,

$$\langle p \rangle = \int_{-\infty}^{+\infty} |P(p)|\, p\, dp \qquad \text{just like for } x.$$

But, if we have $\psi(x)$, how do we switch to p? Well,

$$\langle p \rangle \overset{?}{=} \int_{-\infty}^{+\infty} p\, |\tilde{\psi}(p)|^2\, dp \qquad \text{is it like this? Well, yes.}$$

(Parseval!)

Let's go back to $\langle p \rangle$, and let's obtain it directly in terms of the wavefunction.

$$\langle p \rangle = \int_{-\infty}^{+\infty} dx\, |\psi(x)|^2\, p(x)$$

NO: momentum and position are NOT RELATED!

Let's note that the $\delta(x - x_0)$ could be written as:

$$\delta(x - x_0) = \frac{1}{\sqrt{2\pi}} \int dk\, \tilde{\delta}(k)\, e^{jkx} \qquad \tilde{\delta}(k) \text{ transform of } \delta$$

to represent a δ, we need an (∞) number of plane waves! =C

The magic answer is: $\tilde{\delta}(k) = e^{-jkx_0}$! =)

there is no state with definite position and momentum =C

We need a definition of p given $\psi(x)$. So, hint 1:

$k = \frac{2\pi}{\lambda}$ is associated to a wave, to a particle with $p = \hbar k$, e^{jkx}!

How can I have p appear? Note that $\frac{\partial}{\partial x} e^{jkx} = \partial_x e^{jkx} = jk e^{jkx}$.

So,

$$\frac{\hbar}{j} \partial_x e^{jkx} = \hbar k e^{jkx} = p e^{jkx},$$

that is what we want! =) Moreover, $[\hbar] = [\Delta x\, \Delta p] = m \times v \times x$

p = mass × velocity

So, what putting the exponential the operator

$\frac{\hbar}{j} \partial x$ is somehow producing a momentum o_o

What does momentum have with a derivative, moreover with respect to position! o_o

Another hint is Noether's theorem, from Emmy Noether.

To every symmetry, is associated a conserved quantity.

Symmetries are translation, or rotation.

For instance, to translation, corresponds the conservation of momentum:

$\dot{p} = \frac{\partial p}{\partial t} = 0$. $\quad x \to x + L$

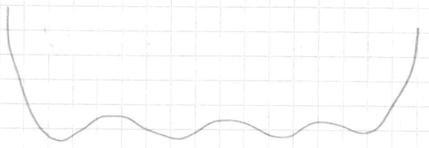
To time translations, $t \to t + T$, Energy is preserved, which is time-independant

To rotation, $\vec{x} \to \text{Rotation}\,\vec{x}$, angular momentum $\dot{\vec{L}} = 0$

Having translational symmetry means translating the whole system and repeating the experiment: nothing changes.

Given a damped particle moving in a potential $U(x)$,

$$\dot{p} = -\nabla U$$



the ∇U is clearly not 0.

Because, potential breaks the symmetry.

Except for constant potential: the only having full translational symmetry.

Less trivial for energy.

What's the relationship between p and a space derivative? Let's define T_L the operation of translating by L:

$T_L f(x) = f(x-L)$.

The $f(x-L)$ can be written as a Taylor expansion around $L=0$ for small L:

$$= f(x) - L\,\partial_x f(x) + \frac{L^2}{2}\partial_x^2 f(x) - \frac{L^3}{6}\partial_x^3 f(x) =$$

$$= \left(1 - L\,\partial_x + \frac{L^2}{2}\partial_x^2 - \frac{L^3}{6}\partial_x^3\right) f(x)$$

this is the Taylor expansion for the exponential: $e^{-L\partial_x} f(x)$!

Derivative exponentiated!

Derivatives w.r.t. x cause translations of L; if L is arbitrarily small we can drop higher order terms, up to $L\partial_x$: infinitesimal translation.

Translations in x are generated by ∂_x.

But, through Noether's theorem, translations in x are associated to momentum conservation.

It should be shocking that ∂_x is related to momentum.

Similarly, translations in t are related to ∂_t, which are associated to energy conservation. $\partial_t \to L$

We saw that translation is somehow related to momentum conservation. Without defining anything!

We declare that in quantum mechanics, $\hat{p}$, the operator $\hat{p}$, is represented by the operator $\frac{\hbar}{j}\partial_x$. This is a Bet, NOT proof.

If we take a state $\psi(x) = e^{jkx}$, momentum $p = \hbar k$, take the operator $\hat{p}$ and apply to our state, what do we get?

$\hat{p}\psi(x) = \hbar k\,\psi_k(x)$ By applying our operator to the state ψ_k, we get back the same state, ψ_k, plus times a constant, that is the momentum we ascribe to that plane wave.

hat $\hat{p}$: operator.

If our state ψ is

$\psi = \frac{1}{\sqrt{2}} e^{jk_1 x} + \frac{1}{\sqrt{2}} e^{jk_2 x}$,

does this state have a definite momentum? No! $\hat{p}\psi$ gives another state

Lecture 5: operators and the Schrödinger equation (Zwiebach)

So far we have learned:

1) that particles or systems are governed, described by wave functions, $\psi(x) \in \mathbb{C}$, complex functions continuous and normalizable. Note that their derivatives are not necessarily continuous

2) there is a probability associated to $\psi(x)$:

$|\psi(x)|^2 dx$ probability of a particle to be in a range from x to $x+dx$: it does not have sense to study probability in a point, but in a range. And thus

$|\psi(x)|^2 dx = |\psi(x)|^2 dx$

3) Superposition principle: particles could be in superpositions, meaning that

$\psi(x) = \alpha\psi_1(x) + \beta\psi_2(x)$

We discussed about operators, and relations between them

We performed an abstraction which led us understanding that somehow the momentum of a particle comes from the operation of an operator on $\psi(x)$ (on the w.f.)

As an aside, p, the momentum of a particle, has been associated to:

$$\hat{p} \longleftrightarrow \frac{\hbar}{j}\frac{\partial}{\partial x} \qquad (1)$$

why partial derivatives? Because ψ depends <u>also</u> on <u>time</u>, not just on x! This is why we don't use $\frac{d}{dx}$ instead

How do we use (1)?

We made (1) in order to work on $\langle p \rangle$, the expected value of the momentum:

$$\langle p \rangle = \int_{-\infty}^{+\infty} dx\, \psi^*(x) \frac{\hbar}{j}\frac{\partial}{\partial x}\psi(x)$$

This is this way because if we try to take a generic w.f. $\psi(x)$, we don't have necessarily (*) by simply applying $\hat{p}$

$$\hat{p}\psi(x) = \frac{\hbar}{j}\frac{\partial}{\partial x}\psi(x)$$

let us take, as a <u>special</u> $\psi(x)$,

$\psi(x) = Ne^{\pm jkx}$ (

$$\hat{p}\psi(x) = \frac{\hbar}{j} jkNe^{jkx} = \hbar k\psi(x)$$

But, Ne^{jkx} has a <u>well</u> <u>specified</u> momentum. Since it is <u>not</u> always the case, we have to perform this averaging.

Now, let us extend this concept to other operators. To other quantities, not just momentum!

"Math interlude"

What is an operator? (math quote)

What do operators have in common with measurable quantities?

There is a simple way of thinking of operators: basically, operators are things that act on objects and scramble them. So, we need to classify on what operators act, and then the operator is some instruction of how to scramble it, producing another object.

A mathematical example of operators and objects is, respectively, matrices and vectors.

Vectors $\leftrightarrow$ objects

matrices $\leftrightarrow$ operators

Example: $\underline{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ object

$\underline{\underline{M}} = \begin{bmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{bmatrix}$ operator

$\underline{\underline{M}}\,\underline{v}$ = vector: $\underline{\underline{M}}$ applied to $\underline{v}$ gives another vector! This is the simplest example of operator acting on object

In quantum mechanics the objects are complex functions of x; operators act on them, transforming them in other functions.

Examples: the operator $\hat{O}$ applied to $f(x)$ returns another function of x.

the simplest operator is $\hat{1}$: the identity

- $\hat{1} f(x) = f(x)$ (2)

  this is like the identity matrix!

- $\frac{\partial}{\partial x}$: the derivative operator! (3)

- $\hat{X}$ is another operator! We just have to define it!

  this is the operator that, given $f(x)$, transforms in $x f(x)$: multiplies by "x" the $f(x)$! (4)

- $\hat{S}_q$: square operator, $\longrightarrow \hat{S}_q f(x) = [f(x)]^2$ (5)

- $\hat{P}_{42}$: $f(x) \to 42$ transforms $f(x)$ in the constant function 42! (6)
  (quite useless)

- $\hat{\delta}_2$ Dirac operator:
  $\hat{\delta}_a f(x) = \delta(x-a) f(x)$ (7)

- A more general one:
  $\hat{O}_{h(x)} \longrightarrow \hat{O}_{h(x)} f(x) = h(x) f(x)$ (8)

There are operators that are particularly nice: linear operators.
If $\hat{O}$ respects superposition, i.e.

$\hat{O}(a f(x) + b g(x)) = a \hat{O} f(x) + b \hat{O} g(x)$,

it is linear. Of our operators, which are? (2), (3), (4) NOT (5),

(5) $S_q(f+g) = f^2 + g^2 + 2fg \neq f^2 + g^2$

NOT (6), and yes $\hat{O}_{h(x)}$

Linear operators are important because of the superposition principle!

Operators have another peculiarity, which can be understood by turning to the simplest objects they can act on.
With matrices, people looks for special vectors. Generally, when you apply a matrix to a vector it changes direction, it jumps from one direction to another. But, there are some funny, special vectors that, after the matrix application, can grow, or become smaller, but they maintain the direction! The eigenvectors! And the constant of proportionality is the eigenvalue.

Operators can have "eigenfunctions": given a linear operator $\hat{A}$,

$\hat{A} f_a(x) = a f_a(x)$

$f_a(x)$ is a pretty unusual function, specific for $\hat{A}$. "a" is the eigenvalue, a complex number. These special things do not necessarily exist, but when they do, they are very useful and nice.

Example:

$\hat{A} \equiv \hat{P}$ $\quad f(x) = e^{jkx}$

$\hat{A} f(x) \longrightarrow \hat{P} e^{jkx} = \hbar k\, e^{jkx}$: $\hbar k$ is the eigenvalue of our e^{jkx}!

For an operator, we can have many eigenvalues and eigenfunctions: even infinite!

Linearity is not necessarily applicable: the sum of eigenvalues/eigenvectors: the sum of two eigenvectors is NOT an eigenvector!

$\hat{A} f_1 = a_1 f_1$
$\hat{A} f_2 = a_2 f_2$ $\longrightarrow \hat{A}(f_1 + f_2) = a_1 f_1 + a_2 f_2 \neq m(f_1 + f_2)$!

An eigenvector cannot be built from other eigenvectors superimposed.

Note: f_a and $3f_a$ is the <u>same</u> eigvc: eigvcs are known less than a constant!

Physics

We know, as postulate: $\hat{p}$, $\hat{x}$. We also have energy postulate: knowing that the energy of a particle is

$E_{kin}+E_{pot}$

$$E = \underbrace{\frac{p^2}{2m}}_{\text{kinetic}} + \underbrace{V(x)}_{\text{potential}}$$

$E_k = \frac{1}{2}mv^2$, but $p = mv$, so $\frac{p^2}{2m}$

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{x})$$

where, $V(\hat{x})$ is obtained putting $\hat{x}$ instead of x, and $\hat{p}^2 = \hat{p}\hat{p} =$

$$= \left(\frac{\hbar}{j}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{j}\frac{\partial}{\partial x}\right) = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$V(\hat{x})$: heuristic of operators for instance, if $V(x) = x^2$,

$V(\hat{x}) = \hat{x}\hat{x}$

So,

$$\hat{E}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)$$

So, the (3) points at the beginning of the lecture are now (4):

(4) To each observable we have associated an operator:

$\hat{A}$ { momentum $\hat{p}$; position $\hat{x}$; energy $\hat{E}$

So, as we did with momentum, we can apply our definition of expectation also:

$$\langle\hat{A}\rangle = \int_{-\infty}^{+\infty} dx\, \psi^*(x)\,\hat{A}\,\psi(x)$$

this is the value we would expect, after many trials, by measuring something on the wave function, the mean.

Other definition: the uncertainty of an operator on ψ:

$$\text{uncertainty } (\Delta\hat{A})_\psi = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}$$

this is the uncertainty of the uncertainty principle.

Another observation, definition, which may be inspired from matrices is the possibility for matrices to commute. We will try to see if the operators associated to position and momentum, the two most important, commute. The order does matter, such as the multiplication order in matrices.

Commutator: $\hat{p}\,\hat{x}$ or $\hat{x}\,\hat{p}$ commute? Does the order matter?

We can not understand clearly just looking at them. Because what operator is clear just when we apply them to <u>functions</u>.

We can <u>test</u> if this, applied on $f(x)$ returns the same:

$$(\hat{p}\hat{x})f(x) \overset{?}{=} (\hat{x}\hat{p})f(x) \quad (?)$$

$$\frac{\hbar}{j}\frac{\partial}{\partial x}\left(x f(x)\right) \quad \times \quad \frac{\hbar}{j}\frac{\partial}{\partial x}f(x)$$

we apply with the different orders, and they are clearly different!

$$\frac{\hbar}{j}f(x) + x\frac{\hbar}{j}\frac{\partial f}{\partial x}$$

This means that

$$\left[\hat{x}\hat{p} - \hat{p}\hat{x}\right]f(x) = -\frac{\hbar}{j}f(x) = j\hbar f(x)$$

This is very strange!

$[\hat{x}\hat{p} - \hat{p}\hat{x}]$, which is the commutator of $\hat{x}\hat{p}$, gives:

$[\hat{x}\hat{p} - \hat{p}\hat{x}] f(x) = j\hbar f(x)$

So,

$[\hat{x}\hat{p} - \hat{p}\hat{x}] = j\hbar \mathbb{I}$ (9)

Apart from Schrödinger equation, this is the most important equation in quantum mechanics: it states that $\hat{x}$ and $\hat{p}$ are incompatible, their application order matters, measuring one confuse the other, so they cannot be measured simultaneously. All of this, is in (9).

This is the way Heisenberg invented quantum mechanics. He called it "matrix mechanics", because he knew that operators were somehow related to matrices.
Today we follow Schrödinger's picture, but this idea is still interesting.

Eq. (9) is deep, and also scary. Scary, for mathematicians: when a mathematician sees (9), he tries to build an example with matrices, like 2x2 matrices, but there is no such example. Neither 3x3, 4x4... except if the matrix is $\infty \times \infty$.

If a physicist sees it, he starts thinking of angular momentum L_i a matrix like it

$[\hat{L}_i, \hat{L}_j] = j\hbar \epsilon_{ijk} \hat{L}_n$ this is easy, to be solved by matrices; ϵ_{ijk} → permutations

NOT (9). (50 min)

Postulate (5)

Upon measuring an observable A associated with the operator $\hat{A}$, two things happen:

(1) - The measured value is a number: one of the eigenvalues of $\hat{A}$. True, both with $\hat{p}$: the observables have associated operators, and their eigenvalues are the measured! In order to be observable, those eigenvalues must be real numbers (even if we said that in general are complex!) So, we will limit the observables to real numbers and the associated operators will be hermitian operators. Special operators that return just real eigenvalues.

(2) After the measure, the eigenfunction goes into the state that is the eigenfunction of the operator. So, since measuring means computing an eigenvalue, the state of the system becomes the eigenfunction. So, after a measure, the system collapses into state ψ_2:

$\hat{A}\psi_2 = a\psi_2$

After measuring momentum, the wavefunction becomes that of the momentum $\hbar k$: if at the beginning the ψ was given by the superposition of many, as Fourier told us, momenta, then after measuring, if we get a constant of momentum, all the others are disappeared.
This is quite a strange thing, almost impossible to explain.

If for instance we have a wavefunction that says that our particle could be everywhere, after we measure position $\hat{x}$, the whole wf becomes a δ function of the measuring position x_0.

Example
Position
Given $\psi(x)$, we measure position and find the value of x_0.
Which is the function best identifying a position eigenstate? The $\delta(x-x_0)$, the function that peaks x_0 and is 0 everywhere else.
So, $\psi(x) \sim \delta(x-x_0)$. But, δ cannot be normalized. Still, we could use one of the limits to represent the δ. But...
Is $\delta(x-x_0)$ an eigenstate of the operator $\hat{x}$? Yes!

$\hat{x}\,\delta(x-x_0) = x\,\delta(x-x_0) = x_0\,\delta(x-x_0)$! Yes!

$\hat{x}\,\delta(x-x_0)$: operator applied to eigenf. $=$ $x_0\,\delta(x-x_0)$: number times eigenfunction → eigenfunction of $\hat{x}$

We could do the same with the momentum! And its eigenfunctions e^{jkx}

Postulate (6)

Given an observable $\hat{A}$ and its eigenfunctions $\psi_n(x)$, where n may run many values, we can expand an arbitrary function in terms of the eigenfunctions of $\hat{A}$, just like we did, with Fourier, with e^{jkx} (eigenf. $\hat{p}$).

An eigenfunction is not determined up to scale, we can normalize them.
Let us normalizing by saying

$$\int dx\ \psi_a^*(x)\ \psi_b(x) = \delta_{ab} \qquad \text{Kronecker delta}$$

We can always do this with eigenfunctions.

Given $\hat{A}$, two things happen

(1) One can expand $\psi(x)$ as

$$\psi(x) = \sum_a C_a\ \psi_a(x) \qquad (10)$$

(2) The probability of measuring A and getting a (a particular state) is given by $|C_a|^2$:

$$P_\psi(a) = |C_a|^2$$

We can illustrate this with δ function.

Example

$\hat{X}$, $\{\delta(x-x_0) \quad \forall x_0\}$, eigenfunctions

$$\psi(x) = \int dx_0\ \psi(x_0)\ \delta(x-x_0)$$

it is just a strange way to write $\psi(x)$ as an integral.
But, this is the analog of (10)! A decomposition in δ functions!

$\delta(x-x_0)$ are the ψ_a, $\psi(x_0)$ are the C_a, and that's it!

So, the probability to find the particle in x_0 is $|\psi(x_0)|^2$

Time evolution Postulate (7)

(7) Schrödinger equation

As happens often in physics, there is experimental evidence and, to build a model, we need a conceptual leap, to suggest the equation.

Planck postulated quantized energies in multiples of $\hbar\omega$. Then Einstein noticed that the energy of the photon is $\hbar\omega$ as well!

photons: $E = \hbar\omega$

momentum: $\vec{p} = \hbar\vec{k}$ (or, 1-d, $p = \hbar k$)

(Planck, Einstein, Compton)

People was not surprised that photons are associated with electromagnetic waves (light is EM), so, vector equation:

$$(E, \vec{p}) = \hbar(\omega, \vec{k})$$

this is a wonderful relativistic equation! Thus $p^\mu = (E, \vec{p})$ is a 4-vector as in relativity!

But then, De Broglie understood that what is good for photons, could be good for all particles: all particles are waves!

$$\psi(x,t) = e^{j(kx-\omega t)} \qquad \text{this is a wave, with } p = \hbar k$$

if $k>0$, $x>0$, this wave moves to the right.

So, if momentum is like that, $p = \hbar k$, momentum must have something does (to, De Broglie) $E = \hbar\omega$.

We already saw that $\hat{p} = \frac{\hbar}{j}\frac{\partial}{\partial x}$

what about energy? If $\hat{E}$ must provide energy, it has to be

$$\hat{E} = j\hbar\frac{\partial}{\partial t}$$

why? Because

$$\frac{\partial}{\partial t}\left[e^{+j(kx-\omega t)}\right] = -j\omega\, e^{+j(kx-\omega t)},$$

so, to have $E = \hbar\omega$,

$$\hat{E}\psi = \cancel{j}\hbar\,\omega\, e^{+j(kx-\omega t)} = \hbar\omega\,\psi = E\psi$$

For this $\psi(x,t) = e^{+j(kx-\omega t)}$ (we already have seen that

$$\frac{\hbar}{j}\frac{\partial}{\partial x}\psi(x,t) = p\,\psi(x,t),$$

and we have just seen that

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = E\,\psi(x,t) \qquad (11)$$

In the first t does not play any role, in the second one yes!

If you know the energy E, you can solve the found differential equation (11), by integrating in time: this is how it evolves in time. Then, Schrödinger came, and completed this equation.

$\hat{E}\psi = E\psi$ — there are two different ways of writing E!

↓ w.r.t. time

↘ w.r.t. $E_K + E_V$

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi(x) \qquad (12)$$

INSPIRATION

This is Schrödinger's equation. No longer found. Energy in fact is no longer a NUMBER, it may change in time.

In general the S. equation (12) is complicated!
First order in time, second in space 3 times

1) This eq. requires complex numbers
2) Is a linear eq.: it satisfies superposition
3) It is deterministic: if you know ψ at $t=0$, you can calculate ψ in each point.

Aside note

If it wasn't clear, what "happens" if you try to "measure" (wrong term as we will see soon) both position and momentum is:

- state 1: wave function → superposition of eigenfunctions (momentum or position)
- state 2: if I measure position, of the bunch of position eigenstates (deltas) I choose 1, discard the other — NO SENSE IN THIS!
- state 3: a δ function has ∞ momenta! White spectrum!

Lecture 6: time evolution and the Schrödinger equation
Allan Adams

We associated operators to observables. Acting on a wave function with an operator is NOT like measuring the observable. It has NOTHING whatsoever to do with measuring the associated observable. It is tempting as a student, but completely wrong. Next lecture.

Review
Postulates

(1) state given by $\psi(x,t)$ = complete specification of state of system

(2) observables are associated to operators, $\hat{A}\varphi_a(x) = a\varphi_a(x)$
they have a natural set of functions, eigenfunctions.

(3) Superpos. Given any two viable wfns, $\psi(x) = \sum_a c_a \varphi_a(x)$,
we can expand it as the superposition of them.
These φ_a may be genuine functions, or eigenfunctions. But, eigenfunctions are more interesting: if $\hat{A} = \hat{p}$ (momentum) over φ_a its eigenfunctions then they are plane waves e^{ikx}. This states that every function can be expanded as sum of eigenfunctions. With respect to other functions, eigenfunctions form a basis, this is a peculiarity of eigenfunctions. Classic example: Fourier

(4) the expansion coefficients are $\mathbb{P}(A=a) = |c_a|^2$,

$$c_a = \langle \varphi_a | \psi \rangle = \int_{-\infty}^{+\infty} dx\, \varphi_a^*(x)\,\psi(x)$$ this is how we find the c_a: as an integral

(was not said in previous lecture) NOTE: this is related to the probabilistic character of quantum: we measure of all possible momenta, just 1.

(5) Collapse: measuring an observable A, we will always measure an eigenvalue a, $\psi(x)$ becomes $\varphi_a(x)$, so the process of measurement changes the state of the system into a single eigenfunction: the former state, given by a bunch of eigenfunctions, collapses into a second, with just (1).

Does it have to be a function of time? No! What happens next!

(6) Schrödinger: given a wave function, we can compute the time derivative

its slope, its "velocity", that is

$$\partial_t \Psi(x,t) = \frac{1}{i\hbar} \hat{E}\, \Psi(x,t) \qquad (1)$$

The time derivative is the rate of variation of $\Psi(x,t)$
So, if we assume that, at $t = t^*$ (t^* a particular time), we know that $\Psi = \Psi(x,t^*)$, we can compute $\partial_t \Psi$ at that moment in time.

We will study how to determine this time evolution.
One of the surprises in quantum mechanics is that time evolution is, in a very specific sense, trivial: it is governed by a linear equation.
This is almost zero! In classical mechanics it's very rare, almost always nonlinear!
For instance, the rate of change of a particle is the product of the force and the force may be a messy function of position, due to capacitors, magnetic fields interacting strange stuff :o

Quantum Zeno problem: a temptation could be to continuously measure the particle, in several times, to see how it evolves. NO! We cannot! If we do, it can NOT evolve! Measure perturbes! Measure changes everything :o Cyndi Lauper said for money.

What about backward evolution? Answer in a second
To get the answer, (1) is: linear, so that the derivative is given by a sum of derivatives the energy computed on a sum of energies!
If Ψ_1, Ψ_2 solve both Sch equation, then $\Psi = \alpha\Psi_1 + \beta\Psi_2$ also solve Sch.

- Unitary: it conserves probability, i.e., knowing everything on Ψ, the integral 1, it must maintain this property. Total probability is 1, always, otherwise things would disappear,
  One theoretical violation is Hawking effect: evaporation of black holes in general relativity, due to quantum effects. Since the black hole sends off radiation, it lose energy and eventually collapses
- if you know initial conditions and derivative, you can study time evolution as solution of an ODE. The system is deterministic. If I know the wave function at some moment of time, I can determine it, unambiguously, at every time. Given full knowledge at a time, I have full knowledge everytime.

Note: evolution is not local, in the sense that time evolution in a point does not depend only on Ψ in that point. This, because of $\hat{E}$, which might be nonlinear (due to strange potentials for example) and "scramble" Ψ too much, making $\partial_t \Psi$ (in a point) depend on several values of Ψ,

The energy operator is a map that, knowing what Ψ is, it tells you how it should be later: but $\hat{E}$ is not "diagonal" in a point-wise sense: several xs could act. (21 min)

Back to the question, we could either back- or for- wood evolve, and integrate forward or backward. But, if at some time we perform a measure, then the wave function collapses, and for evolution will continue starting with this -new- initial condition.
We have two different possibilities of evolution: one is Schrödinger equation, one is collapse to some possible state.

When we "look" at the system, when we measure it, it collapses. When we don't look at it, it follows Schrödinger. This, sounds horrible. This sounds random: the world evolves differently depending on how / when we look at it.
If we simply live with this without concerning about it, the model fits the data, and we can be satisfied just with it. This is the approach of the Copenhagen interpretation: "don't ask, do this, compute this and it's fine": the world is probabilistic, and deterministic if you don't observe. Other people asked the sanity or wisdom to do that.
Cop Out: disavowal of responsability: "not responsible for making sense, just for making predictions"
Recently, the "theory of decoherence" came out (not discussed here) which, roughly, says that when we measure we are interacting with the system with some macroscopic object, washing out quantum effects such as interference fringes.
The question is: if we want to study the system with Schrödinger evolution, it is hard: we have to study motion and trajectory of every particle of the system. If we have a little quantum subsystem that we try to measure, and a "gagillion" of other particles (degrees of freedom), does Schrödinger evolution in the end boil down to collapse for the single quantum microsystem? Yes, but hard to prove.

Let us solve Schrödinger equation (SE)
SE: it is just a linear differential equation.
We have to specify what the energy operator is, just like in $\vec{F} = m\vec{a}$ we have to understand what the force is before solving for p
Strategy (1): use Differential Equation techniques.
Example: the harmonic oscillator

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

The SE for this $\hat{E}$ is:

$$j\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \frac{m\omega^2}{2}x^2\psi(x,t) \qquad (2)$$

we start from knowing an initial condition and solve. Like, NDSolve with Mathematica. We will solve this, in a couple of lectures.
So given $\hat{E}$ for some potential, we end up to an equation somehow similar to (2).

Strategy (2)
Given $\hat{E}$, some specific energy operator, we can solve such PDE in many ways.
In 3 ways:

a) Brute force (Mathematica, or mathematicians...) } quantum physics
b) Extreme cleverness (learning and exploiting physics)
c) Numerically

41 min

As first examples today, we will study energy eigenfunctions
Once we understand how a single energy eigenfunction evolves in time, once we understand that solution, we are going to exploit linearity of SE to write a general solution.
Let us assume that our eigenfunction $\psi(x,t)$ is, at $t=0$, an energy eigenfunction $\phi_E(x)$:

$$\psi(x,0) = \phi_E(x), \qquad (3)$$

→ initial condition of the system.

where, then, $\phi_E(x)$ is such that $\hat{E}\,\phi_E(x) = E\,\phi_E(x)$

this means that if we measure the energy of the system described by $\psi(x,t)$ at $t=0$, we measure energy E with 100% probability: the "superposition" is given by a single contribution (3)!

The Schrödinger equation is:

$$j\hbar \frac{\partial}{\partial t}\psi(x,0) = E\psi(x,0)$$

↳ E is a number!

So,

$$\frac{\partial}{\partial t}\psi(x,0) = -\frac{jE}{\hbar}\psi(x,0)$$ the derivative equal to it self!

$$\rightarrow \boxed{\psi(x,t) = e^{-j\frac{Et}{\hbar}}\psi(x,0)} = e^{-j\frac{Et}{\hbar}}\phi_E(x)$$

What time evolution is? Well, if we start from a state which is on energy eigenstate, remains in an energy eigenstate with the same energy eigenvalue, and just its phase changes, big rotating with constant velocity, $\frac{E}{\hbar}$

Dimensions:

$$\frac{Et}{\hbar}, \quad [\hbar] = [E][t] = pX$$

Note: at $t=0$, we get 1. And energy does not change over time, as well as probability.

Moreover, we could recognize that $E = \hbar\omega$, so $\omega = \frac{E}{\hbar}$, then

$$\frac{Et}{\hbar} = \omega t \; !$$

So, from a state

$$\psi(x,t) = e^{-j\omega t}\phi_E(x),$$

these states are called "stationary states". This because if we are in this state, at a time t, if we measure probability density,

$$\mathbb{P}(x,t) = |\psi(x,t)|^2 = |\phi_E(x)|^2 \; : \text{independent of time!}$$

In this sense, stationary: probability is invariant of time!
Consequences: if we study the expectation value of X,

$$\langle X \rangle_{\psi(x,t)} = \int dx\, \mathbb{P}(x,t)\, x = \int dx\, |\phi_E(x)|^2 x\, dx = \langle X \rangle_{t=0}$$

the expectation value does not change!

Question from Allan: are all systems, always, in an energy eigenstate?
NO! By changing time, we can move so $\langle x \rangle$ changes! And this does not happen in an energy eigenstate!
Other question: are ~~systems~~ any state ever, truly, in energy eigenstates?
Is there any object in the world that is truly described by an energy eigenstate? NO: things do not remain invariant in time!
So, why do we talk about them?
Because we can use them as a basis, by exploiting the superposition principle!
Suppose $\Psi_n(x,t) = e^{-j\omega_n t} \phi_{E_n}(x)$, $E_n = \hbar\omega_n$,
and the subscript n labels different energy eigenfunctions ϕ_{E_n}. So, $\Psi_n(x,t)$ is a solution of SE. So, we can, by linearity,

$$\Psi(x,t) = \sum_n c_n \Psi_n(x,t), \quad (3)$$

and this will be a solution of SE as well

Question from audience: let's say that we measure energy, and the system collapses in an energy eigenstate. Is it ideally possible?
NO! How precisely can we measure energy? Practically, experimentally! There is a fundamental bound, just like for the uncertainty principle!
To measure E we could measure the frequency ω. But, we need to measure for a long time, to be sure that the system doesn't change.
Frequency confidence is bounded by:

$$\Delta\omega\, \Delta t \gtrsim 1 \qquad \text{greater approximately } (\gtrsim) \text{ than } (1)$$

If we multiply both times $\hbar$,

$$\Delta E\, \Delta t \gtrsim \hbar$$

To measure energy with arbitrary precision, we have to wait ... FOREVER!

coming back to (3), another way to say that (3) is a solution of SE, if we know that $\Psi(x,0)$ is equal to

$$\Psi(x,0) = \sum_n c_n \phi_{E_n}(x),$$

then we know that

$$\Psi(x,t) = \sum_n c_n e^{-j\omega_n t} \phi_{E_n}(x)$$

So, having solved once the SE for energy eigenstates, allow to ~~route~~ and exploit the result for general superposition as well.

One more argument: given an energy operator $\hat{E}$, we find, imediately, the set of eigenfunctions $\{\phi_{E_n}\}$, and any $\Psi(x,0)$ can be expanded with them

then we can compute the eigenfunctions just for the initial condition, and then evolve in time just the eigenfunctions!!!
We just need to compute the c_n! The expansion coefficients!
Meanwhile, the $\{c_n\}$ is related to the probability of being in an eigenstate!

As we did for the momentum operator, $\hat{p}$, with its eigenfunctions $\left\{\frac{e^{jkx}}{\sqrt{2\pi}}\right\}$,

$$p = \hbar k,$$

A generic $f(x)$ could be expanded as:

$$f(x) = \int dk \, \frac{1}{\sqrt{2\pi}} e^{jkx} \tilde{f}(k)$$

this is exactly the Fourier theorem

The same is true also for the energy operator. And for all observables in general: the eigenfunctions form a basis on the space of all "good functions", so that an arbitrary function can be expanded in that basis.

Example, position:

$$\hat{x} \longrightarrow \hat{x}\, \delta(x-y) = y\, \delta(x-y)$$

so, $f(x)$ could be represented as:

$$f(x) = \int dy \, \delta(x-y)\, f(y) \qquad \text{(seen lect. 5 also)}$$

Any function can be expanded as a superposition of eigenfunctions of any operator of our choice.
The Fourier theorem is an example!

Example: free particle
The free particle is a particle whose energy operator has no potential whatsoever:

$$\hat{E} = \frac{\hat{p}^2}{2m}$$

Mathematical aside: eigenfunctions do not necessarily live in the space of "non-stupid" smooth, normalizable functions! Think of δ (not even a function) or $\exp(jkx)$ (∞ support).
But, they live in the closure of such state, meaning that we can find a sequence of non-stupid functions that will converge to those silly functions.
For example, for δ, we can build it as a sequence of Gaussian functions!

So, $\hat{E} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

which are the energy eigenfunctions?

$$\hat{E}\,\phi_E = E\,\phi_E \iff -\frac{\hbar^2}{2m}\phi_E''(x) = E\,\phi(x)$$

or

$$\phi''(x) + \frac{2mE}{\hbar^2}\phi(x) = 0$$

We can notice that $\left[\frac{2mE}{\hbar^2}\right] = \frac{1}{m^2}$, so we call $k^2 = \frac{2mE}{\hbar^2}$,

and the solution is:

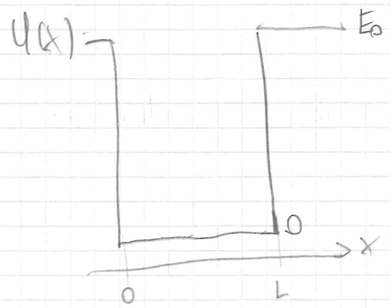
$$\phi_E(x) = Ae^{jkx} + Be^{-jkx} \quad \text{such that} \quad E = \frac{\hbar^2 k^2}{2m}$$

this is the solution of the energy eigenfunction equation

Note that this is NOT the SE! Schroedinger equation is about time, not just about energy eigenfunctions!

One more example: a particle in a box

This is a system with a deep well,



idealization: infinitely high ($E_0 \to \infty$)

and with sharp corners

Let us find the energy eigenfunctions!

What is the probability to find a particle in $x<0$ or $x>L$?
It is 0, because potential is ∞, so it would mean having particles with ∞ energy! And no, not possible.

In this view the boundary condition is $\psi = 0$ outside the box.

So, $\psi(0) = \psi(L) = 0$!

Inside the box, the equation is exactly the same as before, so the solution is the same! with sines and cosines,

$$\phi_E = \alpha\cos(kx) + \beta\sin(kx).$$

If $x=0$, $\psi(0)=0$, $\cos(kx)\neq 0$, so $\alpha = 0$

At $x=L$, $\beta\sin(kx) = 0$ at $x=L$, so

$kx = 0$ @ $x=L$, so $kL = n\pi$, $\boxed{k = \frac{n\pi}{L}}$,

so

$$\phi_{E_n} = A_n \sin\left(\frac{n\pi}{L}x\right),$$

$$E = \frac{\hbar^2 k_n}{2n} = \frac{\hbar\pi^2(n+1)^2}{2nL^2}$$

So, the first eigenfunction is a sine, and its eigenvalue is NOT 0: it is impossible for a particle in a box to have an energy lower than E_0, which is not 0. We can not have lower energy!

Energies are discrete, spaced one from another! This is quite a peculiar fact!

Already in the most trivial examples of solving SE or actually before them, just finding the energy eigenvalues, we discovered that the allowed energies of the particle are discrete, and never 0.

Just like the spectrum of light from an atom of hydrogen: And no one ever found a 0 energy beam of light!

Lecture 7: More on energy eigenstates

Recall:

$$(f|g) = \int_{-\infty}^{+\infty} f^*(x)\, g(x)\, dx \qquad (1)$$

A nice property of our eigenfunctions is that to different eigenvalues correspond different eigenfunctions, i.e., they are orthogonal with regard to the "dot product" (1).

Given for instance φ_{x_0} the eigenfunction of $\hat{x}$ with eigenvalue (position) x_0,

$$\hat{x}\,\varphi_{x_0}(x) = x_0\,\varphi_{x_0}(x), \qquad \left(\varphi_{x_0}(x)\,\middle|\,\varphi_{x_1}(x)\right) = \delta(x_0 - x_1)$$

Similarly,

$$\hat{p}\,\varphi_k(x) = \hbar k\,\varphi_k(x) \longrightarrow \left(\varphi_k(x)\,\middle|\,\varphi_{k'}(x)\right) = \delta(k-k')$$

Note this normalization! Normalized to 1!

Moreover, this (my observation) is quite similar to the duality of Fourier transform

NOTE: different eigenfunctions MAY have the same eigenvalue! (one of the 3 quantum wells!). Several states with same energy! This is:

$$\left.\begin{aligned}\hat{E}\,\varphi_1 &= E_1\varphi_1\\ \hat{E}\,\varphi_2 &= E_1\varphi_2\end{aligned}\right\}\ \text{degenerate eigenfunctions.}$$

Given $\varphi^* = \alpha\varphi_1 + \beta\varphi_2$, φ^* IS an energy eigenfunction!

This is why we said some lecture ago, IS NOT A GENERAL PROPERTY (eigenstate with dimension greater than 1) (eigval multiplicity > 1)

But, it is possible to find a set of orthogonal eigenfunctions even with those degeneracies (not proved here, just, will be assumed): spectral theorem!

Then, as we already have seen, the "spectral theorem" (expansion) =

$$\psi(x) = \int dx_0\, \delta(x-x_0)\, \psi(x_0) \qquad \text{expansion in position eigenfunctions}$$

$$= \int dk\, \frac{1}{\sqrt{2\pi}}\, e^{jkx}\, \tilde{\psi}(k) \qquad \text{" " momentum " (Fourier theorem)}$$

$$= \sum_n c_n\, \varphi_n \qquad \text{" " energy "}$$

But... Why a sum, for energy eigenstates instead that an integral? This will become apparent at the end of today lecture

Sometimes the energies allowed for our system are discrete. This, when we have bound states, that are trapped in some region and cannot escape. Continuous (instead than discrete), when the states can arbitrarily flow away.

Free particle: continuous energy spectrum
Well: discrete

We can also have both of the situations.

We know that $\psi(x,t) = \varphi_n\, e^{-j\frac{E_n t}{\hbar}}$

The fact that these functions have such a well-defined time evolution, allows us to write:

$$\psi(x,t) = \sum_n c_n\, e^{-j\frac{E_n t}{\hbar}}\, \varphi_n(x) \qquad \omega_n := \frac{E_n}{\hbar}$$

So, energy eigenstates are convenient to solve the time problem.

Finite well



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

$$\hookrightarrow \varphi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x), \quad k_n = \frac{(n+1)\pi}{L}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m}$$

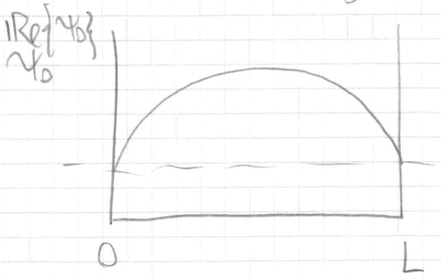
So,

$$\psi(x,0) = \sum_n \varphi_n(x)\, c_n$$

What does this mean. In this system, if I take a particle and throw in here in some arbitrary state, so that at $t=0$ it has that dependence, I can expand it in this way: any function comes from the superposition of such energy eigenstates! Moreover, at time t,

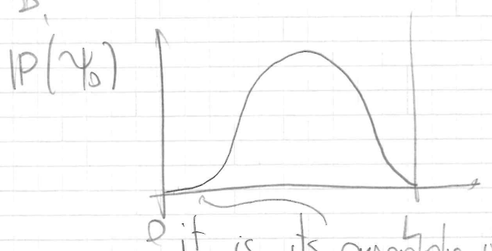
$$\psi(x,t) = \sum_n \varphi_n c_n e^{-j\frac{\pi^2 \hbar^2}{2n} t}$$

Now, let us look at the wave functions and probabilities for the lowest lying states.
For instance, focusing on the ground state $n=0$, ψ_0,



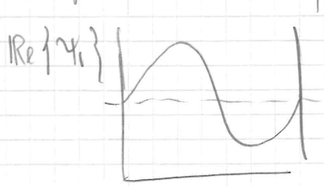
it looks like a sine. It is a sin.

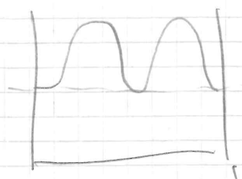
b,



it is its ground state, its square!

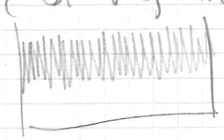
If we take a charged particle and put it in this box, where does it spend most of its time? Well, it has some energy, so it bounces back and forward, but... then, it spends the same amount of time in each position!
INSTEAD, here, the probability distribution is NOT constant!
(the fact that ψ_0 goes to zero at 0, L is related to... the transparency of the diamond!)





even worse! ∅ probability to find in middle

Instead, at very high energies, we will add more and more zeros:



that, effectively (in average), leads to an almost constant probability distribution!

Note: in quantum mechanics, every time something good happens it is because of { interference / superposition } ! =)

Clicker's test !!! min 27.

Answer: (B) : $\hat{E}(\psi_1+\psi_2) = \hat{E}\varphi_1 + \hat{E}\varphi_2 = E_1\varphi_1 + E_2\varphi_2$

Except, we have 0 energy. Is it possible?

Note! $E=0$, is referred to the value of potential energy at infinity: it is a difference to this!
Still, it does not see us!

$$\hat{E}[\psi_1+\psi_2] \neq E_1\psi_1 \quad (E_2=0)\ ! =($$

$$[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} \ ; \ \hat{p}_1$$

$$[\hat{p},\hat{x}] = -[\hat{x},\hat{p}] \quad =)$$

$$i\hat{p} + c\hat{x} = \hat{c}\hat{x} + i\hat{p} \ ! \quad =) \text{ we can apply commutative property!}$$

Non-degenerate: cannot be stationary because the sum of two energy eigenfunctions is NOT an energy eigenfunction, so, NEVER.

It would mean that the sum is NOT an energy eigenstate.

(NO), (it is) (C) : it depends.

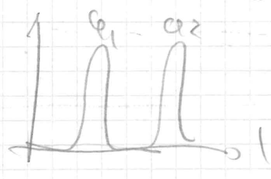
$$\psi(x,t) = \varphi_1(x)e^{-j\omega_1 t} + \varphi_2(x)e^{-j\omega_2 t}$$

$$P(x,t) = \|\psi(x,t)\|_2 = \left(\varphi_1^* e^{+j\omega_1 t} + \varphi_2^* e^{+j\omega_2 t}\right)\left(\varphi_1 e^{-j\omega_1 t} + \varphi_2 e^{-j\omega_2 t}\right) =$$

$$= |\varphi_1|^2 + |\varphi_2|^2 + \varphi_1^*\varphi_2 e^{j(\omega_1-\omega_2)t} + \varphi_2^*\varphi_1 e^{-j(\omega_1-\omega_2)t}$$

Stationary! Constant NOPE!

If φ_1 and φ_2 are non-overlapping in x, first so they sum is stationary!!!!



The product is point-wise 0!

Probability to : $\frac{1}{2}$

Wider well energy of ground state... lower I would say!

Wave function: must be
- smooth
- normalizable
- satisfy problem's boundary conditions!

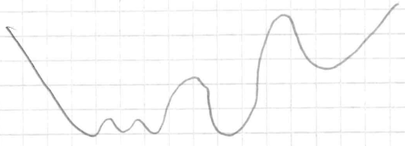
even if it is NOT an energy eigenfunction

End Claver =C

Back to Energy Eigenvalues

Qualitative behavior of energy eigenfunctions: what could we say about its structure? (it's = of an energy eigenstate)

Let's say that someone hands me a certain potential $U(x)$:
we can draw it



what are the energy eigenvalues of this crazy thing?!

We know that the energy eigenvalue equation is:

$$-\frac{\hbar^2}{2m}\varphi_E''(x) + U(x)\varphi_E(x) = E\varphi_E(x)$$

(drop + depedence)

This, cannot be solved analytically.
However, we could say something about how φ_E look like.

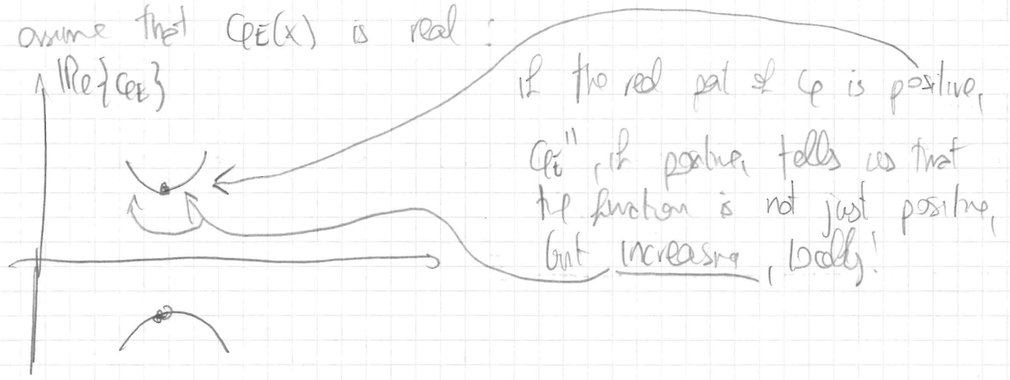
Let us manage this equation into a more convenient form.

$$\frac{\varphi_E''(x)}{\varphi_E(x)} = -\frac{2m}{\hbar^2}\underbrace{\left(E - U(x)\right)}_{\text{RHS}}$$

The second derivative, divided by φ_E, equals this.

The second derivative of a function tells us how the slope of the function changes. So the CURVATURE.

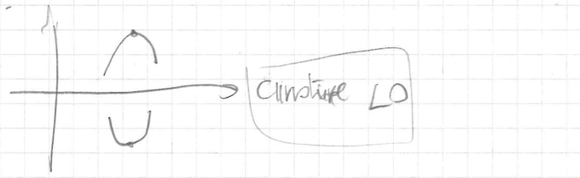
Let us assume that $\varphi_E(x)$ is real:



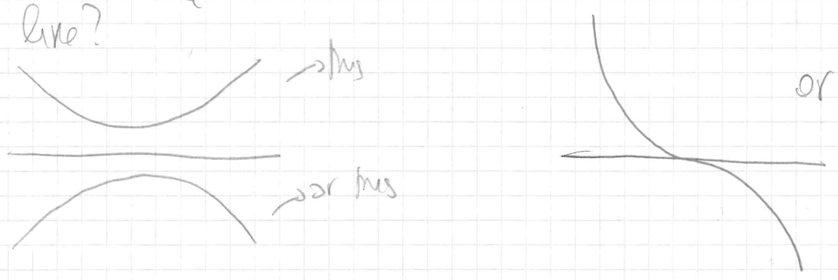
If φ is negative, and the RHS is positive, then φ'' is negative!

$\frac{\varphi_E''}{\varphi_E}$ is the CURVATURE. If positive, the wave function curves away from the axes.

If it is negative,



Imagine that $\frac{\varphi''}{\varphi}$ is constant, positive, K^2 what does the solution look like?

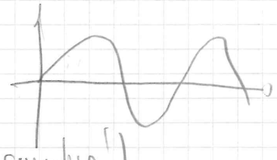


These functions are exponentials: e^{+Kx} or e^{-Kx}, and an arbitrary solution of

$\frac{\varphi''}{\varphi} = K^2$ is $A\underbrace{e^{+Kx}}_{\text{growing exponential}} + B\underbrace{e^{-Kx}}_{\text{collapsing exponential}}$

On the other hand, if we have

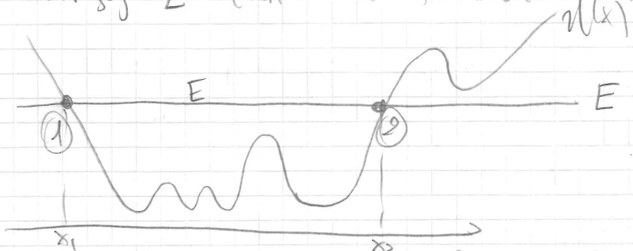
$\frac{\varphi''}{\varphi} = -K^2$, we have negative curvature, so... SINUSOIDS! (always negative curvature!)



And the general solution is

$A e^{jkx} + B e^{-jkx}$

So, coming back to our strange $U(x)$, we have first to pick an energy E (can't find the solution without figuring the energy)(



If we have a classical particle and roll it from 2 (give energy E), it reaches 2 and then go up and down, back and forward. But $x > x_2$ is, classically, a forbidden region!

$x_1 < x < x_2$ is a classically allowed zone, because $E > U(x)$

$x < x_1 \wedge x > x_2$ " " " forbidden " " $E < U(x)$

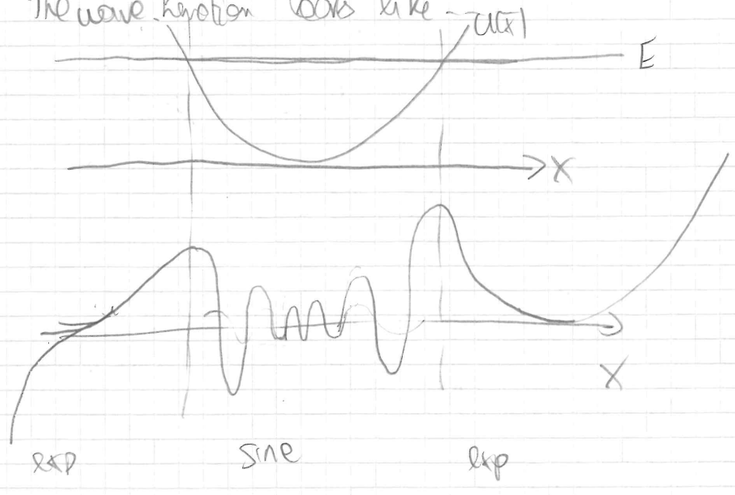
If $E \geq U(x)$, we know that curvature is negative, so the wave function should be sinusoidal.

$E < U(x)$, wave function exponential!

Simple example: a potential that looks like this:



the wave function looks like



For exponentials, the bigger is the difference, the bigger is curvature, so the exp argument. Similarly, for sinusoidals!

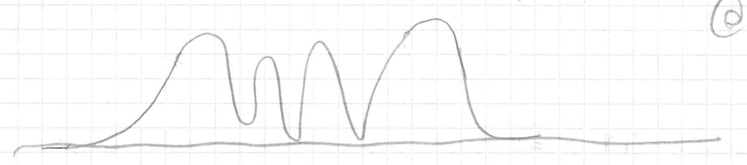
So, in the middle, the wavefunction oscillates rapidly!
When we approach the classical turning point, the variation of the function, so the oscillation rate, becomes less rapid: the slope changes less rapidly. This has two consequences: the wavelenght gets longer (the period), because the curvature is smaller, and the amplitude grows, because it keeps on having a positive/negative slope for longer ranges.
Then we reach the classical turning point!

Since curvature has to be positive, functions will diverge.
@ the turning point, "m" is the same in and out, so both ψ and ψ' must be continuous.

This sketch is bad because of divergence: this wave function diverges so it is NOT normalizable!

So this energy, this function, is not allowable! 1h14

But, if we would reduce E, we would reach (for continuity and for @ turning point),



by matching a (with luck, fortune) a perfect combination of growing and decreasing exponentials that compensate, leading to a normalizable function.
There is provably (!!) very exact values that allows this, an allowed value.
If we do not match that very exact value, the wave function will not have these exact compensations will diverge and then be not normalizable
The allowed, discrete ones are the peculiar values that allow to have normalizable wavefunctions
This is the first step towards understanding why the atom of hydrogen has discrete spectrum. See you next time.

Lecture 8: Quantum Harmonic Oscillator Part 1

Barton Zwiebach

Before starting with the harmonic oscillator, we want to discuss why higher order solutions have more nodes, and arguments for intuition.

If you have a Sch. equation for an energy eigenstate, which has form

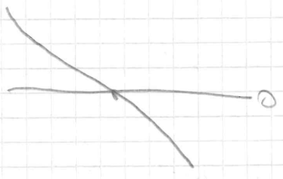
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x), \quad (1)$$

If you look for a bound state, it means that you are looking for a wave function that goes to 0 as $x\to\infty$: a probability function that collapses, that is normalizable, and, if you want to solve (1) to find bound states, you fix E and compute ψ.
But, since you need normalizable solutions, you cannot fix E: E may have very specific values.

If $V(x)$ is a smooth potential, then if $\psi(x_0)=0$ and $\psi'(x_0)=0$, then it means that $\psi(x)=0\ \forall x$: this is a trivial solution, this does not represent a particle!
We cannot have something like



NOT ALLOWED!
Not possible to have both finite and derivative 0.
If we have a 2nd order ODE, ~~and~~ its state is completely determined by knowing those two values. It is an "initial condition"!

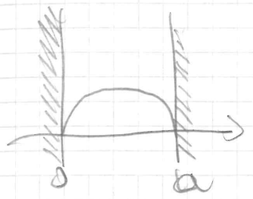


this is a NODE, and it is possible!

Another claim: for bound states in 1 dimension, no degeneracy is possible.
You will never find 2 bound states with the same energy.
Not possible to have DIFFERENT bound states with the same energy.

Not proved here. But very important!

Infinite well



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

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left[(n+1)\frac{\pi}{a}x\right] \qquad E_n = \frac{\hbar^2(n+1)^2}{2ma^2}$$

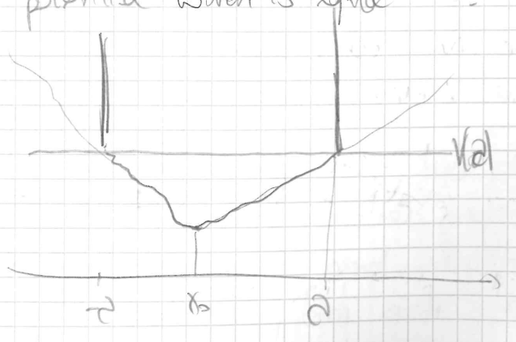
Technically, E_0 has NO NODES! It is 0 just at the extrema! 1 node is something in the middle.
The ground state has no nodes.
E_1, ψ_1 has 1 node, ψ_n has n nodes!
This result is true for extremely general potentials!
This is a very nice result, but hard to prove, so we will study an argument with much physics but not so rigorous.

Given a smooth $V(x)$,
that goes to ∞ when $x\to\infty$,



in this case, you have an ∞ number of bound states. Fact, we will not try to prove it easily.
The ground state will have no nodes, the first will have 1, and so on.
We are going to produce, in order to understand this, what we call "screened potentials".
Let x_0 be the abscissa corresponding to the lowest point of the potential: x_0 : $V(x_0) = \min(V(x))$
The screened potential $V_0(x)$ is a potential which is equal to:

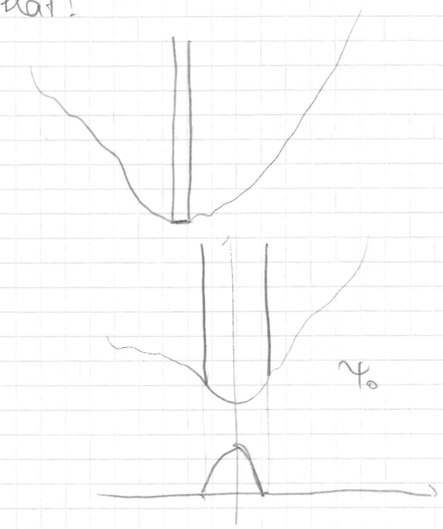
$$V_0(x) = \begin{cases} V(x), & |x| < a \\ \infty, & |x| > a \end{cases}$$



The screened potential is the same, for $-a<x<a$, and ∞ out.

Now, we could try to find the bound states of the screened potential and, as we remove the screen, we would find, for $a \to \infty$, the bound states of the original potential (the $V(x)$ would be more similar to $V(x)$)

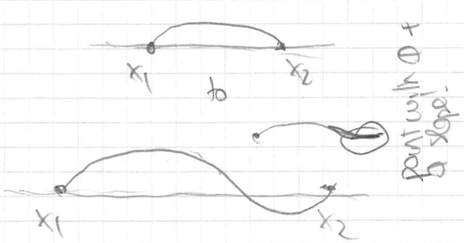
If $a \to 0$, so $a = \varepsilon$, I have a very tiny potential, from $-\varepsilon$ to ε. So, as an approximation, the potential is almost flat: just like the infinitely narrow square well. Being the minimum, 0 denotes it is flat!



Here, we have a tiny ground state, so, as we increase a, the size of the screen, what do we see?

The wave function still must vanish at the screen; and the shape may be more or less close to a sine.

As we have wider screens, is it possible to have a node?
Well, if this would happen, it ~~can~~ must mean to go from

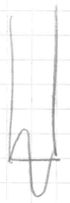


So, by stretching the x_1, x_2 $(-a, a)$ interval, the slope must go down, down, down, until flipping to negative.
So, at some point, the slope must be 0.

And this can not happen, in the same point! No 0 and 0 slope!
This turn can't flip!
Another turn is a Lebesgue like



this. But, our potential is
varying continuously so, at some stage, when we keep stretching the interval, some degeneracy should be born,
but, it is not possible!

There is no way, because, by stretching properly, we would find the evil $\psi' = \psi = 0$!
There is No way to produce a node by stretching!
So, ground state has NO nodes! This is a "physicist proof" =)
For excited states, like, ψ_2  or ψ_1  ,

so we increase them, we cannot create other nodes, for the same reason!

And, does this E_2, E_1 or whatever be greater than the ground state?
Well, with the same screen, ψ_1 has more energy than ψ_0. When we enlarge, this E_1 remains above E_0 when we enlarge the screen because, ~~===~~ in this case, it would have, at some point, the same energy (if the two energies switch, then at some a they are the same, but ~~-~~ NO DEGENERACY IS POSSIBLE! =))
The argument is based on this "continuous deformation" procedure.

$E_n > E_{n'}$, $\quad n > n'$

The more the nodes, the greater is energy.

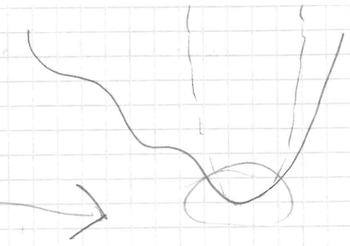
Harmonic Oscillator

This is the most famous quantum mechanics problem because it is useful in many, many applications!
Its characteristic is:

$$\hat{E} = \frac{\hat{p}^2}{2m} + \underbrace{\frac{1}{2} m \omega^2 \hat{x}^2}_{V(x)} \quad (2), \quad [\omega] = \frac{1}{\text{time}} = \frac{2\pi}{T} \qquad T: \text{period of oscillator}$$

in classical mechanics, if oscillates at ω.
ω is the angular velocity, or angular frequency.
What defines an oscillator? The $V(x)$, potential, quadratic in x!
In any sort of arbitrary potential, whenever we have a minimum, or every time that the first derivative vanishes, but not the

2nd derivative. Then we can approximate such potential with that of the harmonic oscillator (qua is this the parabolic approximation?! =))
The real potential is well approximated in a reasonable region



We want to calculate and solve Schrödinger Eq in this case.

Which are its energy eigenstates?
What are the Hamiltonian like (2), which is the ground state?
Well, gotta find it!
But, if you want an approximate value, dimensional analysis will be roughly sufficient! =)
How do we produce an energy, with the constant $\frac{1}{2} m \omega^2 x^2$? Well, $\hbar\omega = E_1$ so, we will actually see that it is actually half of this.
Another interesting quantity is length. How do we construct it? Well, if we know that energies go like

$\frac{\hbar^2}{m a^2}$, and "a" is a length,

$p = \frac{\hbar}{\lambda}$ For De Broglie, so a is a length

But, also, $E = m^2\omega^2 a^2$, so,

$a^4 = \frac{\hbar^2}{m^2\omega^2} \rightarrow \boxed{a^2 = \frac{\hbar}{m\omega}}$ thus a a length!

This is important, because can be used as a length reference.
If someone asks: in the oscillator, in the ground state, how far is the particle oscillating?
Probably about $\sqrt{\frac{\hbar}{m\omega}}$ (and it is about right.

What is Sch. equation?

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi \qquad (3)$$

we don't know neither ψ nor E. How to find them?

Before studying two wonderful strange methods from Allen Adams, we will study one in our life, the direct, uninspired solution method.
This, because knowing a hard, but general method, is useful and very general.
Today we struggle with the differential equation!!!

The (3) is fairly complicated, also due to the presence of all these constants.

First step: cleaning up the equation! Remove units!
Let us clean the right side by cleaning with energies: multiply by

$\frac{2}{\hbar\omega}$

$$= -\frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2} + \frac{m\omega}{\hbar} x^2\psi = \overbrace{\frac{2E}{\hbar\omega}}^{\varepsilon}\psi = \varepsilon\psi$$

Let us call ε the dimensionless value of energy! No units!
Note that $\left[\frac{m\omega}{\hbar}\right] = \frac{1}{[\text{length}]^2}$: we proved $a = \frac{\hbar}{m\omega}$! So, let us say that

$x = au$, with u a new variable!

$$\frac{d}{dx} = \frac{d}{du}\frac{du}{dx} = \frac{d}{du}\left(\frac{dx}{du}\right)^{-1} = \frac{1}{a}\frac{d}{du}$$

$$\frac{d^2}{dx^2} = \frac{d}{dx}\left[\frac{d}{dx}\right] = \frac{d}{dx}\left[\frac{1}{a}\frac{d}{du}\right] = \frac{du}{dx}\frac{d}{du}\left[\frac{1}{a}\frac{d}{du}\right] = \frac{1}{a^2}\frac{d^2}{du^2}$$

So, since $\frac{\hbar}{m\omega} = a^2$, we get (u is a dimensionless quantity!)

$$-\frac{d^2\psi(u)}{du^2} + u^2\psi(u) = \varepsilon\psi(u) \qquad (36)$$

How to solve now this clean equation? Well, we can't fix ε!
How does the solution look as $u \to \infty$? Well, we cannot solve it, but we can understand something. $u^2\psi$ is much greater than $\varepsilon\psi$, so

if we fixed ε, or it is at least small, the equation sort-of becomes

$$\psi'' = u^2 \psi$$

How to solve this is not so obvious: it is not a power of u for sure. Because when we differentiate we should lower the degree rather than increasing it; NOT TRIVIAL to find something that increases the degree (not a polynomial for sure).

Something like

$$e^{u^2} \longrightarrow \frac{d}{du} e^{u^2} = 2u e^{u^2}$$

Something like that.

Let us try something like:

$$\psi(u) = e^{\alpha u^2/2} \qquad \alpha \in \mathbb{R}$$

If we are interested in $u \to \infty$, we can put u^K in front of everything, and the asymptotic behavior will not change!

$$\psi(u) = u^K e^{\frac{\alpha u^2}{2}} \qquad (4)$$

probably, $\alpha < 0$ to have converging functions. However,

$$\psi' = \alpha u u^K e^{\frac{\alpha u^2}{2}} + K u^{K-1} e^{\frac{\alpha u^2}{2}}$$

$$\psi'' = (\alpha u)^2 u^K e^{\frac{\alpha u^2}{2}} + \dots = (\alpha u)^2 \psi + \dots$$

and all these terms, the following ones will surely have lower powers of u, because the first was the main one in this case!

$$= \alpha^2 u^2 u^K e^{\frac{\alpha u^2}{2}} \left[1 + \frac{2K+1}{\alpha} \frac{1}{u^2} + \frac{K(K-1)}{\alpha^2} \frac{1}{u^4} + \dots \right] =$$

$$= \alpha^2 u^2 \psi \left[1 + \frac{2K+1}{\alpha} \frac{1}{u^2} + \dots \right],$$

so, when $u \to \infty$, the solution works, discarding the negligible terms, and then $\alpha^2 = 1$! Our guess, for $\alpha^2 = 1$, is equal to (4)!

But, $\alpha^2 = 1 \Rightarrow \alpha = \pm 1$ (we choose $\alpha = -1$ to have a normalizable solution!

So, for $|u| \to \infty$,

$$\psi(u) = A u^K e^{-\frac{u^2}{2}} + B u^K e^{+\frac{u^2}{2}},$$ we choose $\boxed{B = 0}$:=)

↳ this is the good integral! We want $B = 0$!

How can we use this insight, from these calculations, to compute the solution?

The idea is to change variables a little bit, so write

$$\psi(u) = h(u) e^{-\frac{u^2}{2}}$$

What is $h(u)$? We are just writing ψ, whatever it is, as the product of a certain $h(u)$ times the other! This is a substitution for u^K!

In fact, what we are doing is:

$$\psi(u) = \psi(u) \frac{e^{-\frac{u^2}{2}}}{e^{-\frac{u^2}{2}}} = \frac{\psi(u)}{e^{-\frac{u^2}{2}}} e^{-\frac{u^2}{2}}$$

($\psi(u)$ in the numerator, $e^{-\frac{u^2}{2}}$ in the denominator, $h(u)$ = their ratio)

What we do is: because of this very clever factor $h(u)$, maybe the resulting differential eq. will be simpler! with h unknown function! In practice, $h(u)$ is $\psi(u)$, with some information already included: the asymptotic behavior!

Maybe h is just a polynomial! Who knows!

Plugging into (36), we have (calculations not reported),

$$\frac{d^2 h(u)}{du^2} - 2u \frac{dh(u)}{du} + (\varepsilon - 1) h(u) = 0 \qquad (5)$$

Now, this is a tractable equation! How to solve this? Tractable, but not trivial!

Power series expansion!

$h(u) = a_0 + a_1 u + a_2 u^2 + \cdots$ (1)

and plug just few terms here. We find that a_2 is determined by a_0, a_3 by a_1, and so on. Not trivial, you have to substitute!

It is convenient to see just how works with few terms!

Then, after finding some patterns, start with the sophisticated analysis!

That is:

$$h(u) = \sum_{n=0}^{\infty} a_n u^n$$

$$h'(u) = \sum_{n=0}^{\infty} n\, a_n\, u^{n-1}$$

$$h''(u) = \sum_{n=0}^{\infty} n(n-1)\, a_n\, u^{n-2}$$

$$u\, h'(u) = \sum_{n=0}^{\infty} n\, a_n\, u^n$$

we need these two

But, to have everything function of u^n, is:

$n-2 = m \longrightarrow n = m+2$

Note that

$$\sum_{n=0}^{\infty} n(n-1)\, a_n\, u^{n-2} = \sum_{n=2}^{\infty} n(n-1)\, u^{n-2}$$

$n = m+2$

$$\hookrightarrow h''(u) = \sum_{m=0}^{\infty} (m+2)(m+1)\, u^m = \sum_{n=0}^{\infty} (n+2)(n+1)\, u^n$$

$m \mapsto n$

So, let just plug this in our differential equation (5):

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1)\, a_{n+2} - 2n\, a_n + (\varepsilon - 1) a_n \right] u^n$$

In order to have this whole equation be 0, the coefficient must be 0!

Please note that

$$-2n\, a_n + (\varepsilon - 1) a_n =$$

So

$$a_{n+2}(n+2)(n+1) - (2n+1-\varepsilon)\, a_n = 0$$

So,

$$a_{n+2} = \frac{2n+1-\varepsilon}{(n+1)(n+2)}\, a_n$$

that is effectively a relationship between a_n and a_{n+2}! A very nice recursive relationship!

Then, by defining two values: (a_1, a_0), you can find ALL THE COEFFICIENTS!

$a_0 = h(0)$!

$a_1 = h'(0)$!

Facts (about our solution)

The solution is fixed by providing $h(0)$ and $\left.\frac{dh}{du}\right|_{u=0}$!

Unfortunately, this series has to be compared 'till ∞, and coefficients do not appear to decay so much (a little...). This seems contradictory with our former idea: exponential, times u^k, fixed power (k)! This $h(u)$ seems rather different than just a simple u^k.

What does happen, then, for large n?

$$a_{n+2} \approx \frac{2n}{(n+1)(n+2)}\, a_n \approx \frac{2}{n}\, a_n$$

So: if we take a power series expansion, whose coefficients behave like that, how about is it at ∞? They decay, and ... It has a pretty bad behavior =C

In fact, as "guess", as an intuition, how does e^{u^2} behave? As a power series?

$$e^{u^2} = \sum_{n=0}^{\infty} \frac{1}{n!} (u^2)^n$$

This has just even powers, so, changing letters,

$$= \sum_{\substack{j=0,2,4,\dots \\ \text{even}}} \underbrace{\frac{1}{\left(\frac{j}{2}\right)!}}_{c_j = \frac{1}{\left(\frac{j}{2}\right)!}} u^j$$

this c_j is:

$$\frac{c_{j+2}}{c_j} = \frac{\left(\frac{j}{2}\right)!}{\left(\frac{2+j}{2}\right)!} = \frac{1}{1+\frac{j}{2}} \approx \frac{2}{j}$$

That is exactly the same rate as before!---
So if the series goes to ∞, it has the very same behavior!
Diverging as e^{u^2}!
TERRIBLE!

If this series would not terminate, all this calculation would be pointless
But, happily, the series may terminate! Because "n" are integers!
So maybe for some energies, integer, $2j+1-\varepsilon=0$, so that $a_j=0$,
and from there on, everything is 0: the series may terminate, for some integer ε !!

THIS MAKES US UNDERSTAND WHY ENERGY IS QUANTIZED
The series must terminate, otherwise it blows up!

$2j+1-\varepsilon=0$, makes $a_{j+2}=0$!
And,

$$h(u) = a_j u^j + a_{j-2} u^{j-2} \dots$$

AND THIS IS THE SOLUTION (substitute $j \leftrightarrow n$)

$$h(u) = a_n u^n + \dots$$

The full solution is:

$$\psi(u) = h(u)\, e^{-\frac{u^2}{2}}$$

What about ε?

If $\varepsilon_n = 2n+1$, $= \frac{E_n}{\left(\frac{\hbar\omega}{2}\right)}$,
we just found that

$$E_n = \frac{\hbar\omega}{2}(2n+1) = \hbar\omega\left(n+\frac{1}{2}\right)$$

This is a very famous result: the energy level of the harmonic oscillator!
Moreover, $h(u) = a_n u^n + \dots$
are called Hermite functions! And notation is fixed so that

$$n \longrightarrow 2^n$$

So,

$$h_n(u) \longrightarrow H_n(u) = 2^n u^n + \dots \quad \text{(nice normalization)}$$

The Hermite polynomial is that solving this equation! (5)!

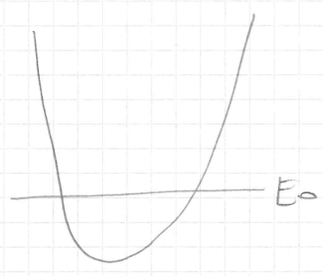
If you want to generate them efficiently, there is the so-called generating function

$$e^{\overbrace{-z^2+2zu}} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(u)$$

power series of z of this stuff, called coefficients in u, and such coefficients are Hermite polynomials!
You can also show that e^{-z^2+2zu} satisfies Hermite equation

$$\frac{d^2 H_n}{du^2} - 2u\frac{dH_n}{du} + 2nH_n = 0 \text{!}$$

Final result: given this potential,



$E_0 = \frac{\hbar\omega}{2}$,
$E_1 = \frac{3}{2}\hbar\omega$, ...

So, the n-th function will be a polynomial, that have n nodes: the "correct" number of nodes! $E_0 \rightarrow$ no nodes
$E_n \rightarrow n$ nodes!

So:

$\psi_n = H_n(u)\, e^{-\frac{u^2}{2}}$ Eigenfunctions

$\psi_n(x) = H_n\left(\frac{x}{a}\right) e^{-\frac{x^2}{2a^2}}$

Eigenvalues: discrete spectrum, even spaced! The most spectrum possible.

Lecture 9: Operator Methods for the Harmonic Oscillator

Allan Adams

A student notes that we use just the even terms $a_0, a_2, a_4 \dots$, not the odd ones. Still, it is a II° order equation.

This, Allan says, is because the other solution of the ode $h(u)$ "simplifies" the $e^{\pm\frac{x^2}{2a^2}}$: from the preliminary asymptotic analysis we extracted a $e^{-\frac{x^2}{2a^2}}$, but there is also the twin solution: that, exponentially growing for increasing x. Well, the $a_1, a_3, a_5 \dots$ terms simplify that!

So, from brute force analysis, we found

$\phi_N = N_N\, e^{-\frac{x^2}{2a^2}}\, H_N\left(\frac{x}{a}\right)$

(N_N: normalization constant)

$E_N = \hbar\omega\left(N + \frac{1}{2}\right)$ evenly spaced

Why are these energies evenly spaced? Well, we found it, but we don't have a deep, physical reason!

Today we will understand this, and apply a method that allows us to understand some of the fine grain structure of the problem.

These moves are general strategies in both quantum mechanics and quantum field theory.

"Operator method"

Let's go back to look at the energy operator:

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

First, let's start with dimensional analysis: life will be better

$[\hbar]$ = momentum × length $(p\,x)$

$[m]$ = mass

$[\omega] = \frac{1}{\text{time}}$

Well, momentum × length, multiplying times a mass we obtain becomes

momentum × (mass × length/time) = momentum × momentum ×

Instead, by doing

$\hbar\omega m$, we have $[\hbar\omega m] = [p]^2$.

Instead,

$\left[\frac{\hbar}{m\omega}\right] = [x]^2$

So, let us define as "scale parameters" these

$x_0 = \sqrt{\frac{2\hbar}{m\omega}}$, $p_0 = \sqrt{2\hbar m\omega}$

So, the scales of our problem will be integer, dimensionless numbers times these scales.

Which is the possible scale of the ground state? More or less, x_0.

We can do the same with energy:

$[E] = \hbar\omega$

So, we can re-write the energy operator as:

$$\hat{E} = \hbar\omega \left[\frac{\hat{p}^2}{p_0^2} + \frac{\hat{x}^2}{x_0^2} \right] \qquad (1)$$

This is just to start studying the operator method with reasonable operators ;-)

Note that

$$x_0 p_0 = 2\hbar$$

So, looking at (1), we see that it is a sum of squares! And, when we see the sum of squares, a tempting step is to factor it! Like with numbers c, d,

$$c^2 + d^2 = (c - jd)(c + jd)$$

Can we do it for operators? Well,

$$\left(\frac{\hat{x}}{x_0} - j\frac{\hat{p}}{p_0} \right)\left(\frac{\hat{x}}{x_0} + j\frac{\hat{p}}{p_0} \right) = \frac{\hat{x}^2}{x_0^2} + \frac{\hat{p}^2}{p_0^2} + \frac{1}{2\hbar}\hat{x}\hat{p} - \frac{1}{2\hbar}\hat{p}\hat{x} =$$

$$= \frac{\hat{x}^2}{x_0^2} + \frac{\hat{p}^2}{p_0^2} + \frac{1}{2\hbar}[\hat{x}, \hat{p}]$$

↳ commutator

Fortunately, this commutator, even if not 0, is simple, and is

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

$$= \frac{\hat{x}^2}{x_0^2} + \frac{\hat{p}^2}{p_0^2} - \frac{1}{2}$$

So, the factorization equals the $\hat{E}$, minus $\frac{1}{2}$.

So,

$$\hat{E} = \hbar\omega \left(\frac{\hat{x}^2}{x_0^2} + \frac{\hat{p}^2}{p_0^2} \right) = \hbar\omega \left[\left(\frac{\hat{x}}{x_0} - j\frac{\hat{p}}{p_0} \right)\left(\frac{\hat{x}}{x_0} + j\frac{\hat{p}}{p_0} \right) + \frac{1}{2} \right]$$

Now, let us define an operator

$$\hat{a} = \frac{\hat{x}}{x_0} + j\frac{\hat{p}}{p_0}, \quad \text{and} \quad \hat{a}^\dagger = \frac{\hat{x}}{x_0} - j\frac{\hat{p}}{p_0}$$

↳ a dagger

We can then write

$$\hat{E} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

This somehow recalls the expression of the energy levels! =)

- Moreover, $\hat{a}^\dagger$ seems somehow something like the "complex conjugate" of $\hat{a}$

What is the "complex conjugate of an operator!? An operator is something that takes an object, a vector, and "rotate" it! What is the complex conjugate of such a thing?! We have to define it!

Math Aside: "complex conjugate" of an operator

Claims, facts

Given any linear operator $\hat{\theta}$, we can build (without any additional assumption or ingredient) another operator, $\hat{\theta}^\dagger$, in the following way:

Consider the inner product of two functions f and g, $(f|g)$,

$$(f|g) = \int dx\, f^* g \qquad \text{(useless, just a reminder)}$$

In a similar way, if, instead of g, we have $\hat{\theta} g$, it becomes

$$(f|\hat{\theta} g) = \int dx\, f^* \hat{\theta} g$$

We define a new operator, by choosing how it acts.

Starting from a modified version of the last equation, $\hat{\theta}^\dagger$ is such that

$$(f|\hat{\theta}^\dagger g) = \int dx\, f^* (\hat{\theta}^\dagger g) = \int dx\, (\hat{\theta} f)^* g = (\hat{\theta} f|g)$$

This new operator, $\hat{\theta}^\dagger$ (θ dagger), is called the "adjoint" of $\hat{\theta}$.

Occasionally, sometimes, "Hermitian adjoint"

Given $\hat{\theta}^\dagger$, applied to g, and doing the inner product with f, we obtain the same as taking $\hat{\theta}$, apply to f, and compute inner product with g.

Examples

Given c a complex number $c^\dagger = ?$

c is a very easy kind of operator (just a number!)

How to find $c^\dagger$?

$$\int dx\, f^* (c^\dagger g) = \int dx\, (cf)^* g = c^* \int dx\, f^* g = \int dx\, f^* (c^* g)$$

$\Rightarrow$ $c^\dagger = c^*$, since this must be true for all f, g (under $\int$)

The adjoint of a complex number is its complex conjugate!

Homework: check that $(\hat{\vartheta}^\dagger)^\dagger = \hat{\vartheta}$

Example 2

What is the adjoint of ∂_x? $\partial_x^\dagger$?

Well,

$$\int dx\, f^* (\partial_x^\dagger g) = \int dx\, (\partial_x f)^* g$$

we apply integration by parts. First,

$$= \int dx\, (\partial_x f)^* g = \int dx\, (\partial_x f^*) g = -\int dx\, f^* \partial_x g \quad + \text{boundary term}$$

$$= \int dx\, f^* (-\partial_x g)$$

$\Rightarrow$ $\boxed{\partial_x^\dagger = -\partial_x}$

What about the boundary term? Well, if we think to work with nice, smooth, but in particular NORMALIZABLE functions (vanishing at $\pm\infty$), the f, g go to 0 at ∞, and the boundary term vanishes as well.

BUT with non-normalizable functions, NO! The adjoint of the derivative is something different!

Example 3

$\hat{x}^\dagger = ?$

Recalling $\hat{x}$, it is: $\hat{x} f = x f$,

$\Rightarrow$, for definition of adjoint

$$\int dx\, f^* (\hat{x}^\dagger g) = \int dx\, (\hat{x} f)^* g = \int dx\, (x f^*)^* g \quad , \text{ but } x \in \mathbb{R}, \text{ so}$$

$$= \int dx\, (x f^*) g = \int dx\, f^* (x g) = \int dx\, f^* (\hat{x} g)$$

$\forall g$,

$\hat{x}^\dagger = \hat{x}$!

Definition

An operator $\hat{\vartheta}$ whose adjoint $\hat{\vartheta}^\dagger$ is equal to $\hat{\vartheta}$, is called Hermitian! (self-adjoint)

For example, a real number is Hermitian. $\hat{x}$ is Hermitian. We can call Hermitian operators "real".

Mathematical fact: a Hermitian operator $\hat{\vartheta}$ has all real (IR) eigenvalues!

Last example.

$\hat{p}^\dagger = ?$

Well,

$$\hat{p} = \frac{\hbar}{i} \partial_x ,$$

well, $\partial_x^\dagger = -\partial_x$, but $i^\dagger = -i$, so $\hat{p}$ is actually Hermitian!

$\hat{p}^\dagger = \hat{p}$! (you can prove it!)

Strong physical fact: all the operators we've created ($\hat{x}, \hat{p}$) are Hermitian

Physical fact: all the observables are real, and, as a corollary, all operators associated to an observable are Hermitian.

This is also connected to the fact that the corresponding eigenvectors suffice to represent any possible function that are a basis.

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end of math. class

Back to our operator $\hat{a} = \frac{\hat{x}}{x_0} + j\frac{\hat{p}}{p_0}$

Well, we proved that $\hat{a}^\dagger$ is effectively that!

$\hat{a}^\dagger = \left(\hat{a}\right)^\dagger$! ;-)

Does $\hat{a}$ correspond to an observable? no! It is not Hermitian, because $\hat{a}^\dagger \neq \hat{a}$!

Does $\hat{a}$ have real eigenvalues? Well, it is not Hermitian. But still it is possible that it has real eigenvalues: it is not mandatory to have an Hermitian operator to have real eigenvalues: there are non-Hermitian operators with real eigenvalues! ;-)

We will discover, at the end of the course, that $\hat{a}$ has a nice set of eigenvectors: what we call "coherent states", useful for lasers. But, the eigenvalues are not, in general, real. So, being complex, we cannot measure them directly, but they are related to something we can measure!

So, why are we interested in $\hat{a}$? Well, because $\hat{E}$ with $\hat{a}$ is very simple, and makes obvious that $\hat{E}$ is Hermitian.

We (can prove) know that

$\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger$, so

$\left(\hat{a}^\dagger\hat{a}\right)^\dagger = \hat{a}^\dagger\hat{a}$

Moreover, very thing: $\hat{a}$ and $\hat{a}^\dagger$ satisfy the simplest commutation relationship in the world! =) (not trivial because)

$$\left[\hat{a}, \hat{a}^\dagger\right] = \left[\left(\frac{\hat{x}}{x_0} + j\frac{\hat{p}}{p_0}\right), \left(\frac{\hat{x}}{x_0} - j\frac{\hat{p}}{p_0}\right)\right] =$$

$$= \left[\frac{\hat{x}}{x_0}, \frac{\hat{x}}{x_0}\right] - j\left[\frac{\hat{x}}{x_0}, \frac{\hat{p}}{p_0}\right] + j\left[\frac{\hat{p}}{p_0}, \frac{\hat{x}}{x_0}\right] + \left[\frac{\hat{p}}{p_0}, \frac{\hat{p}}{p_0}\right]$$

$\left[\frac{\hat{x}}{x_0}, \frac{\hat{x}}{x_0}\right] = 0$ and $\left[\frac{\hat{p}}{p_0}, \frac{\hat{p}}{p_0}\right] = 0$

in fact, $\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$

this becomes:

$$= -\frac{1}{x_0 p_0}\left[\hat{x}, \hat{p}\right] - \frac{1}{x_0 p_0}\left[\hat{x}, \hat{p}\right] \qquad \left(\left[\hat{p}, \hat{x}\right] = -\left[\hat{x}, \hat{p}\right]\right)$$

But $x_0 p_0 = 2\hbar$, and $\left[\hat{x}, \hat{p}\right] = j\hbar$,

so

$$-\frac{1}{2\hbar} \times j\hbar = 1$$

So,

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1$$

Notice that

$\left[\hat{a}^\dagger, \hat{a}\right] = -1$

$\left[\hat{a}, \hat{a}\right] = 0$, $\left[\hat{a}^\dagger, \hat{a}^\dagger\right] = 0$.

Now, we will use these commutator relationships to crush, to submit the problem to our will. It will be like the Romans weeping at the arrival of the Visigoths. It will be DRAMATIC

Two more commutators. This method is powerful because, just by using commutators, and simple relations, we will solve EVERYTHING (just like Barbara in NEGF!!)

$$\left[\hat{E}, \hat{a}\right] = \left[\hbar\omega\,\hat{a}^\dagger\hat{a}, \hat{a}\right] = \left(\hbar\omega\,\frac{1}{2} \text{ is not written because every number commutes with an operator}\right)$$

$$= \hbar\omega\left[\hat{a}^\dagger\hat{a}, \hat{a}\right] = \hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger\hat{a}\right) = \hbar\omega\left(\hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger\right)\hat{a} =$$

$$= \hbar\omega\underbrace{\left[\hat{a}^\dagger, \hat{a}\right]}_{-1}\hat{a} = -\hbar\omega\hat{a}$$

So,

$$\left[\hat{E}, \hat{a}\right] = -\hbar\omega\hat{a}$$

and!

$$\left[\hat{E}, \hat{a}^\dagger\right] = \cdots = +\hbar\omega\hat{a}^\dagger$$

We totally solved the problem. We've just won!

Any time you see something like

$[\hat{O}, \hat{a}^\dagger] = \text{constant} \times \hat{a}^\dagger$

CHEER. You won.

Suppose that we already have access to an eigenfunction of the energy operator: ϕ_E. So,

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

Consider a state $\psi = \hat{a}^\dagger \phi_E$: take the eigenfunction $\hat{a}^\dagger$ acts on it!

However,

$\hat{E}\psi = \hat{E}\hat{a}^\dagger \phi_E$

$\hat{E}$ would love to act on ϕ_E, but there is an $\hat{a}^\dagger$ in the middle. =C

Now,

$\hat{E}\hat{a}^\dagger \phi_E = \left(\hat{E}\hat{a}^\dagger - \hat{a}^\dagger\hat{E} + \hat{a}^\dagger\hat{E}\right) = \left(\left[\hat{E}, \hat{a}^\dagger\right] + \hat{a}^\dagger\hat{E}\right)\phi_E =$

$= \left[\hat{E}, \hat{a}^\dagger\right]\phi_E + \hat{a}^\dagger\hat{E}\,\phi_E$

We commuted the operators! In general, the trick is

$\hat{A}\hat{B}f = \left(\left[\hat{A}, \hat{B}\right] + \hat{B}\hat{A}\right)f,$

so that $\hat{A}$ can act directly on f!

$= \left(-\hbar\omega\hat{a}^\dagger\right)\phi_E + \hat{a}^\dagger\hat{E}\,\phi_E = \left(-\hbar\omega\hat{a}^\dagger + E\hat{a}^\dagger\right)\phi_E =$

($\hat{a}^\dagger\hat{E}\,\phi_E = \hat{a}^\dagger E\,\phi_E$)

$= \left(-\hbar\omega + E\right)\hat{a}^\dagger\phi_E = \left(E - \hbar\omega\right)\hat{a}^\dagger\phi_E = \left(E-\hbar\omega\right)\psi$

What does this mean? If we have a state with energy E, and act on it with $\hat{a}^\dagger$, we get, from ϕ_E, a ψ, new state, also eigenstate of the energy operator, but with a different eigenvalue: decreased of $\hbar\omega$!

This is what we wanted!

From $\hat{E}\,\phi_E \to E\,\phi_E$, $\hat{a}^\dagger\phi_E$ has energy eigenvalue $E-\hbar\omega$!

So, $\psi \propto \phi_{E-\hbar\omega}$! (eigenfunction with energy $E-\hbar\omega$)

proportional, because it must be normalized!

So, energy is: now I start from E, ϕ_E; apply $\hat{a}^\dagger$, find $\phi_{E-\hbar\omega}$, so $E-\hbar\omega$ is the new level. Again, $\hat{a}^\dagger\phi_{E-\hbar\omega}$ is $\phi_{E-2\hbar\omega}$, by the very same argument!

$\hat{a}^\dagger$ has a name! It, basically, lowers energy. So, we will call it "lowering operator": it takes a state with energy E and lowers by $\hbar\omega$.

What about $\hat{a}^\dagger$? Well,

$\hat{E}\psi = \hat{E}\hat{a}^\dagger\phi_E \longrightarrow \left(E \oplus \hbar\omega\right)\phi_E$

So, instead than lowering, it increases energy!

So $\hat{a}$ and $\hat{a}^\dagger$ are the lowering and rising operators!

$\phi_E \to \hat{a}^\dagger\phi_E = \phi_{E+\hbar\omega}$

So, these operators allow us to create a ladder of states. So, why is this ladder evenly spaced?

Well, thanks to $\left[\hat{E}, \hat{a}\right]$ and $\left[\hat{E}, \hat{a}^\dagger\right]$. Because of these commutators!

This can be used in the same way, with Lorentz force: electrons in a magnetic field. The same approach lead to determine the so-called Landau levels!

Does this ladder extend infinitely up? Yes! And down? No!

You can't have energy arbitrarily negative!

In fact, the energy expectation value can be written as

$\langle E\rangle = \int dx\ \phi^* \hat{E}\,\psi = \int dp\ |\psi(p)|^2 \frac{p^2}{2m} + \int dx\ |\psi(x)|^2 \frac{m\omega^2}{2}x^2$

All of these integrands are strictly positive! So, the expectation value is categorically positive, and there is a minimum, E_0: what we called ground state!

Any time you see something like

$[\hat{O}, \hat{a}^\dagger] = \text{constant} \times \hat{a}^\dagger$

CHEER. You won.

Suppose that we already have access to an eigenfunction of the energy operator: ϕ_E. So,

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However,

$\hat{E}\psi = \hat{E}\hat{a}^\dagger\phi_E$

$\hat{E}$ would love to act on ϕ_E, but there is an $\hat{a}^\dagger$ in the middle. =C

Now,

$\hat{E}\hat{a}^\dagger\phi_E = (\hat{E}\hat{a}^\dagger - \hat{a}^\dagger\hat{E} + \hat{a}^\dagger\hat{E})\phi_E = ([\hat{E},\hat{a}^\dagger] + \hat{a}^\dagger\hat{E})\phi_E =$

$= [\hat{E},\hat{a}^\dagger]\,\phi_E + \hat{a}^\dagger\hat{E}\,\phi_E$

we commuted the operators! In general, the trick is

$\hat{A}\hat{B}f = ([\hat{A},\hat{B}] + \hat{B}\hat{A})f$,

so that $\hat{A}$ can act directly on f!

$= (-\hbar\omega\hat{a}^\dagger)\phi_E + \hat{a}^\dagger\underbrace{\hat{E}\phi_E}_{=E\phi_E} = (-\hbar\omega\hat{a}^\dagger + E\hat{a}^\dagger)\phi_E =$

$= (E-\hbar\omega)\hat{a}^\dagger\phi_E = (E-\hbar\omega)\psi$

What does this mean? If we have a state with energy E, and act on it with $\hat{a}^\dagger$, we get, from ϕ_E, a ψ, new state, also eigenstate of the energy operator, but with a different eigenvalue: decreased of $\hbar\omega$!

This is what we wanted!

From $\hat{E}\phi_E \to E\phi_E$, $\hat{a}^\dagger\phi_E$ has energy eigenvalue $E-\hbar\omega$!

So, $\psi \propto \phi_{E-\hbar\omega}$! (eigenvalue with energy $E-\hbar\omega$)

proportional, because it must be normalized!

So, energy is: I start from E, ϕ_E; apply $\hat{a}^\dagger$, find $\phi_{E-\hbar\omega}$, so $E-\hbar\omega$ is the new level. Again, $\hat{a}^\dagger\phi_{E-\hbar\omega}$ is $\phi_{E-2\hbar\omega}$, by the very same argument!

$\hat{a}^\dagger$ has a name! It, basically lowers energy. So, we will call it "lowering operator": it takes a state with energy E and lowers by $\hbar\omega$.

What about $\hat{a}^\dagger$? Well,

$\hat{E}\psi = \hat{E}\hat{a}^\dagger\phi_E \longrightarrow (E+\hbar\omega)\phi_E$

So, instead than lowering, it increases energy!

So $\hat{a}$ and $\hat{a}^\dagger$ are the lowering and rising operators!

$\phi_E \to \hat{a}^\dagger\phi_E = \phi_{E+\hbar\omega}$

So, these operators allow us to create a ladder of states. So, why is this ladder evenly spaced?

Well, thanks to $[\hat{E},\hat{a}]$ and $[\hat{E},\hat{a}^\dagger]$. Because of these commutators!

This can be used in the same way, with Lorentz force, electrons in a magnetic field. The same approach. Lead to determine the so-called Landau levels!

Does this ladder extend infinitely up? Yes! And down? No!

You can't have energy arbitrarily negative!

In fact, the energy expectation value can be written as

$\langle E\rangle = \int dx\, \phi^* \hat{E}\psi = \int dp\, |\tilde{\psi}(p)|^2 \frac{p^2}{2m} + \int dx\, |\psi(x)|^2 \frac{m\omega^2}{2}x^2$

All of these integrands are strictly positive! So, the expectation value is certainly positive, and there is a minimum, E_0: what we called ground state!

This means that, if we continue to lower the ladder with $\hat{a}^\dagger$ at some moment we will find something blocking us!

Well, at some part, if we apply $\hat{a}\,\phi_0$, we would find 0.

The "tower" of states ends at some state such that, further lowering, we find 0

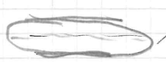
The function 0!

Associated to ϕ_0 there is E_0: ground state!

QUESTION

How do you know that those "ladder" states are ALL states?

Imagine that we have more states than those we found.



We could turn of extra states in the middle.

But, then, by that commutation relation, we must have them another tower. Also this second tower ends. Focusing on ϕ_0, we will have a $\tilde{\phi}_0$. There could be two different states with E_0? Well, the energy of the ground state is: (such that)

$$\hat{E}\,\phi_0 = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\phi_0$$

But $\hat{a}\,\phi_0 = 0$, $\hat{a}$ annihilates ϕ_0, so $\hat{E}\,\phi_0 = \boxed{\frac{1}{2}\hbar\omega}\,\phi_0$

Any state annihilated by $\hat{a}$ must have E_0. This is the only way to be annihilated by $\hat{a}$. But degeneracies are NOT ALLOWED! So energies must be ordered, but we don't have degeneracies.

Now what are the wave functions?

We know that ground state is annihilated by $\hat{a}$: $\hat{a}\,\phi_0 = 0$

But $\hat{a} = \frac{\hat{x}}{x_0} + \frac{\hat{p}}{p_0}$, so, we get

$$\left(\partial_x + \frac{p_0}{\hbar x_0}x\right)\phi_0 = 0$$ first order differential equation, VERY EASY!

$$= \left(\partial_x + \frac{2}{x_0^2}x\right)\phi_0$$

$\hookrightarrow \phi_0 = Ce^{-\frac{x^2}{x_0^2}}$

Then, how to get ϕ_1? Raising operator!

$\hookrightarrow$ change sign! $\partial_x - \frac{2}{x_0^2}x_0\,\phi_0$ just take derivatives and multiply by the constant

The spectrum was obtained just from commutators. Eigenfunctions, with an easy equation.