Seminar 1 (Introduction)

Problem I Dimensional analysis

In cgs units the mass of the electron is $9{,}11\cdot 10^{-28}$ gm., the electric charge is $4{,}8\cdot 10^{-10}$ esu. (electrostatic units) and $\hbar = 1{,}05\cdot 10^{-27}$ erg·sec. Using that $1(\text{esu})^2 = 1$ erg·cm and $1\text{ gm} = 1\text{ erg}\frac{s^2}{cm^2}$, find an estimate for the typical energy of the hydrogen atom. Convert your answer to electron-Volts (eV).

Sense of dimensional analysis is to obtain results up to order, by combining different constants so that resulting combination have dimension we need.

In particular in problem we are given following constants: $m_e = 9{,}11\cdot 10^{-28}$ gm; $e = 4{,}8\cdot 10^{-10}$ esu (electrostatic units); $\hbar = 1{,}05\cdot 10^{-27}$ erg·s; and we are asked to estimate energy of atom in ergs. Note here that, for example, in lectures some other quantaties have been used too. For example speed of light $c = 3\cdot 10^{10}\frac{cm}{s}$ and size of atom $R\sim 1\text{Å}$, but here we will use only data given in problem to have unique way.

First we use that $(1\text{esu})^2 = 1\cdot$erg·cm (remember Coulomb potential $V = \frac{e^2}{r}$) and $1\text{gm} = 1\text{erg}\cdot\frac{s^2}{cm^2}$ (from $E = mc^2$)

So we get: $[c] = \frac{L}{t}$; $[m_e] = \frac{E\cdot t^2}{L^2}$; $[e^2] = E\cdot L$, $[\hbar] = E\cdot t$

So we can now see that $\left[\frac{\hbar^2}{e^4}\right] = \frac{t^2}{L^2}$ so that we are able to cancel $\frac{t^2}{L^2}$ from dimension of mass:

$\left[\frac{m_e\cdot e^4}{\hbar^2}\right] = \frac{E\cdot t^2 L^2}{L^2\cdot t^2} = E$ just as we want. So typical energy in hydrogen atom is

$$E \approx \frac{m_e\cdot e^4}{\hbar^2} = \frac{9{,}11\cdot 10^{-28}\cdot(4{,}8)^4\cdot 10^{-40}}{10^{-54}} \approx 4{,}84\cdot 10^{-11}\text{ erg} = 4{,}84\cdot 6{,}24\text{ eV} \approx 30\text{ eV}$$

② $\boxed{E \approx \frac{m_e \cdot e^4}{\hbar^2} \approx 30\,eV}$, which is close enough to Rydberg constant $Ry = -13{,}6\,eV$ which gives the lowest energy of electron in atom.

Problem II Wien's Law

The Planck modification to the Rayleigh-Jeans spectral emmittance is given by:

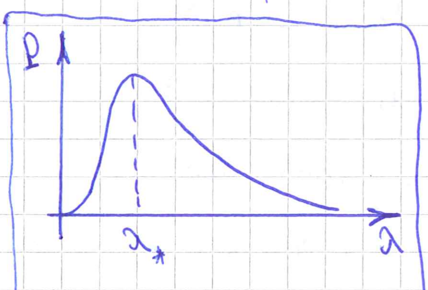
$$P(\lambda, T) = 2\pi \frac{kTc}{\lambda^4} \frac{hc/kT\lambda}{e^{hc/kT\lambda} - 1} = 2\pi \frac{hc^2}{\lambda^5 (e^{hc/kT\lambda} - 1)}$$

Wien's law states that $P(\lambda, T)$ has a peak at $\lambda = \frac{b}{T}$, where $b = \frac{hc}{4{,}956\,k}$; b is called the Wien displacement constant.

(a) Find an equation that the Wien constant satisfies.

Reminder Planck law describes energy emitted by black body per unit area and unit wave length.
Planck modified Rayleigh-Jeans law $P(\lambda, T) = 2\pi \frac{kTc}{\lambda^4}$ which suffers from divergence at $\lambda \to 0$. One of "revolutionary" ideas he introduced resolving this problem was "quanta" of light. It says that radiation comes in discrete packets with energy $\varepsilon = h\nu = \frac{hc}{\lambda}$;

Planck spectra is shown on the picture below (pic 1.)



pic. 1.

It has maximum at some $\lambda_* = \frac{b}{T}$
Let's find equation defining position of this maximum. If we introduce dimensionless quantaty $x = \frac{hc}{kT\lambda}$ we get following formula for distribution:

$P(\lambda, T) \sim \frac{x^5}{e^x - 1}$ where we have omitted overall coefficient that doesn't depend on λ (it won't change position of maximum and will just rescale spectra)

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Now we can write down condition for extremum:

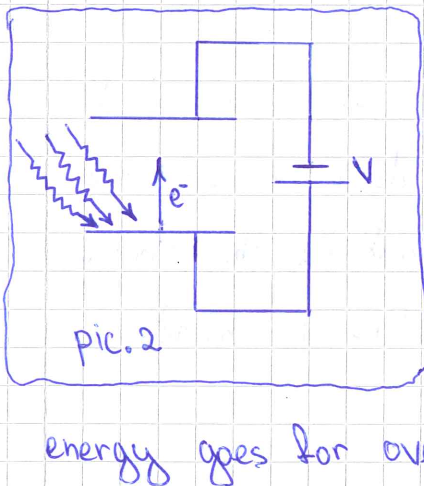
$$\frac{dP}{dx} \sim \frac{5x^4}{e^x-1} - \frac{x^5e^x}{(e^x-1)^2} = \frac{x^4}{(e^x-1)^2}\left((e^x-1)5 - xe^x\right) = 0$$

as $x=0$ mean $\lambda \to \infty$ and we are not satisfied with this solution we are left with

$\boxed{xe^x = 5(e^x-1)}$. This equation is satisfied if $x \approx 5$. As $e^5 \gg 1$ we can write down $xe^x = 5e^x$ which is satisfied when $x=5 \Rightarrow \boxed{\lambda = \frac{hc}{5kT};}$ which is close enough to the one written in text of the problem $\lambda = \frac{hc}{4{,}956kT}$;

Problem III Photo-electric effect

Monochromatic light is shined on a Potassium surface. An experimenter measures the stopping potential to be 1,91 Volts if $\lambda = 3000$ Å and 0,88 Volts if $\lambda = 4000$ Å. Using that the electron charge is $-1{,}6 \cdot 10^{-19}$ Coulombs, find an estimate for Planck's constant from this data. Also find the work function and the threshold wavelength.



pic. 2

Reminder: Scheme of experiment is drawn on (pic. 2). Light hits metalic plate. We can consider light as bunch of photons, with energy $E = h\nu$ each. Photon hit electron and transfers it's energy to it. Part of electron's energy goes for overcoming the potential that keeps the electron in the metal. This part of energy is called work function W.

The potantial applied to the plates attract electrons back to the plate they were emitted from.

Stopping potential is the one that prevents electrons

(4) from reaching opposite plate. Obviously it's given by $|e|V_{stop} = h\nu - W = \frac{hc}{\lambda} - W$.

In our case we have 2 stopping potentials for 2 different wave length : $V_1 = 1{,}91\ V$ for $\lambda_1 = 3\cdot10^3\ \mathring{A}$ and $V_2 = 0{,}88\ V$ for $\lambda_2 = 4\cdot10^3\ \mathring{A}$ so that:

$$|e|V_1 = \frac{hc}{\lambda_1} - W \ ; \ |e|V_2 = \frac{hc}{\lambda_2} - W; \ \text{so}$$

$$hc\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right) = |e|(V_1 - V_2)$$ so that we can find Planck constant:

$$h = \frac{\lambda_1\lambda_2|e|(V_1-V_2)}{c(\lambda_2-\lambda_1)} = \frac{12\cdot10^{6}\mathring{A}^2\ 1{,}03\,eV}{3\cdot10^8\frac{m}{s}\cdot10^3\ \mathring{A}} = 4{,}12\cdot10^{-15}\,eV\cdot s$$

so $$\boxed{h = \frac{\lambda_1\lambda_2|e|(V_1-V_2)}{c(\lambda_2-\lambda_1)} = 4{,}12\cdot10^{-15}\,eV\cdot s\,;}$$

Work function is given by

$$W = -|e|V_1 + \frac{hc}{\lambda_1} = -1{,}91\,eV + \frac{4{,}12\cdot10^{-15}\cdot3\cdot10^8\,eV\cdot m}{3\cdot10^{-7}\ m} = (4{,}12 - 1{,}91)\,eV =$$
$$= 2{,}21\,eV \ , \ \boxed{W = \frac{hc}{\lambda_1} - |e|V_1 = 2{,}21\,eV}$$

Threshold wavelength, i.e. one when energy of photon exacetely equals work function, in our case equals to

$$\boxed{\lambda_t = \frac{hc}{W} = 5600\ \mathring{A}}$$

Important note While doing calculations we have used that $[|e|\cdot V] = eV$ which comes from the definition of the electronvolt as amount of energy gained by the charge of a single electron moved across an electric potential difference of one volt.

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Problem IV De Broglie wave-lengths

Estimate the de Broglie wavelengths for the following:

(a) An average size person walking through Ångstrom laborotory:

Reminder

de Broglie idea was that not only light but any particle is simultaneously wave an particle with the following relation between wavelength and particles momentum: $\boxed{\lambda = \frac{h}{p};}$

For average size person let's take $m = 70\,kg$, $V = 1{,}5\,\frac{m}{s}$, and $p = m \cdot V \approx 100\,kg\,\frac{m}{s}$; then de Broglie wavelength is given by $\boxed{\lambda_h = \frac{h}{p} \approx 6{,}6 \cdot 10^{-36}\,m}$ – very very small wavelength.

(b) Volvo at speed limit on the E4

Speed limit on E4 is $V = 110\,\frac{km}{h} \approx 30\,\frac{m}{s}$, mass of car is about 1 tonn: $m = 10^3\,kg$ then

$$\lambda_v = \frac{h}{p} = \frac{6{,}63 \cdot 10^{-34}\,J \cdot s}{3 \cdot 10^4\,kg\,\frac{m}{s}} \approx 2 \cdot 10^{-38}\,m \quad ; \quad \boxed{\lambda_v = 2 \cdot 10^{-38}\,m}$$

(c) electron at $100\,\frac{km}{s}$

mass of electron is given by $m_e = 9{,}1 \cdot 10^{-31}\,kg \approx 10^{-30}\,kg$ and it is not relativistic since $V = 10^5\,\frac{m}{s} \ll 3 \cdot 10^8\,\frac{m}{s} = c$

so $\lambda_e = \frac{h}{m_e V} = 6{,}63 \cdot 10^{-9}\,m = 66\,\text{Å}$ $\quad \boxed{\lambda_e = 66\,\text{Å}}$

(d) 4 TeV proton at LHC

mass of proton is $m_p c^2 = 1\,GeV \ll 4\,TeV$ so we can take $p = \frac{E}{c}$ and then wave length is given by

$$\lambda_p = \frac{hc}{E} = \frac{4{,}13 \cdot 10^{-15}\,eV \cdot s \cdot 3 \cdot 10^8\,\frac{m}{s}}{4 \cdot 10^{12}\,eV} \approx 3 \cdot 10^{-19}\,m \quad \boxed{\lambda_p \approx 3 \cdot 10^{-19}\,m}$$

⑥ as we see all wavelengths appear to be very small that's wy we think about particles as about localized objects rather than waves.

Note: For numerics you will need Planck constant $h = 6{,}63 \cdot 10^{-34}\ J \cdot s = 4{,}13 \cdot 10^{-15}\ eV \cdot s$.

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Seminar 2 (wave function, expectation values)

Theory reminder

* In quantum mechanics everything has probabilistic nature, so we need to introduce probability amplitude $\Psi(x,t)$, which when squared gives us the probability density $\rho(x,t)$ for particle to be found at point x at time t. We call this probability amplitude the wave-function.

$$\rho(x,t) = \Psi^*(x,t)\,\Psi(x,t) = |\Psi(x,t)|^2$$

* In quantum mechanics we have two kind of objects:

- wave-function $\Psi(x,t)$ discussed above.
- operators $\hat{O}$ acting on this wave-functions. Examples of operators are hamiltonian (energy) operator $\hat{H}$; Operator usually associated with energy is $i\hbar\frac{\partial}{\partial t}$ Another examples is momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$

* Wave-function $\Psi(x,t)$ satisfies S

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

the main equation of quantum mechanics. Important property of Schrödinger equation is it's linearity. I.e. if $\Psi_1(x,t)$ and $\Psi_2(x,t)$ satisfies S. eq. then $\Psi(x,t) = C_1\Psi_1(x,t) + C_2\Psi_2(x,t)$ satisfies S. eq. too.

* Probability should be normalized. As $\int_{-\infty}^{+\infty} dx\,\rho(x) = 1$ (probability to find particle somwhere in space is 1 always) we conclude that $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 = 1$ which we call normalization condition

* we can also derive probability current

$$j(x,t) = \frac{i\hbar}{2m}\left[\left(\frac{\partial}{\partial x}\Psi^*\right)\Psi - \Psi^*\left(\frac{\partial}{\partial x}\Psi\right)\right];$$

② which describes flow of probability through the point x in some direction. That means that probability increases in direction of the flow and decreases in opposite direction.

* In usual probability theory given probability density we can define averages $\langle x\rangle = \int x \rho(x)\,dx$ and standart deviation $\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$. For quantum mechanics this quantaties become:

- expectation value of operator: $\langle O\rangle = \int \Psi^* \hat{O} \Psi\,dx$
- uncertainty: $\sigma_0 = \sqrt{\langle O^2\rangle - \langle O\rangle^2}$

Problem I Consider the wave function $\Psi(x,t) = A e^{-\mu|x|} e^{-i\omega t}$

ⓐ Find A such that the wave-function is properly normalized.

Normalization condition has the following form:

$\int\limits_{-\infty}^{+\infty} |\Psi|^2 dx = 1$, substituting our wave function we get: $|A|^2 \int\limits_{-\infty}^{+\infty} dx\, e^{-2\mu|x|} = 1$, integral gives us:

$$\int\limits_{-\infty}^{+\infty} dx\, e^{-2\mu|x|} = \int\limits_0^{\infty} dx\, e^{-2\mu x} + \int\limits_{-\infty}^{0} dx\, e^{2\mu x} = \int\limits_0^{\infty} dx\, e^{-2\mu x} - \int\limits_{+\infty}^{0} dx\, e^{-2\mu x} =$$

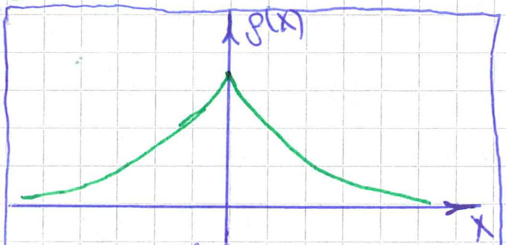
$$= 2\int\limits_0^{\infty} dx\, e^{-2\mu x} = -\frac{1}{\mu} e^{-2\mu x}\Big|_0^{\infty} = \frac{1}{\mu}$$ so normalization condition turns to $|A|^2/\mu = 1 \Rightarrow \boxed{|A| = \sqrt{\mu}}$ note that we are not able to define total phase of wave function as it is unobservable.

ⓑ Sketch the probability density as a function of x.

probability density is given by

$\rho(x) = |\Psi(x,t)|^2 = e^{-2\mu|x|} \cdot |A|^2 = \mu e^{-2\mu|x|}$

and shown on pic. 1



pic. 1.

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ⓒ Find the expectation values for x and x^2 for $\Psi(x,t)$.

Just by definition:

$$\langle x\rangle = \int_{-\infty}^{+\infty} dx\ \Psi^*(x)\, x\, \Psi(x) = \mu \cdot \int_{-\infty}^{+\infty} dx\ x e^{-2\mu|x|}$$

as $f(x) = x e^{-2\mu|x|}$ is odd function $f(x) = -f(-x)$

this integral gives "0": $\boxed{\langle x\rangle = 0}$ – that's always true for symmetric prob. dist.

$\langle x^2\rangle = \int_{-\infty}^{+\infty} dx\ \Psi^*(x)\, x^2\, \Psi(x)$; before taking this integral let's remember some usefull tips about taking integrals.

Note.

We will often meet integrals of the form:

$\int_{-\infty}^{+\infty} dx \cdot x^n e^{-\alpha|x|}$, if n - odd number function in integral is odd and $\int_{-\infty}^{+\infty} dx \cdot x^n e^{-\alpha|x|} = 0$, and if n is even we get:

$$\int_{-\infty}^{+\infty} dx \cdot x^n e^{-\alpha|x|} = 2\int_0^{+\infty} dx \cdot x^n e^{-\alpha x} = 2\cdot(-1)^n \frac{d^n}{d\alpha^n}\int_0^{\infty} dx\, e^{-\alpha x} = 2\cdot(-1)^n \frac{d^n}{d\alpha^n}\cdot\frac{1}{\alpha} =$$

$$= 2\cdot(-1)^n\cdot(-1)^n \frac{d^n}{d\alpha^n}\cdot\frac{1}{\alpha} = 2\frac{n!}{\alpha^{n+1}}$$

. The trick we have used here is called parameter differentiation and this is very useful trick. Note that if you don't have parameter you can introduce it by hands and after perfoming calculations put it to be equal 1 ($\alpha = 1$)

Now we are able to calculate $\langle x^2\rangle$:

$$\langle x^2\rangle = \int_{-\infty}^{+\infty} dx\ \Psi^* x^2 \Psi = \mu\int_{-\infty}^{+\infty} dx\, x^2 e^{-2\mu|x|} = 2\mu\int_0^{\infty} dx\, x^2 e^{-2\mu x} = 2\mu \left.\frac{2}{\alpha^3}\right|_{\alpha=2\mu} =$$

$= \frac{1}{2\mu^2}$, so $\boxed{\langle x^2\rangle = \frac{1}{2\mu^2};}$

ⓓ Find the uncertainty σ_x in the position for $\Psi(x,t)$

By definition

④ $\sigma_x \equiv \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = \frac{1}{\sqrt{2}\mu}$; $\boxed{\sigma_x = \frac{1}{\sqrt{2}\mu};}$

Problem II Suppose you are given the wave-function
$\Psi(x,t) = e^{-i\omega t/2}\, e^{-bmx^2}$

ⓐ Find a potential $V(x)$ and constant b such that $\Psi(x,t)$ will be the solution to Schr. eq.

Schr. eq. looks like $i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x)\,\Psi$.

Let's first find derivatives:

$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \frac{\hbar\omega}{2}\Psi(x,t)$; $\frac{\partial}{\partial x}\Psi(x,t) = -2bmx\,\Psi(x,t)$;

$\frac{\partial^2}{\partial x^2}\Psi(x,t) = (-2bm + 4b^2m^2x^2)\,\Psi(x,t)$ substituting this derivatives into Schr. eq. we get:

$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x) \Rightarrow \frac{\hbar\omega}{2}\Psi = (\hbar^2 b - 2\hbar^2 b^2 m x^2 + V(x))\Psi$

cancelation of constant terms gives us $\hbar^2 b = \frac{1}{2}\hbar\omega \Rightarrow b = \frac{\omega}{2\hbar}$;

and cancelation of x-dependent terms gives

$V(x) = 2\hbar^2 b^2 m x^2 = \frac{1}{2}m\omega^2x^2$;

$$\boxed{\begin{aligned} V(x) &= \tfrac{1}{2}m\omega^2x^2; \\ b &= \tfrac{\omega}{2\hbar}; \end{aligned}}$$

this is potential of harmonic oscillator and the wave-function describes it's ground state.

ⓑ Normalize this wave-function.

Normalization condition is $\int_{-\infty}^{+\infty} dx\, |\Psi(x,t)|^2 = |C|^2 \int_{-\infty}^{+\infty} e^{-2bmx^2}\, dx =$

$= |C|^2\sqrt{\frac{\pi}{2bm}} = 1 \Rightarrow \boxed{|C| = \left(\frac{2bm}{\pi}\right)^{1/4}}$

ⓒ Find the expectation values for x and x^2

By definition:

$\langle x\rangle = \int_{-\infty}^{+\infty} dx\, \Psi^* x \Psi = \int_{-\infty}^{+\infty} dx\, |C|^2 \cdot x\, e^{-2bmx^2}$;

$\langle x^2\rangle = \int_{-\infty}^{+\infty} dx\, \Psi^* x^2 \Psi = \int_{-\infty}^{+\infty} dx\, |C|^2\, x^2\, e^{-2bmx^2}$;

⑤ **Note** Before we proceed let's use parameter differentiation to find general answer for integral $\int_{-\infty}^{+\infty} dx\, x^{2n} e^{-\alpha x^2}$ (obviously $\int_{-\infty}^{+\infty} dx\, x^{2n+1} e^{-\alpha x^2} = 0$ as $x^{2n+1}e^{-\alpha x^2}$ is odd function)

$$\int_{-\infty}^{+\infty} dx\, x^{2n} e^{-\alpha x^2} = (-1)^n \frac{d^n}{d\alpha^n} \int_{-\infty}^{+\infty} dx\, e^{-\alpha x^2} = (-1)^n \frac{d^n}{d\alpha^n} \sqrt{\frac{\pi}{\alpha}} = \sqrt{\pi}\,(-1)^n (-1)^n \frac{1\cdot 3\cdot 5\cdot\ldots}{\alpha^{n+\frac{1}{2}}\cdot 2^n}$$

So $\boxed{\int_{-\infty}^{+\infty} dx\, x^{2n} e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \frac{(2n-1)!!}{(2\alpha)^n}}$

Now we can easily find $\langle x\rangle$ and $\langle x^2\rangle$:

$\langle x\rangle = 0$ since $x e^{-2bmx^2}$ is odd function.

$$\langle x^2\rangle = |C|^2 \int dx \cdot x^2 e^{-2bmx^2} = |C|^2 \sqrt{\frac{\pi}{2bm}} \frac{1}{(4bm)} = \frac{1}{4bm} = \frac{\hbar}{2m\omega}$$

$$\boxed{\begin{aligned}&\langle x\rangle = 0;\\ &\langle x^2\rangle = \frac{\hbar}{2m\omega};\end{aligned}}$$

(d) Find uncertainty.

By definition $\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = \sqrt{\frac{\hbar}{2m\omega}}$

$$\boxed{\sigma_x = \sqrt{\frac{\hbar}{2m\omega}}}$$

Problem III Suppose we are given 2 properly normalized w.f. $\Psi_1(x,t)$ and $\Psi_2(x,t)$ that are solutions to Sch. equation. Hence, the combination $\Psi(x,t) = C\,(\Psi_1(x,t) + e^{i\varphi}\Psi_2(x,t))$ is also a solution. Assume that $\int_{-\infty}^{+\infty} \Psi_1^*(x,t)\Psi_2(x,t)\,dx = 0$;

(a) Find C so that $\Psi(x,t)$ is properly normalized.

normalization condition is

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = |C|^2\left(\int_{-\infty}^{+\infty} |\Psi_1|^2 dx + \int_{-\infty}^{+\infty} |\Psi_2|^2 dx + e^{i\varphi}\int_{-\infty}^{+\infty} \Psi_1^*\Psi_2\, dx + e^{-i\varphi}\int_{-\infty}^{+\infty} \Psi_2^*\Psi_1\, dx\right);$$

now as $\Psi_{1,2}(x,t)$ are normalized properly:

(6) $\int_{-\infty}^{+\infty} |\Psi_{1,2}|^2 dx = 1$ and $\int_{-\infty}^{+\infty} \Psi_1^* \Psi_2 \, dx = \int_{-\infty}^{+\infty} \Psi_2^* \Psi_1 \, dx = 0$ so we get $\int_{-\infty}^{+\infty} |\Psi|^2 dx = |C|^2 \cdot 2 \Rightarrow \boxed{|C| = \frac{1}{\sqrt{2}}}$

(b) Show how the relative phase φ can effect the probability density and position expectation value $\langle x \rangle$

Probability density is

$$\rho(x,t) = |\Psi(x,t)|^2 = |C|^2 \left(|\Psi_1|^2 + |\Psi_2|^2 + \underbrace{e^{i\varphi} \Psi_1^* \Psi_2 + e^{-i\varphi} \Psi_2^* \Psi_1}_{\text{interferation term}} \right)$$

so we see that relative phase φ will give rise to interferation like term $(e^{i\varphi} \Psi_1^* \Psi_2 + e^{-i\varphi} \Psi_2^* \Psi_1)$

For x expectation value we get by definition:

$$\langle x \rangle = \int dx \, \Psi^* x \Psi = \frac{1}{2} \int \Psi_1^* x \Psi_1 dx + \frac{1}{2} \int \Psi_2^* x \Psi_2 dx + \frac{e^{i\varphi}}{2} \int \Psi_1^* x \Psi_2 dx +$$

$$+ \frac{e^{-i\varphi}}{2} \int \Psi_2^* x \Psi_1 dx ;$$ Once again effect of phase is encrypted in last 2 terms.

Problem IV Consider "wave-packet" w.f. $\Psi(x,t)$

$$\Psi(x,t) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{1 + 2ia\hbar t/m}} e^{-\frac{ax^2}{1 + (2ia\hbar t/m)}}$$ where a is constant and m is the particles mass.

(a) Show that $\Psi(x,t)$ is a solution to the Schr. eq. when $V(x) = 0$;

Schr. eq. is given by $i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t)$

First we find derivatives

$$\frac{\partial \Psi}{\partial t} = \frac{2ia\hbar}{m} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \left\{ -\frac{1}{2(1 + 2ia\hbar t/m)^{3/2}} + \frac{ax^2}{(1 + 2ia\hbar t/m)^{5/2}} \right\} \exp\left(-\frac{ax^2}{1 + 2ia\hbar t/m}\right)$$

$$\frac{\partial \Psi}{\partial x} = -\left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{2ax}{(1 + 2ia\hbar t/m)^{3/2}} \exp\left(-\frac{ax^2}{1 + 2ia\hbar t/m}\right);$$

(7) $$\frac{\partial^2\psi}{\partial x^2} = -\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\left[\frac{2a}{(1+2iat\hbar/m)^{3/2}} - \frac{4a^2x^2}{(1+2iat\hbar/m)^{5/2}}\right]\exp\left(-\frac{ax^2}{1+2iat\hbar/m}\right)$$

$$= \frac{2m}{i\hbar}\frac{\partial\psi}{\partial t} \Longrightarrow \boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}}$$

(b) Graph the probability density at $t=0$ and $t=\frac{\sqrt{3}m}{2a\hbar}$.

What's happening to the w.-f. as time evolves.

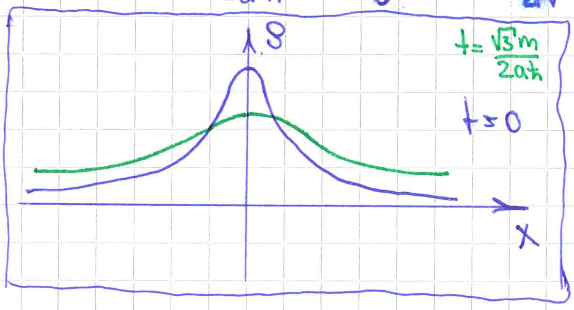
Probability density is given by

$$\rho(x,t) = |\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}}\frac{1}{(1+2iat\hbar/m)^{1/2}(1-2iat\hbar/m)^{1/2}}\exp\left\{-\frac{ax^2}{1+2iat\hbar/m} - \frac{ax^2}{1-2iat\hbar/m}\right\}$$

Then finally:

$$\rho(x,t) = \sqrt{\frac{2a}{\pi}}\frac{1}{(1+4a^2t^2\hbar^2/m^2)^{1/2}}\exp\left[-\frac{2ax^2}{1+4a^2\hbar^2t^2/m^2}\right]$$

* at $t=0$, $\rho(x,t) = \sqrt{\frac{2a}{\pi}}\,e^{-2ax^2}$;
* at $t=\frac{\sqrt{3}m}{2a\hbar}$, $\rho(x,t) = \frac{1}{2}\sqrt{\frac{2a}{\pi}}\,e^{-\frac{1}{2}ax^2} = \sqrt{\frac{a}{2\pi}}\,e^{-\frac{1}{2}ax^2}$



(c) Compute the probability current and show that it is positive when $x>0$ and negative when $x<0$. Explain why this is consistent with conclusions from part (b).

By definition probability current is given by

$$j = \frac{i\hbar}{2m}\left\{\left(\frac{\partial\Psi^*}{\partial x}\right)\cdot\Psi - \Psi^*\left(\frac{\partial\Psi}{\partial x}\right)\right\}$$ if we substitute

expression for derivative we get:

$$\left(\frac{\partial}{\partial x}\Psi^*\right)\Psi = -\frac{2ax}{1-2iat\hbar/m}\Psi^*\Psi$$ then

$$j = \frac{i\hbar}{2m}\left\{\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right\} = -\frac{i\hbar}{2m}\left\{\frac{2ax}{1-2iat\hbar/m} - \frac{2ax}{1+2iat\hbar/m}\right\}|\Psi|^2$$

$$= \frac{i\hbar}{2m}\cdot(-2ax)\cdot 4iat\hbar\cdot\frac{1}{m}|\Psi|^2\cdot\frac{1}{1+4a^2\hbar^2t^2/m^2} = \frac{4a^2\hbar^2tx}{m^2+4a^2\hbar^2t^2}|\Psi|^2$$

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$$\boxed{\begin{array}{l} j = \dfrac{4a^2\hbar^2 t x}{m^2 + 4a^2\hbar^2 t^2} \cdot |\Psi|^2 \\ \text{for} \quad x > 0 \;, \; j > 0; \\ \qquad\; x < 0 \;, \; j < 0; \end{array}}$$

This is consistent with probability density evolution. We can see that it smeared with time and we can see that probability "flows away" from the center which means that $j > 0$ for $x > 0$ (flow to the right) and $j < 0$ for $x < 0$ (flow to the left)

1

Seminar 3 (operators, uncertainty, commutators)

Theory reminder

* All systems in quantum mechanics are described by wave-functions $\psi(x,t)$ which satisfies Sch. eq.:

$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$ ($\hat{H}$ - Hamiltonian operator)

* Observable quantaties are described with operators $\hat{O}$ acting on this w.-f. $\psi(x,t)$

* for states described by w.-f. $\psi(x,t)$ we can write down expectation value of operator $\hat{O}$

$\langle\hat{O}\rangle = \int dx\, \psi^* \hat{O} \psi$

and uncertainty $\sigma_0 = \sqrt{\langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2}$

simple example of operators are $\hat{x}$ and $\hat{p} = -i\hbar\frac{\partial}{\partial x}$;

* Commutator is very important object in QM. If we are given two operators $\hat{A}$ and $\hat{B}$ then their commutator is by definition $[\hat{A},\hat{B}] = \hat{A}\cdot\hat{B} - \hat{B}\hat{A}$

Commutators satisfy following properties:

- Derivation property:

$[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$

proof: $[\hat{A},\hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}C - \hat{B}\hat{C}\hat{A} =$

$= [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$, q.e.d.

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

$[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} = -(\hat{B}\hat{A} - \hat{A}\hat{B}) = -[\hat{B},\hat{A}]$;

In particular it follows that $[\hat{A},\hat{A}] = 0$;

- $[\hat{A}, c] = 0$ if c is usual number (not operator)

* Time evolution of operators

$$\frac{d}{dt}\langle O\rangle = \int\left(\frac{\partial}{\partial t}\psi^* \hat{O}\psi + \psi^*\hat{O}\frac{\partial}{\partial t}\psi\right)dx = \left[\begin{array}{l}\text{using Schr. eq.} \\ \frac{\partial \psi^*}{\partial t} = \frac{i}{\hbar}\hat{H}\psi^*;\ \frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\psi\end{array}\right] =$$

$$= \int\frac{i}{\hbar}\left((H\psi)^*\hat{O}\psi - \psi^*\hat{O}H\psi\right)dx = \int\frac{i}{\hbar}\psi^*[H,\hat{O}]\psi\, dx$$ so we

conclude $\boxed{\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}\langle[H,\hat{O}]\rangle;}$

② * Heisenberg uncertainty principle states that

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2};}$$

* Important commutator is $[\hat{x},\hat{p}]$. Let's consider following quantaty:

$[\hat{x},\hat{p}]\psi = x(-i\hbar\frac{\partial}{\partial x})\psi + i\hbar\frac{\partial}{\partial x}(x\psi) = i\hbar\left(\psi + x\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial x}\right) =$

$= i\hbar\psi$, so we get $[\hat{x},\hat{p}]\psi = i\hbar\psi$. As result is independent of ψ we get $\boxed{[\hat{x},\hat{p}] = i\hbar}$

Problem I Consider the w.-f. from the first exercise of seminar 2 $\Psi(x,t) = \sqrt{\mu}\, e^{-\mu|x|} e^{-i\omega t}$

ⓐ Find the expectation values for p and p^2 for $\Psi(x,t)$

By definition:

$$\langle\hat{p}\rangle = \int_{-\infty}^{+\infty} \Psi^* (-i\hbar)\frac{\partial\Psi}{\partial x} \quad ; \quad \langle\hat{p}^2\rangle = \int_{-\infty}^{+\infty} \Psi^* (-\hbar^2)\frac{\partial^2\Psi}{\partial x^2};$$

Let's find derivatives

$$\frac{\partial\Psi}{\partial x} = -\mu^{3/2}\frac{\partial|x|}{\partial x} e^{-\mu|x|} e^{-i\omega t} \qquad \text{Here } \frac{\partial|x|}{\partial x} = \text{sign}(x) = \begin{cases} +1, & x>0 \\ -1, & x<0 \end{cases}$$

then $\frac{\partial\Psi}{\partial x} = -\mu\cdot\text{sign}(x)\cdot\Psi$ and we get:

$$\langle\hat{p}\rangle = \int_{-\infty}^{+\infty} \Psi^* (-\mu\,\text{sign}(x))\cdot(-i\hbar)\cdot\Psi = +i\mu^2\hbar\int_{-\infty}^{+\infty} dx\, \text{sign}(x)\, e^{-2\mu|x|}$$

as $\text{sign}(x)\, e^{-2\mu|x|}$ is odd function we immedeately get: $\boxed{\langle\hat{p}\rangle = 0;}$

Now we go for $\langle\hat{p}^2\rangle$. $\frac{\partial^2\Psi}{\partial x^2} = -2\mu\,\delta(x)\,\Psi + \mu\,\text{sign}(x)\frac{\partial\Psi}{\partial x} =$

$= -2\mu\delta(x)\Psi + \mu^2\,\text{sign}^2(x)\,\Psi \Rightarrow \frac{\partial^2\Psi}{\partial x^2} = (-2\mu\delta(x) + \mu^2)\Psi(x)$

So that we get

$$\langle\hat{p}^2\rangle = -\hbar^2\int\Psi^*\Psi(-2\mu\delta(x) + \mu^2)\,dx = -\hbar^2\mu^2\underbrace{\int|\Psi|^2 dx}_{1} +$$

$$+ 2\mu\hbar^2\int|\Psi|^2\delta(x)\,dx = -\hbar^2\mu^2 + 2\mu\hbar^2|\Psi(0,t)|^2 = \mu^2\hbar^2 \Rightarrow$$

$$\Rightarrow \boxed{\langle\hat{p}^2\rangle = \hbar^2\mu^2}$$

Note: Delta-function

In the derivation we have used δ-function. Let's

③ remind some facts about it:

Def Delta function is function which is zero everywhere except origin, where it is equal infinity:

$$\delta(x) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases}$$

and which satisfies equation $\int_{-\infty}^{+\infty} \delta(x)\, dx = 1$

* important property we will use is

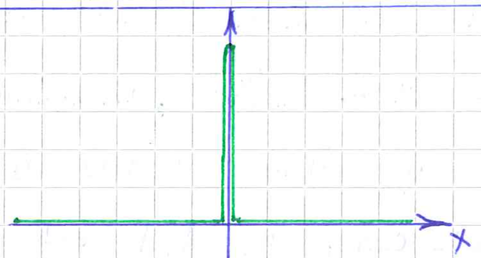
$$\int_{-\infty}^{+\infty} f(x)\delta(x)dx = f(0)$$

* We can define Heaviside step function as integral of delta-function:

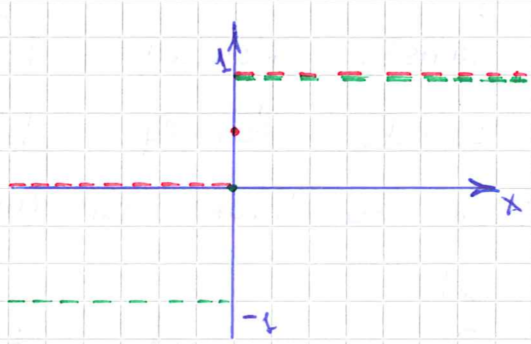
$$H(x) = \int_{-\infty}^{x} \delta(s)\, ds = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}$$

then $\text{sign}(x) = 2H(x) - 1$ and

$$\boxed{\frac{d}{dx}\text{sign}(x) = 2\frac{d}{dx}H(x) = 2\delta(x)}$$



pic1 Dirac δ-function



pic.2 sign(x) function sign(x)=2H(x)-1

H(x) Heaviside function

ⓑ Find the uncertainty σ_p in the momentum for $\Psi(x,t)$

By definition

$$\sigma_p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \hbar\mu \Rightarrow \boxed{\sigma_p = \hbar\mu}$$

Note that on previous class in problem I we have found $\sigma_x = \frac{1}{\sqrt{2}\mu}$ so that $\sigma_p\sigma_x = \frac{\hbar}{\sqrt{2}} > \frac{\hbar}{2} \Rightarrow$ Heisenberg uncertainty principle is satisfied.

④

Problem II In this problem we consider a case where probability is not conserved. This formalism is used to describe the decay of particles. Suppose $\Psi_0(x,t)$ is a normalised solution to Sch. eq. in a potential $V(x)=V_0(x)$. Assume that at $t=0$ we modify potential to

$$V(x) = V_0(x) - \frac{i\Gamma}{2}$$

ⓐ Find the w.-f. $\Psi(x,t)$ for $t\geq 0$ in terms of the original w.-f. $\Psi_0(x,t)$, assuming that $\Psi(x,0)=\Psi_0(x,0)$

Let's say that $\Psi(x,t)=\Psi_0(x,t)\cdot f(x,t)$, so that $f(x,0)=\text{const}=1$. And let's find what equation does $f(x,t)$ satisfy.

Ψ_0 satisfy Sch. eq. $\quad i\hbar\frac{\partial\Psi_0}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} + V_0\Psi_0$

Ψ satisfy Sch. eq. $\quad i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V_0\Psi - \frac{i\Gamma}{2}\Psi$

If we substitute our ansatz $\Psi=\Psi_0 f$ to the second eq. we get:

$$i\hbar\frac{\partial\Psi_0}{\partial t}\cdot f + \Psi_0\, i\hbar\frac{\partial f}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2}f - \frac{\hbar^2}{2m}\Psi_0\frac{\partial^2 f}{\partial x^2} - \frac{\hbar^2}{m}\frac{\partial\Psi_0}{\partial x}\frac{\partial f}{\partial x} +$$
$$+ V_0\Psi_0 f - \frac{i\Gamma}{2}\Psi_0 f \quad \text{or}$$

$$\underbrace{\left(i\hbar\frac{\partial\Psi_0}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\Psi_0}{\partial x^2} - V_0\Psi_0\right)}_{=0 \text{ by Sch. eq. for } \Psi_0}f + \Psi_0\, i\hbar\frac{\partial f}{\partial t} + \frac{i\Gamma}{2}\Psi_0 f + \frac{\hbar^2}{2m}\Psi_0\frac{\partial^2 f}{\partial x^2} +$$
$$+ \frac{\hbar^2}{m}\frac{\partial\Psi_0}{\partial x}\frac{\partial f}{\partial x} = 0$$

Equation will simplify if we assume that f doesn't depend on "x": $f(x,t)=f(t)$. In this case we observe:

$$i\hbar\frac{\partial f}{\partial t} + \frac{i\Gamma}{2}f = 0 \Rightarrow \frac{\partial f}{\partial t} = -\frac{\Gamma}{2\hbar}f \Rightarrow f(t) = e^{-\Gamma t/2\hbar}\cdot C$$

and due to boundary condition $f(0)=C=1$ we finally get $\boxed{f(t) = e^{-\Gamma t/2\hbar}}$ so that resulting w.-f. is given by

$$\boxed{\Psi(x,t) = \Psi_0(x,t)\, e^{-\Gamma t/2\hbar}}$$

(5) (b) Find the total probability that there is a particle somewhere between $-\infty$ and $+\infty$ as a function of t for $t \geq 0$.

This probability is given by:

$$P = \int_{-\infty}^{+\infty} |\Psi|^2 dx = e^{-\Gamma t/\hbar} \int_{-\infty}^{+\infty} |\Psi_0|^2 dx = e^{-\Gamma t/\hbar} \; ; \quad \boxed{P(t) = e^{-\Gamma t/\hbar}}$$

We see the "exponential decay" of probability.

(c) Show that the new potential modifies the current conservation equation.

Current conservation equation is given by

$$\frac{\partial}{\partial t} \rho_0(x,t) + \frac{\partial}{\partial x} J_0(x,t) = 0$$

and $\Psi_0(x,t)$ satisfies it as it satisfies Sch. eq. with hermitian Hamiltonian.

Let's see what will happen if we substitute $\Psi(x,t) = \Psi_0(x,t) \cdot e^{-\Gamma t/2\hbar}$ into this equation:

$$\frac{\partial}{\partial t} \rho(x,t) + \frac{\partial}{\partial x} J(x,t) = ?$$

* Firs of all $J(x,t) \equiv \frac{i\hbar}{2m}\left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^* \frac{\partial \Psi}{\partial x}\right) = \frac{i\hbar}{2m}\left(\frac{\partial \Psi_0^*}{\partial x}\Psi_0 - \Psi_0^* \frac{\partial \Psi_0}{\partial x}\right) \times$
$\times e^{-\Gamma t/\hbar} = J_0(x,t)\, e^{-\Gamma t/\hbar}$ so this part of equation is not changed very much : $\underline{J(x,t) = J_0(x,t)\, e^{-\Gamma t/\hbar}}$

* Now let's take a look on first term:

$$\rho(x,t) \equiv \Psi^* \cdot \Psi = \Psi_0^* \Psi_0 \cdot e^{-\Gamma t/\hbar} = \rho_0(x,t) \cdot e^{-\Gamma t/\hbar}$$ so that :

$$\frac{\partial}{\partial t} \rho(x,t) = \frac{\partial \rho_0}{\partial t} \cdot e^{-\Gamma t/\hbar} - \frac{\Gamma}{\hbar} \rho_0\, e^{-\Gamma t/\hbar}.$$

Putting all together we finally get:

$$\frac{\partial}{\partial t} \rho(x,t) + \frac{\partial}{\partial x} J(x,t) = \underbrace{\left(\frac{\partial \rho_0}{\partial t} + \frac{\partial J_0}{\partial x}\right)}_{0} e^{-\Gamma t/\hbar} - \frac{\Gamma}{\hbar} \rho(x,t)$$

so we see that probability curren is no more conserved:

$$\boxed{\frac{\partial}{\partial t} \rho(x,t) + \frac{\partial}{\partial x} J(x,t) = -\frac{\Gamma}{\hbar} \rho(x,t)}$$

This happens because Hamiltonian of the system is no more hermitian as it has $-\frac{i\Gamma}{2}$ term in it.

⑥ **Problem III** Suppose the Hamiltonian is given by

$$H = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2;$$

ⓐ Find the commutators $[H,\hat{x}]$ and $[H,\hat{p}]$;

Here we will use derivation property of commutator:

$$[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + \hat{B}[\hat{A},\hat{C}]$$ so that

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

$$[\hat{x}^2,\hat{x}] = 2\hat{x}[\hat{x},\hat{x}] = 0$$ due to commutators antisymmetry

$$[\hat{x},\hat{x}] = -[\hat{x},\hat{x}] \Rightarrow [\hat{x},\hat{x}] = 0 \Rightarrow [\hat{x}^n,\hat{x}] = 0 \;\forall n$$

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

$$[\hat{p}^2,\hat{p}] = 0$$

Using all this result's we get:

$$[H,\hat{x}] = \frac{1}{2m}[\hat{p}^2,\hat{x}] + \frac{1}{2}m\omega^2[\hat{x}^2,\hat{x}] = -\frac{2i\hbar\hat{p}}{2m} = -\frac{i\hbar}{m}\hat{p}$$

$$[H,\hat{p}] = \frac{1}{2m}[\hat{p}^2,\hat{p}] + \frac{1}{2}m\omega^2[\hat{x}^2,\hat{p}] = \frac{2i\hbar m\omega^2\hat{x}}{2} = i\hbar m\omega^2\hat{x}$$

$$\boxed{[H,\hat{x}] = -\frac{i\hbar}{m}\hat{p}; \quad [H,\hat{p}] = i\hbar m\omega^2\hat{x};}$$

ⓑ Use result of (a) to find the time rates of change of $\langle x\rangle$ and $\langle p\rangle$

Operators evolution is described by Heisenberg equation $\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}\langle[H,\hat{O}]\rangle$ in particular for $\hat{p}$ and $\hat{x}$ we get:

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{i}{\hbar}\langle[H,\hat{x}]\rangle = \frac{1}{m}\langle\hat{p}\rangle$$

$$\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle[H,\hat{p}]\rangle = -m\omega^2\langle\hat{x}\rangle$$

$$\boxed{\begin{aligned}&\frac{d}{dt}\langle\hat{x}\rangle = \frac{1}{m}\langle\hat{p}\rangle;\\ &\frac{d}{dt}\langle\hat{p}\rangle = -m\omega^2\langle\hat{x}\rangle;\end{aligned}}$$

Note that this equation look's like classical equations of motion $\frac{dx}{dt} = \frac{1}{m}p$; $\frac{d}{dt}p = -m\omega^2 x$; This is called Ehrenfest correspondence principle: operators expectation values satisfy classical equations of motion for corresponding quantaty.

⑦ **Problem IV**

Consider the unnormalized gaussian w.-f. $\Psi(x,0) = e^{-a^2x^2/4}$

ⓐ Find σ_x and σ_p and show that it saturates the Heisenberg uncertainty relation $\sigma_x\sigma_p = \frac{\hbar}{2}$;

* First we should normalize w.-f. because Heisenberg uncertainty is written only for normalized one.

$$\Psi(x) = C\, e^{-a^2x^2/4} \quad ;$$

normalization condition is:

$$1 = \int |\Psi(x)|^2 dx = |C|^2 \int_{-\infty}^{+\infty} e^{-a^2x^2/2} dx = |C|^2 \cdot \sqrt{\frac{2\pi}{a^2}} \Rightarrow \quad |C| = \left(\frac{a^2}{2\pi}\right)^{\frac{1}{4}}$$

* Now we can calculate expectation values we need:

$$\langle \hat{x} \rangle \equiv \int_{-\infty}^{+\infty} \Psi^* \hat{x}\, \Psi\, dx = \int_{-\infty}^{+\infty} |C|^2\, x\, e^{-a^2x^2/2} dx = 0 \quad \text{as } x e^{-a^2x^2/2} \text{ is odd}$$

$$\langle \hat{x}^2 \rangle \equiv \int_{-\infty}^{+\infty} \Psi^* \hat{x}^2 \Psi\, dx = \int_{-\infty}^{+\infty} |C|^2 x^2 e^{-a^2x^2/2} dx = |C|^2 \cdot \sqrt{\frac{2\pi}{a^2}}\, \frac{1}{a^2} = \frac{1}{a^2}$$

$$\langle \hat{p} \rangle \equiv \int_{-\infty}^{+\infty} \Psi^* (-i\hbar) \frac{\partial \Psi}{\partial x} dx = + \frac{i\hbar a^2}{2} \int_{-\infty}^{+\infty} \Psi^* \hat{x}\, \Psi\, dx = 0 \quad \text{as we have seen}$$

$$\langle \hat{p}^2 \rangle \equiv -\hbar^2 \int_{-\infty}^{+\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx \; ; \quad \frac{\partial^2 \Psi}{\partial x^2} = -\frac{a^2 C}{2} \frac{\partial}{\partial x} x e^{-\frac{a^2x^2}{4}} =$$

$$= -\frac{a^2 C}{2}\left(1 - \frac{a^2}{2}x^2\right) e^{-\frac{a^2x^2}{4}} = -\frac{a^2}{2}\left(1 - \frac{a^2x^2}{2}\right)\Psi \quad \text{so that}$$

$$\langle \hat{p}^2 \rangle = (-\hbar^2) \int_{-\infty}^{+\infty} dx\, \Psi^* \left(\frac{a^4x^2}{4} - \frac{a^2}{2}\right)\Psi = (-\hbar^2)\int_{-\infty}^{+\infty} dx\, \Psi^* x^2 \Psi + \frac{\hbar^2 a^2}{2} \int_{-\infty}^{+\infty} dx\, \Psi^* \Psi =$$

$$= -\frac{\hbar^2 a^4}{4} \langle \hat{x}^2 \rangle + \frac{a^2\hbar^2}{2} = \frac{a^2\hbar^2}{4}$$

So we get: $\boxed{\langle \hat{x} \rangle = \langle \hat{p} \rangle = 0; \; \langle \hat{x}^2 \rangle = \sigma_x^2 = \frac{1}{a^2} \; ; \; \langle \hat{p}^2 \rangle = \sigma_p^2 = \frac{a^2\hbar^2}{4}\;;}$

From here we can see that Heisenberg uncertainty is indeed satisfied: $\sigma_x \cdot \sigma_p = \frac{a\hbar}{2} \cdot \frac{1}{a} = \frac{\hbar}{2}$, q.e.d.

ⓑ Now take $\Psi(x,0) = x\, e^{-a^2x^2/4}$. Show that in this case $\sigma_x \sigma_p > \frac{\hbar}{2}$

* First we should normalize w.-f.:

$\Psi(x,0) = |C|\, x\, e^{-a^2x^2/4}$; normalization condition is:

$$1 \equiv \int_{-\infty}^{+\infty} |\Psi|^2 dx = |C|^2 \int_{-\infty}^{+\infty} x^2 e^{-a^2x^2/2} dx = |C|^2 \sqrt{\frac{2\pi}{a^2}}\, \frac{1}{a^2} \Rightarrow \quad |C| = \left(\frac{a^6}{2\pi}\right)^{\frac{1}{4}}$$

* Now we are able to find expectation values for operators:

⑧ $\langle\hat{x}\rangle \equiv \int_{-\infty}^{+\infty} \Psi^* \hat{x} \Psi \, dx = |C|^2 \int_{-\infty}^{+\infty} x^3 e^{-a^2x^2/2} dx = 0$ since $x^3 e^{-a^2x^2/2}$ is odd function.

$$\langle\hat{x}^2\rangle \equiv \int_{-\infty}^{+\infty} \Psi^* \hat{x}^2 \Psi \, dx = |C|^2 \int_{-\infty}^{+\infty} x^4 e^{-a^2x^2/2} dx = \frac{a^3}{\sqrt{2\pi}} \cdot \frac{\sqrt{2\pi}}{a} \cdot \frac{3}{a^4} = \frac{3}{a^2}$$

Before looking on $\langle\hat{p}\rangle$ and $\langle\hat{p}^2\rangle$ let's find $\hat{p}\Psi$ and $\hat{p}^2\Psi$:

$$\hat{p}\Psi \equiv -i\hbar \frac{\partial}{\partial x} |C| x e^{-a^2x^2/4} = -i\hbar|C| \left(1 - \frac{1}{2}a^2x^2\right) e^{-a^2x^2/4} =$$

$$= -i\hbar\left(1 - \frac{1}{2}a^2x^2\right)|C| e^{-a^2x^2/4}$$

$$\hat{p}^2\Psi = -\hbar^2 \frac{\partial^2}{\partial x^2} \Psi = -\hbar^2 \frac{\partial}{\partial x} |C| \left(1 - \frac{1}{2}a^2x^2\right) e^{-a^2x^2/4} =$$

$$= -\hbar^2 |C| \left(-a^2x - \frac{1}{2}a^2x + \frac{1}{4}a^4x^3\right) e^{-a^2x^2/4} \quad \text{so that}$$

$\langle\hat{p}\rangle \equiv \int_{-\infty}^{+\infty} \Psi^* \hat{p} \Psi = -i\hbar|C|^2 \int_{-\infty}^{+\infty} dx \left(1 - \frac{1}{2}a^2x^2\right) x e^{-\frac{1}{2}a^2x^2} = 0$, since $\left(1 - \frac{1}{2}x^2\right) x e^{-\frac{1}{2}a^2x^2}$ is odd function.

$$\langle\hat{p}^2\rangle \equiv \int_{-\infty}^{+\infty} \Psi^* \hat{p}^2 \Psi \, dx = -\hbar^2|C|^2 \int_{-\infty}^{+\infty} dx \left(\frac{1}{4}a^4x^4 - \frac{3}{2}a^2x^2\right) e^{-\frac{1}{2}a^2x^2} =$$

$$= \hbar^2 |C|^2 \frac{3}{2} a^2 \int_{-\infty}^{+\infty} x^2 e^{-\frac{a^2x^2}{2}} dx - \frac{1}{4}\hbar^2 a^4 |C|^2 \int_{-\infty}^{+\infty} dx \, x^4 e^{-\frac{1}{2}a^2x^2} =$$

$$= \frac{3}{2}\hbar^2 a^2 - \frac{1}{4}\hbar^2 a^4 \frac{a^3}{\sqrt{2\pi}} \cdot \frac{\sqrt{2\pi}}{a} \frac{3}{a^4} = \hbar^2 a^2 \left(\frac{3}{2} - \frac{3}{4}\right) = \frac{3}{4} a^2 \hbar^2$$

So we finally get:

$$\boxed{\begin{aligned} &\langle\hat{p}\rangle = \langle\hat{x}\rangle = 0; \\ &\langle\hat{p}^2\rangle = \sigma_p^2 = \tfrac{3}{4}a^2\hbar^2; \\ &\langle\hat{x}^2\rangle = \sigma_x^2 = \tfrac{3}{a^2}; \end{aligned}}$$

$\Rightarrow$ from where we can find that

$$\sigma_x \sigma_p = \frac{\sqrt{3}}{2} a\hbar \frac{\sqrt{3}}{a} = \frac{3}{2}\hbar > \frac{\hbar}{2}, \text{ q.e.d.}$$

$$\boxed{\sigma_x \sigma_p = \frac{3}{2}\hbar > \frac{1}{2}\hbar}$$

Seminar 4 (Solutions of Schr. eq.)

Theory reminder

* W.-f. in QM are found from Schr. eq.

$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$ The way to solve it is to write down $\Psi(x,t) = e^{-\frac{i}{\hbar}Et}\psi(x)$ then E is eignvalue of $\hat{H}$:

$\hat{H}\psi = E\psi$ There is complete set ψ_n of $\hat{H}$ eigenstates and corresponding eigenvalues E_n:

$\hat{H}\psi_n = E_n\psi_n$, then general solution of Sch. eq. due to it's linearity can be written in the following form

$\Psi(x,t) = \sum_n e^{-iE_nt/\hbar} \cdot c_n\psi_n$ from normalization condition we can obtain condition for c_n: $|c_n|^2 = 1$

* Complete set of states ψ_n is orthonormal:

$$\int \psi_n^* \psi_m \, dx = \delta_{nm}$$

* Knowledge of complete set ψ_n of $\hat{H}$ eigenvalues gives us ability to calculate evolution of any given w.-f. in time. The algorithm of doing this is the following:

- Assume we are given $\Psi(x,0) = \psi(x)$ and want to find $\Psi(x,t)$

- First we expand $\psi(x)$ in series of $\hat{H}$ eigenfunctions: $\boxed{\psi(x) = \sum_n c_n\psi_n(x)}$, if we multiply both sides with $\psi_m^*(x)$ and integrate:

$$\int_{-\infty}^{+\infty} \psi_m^* \psi \, dx = \sum_n c_n \int_{-\infty}^{+\infty} \psi_m^* \psi_n dx = \sum_n c_n \delta_{mn} = c_m,$$ so that:

$$\boxed{c_n = \int \psi_n^* \psi \, dx}$$

- Time evolution of the w.-f. is determined by time evolution operator $e^{-\frac{i}{\hbar}\hat{H}t}$

② so that

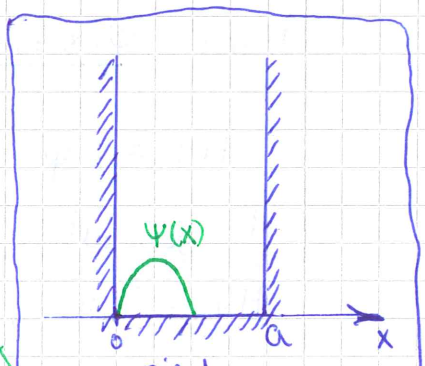
$$\Psi(x,t) = e^{-\frac{i}{\hbar}\hat{H}t} \sum_n c_n \psi_n = \sum_n c_n e^{-\frac{i}{\hbar}\hat{H}t} \psi_n = \sum_n c_n e^{-\frac{i}{\hbar}E_n t} \psi_n$$

$$\boxed{\Psi(x,t) = \sum_n c_n e^{-\frac{i}{\hbar}E_n t} \psi_n ;}$$

Problem I

Consider infinite square well potential

$$V(x) = \begin{cases} 0 , & 0 \leq x \leq a \\ \infty , & x < 0 , \text{ or } x > a ; \end{cases}$$



pic.1

At time $t=0$ the w.-f. is given by

$$\Psi(x,0) = \psi(x) = \begin{cases} c \sin 2\pi x/a , & 0 < x < \frac{a}{2} \\ 0 , & x \leq 0 \text{ or } x \geq \frac{a}{2} \end{cases}$$

About infinite square well potential

In this and next problem we need the set of $\hat{H}$ eigenvalues and eigenfunctions ψ_n of square well potential. Let's write it down:

* First of all there can be no particle outside the well so that $\psi_n(x) = 0$ if $x \in (-\infty, 0) \cup (a, +\infty)$
* For w.f. to be continious we take $\psi_n(0) = \psi_n(a) = 0$
* General solution for Sch. eq. is written as

$$\psi_n(x) = A_n \sin(k_n x) + B_n \cos(k_n x)$$

Substituting this to boundary conditions we get

$$\psi_n(0) = B_n = 0$$

$$\psi_n(a) = A_n \sin(k_n a) = 0 \Rightarrow \quad k_n a = \pi n \Rightarrow k_n = \frac{\pi n}{a} .$$

so $\psi_n(x) = A_n \sin\left(\frac{\pi n x}{a}\right)$

normalization condition for this function reads

$$1 = \int \psi_n^* \psi_n \, dx = \int |A_n|^2 \sin^2\left(\frac{\pi n x}{a}\right) dx = |A_n|^2 \int_0^a \left(\frac{1}{2} - \frac{1}{2} \sin \frac{2\pi n x}{a}\right) dx =$$

$$= |A_n|^2 \frac{a}{2} \Rightarrow \quad A_n = \sqrt{\frac{2}{a}}$$ up to phase. So eigenvalues for this potential are given by:

③ $\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n x}{a}\right);}$ $n=1,2,\ldots$

Some trigonometric identities we will be using:

$\sin^2 x = \frac{1}{2}(1-\cos 2x)$; $\sin x \cdot \sin y = \frac{1}{2}(\cos(x-y) - \cos(x+y))$

$\cos^2 x = \frac{1}{2}(1+\cos 2x)$; $\cos x \cdot \cos y = \frac{1}{2}(\cos(x+y) + \cos(x-y))$

$\cos x \cdot \sin y = \frac{1}{2}(\sin(x+y) - \sin(x-y))$;

* Energy corresponding to ψ_n is given by:

$$E_n\psi_n = \hat{H}\psi_n = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} = -\frac{\hbar^2}{2m}\cdot\left(\frac{\pi n}{a}\right)^2\cdot\left(-\sqrt{\frac{2}{a}}\sin\left(\frac{\pi n x}{a}\right)\right) =$$

$$= \frac{\pi^2 n^2 \hbar^2}{2ma^2}\psi_n \text{ , so that } \boxed{E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2},\ n=1,2,\ldots}$$

* Usefull thing to know how solution looks like for "shifted" potential of form:

$$V = \begin{cases} 0 & , -\frac{a}{2} \leq x \leq \frac{a}{2} \\ \infty & , |x| > \frac{a}{2} \end{cases}$$

obviously we should just replace $x \to x + \frac{a}{2}$ to get new. w.-f.:

$$\psi(x) \to \psi(x+\tfrac{a}{2}) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}(x+\tfrac{a}{2})\right) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}x + \frac{\pi n}{2}\right) =$$

$$= \sqrt{\tfrac{2}{a}}\cos\frac{\pi n x}{a},\ n=1 \bmod 4;\quad -\sqrt{\tfrac{2}{a}}\cos\frac{\pi n x}{a},\ n=3 \bmod 4;$$
$$-\sqrt{\tfrac{2}{a}}\sin\frac{\pi n x}{a},\ n=2 \bmod 4;\quad \sqrt{\tfrac{2}{a}}\sin\frac{\pi n x}{a},\ n=0 \bmod 4;$$

"–" in the w.-f. doesn't play role as it's unobservable and we can absorb it into the definition of w.-f.

So we are left with 2 kind of solutions:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\cos\frac{\pi n x}{a},\ n \text{ odd}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{\pi n x}{a},\ n \text{ even}$$

or written in another way

even: $\psi_{n+}(x) = \sqrt{\frac{2}{a}}\cos\frac{(2n-1)\pi x}{a};\ n=1,2,\ldots$

odd: $\psi_{n-}(x) = \sqrt{\frac{2}{a}}\sin\frac{2\pi n x}{a};\ n=1,2,\ldots$

$\pm$ signs denote that solutions are even or odd under $x \to -x$ transformations.

Having all this information we can finally start with

④ problem:

ⓐ Find C in terms of a so that $\psi(x)$ is properly normalized.

Normalization condition is as usally given by

$$1=\int|\psi(x)|^2dx = |C|^2\int_0^{a/2}\sin^2\frac{2\pi x}{a} = |C|^2\int_0^{a/2}\left(\frac{1}{2}-\frac{1}{2}\cos\frac{4\pi x}{a}\right)dx =$$

$$= |C|^2\left(\frac{1}{2}x-\frac{a}{8\pi}\sin\frac{4\pi x}{a}\right)\Big|_0^{\frac{a}{2}} = |C|^2\cdot\frac{a}{4}$$ so we conclude

$\boxed{C=\frac{2}{\sqrt{a}}}$ up to unobservable phase.

ⓑ Find $\langle E\rangle$;

By definition $\langle E\rangle = \int\psi^*\hat{H}\psi\,dx$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}C\cdot\sin\frac{2\pi x}{a} = \frac{\hbar^2}{2m}\cdot C\cdot\frac{4\pi^2}{a^2}\sin\frac{2\pi x}{a} = \frac{4\pi^2\hbar^2}{2ma^2}\psi$$

so that

$$\langle E\rangle = \frac{2\pi^2\hbar^2}{ma^2}\int\psi^*\psi\,dx = \frac{2\pi^2\hbar^2}{ma^2};$$ so that $\boxed{\langle E\rangle = \frac{2\pi^2\hbar^2}{ma^2}}$

ⓒ Find $\psi(x)$ in terms of the eigenfunctions of H.

As we have seen the eigenfunction of $\hat{H}$ in square well potential is

$$\psi_n(x) = \begin{cases} A_n\sin\frac{\pi n x}{a}, & 0<x<a; \\ 0, & x\geq a,\ x\leq 0; \end{cases}$$ with corresponding energy being $E_n=\frac{\hbar^2\pi^2n^2}{2ma^2}$;

We should follow algorithm we have described in theory part:

- first we expand $\Psi(x,0)=\psi(x)$ in terms of $\psi_n(x)$ eigenfunctions:

$$\psi(x)=\sum_n c_n\psi_n(x)$$ with c_n given by:

$$c_n=\int\psi_n^*(x)\,\psi(x)$$ if we find c_n we get:

$$c_n=\frac{2\sqrt{2}}{a}\int_0^{\frac{a}{2}}dx\,\sin\left(\frac{\pi n x}{a}\right)\cdot\sin\left(\frac{2\pi x}{a}\right) = \frac{\sqrt{2}}{a}\int_0^{\frac{a}{2}}dx\left[\cos\frac{\pi(n-2)x}{a}-\cos\frac{\pi(n+2)x}{a}\right]=$$

⑤

$$= \frac{\sqrt{2}}{a}\left\{\sin\frac{\pi(n-2)x}{a}\cdot\frac{a}{\pi(n-2)} - \frac{a}{\pi(n+2)}\cdot\sin\frac{\pi(n+2)x}{a}\right\}\Bigg|_0^{a/2} =$$

$$= \frac{\sqrt{2}}{a}\left\{\frac{a}{\pi(n-2)}\sin\frac{\pi(n-2)}{2} - \frac{a}{\pi(n+2)}\cdot\sin\frac{\pi(n+2)}{2}\right\}$$

Here we have 2 different cases:

Ⓘ n is even ($n=2k$) then $\sin\frac{2\pi(k-1)}{2} = \sin\frac{2\pi(k+1)}{2} = 0$;

Ⓘⓘ n is odd ($n=2k+1$) then $\sin\left(\frac{\pi n}{2}-\pi\right) = \sin\left(\frac{\pi n}{2}+\pi\right) =$

$= -\sin\frac{\pi n}{2} = -\sin\frac{\pi(2k+1)}{2} = (-1)^k$ then

Case $n=2$ should be considered separately:

$$C_2 = \frac{2\sqrt{2}}{a}\int_0^{a/2} dx \sin^2\frac{2\pi x}{a} = \frac{2\sqrt{2}}{a}\left(\frac{a}{4} + \frac{a}{8\pi}\sin\frac{4\pi x}{a}\Big|_0^{a/2}\right) = 1/\sqrt{2}$$

$\underline{C_2 = 1/\sqrt{2}}$

$$C_n = \begin{cases} 0, & n=2k, k\neq 1 \text{ (n is even)} \\ \frac{(-1)^k\cdot 4\sqrt{2}}{\pi(n^2-4)}, & \text{if } n=2k+1 \text{ (n is odd)} \\ \frac{1}{\sqrt{2}}, & n=2 \end{cases}$$

So that

$$\psi(x) = \begin{cases} \sum_{n=2k+1}\frac{(-1)^k 4\sqrt{2}}{\pi(n^2-4)}\cdot\sqrt{\frac{2}{a}}\sin\frac{\pi n x}{a} + \frac{1}{\sqrt{2}}\cdot\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}; & 0<x<a \\ 0, & x\geqslant a,\ x\leqslant 0; \end{cases}$$

ⓓ Find $\langle E\rangle$ using the results from (c). You should end up with an infinite sum and show that this is equal to the value you found in (B).

By definition $\langle E\rangle$ is given by:

$\langle E\rangle \equiv \int dx\, \psi^* \hat{H}\psi$ if we substitute eigenfunction expansion $\psi = \sum_n C_n\psi_n$ into this formula we get:

$$\langle E\rangle = \int dx \sum_n\sum_m C_n^* C_m \psi_n^* \underbrace{\hat{H}\psi_m}_{E_m\psi_m} = \sum_{n,m} C_n^* C_m E_m \int dx \underbrace{\psi_n^*\psi_m}_{\delta_{mn}} =$$

$= \sum_n |C_n|^2 E_n$ so we end up with the following formula:

$$\boxed{\langle E\rangle = \sum_n |C_n|^2 E_n}$$

the same formula is valid for any operator $\hat{O}$ if O_n and ψ_n are eigenvalues and eigenstates of this operator.

ⓑ using this formula, result for c_n coefficients from part ⓒ and energy levels $E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2}$ we get:

$$\langle E \rangle = \sum_{n\,\text{odd}}' \frac{16\cdot 2}{\pi^2 (n^2-4)^2}\cdot \frac{\pi^2 n^2 \hbar^2}{2ma^2} + \frac{E_2}{2} = \frac{16\hbar^2}{ma^2}\sum_{n\,\text{odd}}' \frac{n^2}{(n^2-4)^2} + \frac{2\pi^2\hbar^2}{2ma^2}$$

Finding this summ is a little bit tricky:

$$\sum_{n\,\text{odd}}' \frac{n^2}{(n^2-4)^2} = \sum_{n\,\text{odd}}' n\cdot\left(\frac{n}{(n-2)^2(n+2)^2}\right) = \sum_{n\,\text{odd}}' \frac{1}{8} n \cdot \left(\frac{1}{(n-2)^2} - \frac{1}{(n+2)^2}\right) =$$

$$= \frac{1}{8}\sum_{n\,\text{odd}}' \frac{n}{(n-2)^2} - \frac{1}{8}\sum_{n\,\text{odd}}' \frac{n}{(n+2)^2};$$

$$\sum_{n\,\text{odd}}' \frac{n}{(n-2)^2} = \sum_{n\,\text{odd}}' \frac{1}{n-2} + 2\sum_{n\,\text{odd}}' \frac{1}{(n-2)^2} = \sum_{n\,\text{odd}}' \frac{1}{n-2} + 2\sum_{n\,\text{odd}}' \frac{1}{n^2} + 2 =$$

$$= \sum_{n\,\text{odd}}' \frac{1}{n} + 2\sum_{n\,\text{odd}}' \frac{1}{n^2} - 1 + 2 = \sum_{n\,\text{odd}}' \frac{1}{n} + 2\sum_{n\,\text{odd}}' \frac{1}{n^2} + 1;$$

We have used here shift of "n" in summation:

$$\sum_{n\,\text{odd}}' \frac{1}{n-2} = [n-2=n'] = \sum_{\substack{n'=-1\\ \text{odd}}}^{\infty} \frac{1}{n'} = \sum_{n'\,\text{odd}}' \frac{1}{n'} - 1;$$

$$\sum_{n\,\text{odd}}' \frac{1}{(n-2)^2} = [n-2=n'] = \sum_{n'=-1}^{\infty} \frac{1}{n'^2} = \sum_{n'\,\text{odd}}' \frac{1}{n'^2} + 1;$$

In the same way we operate with the second sum:

$$\sum_{n\,\text{odd}}' \frac{n}{(n+2)^2} = \sum_{n\,\text{odd}}' \frac{1}{n+2} - 2\sum_{n\,\text{odd}}' \frac{1}{(n+2)^2} = \sum_{n\,\text{odd}}' \frac{1}{n} - 1 - 2\sum_{n\,\text{odd}}' \frac{1}{n^2} + 2$$

Here we have used shifts of n in summation too:

$$\sum_{n\,\text{odd}}' \frac{1}{n+2} = [n+2=n'] = \sum_{n'=3}' \frac{1}{n'} = \sum_{n'\,\text{odd}}' \frac{1}{n'} - 1$$

$$\sum_{n\,\text{odd}}' \frac{1}{(n+2)^2} = [n+2=n'] = \sum_{n'=3}' \frac{1}{n'^2} = \sum_{n'\,\text{odd}}' \frac{1}{n'^2} + 2$$

So, taking all results together we get:

$$\sum' \frac{n^2}{(n^2-4)^2} = \frac{1}{8}\left(\sum' \frac{n}{(n-2)^2} - \sum' \frac{n}{(n+2)^2}\right) = \frac{1}{8}\left(2\sum' \frac{1}{n^2} + \cancel{\sum' \frac{1}{n} + 1} + 2\sum' \frac{1}{n^2} - \cancel{\sum' \frac{1}{n} - 1}\right) =$$

$= \frac{1}{2}\sum' \frac{1}{n^2}$, so we get:

$$\boxed{\sum_{n\,\text{odd}}' \frac{n^2}{(n^2-4)^2} = \frac{1}{2}\sum_{n\,\text{odd}}' \frac{1}{n^2}}$$

(7) Before we find $\sum_{n\,odd} \frac{1}{n^2}$ let's find sum ovel all natural numbers (not only odd one). Let's for this expand x^2 in Fourier series:

$$x^2 = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx)$$

$b_n = 0$ as x^2 is even function of x: $x^2 = (-x)^2$;

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} x^2 dx = \frac{1}{3\pi} x^3\Big|_{-\pi}^{\pi} = \frac{2\pi^2}{3};$$

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} x^2 \cos nx\, dx = \underbrace{\frac{1}{\pi n} x^2 \sin(nx)\Big|_{-\pi}^{\pi}}_{0} - \frac{2}{\pi n}\int_{-\pi}^{\pi} x \sin nx =$$

$$= \frac{2}{\pi n^2} x \cos nx\Big|_{-\pi}^{\pi} - \frac{2}{\pi n^2}\int_{-\pi}^{\pi} dx \cos nx = \frac{4}{n^2}(-1)^n - \frac{2}{\pi n^3} \sin nx\Big|_{-\pi}^{\pi} = \frac{4}{n^2}(-1)^n$$

So we get:

$$x^2 = \frac{\pi^2}{3} + 4\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2}\cos(nx)$$, substituting $x = \pi$ into this equation we get $\cos(\pi n) = (-1)^n \Rightarrow$

$$\pi^2 = \frac{\pi^2}{3} + 4\sum_{n=1}^{\infty}\frac{1}{n^2}$$ so that $$\boxed{\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}}$$

Now let's write down the sum over odd n as difference between complete sum and sum over even n

$$\sum_{n\,odd} \frac{1}{n^2} = \sum_{n}' \frac{1}{n^2} - \sum_{n=2k}' \frac{1}{n^2} = \sum_{n}' \frac{1}{n^2} - \sum_{k}' \frac{1}{4k^2} = \frac{3}{4}\sum_{n}' \frac{1}{n^2} = \frac{\pi^2}{8}$$ so we get:

$$\boxed{\sum_{n\,odd} \frac{n^2}{(n^2-4)^2} = \frac{1}{2}\sum_{n\,odd}\frac{1}{n^2} = \frac{\pi^2}{16}}$$

Finally substituting this sum into obtained expression for ⟨E⟩ we get:

$$\langle E \rangle = \frac{16\hbar^2}{ma^2}\sum_{n\,odd}' \frac{n^2}{(n^2-4)^2} + \frac{\pi^2\hbar^2}{ma^2} = \frac{2\pi^2\hbar^2}{ma^2};$$ $$\boxed{\langle E \rangle = \frac{2\pi^2\hbar^2}{ma^2}}$$ which

coinsides with the result obtained in part (b) of the problem

8 ⓔ Find $\Psi(x,t)$, simplifying as much as possible.

As we have seen in "theory" part, time dependent w.-f. is given by:

$\Psi(x,t) = \sum_n C_n e^{-iE_n t/\hbar} \psi_n$ where ψ_n are eigenstates of $\hat{H}$. In our case $\psi_n = \sqrt{\frac{2}{a}} \sin\frac{\pi n x}{a}$;

$$E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2};$$

$$C_n = \frac{(-1)^k 4\sqrt{2}}{\pi(n^2-4)}; \ n = 2k+1, \text{ or } \frac{1}{\sqrt{2}} \text{ for } n=2$$

So all together they give:

$$\Psi(x,t) = \sum_{n=2k+1} \frac{(-1)^k 4\sqrt{2}}{\pi(n^2-4)} e^{-\frac{i\pi^2 n^2 \hbar^2 t}{2\hbar m a^2}} \sqrt{\frac{2}{a}} \sin\frac{\pi n x}{a} + \frac{1}{\sqrt{a}} e^{-i\frac{2\pi^2\hbar^2 t}{ma^2}} \sin\frac{2\pi x}{a}, \ 0<x<a$$

$$\boxed{\Psi(x,t) = \sum_{n=2k+1} \frac{(-1)^k 8}{\pi\sqrt{a}(n^2-4)} e^{-\frac{i\pi^2 n^2 \hbar t}{2ma^2}} \sin\left(\frac{\pi n x}{a}\right) + \frac{1}{\sqrt{a}} e^{-\frac{i 2\pi^2 \hbar^2 t}{ma^2}} \sin\frac{2\pi x}{a}; \ 0<x<a}$$

Problem II (compendium N2)

Consider a particle with mass m in the 1d infinite square well potential:

$$V(x) = \infty, \quad |x| > a$$
$$V(x) = 0, \quad |x| \leq a$$

At $t=0$ w.-f. for the particle is $\psi(x) = A(a-|x|)$

ⓐ Find the coefficient A so that $\psi(x)$ is properly normalized.

Normalization condition as usually reads:

$$1 = \int_{-\infty}^{+\infty} |\Psi|^2 dx = |A|^2 \int_{-a}^{a} (a-|x|)^2 dx = |A|^2 \int_{-a}^{a} (a^2 - 2a|x| + |x|^2)\, dx =$$

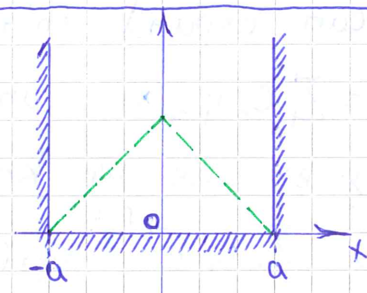
$$= 2|A|^2 \int_0^a (a-x)^2 dx = -\frac{2}{3}|A|^2 (a-x)^3 \Big|_0^a = \frac{2}{3}|A|^2 a^3 \Rightarrow$$

$$\Rightarrow |A| = \sqrt{\frac{3}{2a^3}} \quad \text{or} \quad \boxed{A = \sqrt{\frac{3}{2a^3}}} \quad \text{up to unobservable phase}$$

9

(b) Determine the time dependent w.-f. $\Psi(x,t)$. Your answer should be expressed as infinite sum.

One more time we should follow our algorithm - first we expand in eigenstates of $\hat{H}$. For the potential in the problem eigenstates, as we have found are given by even and odd parts:



pic. 2

even: $\psi_{n+} = \sqrt{\frac{1}{a}} \cos \frac{(2n-1)\pi x}{2a}$, $n=1,2,\ldots$

odd: $\psi_{n-} = \sqrt{\frac{1}{a}} \sin \frac{\pi n x}{a}$, $n=1,2,\ldots$, corresponding to the energy E_{2n-1} E_{2n} $\left(E_n = \frac{\pi^2 n^2 \hbar^2}{8ma^2}\right)$; Wee need to expand only in even functions, as coefficients of expansion in odd functions are automatically zero:

$C_{n-} = \int \psi^*_{n-} \psi = 0$. So that $\psi = \sum_n C_n \psi_{n+}$ where expansion coeffisients are given by:

$$C_n = \int \psi^*_{n+} \psi = \sqrt{\frac{1}{a}} \cdot \sqrt{\frac{3}{2a^3}} \int_{-a}^{a} \cos\left(\frac{(2n-1)\pi x}{2a}\right) \cdot (a-|x|)\, dx =$$

$$= \frac{\sqrt{3}}{\sqrt{2}a^2} \cdot 2 \int_0^a dx \cos\left(\frac{(2n-1)\pi x}{2a}\right) \cdot (a-x);$$

$$\int_0^a dx \cos\left(\frac{\pi x}{a}\left(n-\tfrac{1}{2}\right)\right) = \frac{a}{\pi\left(n-\frac{1}{2}\right)} \sin\left(\frac{\pi x}{a}\left(n-\tfrac{1}{2}\right)\right)\Big|_0^a = \frac{a}{\pi\left(n-\frac{1}{2}\right)} \sin\left(\pi n - \frac{\pi}{2}\right) =$$

$$= -\frac{a}{\pi\left(n-\frac{1}{2}\right)} \cos \pi n = \frac{a(-1)^{n+1}}{\pi\left(n-\frac{1}{2}\right)}$$

$$\int_0^a dx \cdot x \cos\left(\frac{\pi x}{a}\left(n-\tfrac{1}{2}\right)\right) = \frac{a}{\pi\left(n-\frac{1}{2}\right)} x \sin\left(\frac{\pi x}{a}\left(n-\tfrac{1}{2}\right)\right)\Big|_0^a -$$

$$- \frac{a}{\pi\left(n-\frac{1}{2}\right)} \int_0^a dx \sin\left(\frac{\pi x}{a}\left(n-\tfrac{1}{2}\right)\right) = \frac{a^2}{\pi\left(n-\frac{1}{2}\right)} \sin\left(\pi\left(n-\tfrac{1}{2}\right)\right) + \frac{a^2}{\pi^2\left(n-\frac{1}{2}\right)^2} \times$$

$$\times \cos\left(\frac{\pi x}{a}\left(n-\tfrac{1}{2}\right)\right)\Big|_0^a = \frac{a^2(-1)^{n+1}}{\pi\left(n-\frac{1}{2}\right)} - \frac{a^2}{\pi^2\left(n-\frac{1}{2}\right)^2}$$

Taking this two terms together we get:

(10)

$$C_n = \frac{\sqrt{6}}{a^2}\left(\frac{a^2(-1)^{n+1}}{\pi(n-\frac{1}{2})} - \frac{a^2(-1)^{n+1}}{\pi(n-\frac{1}{2})} + \frac{a^2}{\pi^2(n-\frac{1}{2})^2}\right)$$

$$\boxed{C_n = \frac{\sqrt{6}}{\pi^2(n+\frac{1}{2})^2};}$$

So we can expand initial wave function as:

$\Psi(x,0) = \sum C_n \psi_{n+}(x)$ and in this case time-dep. w.-f. is given, as we know, by:

$$\Psi(x,t) = \sum_n C_n e^{-i\frac{E_n t}{\hbar}} \psi_{n+}(x)$$

E_n here is formal note, really - this is energy corresponding to ψ_{n+} eigenstate, i.e. $E_n \equiv E_{2n-1} = \frac{\pi^2\hbar^2}{2ma^2}(n-\frac{1}{2})^2$;

and then we finally get time-dependent state:

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} \frac{\sqrt{6}}{\pi^2(n-\frac{1}{2})^2} \cdot \exp\left(-\frac{i\pi^2\hbar t}{2ma^2}(n-\frac{1}{2})^2\right)\cos\left(\frac{\pi x}{a}(n-\frac{1}{2})\right);}$$

(c) What is the w.-f. after a time $t = 2ma^2/\hbar\pi$ has elapsed?

Let's write down standard formula for time-dep. w.-f.

$\Psi(x,t) = \sum_{n=1}^{\infty} C_n e^{-iE_n t/\hbar} \psi_n$ and consider time dependent exponent for our particular case with $E_n = \frac{\pi^2\hbar^2}{2ma^2}(n-\frac{1}{2})^2$

then if we substitute $t = \frac{2ma^2}{\pi\hbar}$ we get

$$\exp\left(-\frac{iE_n t}{\hbar}\right) = \exp\left(-i\frac{\pi^2\hbar}{2ma^2}(n-\frac{1}{2})^2 \cdot \frac{2ma^2}{\pi\hbar}\right) = \exp\left(-i\pi(n-\frac{1}{2})^2\right) =$$

$= \underbrace{e^{-i\pi n^2}}_{(-1)^n} \underbrace{e^{i\pi n}}_{(-1)^n} e^{-i\frac{\pi}{4}} = e^{-i\frac{\pi}{4}}$ Then for w.-f. we get:

$$\Psi(x,t) = \sum_{n=1}^{\infty} C_n e^{-i\frac{\pi}{4}}\psi_n = e^{-i\frac{\pi}{4}}\sum_{n=1} C_n\psi_n = e^{-i\frac{\pi}{4}}\Psi(x,0) \text{ so}$$

$$\boxed{\Psi(x,t) = e^{-i\frac{\pi}{4}}\sqrt{\frac{3}{2a^3}}(a-|x|);}$$

(d) Does this state have definite parity? If so what is the parity?

(11) We say that state have definete parity $P=+1\ (-1)$ if it satisfies following equation:

$\psi(x) = +1\,(-1)\cdot\psi(-x)$, i.e. if it changes sign or not after reflection $x \to -x$.

In our case

$$\Psi(-x,t) = \sum_n C_n e^{-iE_n t/\hbar}\,\psi_{n,+}(-x) = \sum_n C_n e^{-iE_n t/\hbar}\,\psi_{n,+}(x) = \Psi(x,t)$$

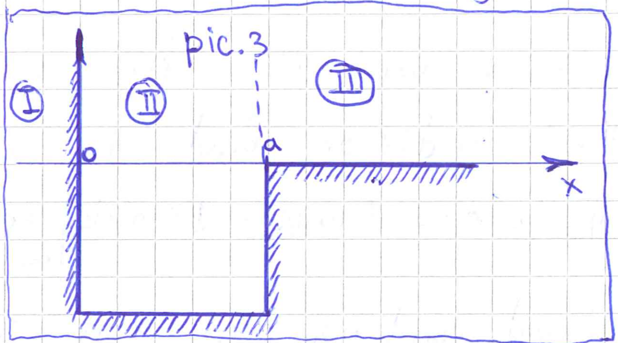
so we conclude that this state has parity $\boxed{P=+1}$

Problem III Consider 1d potential:

$V(x)=0 \qquad x>a$

$V(x)=-V_0 \qquad 0<x<a$

$V(x)=\infty \qquad x<0$



ⓐ Write down the w.-f. and boundary conditions (b.c.) that need to be satisfied at $x=0$ and $x=a$.

Let's consider 3 regions:

I $x<0$; II $0<x<a$ III $x>a$

I $x<0$. In this region $V(x)=\infty$ so that w.-f. should be 0 as no particle can be observed in this region

$\psi_{I}(x)=0$

II $0<x<a$, Sch. eq. reads:

$$E\psi_{II} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{II} - V_0\psi_{II}$$ solution to this equation is:

$$\frac{d^2}{dx^2}\psi_{II} = -\frac{2m}{\hbar^2}(E+V_0)\psi_{II} \Rightarrow \boxed{\psi_{II}(x) = Ae^{ikx} + Be^{-ikx};\ k=\frac{\sqrt{2m(E+V_0)}}{\hbar}}$$

III $x>a$, Sch. eq. is:

$$E\psi_{III} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{III};\ \Rightarrow \boxed{\psi_{III}(x) = Ae^{\varkappa x} + Be^{-\varkappa x};\quad \varkappa = \frac{\sqrt{-2mE}}{\hbar}}$$

We have written solution in this form as we will consider solutions with negative energy $E<0$ further. If $E>0$ this solution is oscillatory.

(12) Now we want w.f. to be smooth continious function. For this we put the following conditions:

(I) at $x=0$ we want $\psi_{II}(x=0)=0$ for function to be continious

(II) at $x=a$ we take

$$\psi_{II}(x=a) = \psi_{III}(x=a)$$

$$\frac{d}{dx}\psi_{II}(x=a) = \frac{d}{dx}\psi_{III}(x=a)$$ so that w.f. is

continious with it's first x-derivative.

First condition leads to

$$\psi_{II}(x=0) = A\cos(xk) + B\sin(xk)\Big|_{x=0} = 0 \Rightarrow A=0$$

Second condition at $x=a$ gives:

$$\psi_{II}(a) = B\sin(ka) = \psi_{III}(a) = Ce^{-\varkappa a}$$

$$\frac{d\psi_{II}}{dx}\Big|_{x=a} = kB\cos(ka) = \frac{d\psi_{III}}{dx}\Big|_{x=a} = -\varkappa C e^{-\varkappa a};$$

Note that we have taken $\psi_{III}(x) = Ce^{-\varkappa x}$ and ommited $e^{+\varkappa x}$ part, because it blows up at infinity and w.-f. appears to be unnormalizable.

So boundary conditions give:

$$\boxed{\begin{aligned} B\sin(ka) &= Ce^{-\varkappa a}; \\ kB\cos(ka) &= -\varkappa C e^{-\varkappa a}; \end{aligned}} \qquad \begin{aligned} \psi_{II} &= B\sin(kx); \\ \psi_{III} &= Ce^{-\varkappa x}; \end{aligned}$$

(b) Draw a graphical solution for the energy values of the bound states.

Deviding first eq. with second we get:

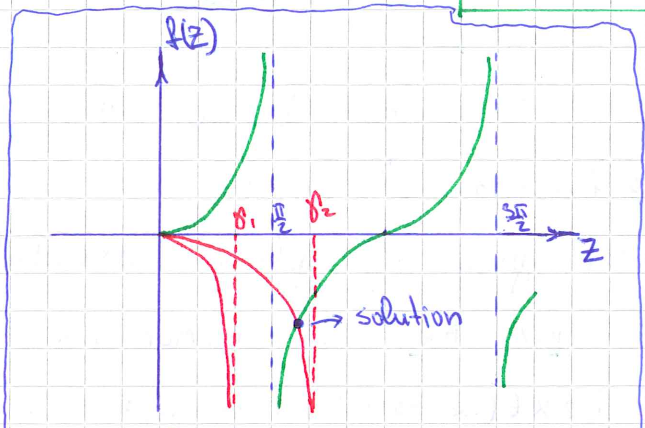
$$\frac{B\sin(ka)}{kB\cos(ka)} = \frac{Ce^{-\varkappa a}}{-\varkappa C e^{-\varkappa a}} \Rightarrow \boxed{\tan(ka) = -\frac{k}{\varkappa}}$$

This equation is hard to solve. But we can draw graphs of functions so that we can do conclusions about solutions of this equation.

13

Now if we denote $ka = z$ and $\varkappa a = \sqrt{\gamma^2 - z^2}$; where $\gamma = \frac{\sqrt{2mV_0}}{\hbar} a$; Then:

$$\boxed{\tan z = -\frac{z}{\sqrt{\gamma^2 - z^2}};}$$



pic. 4

Graphically we draw l.h.s. and r.h.s. of equation above on (pic.4) Intersection give you value of z corresponding to energy level.

(c) Find a condition that V_0 and a must satisfy in order for there to be at least one bound state.

note from pic.4, that if $\gamma < \frac{\pi}{2}$ no intersection of two graphs happens. And when $\gamma \to \frac{\pi}{2}$ they intersect as both goes to infinity. This one intersection moves then to the right while γ increases and when γ approaches $\frac{3\pi}{2}$ second intersection appears and we have 2 levels in the well. And so on. So, relation to observe one level is

$$\gamma = \frac{\pi}{2} \quad \text{or} \quad \frac{2mV_0a^2}{\hbar^2} = \frac{\pi^2}{4} \Rightarrow \boxed{V_0 a^2 = \frac{\pi^2\hbar^2}{8m};}$$

Problem IV Consider a free particle on a circle with circumferenee L. At time $t=0$ the w.-f. is

$$\psi(x) = \begin{cases} C, & -\frac{a}{2} < x < \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$$

Normalize the w.-f. and find $\psi(x)$ in terms of eigenfunctions of. p.

System on the circle is periodic, i.e. we identify points $x \sim x + n \cdot L$, $n \in \mathbb{Z}$. That makes some effects more interesting. In particular as we will see momentum is quatized for the particle on a circle.

(14) Normalization condition as usually reads:

$$1=\int_{-\frac{L}{2}}^{\frac{L}{2}}\psi^*(x)\,\psi(x) = |C|^2\int_{-\frac{a}{2}}^{\frac{a}{2}}dx = |C|^2 a \Rightarrow \boxed{C=\frac{1}{\sqrt{a}} \text{ up to unobservable phase.}}$$

Note that we integrate over one circumference only.

* Now let's write down eigenfunctions of $\hat{p}$ on a circle. As usually they are given by plane waves. Indeed:

$$-i\hbar\frac{d}{dx}e^{ipx/\hbar} = +p\,e^{ipx/\hbar}, \text{ so } \underline{\psi_p(x) = Ae^{ipx}} \text{ is momentum}$$

eigenstate. On real line (i.e. $x\in(-\infty,+\infty)$) it is not normalizable, at least straightforward. But on a circle it is. Indeed we can impose our usual normalization condition:

$$1=\int_{-\frac{L}{2}}^{L/2}dx\,|A|^2\,|e^{ipx/\hbar}|^2 = |A|^2\cdot L \Rightarrow \boxed{A=\frac{1}{\sqrt{L}}} \text{ up to phase as usually}$$

* One new thing for the circle with comparison to the line is quantization of momentum, due to periodicity:

$$\psi(x+L)=\psi(x) \Rightarrow Ae^{ipx\frac{i}{\hbar}} = Ae^{\frac{i}{\hbar}px+\frac{i}{\hbar}pL} \Rightarrow e^{\frac{i}{\hbar}pL}=1 \text{ so}$$

we get $pL = 2\pi n\hbar \Rightarrow \boxed{p_n = \frac{2\pi n\hbar}{L};}$

* To rewrite $\psi(x)$ in terms of plane waves we should Fourier-expand it:

$$\psi(x) = \sum_{n=-\infty}^{+\infty} C_n\, e^{ip_nx/\hbar}\cdot A \quad \text{to find coefficient of expansion}$$

C_n we should multiply both sides of expansion with

$$e^{-ip_mx/\hbar}; \qquad \psi(x)\,e^{-i2\pi m\frac{x}{L}} = \sum_n C_n\, e^{i2\pi(n-m)\frac{x}{L}}A$$

We know from analysis that $\int_{-\frac{L}{2}}^{L/2}dx\,e^{i(n-m)2\pi\frac{x}{L}} = \delta_{n,m}L$

So that we integrate last equation and get:

$$\int\psi(x)\,e^{-2\pi im\frac{x}{L}} = LA\sum_n C_n\,\delta_{n,m} \quad \text{so finally}$$

(15)

$$\boxed{C_m = \frac{1}{\sqrt{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx\, \psi(x)\, e^{-2\pi i m \frac{x}{L}};}$$

In our case:

$$C_n = \frac{1}{\sqrt{L}} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx\, C\, e^{-i2\pi n \frac{x}{L}} = \frac{C}{\sqrt{L}} \frac{iL}{2\pi n} e^{-i2\pi n \frac{x}{L}} \Big|_{-\frac{a}{2}}^{\frac{a}{2}} =$$

$$= \frac{i}{2\pi n} \sqrt{\frac{L}{a}} \left(e^{-in\frac{\pi a}{L}} - e^{in\frac{\pi a}{L}} \right) = \frac{1}{\pi n} \sqrt{\frac{L}{a}} \sin\left(\frac{\pi n a}{L}\right)$$

So we finally get:

$$\boxed{\psi(x) = \sum_{n=-\infty}^{+\infty} \frac{1}{\sqrt{a}\,\pi n} \sin\left(\frac{\pi n a}{L}\right) e^{i2\pi n \frac{x}{L}};}$$

Problem V Consider the wave packet of a free particle at $t=0$

$\Psi(x,0) = \psi(x)$

$$\psi(x) = \begin{cases} C \sin\left(\frac{2\pi x}{a}\right), & 0 < x < \frac{a}{2}. \\ 0, & x \leq 0,\ x \geq \frac{a}{2}. \end{cases}$$

Normalize the w.-f. and find the time development of the packet.

We have already normalized this w.-f. in problem I:

$$\boxed{C = \frac{2}{\sqrt{a}};}$$

To find time evolution of the package we should

- expand into plane waves $e^{ipx/\hbar}$ (which are the eigenstates of free particle Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$

To do this we should fourier transform of $\psi(x)$:

$$\psi(x) = \int \frac{dp}{2\pi\hbar} e^{ipx/\hbar} \phi(p), \quad \text{where} \quad \phi(p) = \int dx\, e^{-ipx/\hbar} \psi(x);$$

- apply time evolution operator $e^{-i\hat{H}t/\hbar}$ to this expanded w.-f.

$$\Psi(x,t) \equiv e^{-i\hat{H}t/\hbar} \psi(x) = \int \frac{dp}{2\pi\hbar} e^{-i\hat{H}t/\hbar} \psi_p(x)\, \phi(p) \quad \text{as} \quad \hat{H}\psi_p(x) = \frac{p^2}{2m}\psi_p(x)$$

we find: $\Psi(x,t) = \int \frac{dp}{2\pi\hbar} e^{-ip^2 t/2m\hbar} e^{ipx/\hbar} \phi(p);$

Let's follow this algorithm:

(16) * Let's find Fourier of $\psi(x)$, $\phi(p)$

$$\phi(p) = \int_0^{a/2} dx\, C\cdot e^{-ipx/\hbar} \sin\frac{2\pi x}{a} = \frac{C}{2i}\int_0^{a/2} dx \left\{ e^{i\left(\frac{2\pi}{a}-\frac{p}{\hbar}\right)x} - e^{-i\left(\frac{2\pi}{a}+\frac{p}{\hbar}\right)x} \right\} =$$

$$= \frac{C}{2i}\left\{ \frac{1}{i\left(\frac{2\pi}{a}-\frac{p}{\hbar}\right)} e^{i\left(\frac{2\pi}{a}-\frac{p}{\hbar}\right)x} + \frac{1}{i\left(\frac{2\pi}{a}+\frac{p}{\hbar}\right)} e^{-i\left(\frac{2\pi}{a}+\frac{p}{\hbar}\right)x} \right\}\Bigg|_0^{\frac{a}{2}} =$$

$$= \frac{C}{2i}\left\{ \frac{1}{i\left(\frac{2\pi}{a}-\frac{p}{\hbar}\right)} \left(\underbrace{e^{i\pi}}_{-1} e^{-ipa/2\hbar} - 1 \right) + \frac{1}{i\left(\frac{2\pi}{a}+\frac{p}{\hbar}\right)} \left(\underbrace{e^{-i\pi}}_{-1} e^{-ipa/2\hbar} - 1 \right) \right\} =$$

$$= -\frac{C}{2}\cdot\frac{2\pi}{a}\cdot\frac{1}{\frac{4\pi^2}{a^2}-\frac{p^2}{\hbar^2}}\left(-e^{-i\frac{pa}{2\hbar}} - 1\right)$$ so we finally get:

$$\boxed{\begin{gathered} \psi(x) = \int \frac{dp}{2\pi\hbar} e^{ipx/\hbar}\, \phi(p); \\ \phi(p) = \frac{C\pi}{a}\frac{1}{\frac{4\pi^2}{a^2}-\frac{p^2}{\hbar^2}}\left(1 + e^{-i\frac{pa}{2\hbar}}\right); \end{gathered}}$$

* Now we can write down time-dependent w.-f.:

$$\Psi(x,t) = \int \frac{dp}{2\pi\hbar} e^{ipx/\hbar} e^{-i\frac{p^2 t}{2m}} \frac{2}{a^{3/2}} \frac{1}{\frac{4\pi^2}{a^2}-\frac{p^2}{\hbar^2}}\left(1+e^{-i\frac{pa}{2\hbar}}\right)$$

$$\boxed{\Psi(x,t) = \int \frac{dp}{a^{3/2}\pi\hbar}\cdot\frac{1}{\frac{4\pi^2}{a^2}-\frac{p^2}{\hbar^2}}\cdot e^{i\frac{px}{\hbar}} e^{-i\frac{p^2 t}{2m}}\left(1+e^{-i\frac{pa}{2\hbar}}\right);}$$

Unfortunately we can't take this integral without some special knowledge of complex analysis and it is enough to leave this answer in such form.

1

Seminar 5 (examples of scattering and bound states in different potentials)

Theoretical reminder: * main object we deal with in quantum mechanics is wave-function $\psi(x,t)$ which describes probability density $\rho(x,t) = |\psi(x,t)|^2$

* w.-f. $\psi(x,t)$ obeys Schr. eq.

$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$ where $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ is Hamiltonian operator

If we split $\psi(x,t) = e^{-iEt/\hbar}\varphi(x)$ we obtain stationary Schr. eq.: $\hat{H}\varphi = E\varphi$ → thus φ is eigenstate and E is eigenvalue of Hamiltonian

* Due to linearity of Sch. eq. any time-dependent solution can be written in terms of eigenstates and eigenvalues of $\hat{H}$:

$$\boxed{\psi(x,t) = \sum_n e^{-iE_n t/\hbar}\varphi_n(x)} \quad \text{where} \quad \hat{H}\varphi_n = E_n\varphi_n;$$

* Important condition, w.-f. should satisfy is continuity ($\psi(x,t)$ is single-valued) and continuity of derivative ($\psi'(x,t)$ is single-valued everywhere)

* If $V = V_0 = \text{const}$, then Schr. eq. reads

$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = (E - V_0)\varphi$ and general solution takes form $\varphi(x) = Ae^{ikx} + Be^{-ikx}$, $k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

** This general solution is valid even if $E < V_0$. In this case we get two real exponents and choose solution that decays on $x \to \pm\infty$, in order for w.-f. to be normalizable.

** This general solution is only plane wave normalizable for the case $E > V_0$;

② Problem I (Scattering on the potential step)

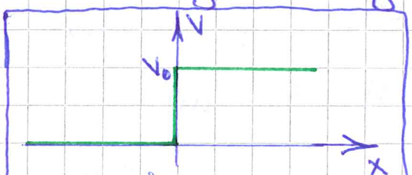
Suppose an electron hits a potential step with height $V_0 = 5eV$. Find the reflection and transmission coefficients, R and T when electon energy is:

ⓐ $E = 2{,}5eV$; ⓑ $E = 7{,}5eV$; ⓒ $E = 5eV$;

Theory reminder: Before substituting particular numbers into expressions you know from lecture let's refresh solution in memory:

Step potential is the one given by

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



pic. 1

In such kind of problems we consider separetly several regions:

(I): $x<0$ and (II) $x>0$;

For $V = const$ we know general solution of form

$\psi = Ae^{ikx} + Be^{-ikx}$, $k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

Let's consider 2 cases separately:

ⓐ $E > V_0$

in region (I) general solution is

$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$, containing both e^{ikx} (plane wave coming from $-\infty$) and e^{-ikx} (plane wave reflected from step and coming back to $-\infty$) and k is given by $k = \frac{\sqrt{2mE}}{\hbar}$;

in region (II) we write solution as:

$\psi_{II}(x) = Ce^{ik'x}$, where $k' = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ so we obtain only wave going away of the step towards infinity

3

Now applying continuity conditions we get at $x=0$

$$\psi_I(0) = \psi_{II}(0) \Rightarrow A + B = C$$

$$\left.\frac{d}{dx}\psi_I(x)\right|_{x=0} = \left.\frac{d}{dx}\psi_{II}(x)\right|_{x=0} \Rightarrow k(A-B) = k'C$$

Now we can express B and C coefficients through A:

$$k(A-B) = k'(A+B); \Rightarrow \boxed{B = \frac{k-k'}{k+k'}A;}$$

$$C = B + A = \frac{2k}{k+k'}A \Rightarrow \boxed{C = \frac{2k}{k+k'}A;}$$

Then reflection and transition coeff are given by

$$\boxed{R = \frac{|B|^2}{|A|^2} = \frac{(k-k')^2}{(k+k')^2}; \quad T = \frac{|C|^2}{|A|^2} \cdot \frac{k'}{k} = \frac{4kk'}{(k+k')^2};}$$

This expressions come from relations between currents. In particular

$\psi = Ae^{ikx}$ brings current $J(x,t) = \frac{k\hbar}{m}|A|^2;$

$\psi = Be^{-ikx}$ —— || —— $J(x,t) = -\frac{k\hbar}{m}|B|^2;$

B now if $E < V_0$:

in region I everything stays the same

but in region II we get:

$\psi_{II} = Ce^{-\varkappa x} + De^{\varkappa x}$ where $\varkappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$. In order to make this w.f. normalizable we choose $D=0$ and get $\psi_{II} = Ce^{-\varkappa x}$. Current corresponding to this solution is given by:

$$J(x,t) \equiv \frac{i\hbar}{2m}\left(\left(\frac{\partial}{\partial x}\psi^*\right)\psi - \psi^*\left(\frac{\partial}{\partial x}\psi\right)\right) = \frac{i\hbar}{2m}|C|^2(-\varkappa+\varkappa)e^{-2\varkappa x} = 0$$

So we see that there is no wave going through step so that $\boxed{R = 1, T = 0;}$

C in case $E = V_0$ w.f. in region II is $\psi_{II} = C = \text{const}$ and thus $J(x,t) = 0$ for $x > 0$ and we get the same result as in the case B

④ Now we can put numerical values of E and V_0 into this answers:

ⓐ $E = 2{,}5\,eV < V_0 \Rightarrow$ $\underline{R=1,\ T=0}$;

ⓑ $E = 5eV = V_0 \Rightarrow$ $\underline{R=1,\ T=0}$;

ⓒ $E = 7{,}5\,eV$, $R = \frac{(k-k')^2}{(k+k')^2} = \frac{(\sqrt{E}-\sqrt{E-V_0})^2}{(\sqrt{E}+\sqrt{E-V_0})^2} = \frac{\left(1-\sqrt{1-\frac{2}{3}}\right)^2}{\left(1+\sqrt{1-\frac{2}{3}}\right)^2}$

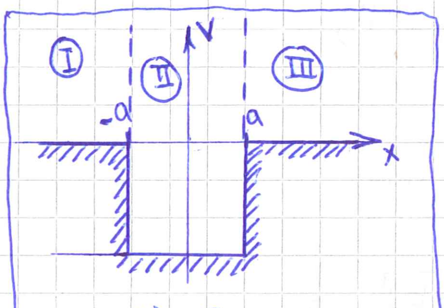
$\underline{R = 0{,}071;\quad T = 1-R = 0{,}929\,eV}$;

Problem II (finite square well)

Consider the finite square well

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

Solve graphically for the odd parity bound state solutions. What condition must be satisfied for there to be at least one such state.



pic. 2

Even parity bound states are found in lecture notes. Now we do the same procedure for states. In regions Ⓘ Ⓘⓘ and Ⓘⓘⓘ we obtain:

$$\begin{cases} \psi_I = Ae^{\varkappa x}; & x<-a; \\ \psi_{II} = B\sin kx + C\cdot\cos kx; & -a<x<a; \\ \psi_{III} = De^{-\varkappa x}; & x>a; \end{cases} \qquad \text{where} \quad \varkappa = \frac{\sqrt{-2mE}}{\hbar}; \quad k = \frac{\sqrt{2m(E+V_0)}}{\hbar};$$

Note that ψ_I and ψ_{II} are chosen to be normalizable, i.e. $\psi_I \to 0$, when $x \to -\infty$ and ψ_{III}, when $x \to +\infty$;

* Firs simplification comes from antisymmetry of w.f.:

$\psi_I(x) = -\psi_{III}(-x) \Rightarrow \quad Ae^{\varkappa x} = -De^{\varkappa x} \Rightarrow \quad \underline{A=D}$

$\psi_{II}(x) = -\psi_{II}(-x) \Rightarrow \quad B\sin kx + C\cdot\cos kx = B\sin kx - C\cos kx \Rightarrow$

$\Rightarrow C=0$. Finally we obtain following w.f.:

(5)

$$\boxed{\psi_I = -Ae^{\varkappa x}; \quad \psi_{II} = B\sin kx; \quad \psi_{III} = Ae^{-\varkappa x};}$$

* Now we can apply continuity conditions on the edges of square well:

$$\begin{cases} \psi_{II}(a) = \psi_{III}(a); \\ \frac{d}{dx}\psi_{II}(a) = \frac{d}{dx}\psi_{III}(a); \end{cases} \Rightarrow \begin{cases} B\sin ka = Ae^{-\varkappa a} \\ kB\cos ka = -\varkappa A e^{-\varkappa a} \end{cases}$$

conditions in $x=-a$ are satisfied then automatically due to antisymmetry of w.f.

Now deviding first equation with second one we get: $\frac{1}{k}\,tg\,ka = -\frac{1}{\varkappa} \Rightarrow \boxed{tg\,ka = -\frac{k}{\varkappa};}$

* This equation is transcendental and we can't find solution analytically but we can do it graphically (at least understand what is going on qualitavely.

Let's write down level equations through $ka = z$ variable.

Then $\varkappa a = \frac{\sqrt{2ma^2(V_0 - V_0 + E)}}{\hbar} = \sqrt{\gamma^2 - z^2}$ where $\gamma = \frac{\sqrt{2mV_0}\,a}{\hbar}$;

Thus equation finally looks like:

$$\boxed{tg\,z = -\frac{z}{\sqrt{\gamma^2 - z^2}}}$$ – odd levels

Equation for even levels was found on lecture

$$\boxed{z\,tg\,z = \sqrt{\gamma^2 - z^2}}$$ – even levels

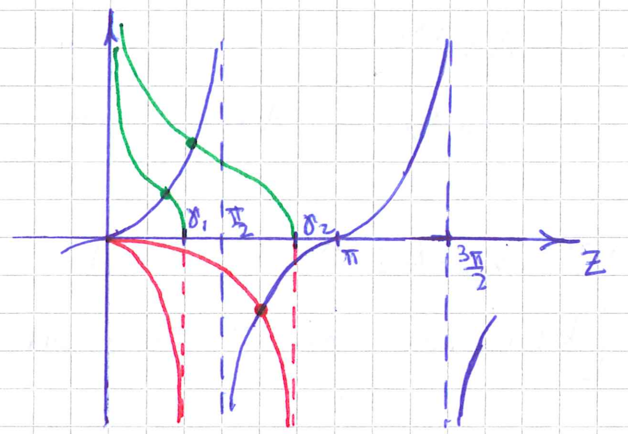
To draw graphical solution we shold draw $\frac{\sqrt{\gamma^2 - z^2}}{z}$ and $-\frac{z}{\sqrt{\gamma^2 - z^2}}$ functions. But as we should do it only qualitavly it's enough to know theirs asymptotes:

** $\frac{\sqrt{\gamma^2 - z^2}}{z} \to +\infty$ as $z \to 0$ and $\frac{\sqrt{\gamma^2 - z^2}}{z} = 0$ at $z = \gamma$

** $-\frac{z}{\sqrt{\gamma^2 - z^2}} = 0$ at $z = 0$ and $-\frac{z}{\sqrt{\gamma^2 - z^2}} \to -\infty$ at $z = \gamma$

So solutions we get are the following: (see pic.3)

⑥



pic. 3

Red lines on (pic. 3) shows $-\frac{z}{\sqrt{\gamma^2-z^2}}$ function and intersection with $tg\,z$ shows solution for odd-parity bound state. Note that

if $0<\gamma<\pi$ – there is 1 even solution

$\pi<\gamma<2\pi$ – 2 even solutions

$\boxed{\pi(n-1)<\gamma<\pi n \text{ – } n \text{ even solutions}}$

$0<\gamma<\frac{\pi}{2}$ – no solutions (odd)

$\frac{\pi}{2}<\gamma<\frac{3\pi}{2}$ – 1 odd solution

$\boxed{\frac{\pi}{2}(2n+1)<\gamma<\frac{\pi}{2}(2n+3) \text{ – } (n-1) \text{ odd solutions}}$

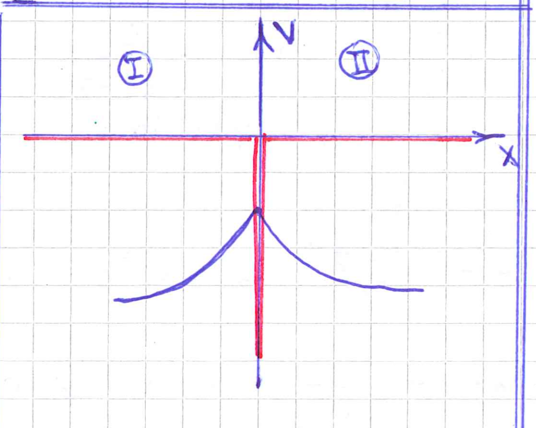
* We now have seen that odd solutions exist only if $\gamma>\frac{\pi}{2} \Rightarrow \boxed{V_0 a^2 \geqslant \frac{\pi^2\hbar^2}{8m}}$

<u>Problem III</u> <u>(Delta function potential)</u>

Consider the δ-function potential

$$V(x) = -\alpha\delta(x),$$

where $\alpha>0$. Find normalized w.f and energies of bound states



pic. 4 δ-potential

Before sol ing this problem let's refresh our knowledge about δ-functions and their role in quantum mechanics.

7

- $\delta(x) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases}$
- $\int_{-a}^{a} \delta(x) = 1 \quad \forall a$
- $\int_{-a}^{a} \delta(x) f(x) = f(0) \ \forall a.$
- assume we have potential proportional to $\delta(x)$ in Sch. eq. Obviously as it's 0 everywhere except $x=0$ it doesn't effect solutions at $x \neq 0$.

To understand what is going on at $x=0$ let's integrate Sch. eq. near $x=0$ (i.e. $\int_{-\varepsilon}^{\varepsilon}$ + limit $\varepsilon \to 0$)

$$\int_{-\varepsilon}^{\varepsilon} \left(-\frac{\hbar^2}{2m}\right) \frac{d^2\psi}{dx^2} + \int_{-\varepsilon}^{\varepsilon} V(x)\psi(x) = E\int_{-\varepsilon}^{\varepsilon} \psi(x)$$

- as function ψ is continious we have:

$$\lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \psi(x)dx = 0$$

- $\int_{-\varepsilon}^{\varepsilon} V(x)\psi(x) = -\alpha \int_{-\varepsilon}^{\varepsilon} \delta(x)\psi(x)dx = -\alpha\psi(0)$
- $\int_{-\varepsilon}^{\varepsilon} \left(-\frac{\hbar^2}{2m}\right) \frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m} \left.\frac{d\psi}{dx}\right|_{-\varepsilon}^{\varepsilon} = \frac{\hbar^2}{2m}\left(\psi'(-\varepsilon) - \psi'(+\varepsilon)\right)$

So we eventually get out of Sch. eq. boundary condition for w.f. derivatives:

$$\boxed{-\frac{\hbar^2}{2m} \left.\frac{d\psi}{dx}\right|_{-\varepsilon}^{\varepsilon} = \alpha\psi(0)}$$

This is good thing to remember:
δ-function leave w.f. continious but imply discontinuity in w.f. derivatives

Now we can consider problem in usual way:

* we have regions I ($x<0$) and II ($x>0$) where solution for bound states ($E<0$) w.f. is given by

$\psi_I = Ae^{\varkappa x}$ — here we have ommited unnormalizable
$\psi_{II} = Be^{-\varkappa x}$ exponent already.

(8) * continuity of w.f. give:

$A = B$ as $\psi_I(0) = \psi_{II}(0)$ so we obtain w.f.:

$\psi_I = A e^{\varkappa x}$, $\psi_{II} = A e^{-\varkappa x}$ where $\varkappa = \frac{\sqrt{-2mE}}{\hbar}$

* Now we can apply boundary condition for w.f. derivatives at $x=0$:

$$-\frac{\hbar^2}{2m}\left(\frac{d\psi_{II}}{dx}\Big|_{x=0} - \frac{d\psi}{dx}\Big|_{x=0}\right) = \alpha\, \psi(0) = \alpha A$$

substituting ψ_I and ψ_{II} we obtain:

$$-\frac{\hbar^2}{2m} A(-2\varkappa) = \alpha A \quad \Rightarrow \quad \varkappa = \frac{m\alpha}{\hbar^2} \quad \Rightarrow \quad \frac{-2mE}{\hbar^2} = \frac{\alpha^2 m^2}{\hbar^4} \quad \text{so}$$

we get bound energy state $\boxed{E = -\frac{m\alpha^2}{2\hbar^2}}$

* finally we should normalize w.f. Normalization condition as usually reads:

$$1 = \int_{-\infty}^{+\infty} |\psi|^2 dx = |A|^2 \int_{-\infty}^{\infty} e^{-\varkappa|x| \cdot 2} = 2|A|^2 \int_0^\infty dx\, e^{-2\varkappa x} = -\frac{2|A|^2}{2\varkappa} e^{-2\varkappa x}\Big|_0^\infty =$$

$= \frac{|A|^2}{\varkappa}$ so that we get $A = \sqrt{\varkappa}$ up to an unobservable phase. So normalized w.f. is given by

$$\boxed{\psi(x) = \sqrt{\varkappa}\, e^{-\varkappa|x|}; \quad \varkappa = \frac{\sqrt{-2mE}}{\hbar}; \quad E = -\frac{m\alpha^2}{2\hbar^2};}$$

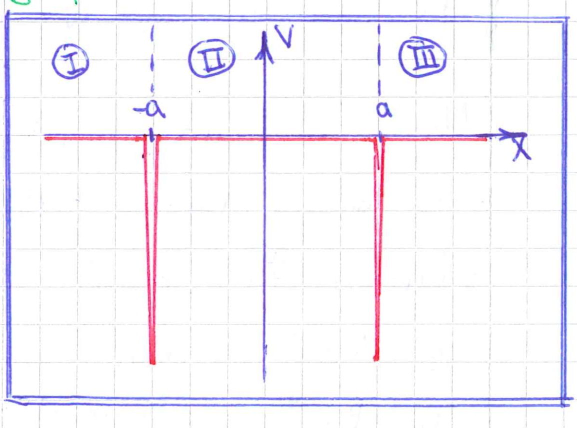
Note that there is only one bound state.

Problem IV (Compendium N3) scattering on two Delta-functions

Suppose that particles with energy $E>0$ and mass m are coming in from the left where they pass over the 1D double δ-function potential:

$$V(x) = -\frac{\hbar^2 b}{2m}\left(\delta(x+a) + \delta(x-a)\right)$$

where $b>0$



(a) Find the wave number k in terms of E

As δ-functions don't effect

(9) solutions expect 2 points $x=\pm a$; we can immedeately write $\boxed{k=\frac{\sqrt{2mE}}{\hbar}}$ – the same relation as for free particles.

(b) Find the reflection coefficient as a function of the wave number $k, m, \hbar, \beta$ and a.

* We, as usually, devide space into several regions:

(I) $x<-a$; (II) $-a<x<a$; (III) $x>a$;

Solution in this regions look as usually:

$$\begin{cases} \psi_I(x) = Ae^{ikx} + Be^{-ikx}; \\ \psi_{II}(x) = Ce^{ikx} + De^{-ikx}; \\ \psi_{III}(x) = Fe^{ikx}; \end{cases}$$

In regions I and II we have both incoming (e^{ikx}) and reflected (e^{-ikx}) waves, while there can be no incoming wave for $x>a$ (region III)

* Now we apply boundary conditions in $x=\pm a$;

continuity condition gives:

$x=-a$: $\quad Ae^{-ika} + Be^{ika} = Ce^{-ika} + De^{ika}$;

$x=+a$: $\quad Ce^{ika} + De^{-ika} = Fe^{ika}$;

Derivatives of w.f. are not continious. Boundary conditions are:

$x=-a$; $\psi_I'(-a) - \psi_{II}'(-a) = \beta\,\psi(-a) \Rightarrow$

$\Rightarrow ik(Ae^{-ika} - Be^{ika}) - ik(Ce^{-ika} - De^{ika}) = \beta(Ae^{-ika} + Be^{ika})$

$x=a$; $\psi_{II}'(a) - \psi_{III}'(a) = \beta\,\psi(a) \Rightarrow$

$\Rightarrow ik(Ce^{ika} - De^{-ika}) - ikFe^{ika} = \beta Fe^{ika}$

So we get system of 4 equations:

$$\boxed{\begin{aligned} &(I)\ Ae^{-ika} + Be^{ika} = Ce^{-ika} + De^{ika}; \\ &(II)\ Ce^{ika} + De^{-ika} = Fe^{ika}; \\ &(III)\ Ae^{-ika} - Be^{ika} - Ce^{-ika} + De^{ika} = \frac{\beta}{ik}(Ae^{-ika} + Be^{ika}); \\ &(IV)\ Ce^{ika} - De^{-ika} = F\left(\frac{\beta}{ik}+1\right)e^{ika}; \end{aligned}}$$

Let's denote $\alpha = \frac{\beta}{ik}$

(10) $Ce^{ika} - De^{-ika} = (\alpha+1)(Ce^{ika} + De^{-ika})$ so

$C = -\left(\frac{2}{\alpha}+1\right)e^{-2ika}D$; substituting this into eq. (I) we get:

$$Ae^{-ika} + Be^{ika} = De^{ika}\left(1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}\right) \quad (\text{V})$$

And substitution into eq. (III) gives:

$$Ae^{-ika}(1-\alpha) - Be^{ika}(1+\alpha) + De^{ika}\left(1 + \left(\frac{2}{\alpha}+1\right)e^{-4ika}\right) = 0; \quad (\text{VI})$$

Now if we expres D throug A and B using eq (V):

$$D = \frac{(Ae^{-ika} + Be^{ika})e^{-ika}}{1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}};$$ and substitute this into

eq. (VI) we get:

$$A\,e^{-ika}(1-\alpha) - B\,e^{ika}(1+\alpha) + (Ae^{-ika} + Be^{ika})\frac{1 + \left(\frac{2}{\alpha}+1\right)e^{-4ika}}{1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}} = 0;$$

Coefficient in front of Ae^{-ika}: $1-\alpha + \frac{1 + \left(\frac{2}{\alpha}+1\right)e^{-4ika}}{1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}} =$

$$= \frac{2 - \alpha + (2+\alpha)e^{-4ika}}{1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}};$$

Coefficient in front of Be^{ika}: $-(1+\alpha) + \frac{1 + \left(\frac{2}{\alpha}+1\right)e^{-4ika}}{1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}}$

$$= \frac{+2\left(\frac{2}{\alpha}+1\right)e^{-4ika} + \alpha - (2+\alpha)e^{-4ika}}{1 - \left(\frac{2}{\alpha}+1\right)e^{-4ika}}$$

So we get:

$$Ae^{-ika}\left(2 - \alpha + (2+\alpha)e^{-4ika}\right) = Be^{ika}\left(-\left(\frac{2}{\alpha}+1\right)2e^{-4ika} + \alpha - (2+\alpha)e^{-4ika}\right)$$

thus

$$\frac{B}{A} = e^{-2ika}\frac{e^{-2ika}(4\cos(2ka) - 2i\alpha\sin(2ka))}{e^{-4ika}\left(-\frac{4}{\alpha} - \alpha\cdot -4 + \alpha\, e^{4ika}\right)}$$ thus

$$\frac{B}{A} = \frac{4\cos(2ka) - \frac{2\beta}{k}\sin(2ka)}{\frac{\beta}{ik}\left(\frac{4k^2}{\beta^2} - 1 + e^{4ika} - \frac{4ik}{\beta}\right)}$$ and finally

$$\frac{B}{A} = \frac{i\beta(4k\cos(2ka) - 2\beta\sin(2ka))}{k(k-i\beta) + \beta^2(e^{4ika} - 1)}$$

Reflection coefficient is then given by:

(11)

$$R \equiv \left|\frac{B}{A}\right|^2 = \frac{\beta^2\left(4k\cos(2ka) - 2\beta\sin(2ka)\right)^2}{|k(k-i\beta) + \beta^2(e^{4ika}-1)|^2}$$

Using:

$$k(k-i\beta) + \beta^2(e^{4ika}-1) = k^2 - \beta^2(1-\cos 4ka) - i(k\beta - \beta^2\sin 4ka) =$$

$$= k^2 - 2\beta^2\sin^2(2ka) - i\beta(k - \beta\sin 4ka)$$ we get:

$$\boxed{R = \frac{\beta^2\left(4k\cos(2ka) - 2\beta\sin(2ka)\right)^2}{\left(k^2 - 2\beta^2\sin^2(2ka)\right)^2 + \beta^2(k - \beta\sin 4ka)^2};}$$

(c) Find a relation between k, β, and a that gives zero for the reflection coefficient.

R is "0" when numerator is zero, i.e.:

$$4k\cos(2ka) = 2\beta\sin(2ka) \Rightarrow \boxed{tg(2ka) = \frac{2k}{\beta};}$$

Problem V (S-matrix)

Suppose we have potential $V(x)$ such that $V(x)=0$ as $x \to \pm\infty$ but is otherwise arbitrary. A solution to Sch eq. is then

$$\psi(x) \approx Ae^{ikx} + Be^{-ikx}, \quad x \ll 0$$

$$\psi(x) \approx Ce^{ikx} + De^{-ikx}, \quad x \gg 0$$

Note that A and D components are incoming waves and the B and C are outgoing waves. The S-matrix is defined as

$$\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}\begin{pmatrix} A \\ D \end{pmatrix}$$

Show that S is unitary ($SS^+ = 1$), and $S(-k) = S^+(k)$

* Let's consider currents for $x \gg 0$ and $x \ll 0$

For w.f. $\psi(x) = Ae^{ikx} + Be^{-ikx}$ current is given by

$$J(x,t) \equiv \frac{i\hbar}{2m}\left(\frac{\partial\psi^*}{\partial x}\psi - \psi^*\frac{\partial\psi}{\partial x}\right) = \frac{i\hbar}{2m} ik\Big(\left(-A^*e^{-ikx} + B^*e^{ikx}\right)\left(Ae^{ikx} + Be^{-ikx}\right)$$

$$- \left(A^*e^{-ikx} + B^*e^{ikx}\right)\left(Ae^{ikx} - Be^{-ikx}\right)\Big) = -\frac{k\hbar}{2m}\Big(-|A|^2 + |B|^2 +$$

$$+ \cancel{B^*A}e^{2ikx} - \cancel{BA^*}e^{-2ikx} - |A|^2 + |B|^2 + \cancel{A^*B}e^{-2ikx} - \cancel{B^*A}e^{2ikx}\Big) \Rightarrow$$

(12) $\Rightarrow$ $J(x,t) = \frac{k\hbar}{m}(|A|^2 - |B|^2)$, so that:

$x \gg 0$: $J(x,t) = \frac{k\hbar}{m}(|C|^2 - |D|^2)$;

$x \ll 0$: $J(x,t) = \frac{k\hbar}{m}(|A|^2 - |B|^2)$;

and they should be equal (probability current conservation) so we get:

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

Let's look on $\begin{pmatrix} A \\ D \end{pmatrix}$ and $\begin{pmatrix} C \\ B \end{pmatrix}$ as on vectors. Then

$$|C|^2 + |B|^2 \equiv (C^* \; B^*)\begin{pmatrix} C \\ B \end{pmatrix} = (A^* \; D^*)\, S^+ S \begin{pmatrix} A \\ D \end{pmatrix} = (A^* \; D^*)\begin{pmatrix} A \\ D \end{pmatrix} = |A|^2 + |D|^2$$

so that $(A^* \; D^*)(S^+S - \mathbb{1})\begin{pmatrix} A \\ D \end{pmatrix} = 0$ as $\begin{pmatrix} A \\ D \end{pmatrix}$ is random

we conclude that $\boxed{S^+S = \mathbb{1}, \text{ q.e.d.}}$

So unitary matricies are one preserving length of complex vector (i.e. $|A|^2 + |D|^2$ is length of $\begin{pmatrix} A \\ D \end{pmatrix}$)

* Now we should show that $S(-k) = S^+(k)$

If we change $k \to -k$ it is equivalent to the change of incoming and outcoming waves: $\begin{pmatrix} C \\ B \end{pmatrix} \longleftrightarrow \begin{pmatrix} A \\ D \end{pmatrix}$

So our "new" S-matrix will be given by:

$$\begin{pmatrix} C' \\ B' \end{pmatrix} = S(-k)\begin{pmatrix} A' \\ D' \end{pmatrix} \Rightarrow \begin{pmatrix} A \\ D \end{pmatrix} = S(-k)\begin{pmatrix} C \\ B \end{pmatrix} \Rightarrow \begin{pmatrix} C \\ B \end{pmatrix} = S^{-1}(-k)\begin{pmatrix} A \\ D \end{pmatrix} \text{ and}$$

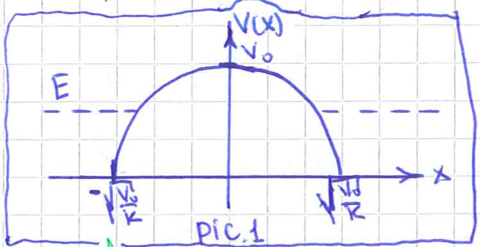
we conclude that $S^{-1}(-k) = S(k) \Rightarrow \boxed{S(-k) = S^{-1}(k)}$ q.e.d.

1

Seminar 6 (Postulates of QM)

Problem I (Tunneling). Suppose there is a potential barrier with the potential given by

$$V(x) = \begin{cases} V_0 - Kx^2 & , |x| < \sqrt{\frac{V_0}{K}} \\ 0 & , |x| > \sqrt{\frac{V_0}{K}} \end{cases}$$



pic.1

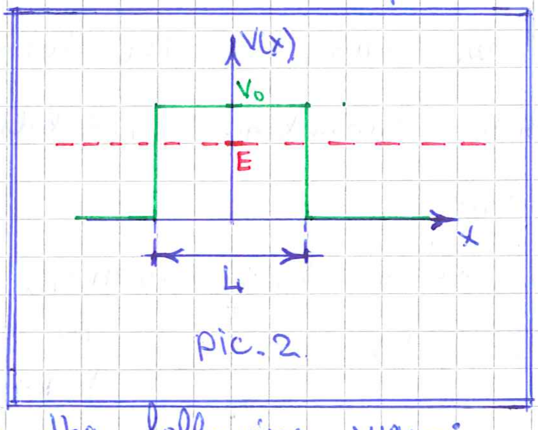
Estimate the tunneling probability for a particle of mass m and energy E assuming that $0 < E < V_0$;

Theory reminder. On the lecture you have obtained that for simple square barrier tunneling probability (which is just equal to usual T – the transition coefficient for incoming wave e^{ikx}) is given by

$$\boxed{T \approx \frac{4E(V_0 - E)}{V_0^2} e^{-2\varkappa L}} \; ; \; \varkappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

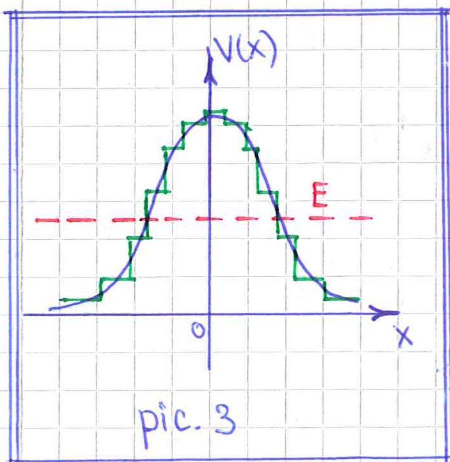
and assumption is $\varkappa L \gg 1$ (true almost alway for semi-classical potentials)

Corresponding barrier is shown on pic.2. Now we want to write down estimate for potential of general form, not only square barrier.



pic.2

We do it in the following way:



pic. 3

* assume there is some random potential such that $V(x) \to 0 \quad x \to \pm\infty$ and approximate it as series of N steps of width L each of them
* for each step transition coefficient is given by usual formula for tunneling through square barrier:

(2) $T_j \sim e^{-2\varkappa_j \Delta L}$; $\varkappa_j = \frac{\sqrt{2m(V(x_j)-E)}}{\hbar}$; $j = 1,\dots,N$, N is number of steps for which $V>E$;

we have ommited pre-exponential factor as any way it is of order 1, while expontial suppression is strong enough as $\varkappa \Delta L \gg 1$.

* Total probability of tunneling will be given by product of T_j probabilities:

$$T \sim \prod_{j=1}^{N} T_j \sim \prod_{j=1}^{N} e^{-2\varkappa_j \Delta L} = \exp\left(-\frac{2}{\hbar}\sum_{j=1}^{N}\sqrt{2m(V(x_j)-E)}\,\Delta L\right)$$

Now if we go to continious limit $N\to\infty$, $\Delta L \to 0$ we should replace the sum with integral:

$$\boxed{T \sim \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2}\sqrt{2m(V(x)-E)}\,dx\right)}$$ where x_1 and x_2 are points satisfying eq. $V(x)=E$ and called classical turning points.

Now we can use the formula we have observed to estimate tunneling probability for our particular potential:

* first we find turning points, by defenition:

$E = V_0 - Kx^2 \Rightarrow$ $\boxed{x_{1,2} = \pm\sqrt{\frac{V_0-E}{K}}\,;}$ $\to$ this are turning points we need.

* now we can take integral standing in exponent:

$$\int_{x_1}^{x_2}\sqrt{2m(V(x)-E)}\,dx = \int_{x_1}^{x_2}\sqrt{2m(V_0-E)-2mKx^2}\,dx =$$

$$= \sqrt{2m(V_0-E)}\int_{x_1}^{x_2}\sqrt{1-\frac{K}{V_0-E}x^2}\,dx = \left[\begin{matrix}\text{after change}\\ t=\sqrt{\frac{K}{V_0-E}}\,x\end{matrix}\right] =$$

$$= \sqrt{2m(V_0-E)}\sqrt{\frac{V_0-E}{K}}\int_{t_1}^{t_2}\sqrt{1-t^2}\,dt$$ where $t_{1,2} = x_{1,2}\sqrt{\frac{K}{V_0-E}} = \mp 1$

so we get:

③ $$\int_{-1}^{1}\sqrt{1-t^2}\,dt = 2\int_{0}^{1}\sqrt{1-t^2}\,dt = \left[\begin{matrix} t=\sin \\ t(0,\frac{\pi}{2})\end{matrix}\right] = 2\int_{0}^{\frac{\pi}{2}}\cos^2\, d =$$

$$= \int_{0}^{\frac{\pi}{2}}(1+\cos 2u)\,du = \frac{\pi}{2}$$

So taking everything together we get:

$$\int_{x_1}^{x_2}\sqrt{2m(V(x)-E)}\,dx = \sqrt{\frac{2m}{K}}(V_0-E)\frac{\pi}{2}$$ and probability

of tunneling is then:

$$\boxed{T \sim \exp\left(-\frac{\pi(V_0-E)}{\hbar}\sqrt{\frac{2m}{K}}\right);}$$

Postulates of quantum mechanics (theory)

(I) Now we will introduce "bra" and "ket" vectors describing states:

* $\langle\psi|$ - bra , $|\psi\rangle$ - ket

* There exist inner product of bra and ket

$$\langle\psi_1|\psi_2\rangle \equiv \int \psi_1^*\psi_2\,dx \quad ; \quad \langle\psi_1|\psi_2^*\rangle = \langle\psi_2|\psi_1\rangle$$

This product is

- bilinear: $\langle\psi_1|a_2\psi_2 + a_3\psi_3\rangle = a_2\langle\psi_1|\psi_2\rangle + a_3\langle\psi_1|\psi_3\rangle$

$$\langle a_1\psi_1 + a_2\psi_2|\psi_3\rangle = a_1^*\langle\psi_1|\psi_3\rangle + a_2^*\langle\psi_2|\psi_3\rangle$$

- satisfy Shwarz identity:

$$\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_1\rangle \leq \langle\psi_1|\psi_1\rangle\langle\psi_2|\psi_2\rangle$$

Note: * ket's and bra's for problems with finite number of states can be thought about just as vectors, and inner product as scalar product of this vectors:

$$\langle u|v\rangle = u_1^*v_1 + u_2^*v_2 + \ldots + u_n^*v_n$$

* Physically ket describe state of system. It's almost the same as wave function $\psi(x)$ but little more abstract thing.

④ (II) Other groundstone object of QM are operators $\hat{O}$ acting on states $|\psi\rangle$. We have already seen examples of operators acting on $\psi(x)$. Now we generalize it on ket formalism:

$$\hat{O}|\psi\rangle \equiv |\hat{O}\psi\rangle = |\chi\rangle \; ; \quad \hat{O}|\psi_1+\psi_2\rangle = \hat{O}|\psi_1\rangle + \hat{O}|\psi_2\rangle$$ - operators are linear

* conjugate operator is defined by acting on bra:

$$\langle\psi|\hat{O}^+ \equiv \langle O\psi| = \langle\chi| \; ; \quad \langle\psi_1+\psi_2|\hat{O}^+ = \langle\psi_1|O^+ + \langle\psi_2|O^+ \; ;$$

Operators have eigenstates $|\psi_n\rangle$ and corresponding

* eigenvalues α_n defined as: $\boxed{\hat{O}|\psi_n\rangle = \alpha_n|\psi_n\rangle;}$

* Operator eigenstates form complete set of states. I.e. any state $|\psi\rangle$ can be written as expansion in $|\psi_n\rangle$:

$|\psi\rangle = \sum_n c_n|\psi_n\rangle$; (remember we have used formula $\psi(x) = \sum_n c_n\psi_n(x)$)

$c_n = \langle\psi_n|\psi\rangle$;

(III) Just in the same way as we can write down time evolution of state:

$$\boxed{|\psi,t\rangle = \sum_n c_n e^{-itE_n/\hbar}|\psi_n\rangle;}$$

Where ψ_n are eigenstates of Hamiltonian $\hat{H}$: $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$;

(IV) Measurment

* Measurment of physical quantaties differs in QM from classical picture.

* Assume we have system described by state $|\psi\rangle$ and we want to measure some quantaty "O" for this system

* First of all we introduce hermitian (i.e. $\hat{O}^+ = \hat{O}$, in order to have real eigenvalues) operator $\hat{O}$ corresponding to this physical quantaty. It hase some eigen spectrum $\hat{O}|\psi_n\rangle = \alpha_n|\psi_n\rangle$

(5) * Measurement postulate states that

- when we measure value of "O" in the system described by $|\psi\rangle$ we observe one of the $\hat{O}$'s eigenvalues λ_n with probability $P = |\langle\psi|\psi_n\rangle|^2$;
- after measurment state is changed to the eigenstate $|\psi_n\rangle$ corresponding to the observed eigenvalue λ_n;

Schematically it looks like the following:

$$|\psi\rangle \xrightarrow{\qquad\qquad} |\psi_n\rangle$$

initial state — observation made λ_n is observed — final state after measur.

Problem II (Degenerate states)

Suppose there are two independent states $|\psi_1\rangle$ and $|\psi_2\rangle$ that are both eigenstates of Hamiltonian H with the same eigenvalue E.

(a) Show that any linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ is also eigenstate of $\hat{H}$;

General linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ looks like $|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$. Let's act with Hamiltonian on this state: $\hat{H}|\psi\rangle = \hat{H}c_1|\psi_1\rangle + \hat{H}c_2|\psi_2\rangle = c_1E|\psi_1\rangle + c_2E|\psi_2\rangle = E|\psi\rangle$

so we have shown $\boxed{\hat{H}|\psi\rangle = E|\psi\rangle\text{, q.e.d.}}$

(b) Assume that $\langle\psi_1|\psi_2\rangle = \lambda$ and $\langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1$, where λ is complex. Find two linear independent eigenstates $|\varphi_1\rangle$ and $|\varphi_2\rangle$ such that $\langle\varphi_n|\varphi_m\rangle = \delta_{mn}$

In general states $|\varphi_1\rangle$ and $|\varphi_2\rangle$ can be written as $|\varphi_1\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle$; $|\varphi_2\rangle = b_1|\psi_1\rangle + b_2|\psi_2\rangle$;

⑥ But it will be a bit difficult to solve system of equations

$\langle\varphi_n|\varphi_m\rangle = \delta_{nm} \Rightarrow \quad \langle\varphi_1|\varphi_1\rangle = \langle\varphi_2|\varphi_2\rangle = 1; \; \langle\varphi_1|\varphi_2\rangle = 0$

Instead we will simplify our work and follow what is called Gramm - Schmidt process wich you can be familiar with from linear algebra.

* Let's choose $|\varphi_1\rangle$ in simplies form:

$|\varphi_1\rangle = |\psi_1\rangle$ it's already normalized

* Now we should build $|\varphi_2\rangle$ orthogonal to $|\varphi_1\rangle$:

in general $|\varphi_2\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$ as $\langle\varphi_2|\varphi_1\rangle = 0$ we get equation:

$$c_1\underbrace{\langle\psi_1|\psi_1\rangle}_{1} + c_2\underbrace{\langle\psi_1|\psi_2\rangle}_{\lambda} = 0 \Rightarrow c_1\cdot 1 + c_2\cdot\lambda = 0 \Rightarrow$$

$c_1 = -c_2\lambda$ and we get: $\quad |\varphi_2\rangle = c_2(|\psi_2\rangle - \lambda|\psi_1\rangle)$

* finally we can normalize $|\varphi_2\rangle$: Normalization condition as usually reads:

$$\langle\varphi_2|\varphi_2\rangle = |c_2|^2\left(\langle\psi_2| - \lambda^*\langle\psi_1|\right)\left(|\psi_2\rangle - \lambda|\psi_1\rangle\right) =$$

$$= |c_2|^2\Big(\underbrace{\langle\psi_2|\psi_2\rangle}_{1} - \lambda^*\underbrace{\langle\psi_1|\psi_2\rangle}_{\lambda} - \lambda\underbrace{\langle\psi_2|\psi_1\rangle}_{\lambda^*} + |\lambda|^2\underbrace{\langle\psi_1|\psi_1\rangle}_{1}\Big) =$$

$$= |c_2|^2(1 - |\lambda|^2) \Rightarrow \quad c = \frac{1}{\sqrt{1-|\lambda|^2}}$$ up to unobservable phase.

So we eventually get

$$\boxed{\begin{aligned} |\varphi_1\rangle &= |\psi_1\rangle \\ |\varphi_2\rangle &= \frac{1}{\sqrt{1-|\lambda|^2}}\left(|\psi_2\rangle - \lambda|\psi_1\rangle\right) \end{aligned}}$$

In principle if we had more vectors (i.e. states $|\psi\rangle$) we can go on. Building orthogonal combinations in very same way (see Gramm - Schmidt orthogonalisation in any book on linear algebra).

Problem III (Measurment)

Suppose we have 2 observables A and B with corresponding operators $\hat{A}$ and $\hat{B}$. Suppose further that $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthonormal states and are also eigenstates of $\hat{A}$ with eigenvalues a_1 and a_2 respectively. Assume that $|\varphi_1\rangle = 2|\psi_1\rangle + |\psi_2\rangle$ and $|\varphi_2\rangle = |\psi_1\rangle - 2|\psi_2\rangle$ are eigenstates of $\hat{B}$ with eigenvalues b_1 and b_2 respectively.

a) Normalize the eigenstates of $\hat{B}$.

Normalization condition reads as usually:

$$1 = \langle\varphi_1|\varphi_1\rangle = |c_1|^2 (2\langle\psi_1| + \langle\psi_2|)(2|\psi_1\rangle + |\psi_2\rangle) =$$

$$= |c_1|^2 (4\langle\psi_1|\psi_1\rangle + \langle\psi_2|\psi_2\rangle + 2\langle\psi_1|\psi_2\rangle + 2\langle\psi_2|\psi_1\rangle)$$

due to orthonormality $\langle\psi_n|\psi_m\rangle = \delta_{nm}$ we have

$\langle\psi_1|\psi_1\rangle = 1$; $\langle\psi_2|\psi_2\rangle = 1$; $\langle\psi_2|\psi_1\rangle = 0$; so we get:

$\langle\varphi_1|\varphi_1\rangle = (4+1)|c_1|^2 = 1 \Rightarrow$ $c_1 = \frac{1}{\sqrt{5}}$ up to unobservable phase.

In the same way for $|\varphi_2\rangle$ we get:

$$1 = \langle\varphi_2|\varphi_2\rangle = |c_2|^2 (\langle\psi_1| - 2\langle\psi_2|)(|\psi_1\rangle - 2|\psi_2\rangle) =$$

$$= |c_2|^2 (\langle\psi_1|\psi_1\rangle + 4\langle\psi_2|\psi_2\rangle - 2\langle\psi_2|\psi_1\rangle - 2\langle\psi_1|\psi_2\rangle) = 5|c_2|^2 \Rightarrow$$

$\Rightarrow c_2 = \frac{1}{\sqrt{5}}$ up to unobservable phase

So eventally we get following normalized eigenstates of $\hat{B}$:

$$\boxed{\begin{aligned} |\varphi_1\rangle &= \frac{1}{\sqrt{5}}|\psi_2\rangle + \frac{2}{\sqrt{5}}|\psi_1\rangle; \\ |\varphi_2\rangle &= \frac{1}{\sqrt{5}}|\psi_1\rangle - \frac{2}{\sqrt{5}}|\psi_2\rangle; \end{aligned}}$$

b) Suppose one starts with the state $|\psi_1\rangle$. What is probability of measuring a_1 and a_2 for A?

(b) as we have mentioned in theory part, when we do measurement we obtain eigenvalues α_n of correspon-ding operator $\hat{A}$ with probability given by
$P = |\langle\psi_n|\psi\rangle|^2$, $|\psi_n\rangle$ - eigenstate corresponding to α_n;

So probability to observe a_1 is $P_1 = |\langle\psi_1|\psi_1\rangle|^2 = 1$
———————— " ———————— a_2 is $P_2 = |\langle\psi_1|\psi_2\rangle|^2 = 0$

(c) Immediately after the measurement of A, B is measured. What is the probability for measuring b_1 and b_2?

After measurement of $\hat{A}$ we still have $|\psi_1\rangle$ state.
No collapse take place, as $|\psi_1\rangle$ is $\hat{A}$ eigenstate anyway.
So probabilities for measuring b_1 and b_2 are given by:

$$P_{b_1} = |\langle\phi_1|\psi_1\rangle|^2 = \left|\tfrac{1}{\sqrt{5}}(2\langle\psi_1| + \langle\psi_2|)|\psi_1\rangle\right|^2 = \tfrac{1}{5}\cdot|(2\langle\psi_1|\psi_1\rangle + \langle\psi_2|\psi_1\rangle)|^2 = \tfrac{4}{5};$$

$$P_{b_2} = |\langle\phi_2|\psi_1\rangle|^2 = \left|\tfrac{1}{\sqrt{5}}(\langle\psi_1| - 2\langle\psi_2|)|\psi_1\rangle\right|^2 = \tfrac{1}{5}|\langle\psi_1|\psi_1\rangle - 2\langle\psi_2|\psi_1\rangle|^2 = \tfrac{1}{5}$$

so we eventually get: $\boxed{P_{b_1} = \tfrac{4}{5};\ P_{b_2} = \tfrac{1}{5};}$

(d) Assuming that b_1 was measured for B, a measurement of A is now made. What are the probabilities for finding a_1 and a_2?

If b_1 was measured for B following state collapse take place: $|\psi_1\rangle \to |\phi_1\rangle$ and after measurement state of our system is $|\phi_1\rangle$. Then, if we again measure A probabilities to obtain a_1 and a_2 are the following:

$$P_{a_1} = |\langle\phi_1|\psi_1\rangle|^2 = P_{b_1} = \tfrac{4}{5};\quad P_{a_2} = |\langle\phi_1|\psi_2\rangle|^2 = \left|\tfrac{1}{\sqrt{5}}(2\langle\psi_1| + \langle\psi_2|)|\psi_2\rangle\right|^2 =$$

$$= \tfrac{1}{5}|2\underbrace{\langle\psi_1|\psi_2\rangle}_{0} + \langle\psi_2|\psi_2\rangle|^2 = \tfrac{1}{5};\quad \boxed{P_{a_1} = \tfrac{4}{5};\ P_{a_2} = \tfrac{1}{5};}$$

Note: We could avoid calculating P_{a_2} directly as we know that $P_{a_1} + P_{a_2} = 1$ (no other possible results then a_1 and a_2)

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Problem IV (Uncertainty)

Consider a particle with mass m in 1d potential $V(x) = \lambda x^4$ where $\lambda > 0$. Using the Heisenberg uncertainty relation $(\Delta x \Delta p \geq \frac{\hbar}{2})$, estimate the ground state energy of the particle as function of $m, \hbar$ and λ.

Let's consider Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \Rightarrow$

$\Rightarrow \quad \hat{H} = \frac{\hat{p}^2}{2m} + \lambda \hat{x}^4;$

Ground state energy is given by the following expectation value:

$\langle \psi_0 | \hat{H} | \psi_0 \rangle \equiv \langle \hat{H} \rangle = \frac{\langle \hat{p}^2 \rangle}{2m} + \lambda \langle \hat{x}^4 \rangle$ where $|\psi_0\rangle$ is ground state. We don't know this ground state but we are still able to evaluate $\langle H \rangle$ bound from below:

* First let's notice the following facts

$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 \Rightarrow \quad \langle p^2 \rangle = \sigma_p^2 + \langle p \rangle^2 \geq \sigma_p^2$ as $\langle p \rangle^2 \geq 0$

same is valid for $\langle x^2 \rangle$: $\langle x^2 \rangle = \sigma_x^2 + \langle x \rangle^2 \geq \sigma_x^2$ as $\langle x \rangle^2 \geq 0$

So we can rewrite Heisenberg uncertainty in the following way: $\quad \sigma_x^2 \sigma_p^2 \geq \frac{\hbar^2}{4} \Rightarrow \quad \underline{\langle \hat{p}^2 \rangle \langle \hat{x}^2 \rangle \geq \frac{\hbar}{4};}$

<u>Note</u> Case of ground state in symmetric potential is special:

- We know that in symmetric potentials w.f. are either symmetric or antisymmetric.

- There is theorem (we will not proove it here) that symmetric state has lower energy then antisymmetric. And thus <u>lowest energy state is always symmetric.</u>

And we know that for symmetric w.f.:

$\langle x \rangle = \int \underbrace{\psi^*(x) \cdot x \cdot \psi(x)}_{\text{odd funct}} = 0$ and same for $\langle p \rangle$

(10) The same thing can be understood qualitively. In ground state particle shouldn't move anywhere ($\langle p\rangle=0$) and should be placed at minimum of potential, i.e. $\langle x\rangle=0$; So for symmetric potential we get: $\sigma_x^2=\langle\hat{x}^2\rangle$; $\sigma_y^2=\langle\hat{p}^2\rangle \Rightarrow \langle\hat{x}^2\rangle\langle\hat{p}^2\rangle \geq \frac{\hbar^2}{4}$;

* Now we can set lowest bound for $\langle\hat{x}^4\rangle$:

$\langle\hat{x}^4\rangle-\langle\hat{x}^2\rangle^2=(\Delta x^2)^2$ this is definition of average square deviation. We see that:

$\underline{\langle\hat{x}^4\rangle \geq \langle x^2\rangle^2}$. So we rewrite for Hamiltonian expectation value:

$\langle H\rangle \geq \frac{\langle p^2\rangle}{2m}+\lambda\langle x^2\rangle^2$ now from Heisenberg uncertainty we have $\langle p^2\rangle\langle x^2\rangle \geq \frac{\hbar^2}{4} \Rightarrow \langle p^2\rangle \geq \frac{\hbar^2}{4\langle x^2\rangle}$ so that

$$\langle H\rangle \geq \frac{\hbar^2}{8m\langle x^2\rangle}+\lambda\langle x^2\rangle^2$$

* now we can minimiz (i.e. find minimum) function on r.h.s. of obtained inequality:

$$\frac{d}{d\langle x^2\rangle}\left(\frac{\hbar^2}{8m\langle x^2\rangle}+\lambda\langle x^2\rangle^2\right)=-\frac{\hbar^2}{8m\langle x^2\rangle^2}+2\lambda\langle x^2\rangle=0 \Rightarrow$$

$$\Rightarrow \langle x^2\rangle=\left(\frac{\hbar^2}{16m\lambda}\right)^{\frac{1}{3}}; \text{ so that } \langle x^2\rangle_{min}=\frac{1}{2}\left(\frac{\hbar^2}{2m\lambda}\right)^{\frac{1}{3}}$$

Substituting this back we get lowest bound for energy:

$$\langle H\rangle \geq \frac{\hbar^2}{8m}\cdot 2\left(\frac{2m\lambda}{\hbar^2}\right)^{\frac{1}{3}}+\frac{\lambda}{4}\left(\frac{\hbar^2}{2m\lambda}\right)^{\frac{2}{3}}=\frac{1}{4}\left(\frac{\hbar^6\cdot 2m\lambda}{\hbar^2 m^3}\right)^{\frac{1}{3}}+\frac{1}{4}\left(\frac{\lambda^3\hbar^4}{4m^2\lambda^2}\right)^{\frac{1}{3}} \Rightarrow$$

$$\Rightarrow \langle H\rangle \geq \frac{3}{4}\left(\frac{\hbar^4\lambda}{4m^2}\right)^{\frac{1}{3}}.$$ This gives good estimation for ground state energy:

$$\boxed{E_0=\frac{3}{4}\left(\frac{\hbar^4\lambda}{4m^2}\right)^{\frac{1}{3}};}$$

Seminar 7 (Finite-dimensional Hilbert spaces)

Theory reminder

Finite dimensional state space system is familiar to us from linear algebra. The following correspondences should be made to obtain this:

I. State is denoted by bra and ket vectors $\langle\psi|$ and $|\psi\rangle$ (remember that $\langle\psi| \equiv (|\psi\rangle)^{+}$). So for finite (say "n") dimensional space of states:

$$|\psi\rangle = \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix} \text{ and thus } \langle\psi| = [c_1 \dots c_n];$$

II. Operators acting on bra and ket states give another bra or ket:

$$\hat{M}|u\rangle = |v\rangle. \Rightarrow \hat{M}\cdot\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix};$$ this should lead

to the conclusion that $\hat{M}$ is just matrix:

$$M = \begin{bmatrix} M_{11} & M_{12} & \dots & M_{1N} \\ M_{21} & M_{22} & \dots & M_{2N} \\ \vdots & \vdots & & \vdots \\ M_{N1} & M_{N2} & \dots & M_{NN} \end{bmatrix}$$ And action on state is given jus by usual matrix

multiplication:

$$\hat{M}|u\rangle = \begin{bmatrix} M_{11} & M_{12} & \dots & M_{1N} \\ \dots & \dots & \dots & \dots \\ M_{N1} & M_{N2} & \dots & M_{NN} \end{bmatrix}\begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix}.$$

III. Inner product of states is equivalent to simply scalar product of vectors:

$$\langle u|v\rangle = [u_1^+ u_2^+ \dots u_N^+]\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix} = u_1^+ v_1 + u_2^+ v_2 + \dots + u_N^+ v_N$$

IV. We can introduce basis of states as

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \dots \; |n\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \dots \; |N\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \end{bmatrix};$$ we can always make such choise.

(2) Then matrix element's have the following simple form: $\boxed{M_{nm} = \langle n | M | m \rangle;}$

(VI) The most important part in QM, as we know are eigenvalues and eigenstates of operators, satisfying:

$\hat{M}|u_i\rangle = u_i|u_i\rangle$ where u_i is eigenvalue (number) corresponding to eigenstate $|u_i\rangle$. In finite dimensional space of states this turns into equation for eigenvalues and eigenvectors of M matrix:

$\boxed{M \cdot \bar{u}_i = u_i \cdot \bar{u}_i}$ Solution of this equation exist only if

$\underline{\det(\hat{M} - u_i \cdot \hat{I}) = 0}$ → in this way we find u_i, then we solve equation $\underline{(\hat{M} - u_i \hat{I})\, \bar{u}_i = 0}$ to find eigenvector $\bar{u}_i$;

Problem I (Compendium 6)

Consider a two-state system with normalized states given by:

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}; \quad |2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix};$$

The Hamiltonian H and another operator U are given by

$$H = \lambda \begin{bmatrix} 3 & -4i \\ 4i & -3 \end{bmatrix}; \quad U = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix};$$

where λ is positive.

(a) Find eigenvalues of H.

We find it in usual way as we always do it for matricies:

* first we write down secular equation:

$$0 = \det(H - \varepsilon I) = \begin{Vmatrix} 3\lambda - \varepsilon & -4i\lambda \\ 4i\lambda & -3\lambda - \varepsilon \end{Vmatrix} = \varepsilon^2 - 9\lambda^2 - 16\lambda^2 = \varepsilon^2 - 25\lambda^2 = 0$$

so that $\boxed{\varepsilon_{\pm} = \pm 5\lambda;}$ - this are eigenvalues of our

③ Hamiltonian, which give us values of energy for stationary states.

ⓑ Find the normalized eigenstates for H

Eigenstates (which are basically eigenvectors of matrix H) can be found from equations:

$(\hat{H} - \varepsilon_\pm \hat{I})|\psi_\pm\rangle = 0$. In particular:

* for $\varepsilon_+ = 5\alpha$, $(\hat{H} - \varepsilon_+ \hat{I}) = \begin{bmatrix} -2 & -4i \\ 4i & -8 \end{bmatrix}\alpha$.

Next step - we should take general form of $|\psi_+\rangle$:

$|\psi_+\rangle = \begin{bmatrix} a_+ \\ b_+ \end{bmatrix}$. Then we get:

$$\alpha \begin{bmatrix} -2 & -4i \\ 4i & -8 \end{bmatrix} \begin{bmatrix} a_+ \\ b_+ \end{bmatrix} = \alpha \begin{bmatrix} -2a_+ - 4ib_+ \\ 4ia_+ - 8b_+ \end{bmatrix} = 0 \Rightarrow a_+ = -2ib_+ \text{ so that}$$

$|\psi_+\rangle = b_+ \begin{bmatrix} -2i \\ 1 \end{bmatrix}$;

normalization condition as usually reads:

$$1 = \langle\psi_+|\psi_+\rangle = |b_+|^2 \,[2i \;\; 1] \begin{bmatrix} -2i \\ 1 \end{bmatrix} = |b_+|^2 (4+1) = 5|b_+|^2$$

so we get $b_+ = \frac{1}{\sqrt{5}}$ up to unobservable phase

then finally:

$$\boxed{|\psi_+\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} -2i \\ 1 \end{bmatrix} = \frac{1}{\sqrt{5}}(-2i|1\rangle + |2\rangle); \quad \varepsilon_+ = 5\alpha;}$$

* for $\varepsilon_- = -5\alpha$: $(\hat{H} - \varepsilon_- \hat{I}) = \alpha \begin{bmatrix} 8 & -4i \\ 4i & 8 \end{bmatrix} \Rightarrow$ if $|\psi\rangle = \begin{bmatrix} a_- \\ b_- \end{bmatrix}$

Then $\begin{bmatrix} 8 & -4i \\ 4i & 8 \end{bmatrix} \begin{bmatrix} a_- \\ b_- \end{bmatrix} = 0 \Rightarrow b_- = -2ia_-$ so that

$|\psi_-\rangle = a_- \begin{bmatrix} 1 \\ -2i \end{bmatrix}$; Normalization condition gives

$\langle\psi_-|\psi_-\rangle = |a_-|^2 + |b_-|^2 = 1 \Rightarrow |a_-|^2 \cdot 5 = 1$ so $a_- = \frac{1}{\sqrt{5}}$ up to phase

So in the end we get:

$$\boxed{|\psi_-\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ -2i \end{bmatrix} = \frac{1}{\sqrt{5}}(|1\rangle - 2i|2\rangle); \quad \varepsilon_- = -5\alpha;}$$

④ ⓒ What is the probability that a measurement of U will be +1 if the system is in the lower energy state?

Let's remember how measurement is done in QM:

① When we measure value of some operator $\hat{U}$ in system described by state $|\psi\rangle$ we get as the result eigenvalues u_n of $\hat{U}$ with probability $P = |\langle\psi|u_n\rangle|^2$ where $|u_n\rangle$ is corresponding eigenstate of $\hat{U}$

② after value u_n is measured w.f. of system becomes $|u_n\rangle$ (collapse of w.f.)

$\hat{U}$ is already diagonal in basis of $|1\rangle$ and $|2\rangle$

so $\hat{U}|1\rangle = +|1\rangle$; $\hat{U}|2\rangle = -|2\rangle$ $\Rightarrow$ $|1\rangle$, $|2\rangle$ are eigenstates of $\hat{U}$ with eigenvalues +1 and -1 correspondingly. $\underline{|u_+\rangle = |1\rangle ; |u_-\rangle = |2\rangle}$;

So, probability we are interested in is given by

$$P_+ = |\langle u_+|\psi_-\rangle|^2 = |\langle 1|\psi_-\rangle|^2 = \left|\frac{1}{\sqrt{5}}[1\ 0]\begin{bmatrix}1\\-2i\end{bmatrix}\right|^2 = \frac{1}{5}.$$

So probability is $\boxed{P_+ = \frac{1}{5};}$

ⓓ What is the expectation value of U for the system in the lower energy state?

Lower energy state is given by $|\psi_-\rangle = \frac{1}{\sqrt{5}}\begin{bmatrix}1\\-2i\end{bmatrix}$;

Expectation velue of U in this state is given by:

$$\langle\hat{U}\rangle = \langle\psi_-|\hat{U}|\psi_-\rangle = \frac{1}{5}[1\ 2i]\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}1\\-2i\end{bmatrix} = \frac{1}{5}[1\ 2i]\begin{bmatrix}1\\2i\end{bmatrix} = \frac{1}{5}(1-4)$$

$\Rightarrow$ $\boxed{\langle\hat{U}\rangle = -\frac{3}{5}}$

(5)

Problem II (Compendium 7)

Consider the 3 state system with normalized state given by

$$|1\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix}; \quad |2\rangle = \begin{bmatrix}0\\1\\0\end{bmatrix}; \quad |3\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix};$$

and a Hamiltonian given by:

$$H = \alpha \begin{bmatrix} 1 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 \end{bmatrix}$$

where $\alpha > 0$

(a) find 3 energy eigenvalues for this system.

As usually to find eigenvalues of matricies we should write down secular equation:

$$\det(\hat{H} - \varepsilon_i \hat{I}) = 0 \Rightarrow \left\| \begin{matrix} \alpha-\varepsilon_i & \alpha/\sqrt{2} & 0 \\ \alpha/\sqrt{2} & \alpha-\varepsilon_i & \alpha/\sqrt{2} \\ 0 & \alpha/\sqrt{2} & \alpha-\varepsilon_i \end{matrix} \right\| = (\alpha-\varepsilon_i)^3 - 2\frac{\alpha^2}{2}(\alpha-\varepsilon_i) =$$

$$= (\alpha-\varepsilon_i)\left((\alpha-\varepsilon_i)^2 - \alpha^2\right) = \varepsilon_i(\varepsilon_i-\alpha)(\varepsilon_i-2\alpha) = 0$$

So we get 3 eigenvalues of Hamiltonian (energy levels):

$$\boxed{\varepsilon = 0; \ \varepsilon = \alpha; \ \varepsilon = 2\alpha;}$$

(b) Find the normalized energy eigenstates

To find eigenstates we should solve equation $(\hat{H} - \varepsilon_i \hat{I})|\psi_i\rangle = 0$:

* for $\varepsilon_0 = 0$

$$\alpha \begin{bmatrix} 1 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 \end{bmatrix} \begin{bmatrix} a_0 \\ b_0 \\ c_0 \end{bmatrix} = 0 \quad \text{where } |\psi_0\rangle = \begin{bmatrix} a_0 \\ b_0 \\ c_0 \end{bmatrix}$$

from this equation we get: $b_0 = -\sqrt{2}a_0$; $b_0 = -\sqrt{2}c_0$; $a_0 = c_0$;

and from normalization condition:

$$\langle\psi_0|\psi_0\rangle = |a_0|^2 + |b_0|^2 + |c_0|^2 = c_0^2(1+1+2) = 4c_0^2 = 1 \Rightarrow$$

$\Rightarrow c_0 = \frac{1}{2}$ up to phase.

$$\boxed{\varepsilon_0 = 0; \ |\psi_0\rangle = \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix}\frac{1}{2};}$$

ⓑ * for $\varepsilon_1 = \alpha$; We take general $|\psi_1\rangle$:

$|\psi_1\rangle = \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix}$ then it should satisfy following equation:

$$\alpha \begin{bmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \end{bmatrix} \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix} = 0 \Rightarrow$$

$b_1 = 0$; and normalization condition

$a_1 = -c_1$; gives: $|a_1|^2 + |b_1|^2 + |c_1|^2 = 2|c_1|^2 = 1$

$\Rightarrow c_1 = \frac{1}{\sqrt{2}}$ up to phase so that

$$\boxed{\varepsilon_1 = \alpha; \ |\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}}$$

* for $\varepsilon_2 = 2\alpha$; general $|\psi_2\rangle$ is given by $|\psi_2\rangle = \begin{bmatrix} a_2 \\ b_2 \\ c_2 \end{bmatrix}$;

$$\alpha \begin{bmatrix} -1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -1 \end{bmatrix} \begin{bmatrix} a_2 \\ b_2 \\ c_2 \end{bmatrix} = 0$$

$b_2 = \sqrt{2} a_2$; $b_2 = \sqrt{2} c_2$ and from normalization:

$1 = |a_2|^2 + |b_2|^2 + |c_2|^2 = 4|c_2|^2 = 1 \Rightarrow$

$\Rightarrow c_2 = \frac{1}{2}$ up to phase. so finally we get:

$$\boxed{\varepsilon_2 = 2\alpha; \ |\psi_2\rangle = \frac{1}{2} \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix};}$$

ⓒ If the system is in the ground state, what is probability that it is in state $|1\rangle$?

Ground state (i.e. state with the lowest energy) in our case is $|\psi_0\rangle = \frac{1}{2} \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix}$; then probability for system to be found in state $|1\rangle$ is given by inner product:

$P_1 = |\langle 1 | \psi_0 \rangle|^2 = \left| \frac{1}{2} [1 \ 0 \ 0] \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} \right|^2 = \frac{1}{4}$; so $\boxed{P_1 = \frac{1}{4};}$

ⓓ If the system starts in state $|1\rangle$ with probability 1 at time $t=0$, what is the probability that it is in state $|3\rangle$ at time $t = \frac{\pi \hbar}{\alpha}$?

To find time evolution we should proceed as follows:

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* expand $|\psi\rangle$ in system of Hamiltonian eigenstates $|\psi_n\rangle$: $\underline{|\psi\rangle = \sum_n c_n|\psi_n\rangle}$ where c_n is given by $\underline{c_n = \langle\psi_n|\psi\rangle}$

* apply time-evolution operator $e^{-\frac{i}{\hbar}\hat{H}t}$. As $|\psi_n\rangle$ is eigenstate of $\hat{H}$: $e^{-\frac{i}{\hbar}\hat{H}t}|\psi_n\rangle = e^{-\frac{i}{\hbar}E_n t}|\psi_n\rangle$;

So that: $\underline{|\psi, t\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi, t=0\rangle = \sum_{n=0}^{\infty} c_n e^{-\frac{i}{\hbar}E_n t}|\psi_n\rangle}$;

That means that for applying last formula we need to know eigenvalues of Hamiltonian and coefficients of expansion c_n.

In our case:

$|\psi, t=0\rangle = |1\rangle$

Coefficients of expansion are given by:

$$c_0 = \langle\psi_0|\psi\rangle = \frac{1}{2}\begin{bmatrix}1 & -\sqrt{2} & 1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix} = \frac{1}{2};$$

$$c_1 = \langle\psi_1|\psi, t=0\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0 & -1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix} = \frac{1}{\sqrt{2}};$$

$$c_2 = \langle\psi_2|\psi, t=0\rangle = \frac{1}{2}\begin{bmatrix}1 & \sqrt{2} & 1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix} = \frac{1}{2};$$

So that: $|\psi, t=0\rangle = \frac{1}{2}|\psi_0\rangle + \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{2}|\psi_2\rangle$; and time-dependent wave function is given by:

$$|\psi, t\rangle = \frac{1}{2}e^{-\frac{i}{\hbar}\varepsilon_0 t}|\psi_0\rangle + \frac{1}{\sqrt{2}}e^{-\frac{i}{\hbar}\varepsilon_1 t}|\psi_1\rangle + \frac{1}{2}e^{-\frac{i}{\hbar}\varepsilon_2 t}|\psi_2\rangle$$

in particular for $t = \frac{\pi\hbar}{2}$: $\varepsilon_0 t = 0$; $\varepsilon_1 t = \pi\hbar$; $\varepsilon_2 t = 2\pi\hbar$

and thus

$$|\psi, t=\frac{\pi\hbar}{2}\rangle = \frac{1}{2}|\psi_0\rangle + \frac{1}{\sqrt{2}}e^{-i\pi}|\psi_1\rangle + \frac{1}{2}e^{-2\pi i}|\psi_2\rangle$$

$$|\psi, t=\frac{\pi\hbar}{2}\rangle = \frac{1}{2}|\psi_0\rangle - \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{2}|\psi_2\rangle = \frac{1}{4}\begin{bmatrix}1\\-\sqrt{2}\\1\end{bmatrix} + \frac{1}{4}\begin{bmatrix}1\\\sqrt{2}\\1\end{bmatrix} - \frac{1}{2}\begin{bmatrix}1\\0\\-1\end{bmatrix} =$$

$$= \begin{bmatrix}0\\0\\1\end{bmatrix} = |3\rangle; \quad |\psi, t=\frac{\pi\hbar}{2}\rangle = |3\rangle$$

Thus probability for system to be found in state $|3\rangle$ at $t = \frac{\pi\hbar}{2}$ is $P_3 = |\langle 3|\psi, t=\frac{\pi\hbar}{2}\rangle|^2 = |\langle 3|3\rangle|^2 = 1$; $\boxed{P_3 = 1}$

⑧ Problem III

In the notes we gave the example of a two state system with states $|\uparrow\rangle$ and $|\downarrow\rangle$. Now suppose that we have a tensor product of 2 such states such that there are 4 states in total:

$$|\uparrow\uparrow\rangle \; ; \; |\uparrow\downarrow\rangle ; \; |\downarrow\uparrow\rangle \; ; \; |\downarrow\downarrow\rangle$$

Let A_1 be an operator that measures the sign of the first arrow (+1 for $\uparrow$ and -1 for $\downarrow$) and A_2 - the same for second arrow. F_1 and F_2 are operators flipping first and second arrows.

ⓐ write A_1, A_2, F_1 and F_2 as 4x4 matricies.

Let's choose basis of vectors in the following way:

$$|1\rangle = |\uparrow\uparrow\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix} ; \quad |2\rangle = |\uparrow\downarrow\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix} ; \quad |3\rangle = |\downarrow\uparrow\rangle = \begin{bmatrix}0\\0\\1\\0\end{bmatrix} ; \quad |4\rangle = |\downarrow\downarrow\rangle = \begin{bmatrix}0\\0\\0\\1\end{bmatrix} ;$$

we are always free to choose basis as we want.

Then A and F operators act on this bassis as follows:

$$A_1|1\rangle = A_1|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle = |1\rangle ; \qquad A_2|1\rangle = A_2|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle = |1\rangle ;$$

$$A_1|2\rangle = A_1|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle = |2\rangle ; \qquad A_2|2\rangle = A_2|\uparrow\downarrow\rangle = -|\uparrow\downarrow\rangle = -|2\rangle ;$$

$$A_1|3\rangle = A_1|\downarrow\uparrow\rangle = -|\downarrow\uparrow\rangle = -|3\rangle ; \qquad A_2|3\rangle = A_2|\downarrow\uparrow\rangle = |\downarrow\uparrow\rangle = |3\rangle ;$$

$$A_1|4\rangle = A_1|\downarrow\downarrow\rangle = -|\downarrow\downarrow\rangle = -|4\rangle ; \qquad A_2|4\rangle = A_2|\downarrow\downarrow\rangle = -|\downarrow\downarrow\rangle = -|4\rangle ;$$

$$F_1|1\rangle = F_1|\uparrow\uparrow\rangle = |\downarrow\uparrow\rangle = |3\rangle ; \qquad F_2|1\rangle = F_2|\uparrow\uparrow\rangle = |\uparrow\downarrow\rangle = |2\rangle ;$$

$$F_1|2\rangle = F_1|\uparrow\downarrow\rangle = |\downarrow\downarrow\rangle = |4\rangle ; \qquad F_2|2\rangle = F_2|\uparrow\downarrow\rangle = |\uparrow\uparrow\rangle = |1\rangle ;$$

$$F_1|3\rangle = F_1|\downarrow\uparrow\rangle = |\uparrow\uparrow\rangle = |1\rangle ; \qquad F_2|3\rangle = F_2|\downarrow\uparrow\rangle = |\downarrow\downarrow\rangle = |4\rangle ;$$

$$F_1|4\rangle = F_1|\downarrow\downarrow\rangle = |\uparrow\downarrow\rangle = |2\rangle ; \qquad F_2|4\rangle = F_2|\downarrow\downarrow\rangle = |\downarrow\uparrow\rangle = |3\rangle ;$$

As we have already mentioned if we have some basis $\{|n\rangle\}$ operator matrix elements are given by

⑨

$$\boxed{M_{mn} = \langle \underset{\text{row\#}}{m} | M | \underset{\text{array\#}}{n} \rangle}$$

Let's consider what this formula gives us:

* A_1 operator

As $\langle n|m\rangle = \delta_{nm}$ nonzero components of A_1 are

$\langle 1|A_1|1\rangle = 1$; $\langle 2|A_1|2\rangle = (A_1)_{22} = 1$;

$\langle 3|A_1|3\rangle \equiv (A_1)_{33} = -1$; $\langle 4|A_1|4\rangle = (A_1)_{44} = -1$;

So A_1 matrix is given by:

$$\boxed{A_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix};}$$

* A_2 operator: in the same way nonzero comp. are:

$\langle 1|A_2|1\rangle \equiv (A_2)_{11} = 1$; $\langle 2|A_2|2\rangle \equiv (A_2)_{22} = -1$;

$\langle 3|A_2|3\rangle \equiv (A_2)_{33} = 1$; $\langle 4|A_2|4\rangle \equiv (A_2)_{44} = -1$; so that

$$\boxed{A_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix};}$$

* F_1 operator. Nonzero components are:

$\langle 3|F_1|1\rangle = \langle 1|F_1|3\rangle = 1 \Rightarrow (F_1)_{13} = (F_1)_{31} = 1$;

$\langle 2|F_1|4\rangle = \langle 4|F_1|2\rangle = 1 \Rightarrow (F_1)_{24} = (F_1)_{42} = 1$; so that:

$$\boxed{F_1 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix};}$$

* F_2 operator Nonzero components are:

$\langle 1|F_2|2\rangle = \langle 2|F_2|1\rangle = 1 \Rightarrow (F_2)_{12} = (F_2)_{21} = 1$;

$\langle 3|F_2|4\rangle = \langle 4|F_2|3\rangle = 1 \Rightarrow (F_2)_{34} = (F_2)_{43} = 1$; so that:

$$\boxed{F_2 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix};}$$

Second way to obtain expressions for matricies (if you forget formula or confused about raw and array numbers)

(10) is the following:

* assume F_1 is in general form:

$$F_1 = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix};$$

* now let's act with it on basis vectors:

• $F_1|1\rangle = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} = |3\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ so we get:

$a_{11} = a_{21} = a_{41} = 0;\ a_{31} = 1;$

• $F_1|2\rangle = \begin{bmatrix} 0 & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 1 & a_{32} & a_{33} & a_{34} \\ 0 & a_{42} & a_{43} & a_{44} \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{bmatrix} = |4\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ so that:

$a_{12} = a_{22} = a_{32} = 0;\ a_{42} = 1;$

• $F_1|3\rangle = \begin{bmatrix} 0 & 0 & a_{13} & a_{14} \\ 0 & 0 & a_{23} & a_{24} \\ 1 & 0 & a_{33} & a_{34} \\ 0 & 1 & a_{43} & a_{44} \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \\ a_{43} \end{bmatrix} = |1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ so that:

$a_{13} = 1;\ a_{23} = a_{33} = a_{43} = 0;$

• $F_1|4\rangle = \begin{bmatrix} 0 & 0 & 1 & a_{14} \\ 0 & 0 & 0 & a_{24} \\ 1 & 0 & 0 & a_{34} \\ 0 & 1 & 0 & a_{44} \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} a_{14} \\ a_{24} \\ a_{34} \\ a_{44} \end{bmatrix} = |2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ so that

$a_{14} = a_{34} = a_{44} = 0;\ a_{24} = 1;$ and finally we get:

$$\boxed{F_1 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}}$$

; which coinsides with answer observed previously. The same can be done for other 3 operators.

(b) find F_1F_2 as a 4x4 matrix.

There are 2 ways to observe F_1F_2 as 4x4 matrix:

First way is physical. Operator $F_1 \cdot F_2$ is the one that flips both spins. Let's look how it acts on basis

11

states:

$F_1F_2|1\rangle = F_1F_2|\uparrow\uparrow\rangle = |\downarrow\downarrow\rangle = |4\rangle$;

$F_1F_2|2\rangle = F_1F_2|\uparrow\downarrow\rangle = |\downarrow\uparrow\rangle = |3\rangle$;

$F_1F_2|3\rangle = F_1F_2|\downarrow\uparrow\rangle = |\uparrow\downarrow\rangle = |2\rangle$;

$F_1F_2|4\rangle = F_1F_2|\downarrow\downarrow\rangle = |\uparrow\uparrow\rangle = |1\rangle$;

So nonzero elements of F_1F_2 matrix are given by.

$(F_1F_2)_{14} = (F_1F_2)_{41} = \langle 4|F_1F_2|1\rangle = 1$

$(F_1F_2)_{23} = (F_1F_2)_{32} = \langle 2|F_1F_2|3\rangle = 1$, so matrix F_1F_2 is:

$$\boxed{F_1F_2 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix};}$$

Second way is streighforward. For finite dimensional space of states product of operators is given by usual product of corresponding matricies:

$$F_1 \cdot F_2 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$ so we finally get

the same answe as the one obtained above.

c) Find eigenvalues and eigenstates of F_1F_2. Are there any degeneracies?

To find eigenvalues we should as usually write down secular equation:

here we use expansion of determinant in first raw

$$\det(\hat{F}_1 \cdot \hat{F}_2 - \lambda \hat{I}) = \begin{vmatrix} -\lambda & 0 & 0 & 1 \\ 0 & -\lambda & 1 & 0 \\ 0 & 1 & -\lambda & 0 \\ 1 & 0 & 0 & -\lambda \end{vmatrix} = -\lambda \begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{vmatrix} - \begin{vmatrix} 0 & -\lambda & 1 \\ 0 & 1 & -\lambda \\ 1 & 0 & 0 \end{vmatrix} =$$

$$= -\lambda(-\lambda^3 + \lambda) - (\lambda^2 - 1) = (\lambda^2 - 1)^2 = (\lambda - 1)^2(\lambda + 1)^2$$

so we get eigenvalues:

$\boxed{\lambda = \pm 1 \text{ - both are double degenerate}}$ as in secular equation we have terms of second power: $(\lambda-1)^2$, so we get same eigenvalue twice.

(12) (d) Which eigenstates of F_1F_2 are not eigenstates of F_1 and F_2 individually?

Let's do opposite - find simultaneous eigenstates of F_1F_2, F_1 and F_2.

* First let's find eigenstates of $F_1 \cdot F_2$ operator

• $\lambda = +1$

Equation $(\hat{F}_1 \cdot \hat{F}_2 - \lambda \hat{I})|\psi_+\rangle = 0$ takes form:

$$\begin{bmatrix} -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} a_+ \\ b_+ \\ c_+ \\ d_+ \end{bmatrix} \text{ so where } |\psi_+\rangle = \begin{bmatrix} a_+ \\ b_+ \\ c_+ \\ d_+ \end{bmatrix};$$

so we get:

$a_+ = d_+$
$b_+ = c_+$

so general eigenstate is given by:

$$\boxed{|\psi_+\rangle = \begin{bmatrix} a_+ \\ b_+ \\ b_+ \\ a_+ \end{bmatrix};\ \lambda = +1;}$$

Note that we havn't normalized state yet.

• $\lambda = -1$;

Equation for eigenstates is given by:

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} a_- \\ b_- \\ c_- \\ d_- \end{bmatrix} \text{ so where } |\psi_-\rangle = \begin{bmatrix} a_- \\ b_- \\ c_- \\ d_- \end{bmatrix}$$

so we get:

$a_- = -d_-$; $b_- = -c_-$, and thus

$$\boxed{|\psi_-\rangle = \begin{bmatrix} a_- \\ b_- \\ -b_- \\ -a_- \end{bmatrix};\ \lambda = -1;}$$

Note that both eigenstates we have found are linear combinations of 2 (equals # of degeneracy) linearly independent states:

for $\lambda = +1$ these are: $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$;

for $\lambda = -1$: $\begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix}$;

* Now we can find how F_1 and F_2 operators act on $|\psi_+\rangle$ and $|\psi_-\rangle$ states:

- $|\psi_+\rangle$ state:

$$F_2|\psi_+\rangle \equiv \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a_+ \\ b_+ \\ b_+ \\ a_+ \end{bmatrix} = \begin{bmatrix} b_+ \\ a_+ \\ a_+ \\ b_+ \end{bmatrix} = c \begin{bmatrix} a_+ \\ b_+ \\ b_+ \\ a_+ \end{bmatrix}$$

as $\hat{F}_2^2 = \hat{I}$ (check it by matrix multiplication, physically this mean that we flip first spin twice and come back to initial state) it's eigen values can be +1 or -1. Indeed

$$F_2|\lambda\rangle = \lambda|\lambda\rangle \; ; \quad F_2^2|\lambda\rangle = \lambda F_2|\lambda\rangle = \lambda^2|\lambda\rangle = \hat{I}|\lambda\rangle = 1|\lambda\rangle$$

so $\lambda^2 = 1 \Rightarrow \lambda = \pm 1$. Let's consider this 2 cases (further we denote eigenvalues of $\hat{F}_1$ and $\hat{F}_2$ as f_1 and f_2):

- $f_2 = +1$ then we want $c = +1$ in obtained equation so that $b_+ = a_+$ and corresponding eigenstate is $\boxed{|\varphi_1\rangle = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} ; \; f_2 = +1 ; \; f_{12} = +1}$

Note: Let's proove that f_{12} (eigenvalue of $F_1 \cdot F_2$) is simply given by product of f_1 and f_2 - eigenvalues of F_1 and F_2 operators. Indeed let's assume that just as we have $|\varphi\rangle$ is eigenstate of $F_1 \cdot F_2 = F_2 F_1$ and F_1 then $F_2 F_1 |\varphi\rangle \equiv f_{12}|\varphi\rangle = F_2 \cdot f_1 |\varphi\rangle$ in order for this to be satisfied we need $|\varphi\rangle$ to be eigenstate of F_2 with the eigenvalue f_2, satisfying $f_{12} = f_1 \cdot f_2$; q.e.d.

We can check this for $|\varphi_1\rangle$:

$$F_1|\varphi_1\rangle \equiv \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \Rightarrow$$ $|\varphi_1\rangle$ is eigenstate of F_1 with eigenvalue $f_1 = +1$;

- $f_2 = -1$ if we choose $b_+ = -a_+$ we get $c = -1$ so

(14) so $$\boxed{|\varphi_2\rangle = \frac{1}{2}\begin{bmatrix}1\\-1\\-1\\1\end{bmatrix} \; ; \quad f_1 = -1;\ f_2 = -1;\ f_{12} = +1;}$$

• now we go for $|\psi_-\rangle$ state:

$$F_2|\psi_-\rangle = \begin{bmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}\begin{bmatrix}a_-\\b_-\\-b_-\\a_-\end{bmatrix} = \begin{bmatrix}b_-\\a_-\\-a_-\\-b_-\end{bmatrix} = f_2\begin{bmatrix}a_-\\b_-\\-b_-\\-a_-\end{bmatrix}$$

here 2 eigenvalues possible:

- $f_2 = +1$: implies $a_- = b_-$ so we get following state: $$\boxed{|\varphi_3\rangle = \frac{1}{2}\begin{bmatrix}1\\1\\-1\\-1\end{bmatrix} \; ; \quad \begin{matrix}f_{12} = -1\\ f_2 = +1\end{matrix} \Rightarrow f_1 = -1;}$$

- $f_2 = -1$ implies $a_- = -b_-$ so that: $$\boxed{|\varphi_4\rangle = \frac{1}{2}\begin{bmatrix}1\\-1\\1\\-1\end{bmatrix} \; ; \quad \begin{matrix}f_{12} = -1\\ f_2 = -1\end{matrix} \Rightarrow f_1 = +1;}$$

So we have four simultaneous eigenstates of F_1F_2, F_1, and F_2 given by $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, |\varphi_4\rangle$. All other eigenstates of F_1F_2 (there is infinite number of them) are not simultaneously eigenstates of F_1 and F_2.

Example of eigenstate of F_1F_2 but not of F_1 and F_2 is for example state $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\1\end{bmatrix} = \frac{1}{\sqrt{2}}(|1\rangle + |4\rangle) = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$

This can be understood physically: if we flip both arrows this state goes to itself, while flipping only one of arows give $F_1(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) = |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle$; completely different state.

(e) For one of the eigenstates in (d), describe what happens for a measurement of A_2 after measurment is made for A_1.

(15) Let's take for example state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ it is eigenstate of F_1F_2 but not of F_1 and F_2:

$F_1F_2(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle$ - initial state.

$F_1(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = |\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle$; $F_2(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$.

Let's remind that after measurment state of system $|\psi\rangle$ collapses to one of the eigenstates of operator we are measuring, with probability $P = |\langle\psi|\psi_n\rangle|^2$;

Assume we measure A_1 first:

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \xrightarrow[\text{collapse}]{} \begin{cases} |\uparrow\downarrow\rangle \text{ with probability } P=\frac{1}{2}, & A_1=+1; \\ |\downarrow\uparrow\rangle \text{ ——— '' ——— } P=\frac{1}{2}, & A_1=-1; \end{cases}$$

Then if we measure A_2 after A_1 we $\boxed{\text{necesarily}}$ get $A_2=-1$ (if $A_1=+1$ was obtained) or $A_2=+1$ (if $A_1=-1$ was observed). So measurements of A_1 and A_2 are strongly correlated. This kind of states are called entangled, and they are important in quantum information theory.

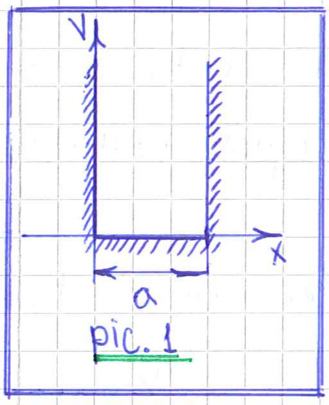
Seminar 8 (more problems)

During this class we will remember main points we have learned in first part of course

Problem I (An electron in square well)

Consider an electron in an infinite square well with width $1 Å = 10^{-10}$ m and mass $m = 9{,}11 \cdot 10^{-28}$ kg.

ⓐ Find the speed of the electron for each energy level.



pic. 1

We have already solved problems on levels in infinite square well before (see lecture N4 and problem set N4 solutions for details)

Solution to particle in the box is the following:

* first we write Sch. eq. as usually:

$$E_n \psi_n = -\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2}, \text{ for } 0 < x \leq a; \quad \psi_n(x) = 0 \text{ outside the box}$$

as potential there is infinite and particles can't be observed there.

* Due to continuity of w.f. we put boundary conditions $\psi(0) = \psi(a) = 0$;
* General solution to Sch. eq. satisfying b.c. is

$$\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin\frac{\pi n x}{a}; \quad E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2}, \ n = 1, 2, 3 \ldots}$$

From here we can estimate velocity of the electron using classical formulas:

$\frac{mv_n^2}{2} = T_n$; where T_n is kinetic energy of electron on level n.
($T_n = E_n$ as $V = 0$ for $0 < x < a$)

The way to justify this equation we can use Ehrenfest theorem, that states relation between classical mechanics relations with corresponding

② relations for expectation values. In particular we can use Heisenberg equation:

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}[H,\hat{x}] = \frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m},\hat{x}\right] = \frac{i}{\hbar m}\hat{p}\underbrace{[\hat{p},\hat{x}]}_{-i\hbar} = \frac{\hat{p}}{m} \quad \text{so}$$

that $\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m}$ - Heisenberg picture.

Now if we evaluate $\left\langle\frac{d\hat{x}}{dt}\right\rangle = \frac{1}{m}\langle\hat{p}\rangle$ then we get $\langle p\rangle_n = \int_{-\infty}^{+\infty} dx\, \psi_n^*(x)\left(-i\hbar\frac{d}{dx}\right)\psi_n(x) = 0$ as $\psi(x) = -\psi(-x)$

and thus: $\psi_n^*(-x)\left(-i\hbar\frac{d}{d(-x)}\right)\psi_n(-x) = \psi_n^*(x)\, i\hbar\frac{d}{dx}\psi_n(x)$

So that $\left\langle\frac{d\hat{x}}{dt}\right\rangle_n = 0$. This is reasonable, as particle in a box moves to the right and left with equal probability, and velocity in average is 0.

Proper quantaty that gives velocity of electron is then:

$$\left\langle\left(\frac{d\hat{x}}{dt}\right)^2\right\rangle = \frac{1}{m^2}\langle\hat{p}^2\rangle = \frac{2}{m}\langle E\rangle$$ so that velocity

of electron on level n is:

$$V_n = \sqrt{\left\langle\left(\frac{d\hat{x}}{dt}\right)^2\right\rangle_n} = \sqrt{\frac{2E_n}{m}} = \sqrt{\frac{\pi^2 n^2\hbar^2}{m^2a^2}}; \quad V_n = \frac{\pi n\hbar}{ma};$$

$$V_n = \frac{3{,}14\cdot 6{,}63\cdot 10^{-34}\,\frac{kg\cdot m^2}{s^2}\cdot n}{9{,}1\cdot 10^{-28}\,kg\cdot 10^{-10}\,m} = 2{,}3\cdot n\cdot 10^4\,\frac{m}{s}; \quad \text{finally}$$

$$\boxed{V_n = \frac{\pi\hbar n}{ma} = 2{,}3\cdot n\cdot 10^4\,\frac{m}{s};}$$

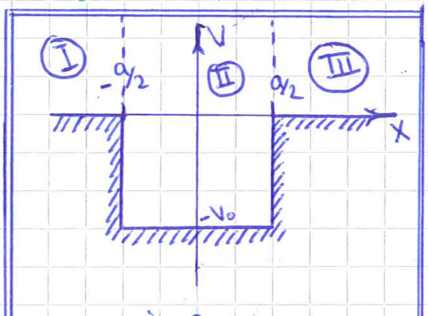
Ⓑ At what value of n would the electron surpass the speed of light?

Let's just substitute c instead of V_n into the formula above: $c = \frac{\pi\hbar n}{ma} \Rightarrow n = \left[\frac{mac}{\pi\hbar}\right] = \left[\frac{3\cdot 10^8}{2{,}3\cdot 10^4}\right] \approx 1{,}3\cdot 10^4$

So for all levels $n > 1{,}3\cdot 10^4$ velocity of electron will be bigger then speed of light c. This happens because Sch. eq. (and all QM we consider in this course) is non-relativistic and should be modified.

③

ⓒ Now instead of an infinite well assume that it is a finite square well with depth V_0. At what value of V_0 would there be a bound state where the electron is surpassing the speed of light?



pic. 2

Before doing this problem let's remind solution of energy level problem for finite square well. (this was done in Lecture 5 and problem 2 of set 5)

* first we devide space into 3 regions and write down general solution for Sch. eq. in this 3 regions:

$$\begin{cases} \psi_I = Ae^{\varkappa x}; \; x < -\frac{a}{2} \quad \text{where} \quad \varkappa = \frac{\sqrt{-2mE}}{\hbar}; \\ \psi_{II} = B\sin kx + C\cdot\cos kx; \; -\frac{a}{2} < x < \frac{a}{2} \quad ; \quad k = \frac{\sqrt{2m(E+V_0)}}{\hbar}; \\ \psi_{III} = De^{-\varkappa x}; \; x > \frac{a}{2}; \end{cases}$$

*Then using boundary conditions:

- $\psi_{II}\left(\frac{a}{2}\right) = \psi_{III}\left(\frac{a}{2}\right); \quad \left.\frac{d\psi_{II}}{dx}\right|_{x=a/2} = \left.\frac{d\psi_{III}}{dx}\right|_{x=a/2};$

- $\psi_I\left(-\frac{a}{2}\right) = \psi_{II}\left(-\frac{a}{2}\right); \quad \left.\frac{d\psi_I}{dx}\right|_{x=-\frac{a}{2}} = \left.\frac{d\psi_{II}}{dx}\right|_{x=-a/2};$

we write down equations that define energy levels in well.

$$\boxed{\begin{array}{ll} \operatorname{tg} z = -\frac{z}{\sqrt{\gamma^2 - z^2}}; \; - \text{odd levels.} & \text{Here } \frac{1}{2}ka = z; \\ & \frac{1}{2}\varkappa a = \sqrt{\gamma^2 - z^2}; \; \gamma = \sqrt{2mV_0}\frac{a}{2\hbar}; \\ z\cdot\operatorname{tg} z = \sqrt{\gamma^2 - z^2}; \; - \text{even levels.} & \end{array}}$$

This equations can be solved graphically (see pic. 3)

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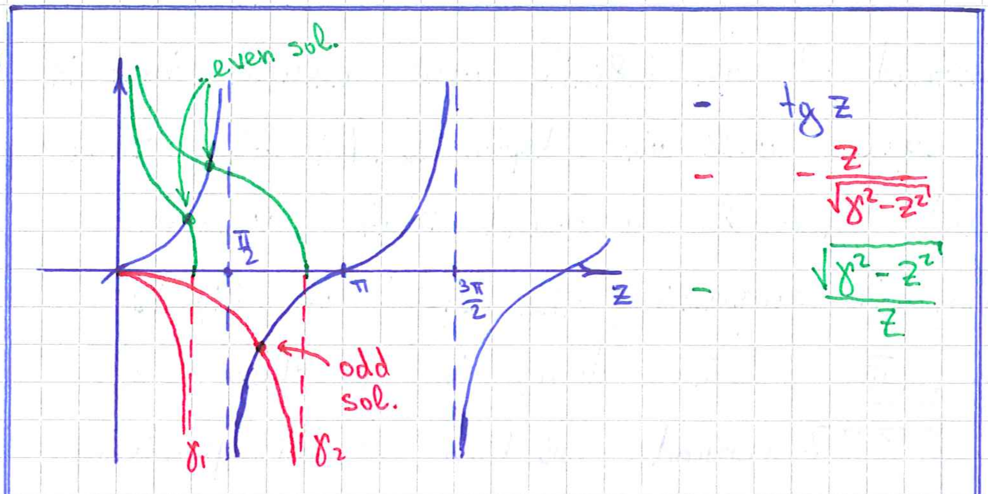


pic. 3

From this graphical solutions we conclude:

if $0<\gamma<\pi$ - there is 1 even solution;

$\pi<\gamma<2\pi$ - 2 even solutions;

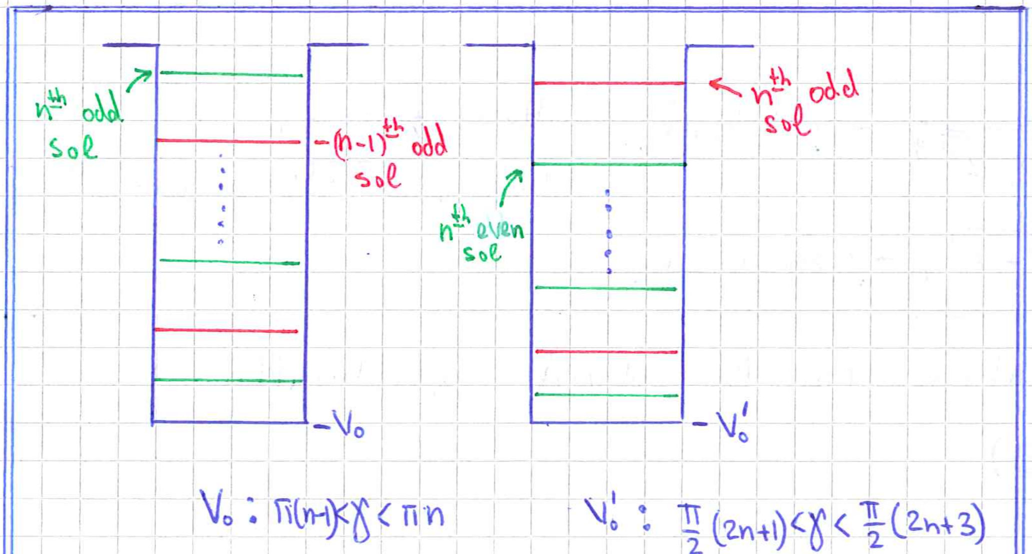
$\boxed{\pi(n-1)<\gamma<\pi n \text{ - n even solutions}}$

$0<\gamma<\frac{\pi}{2}$ - no odd solutions;

$\frac{\pi}{2}<\gamma<\frac{3\pi}{2}$ - 1 odd solution;

$\boxed{\frac{\pi}{2}(2n+1)<\gamma<\frac{\pi}{2}(2n+3) \text{ - (n-1) odd solutions}}$

What happens if we make well deeper and deeper? Deeper well means that γ becomes larger and as we see from pic.3 new levels (even and odd in turn) will be appearing (see pic. 4)



pic 4

(5) For estimation of highest level in finite well thus we can assume $E \approx 0$ (if you look on graphical solution we can see that when new level just appears $z \approx \gamma \Rightarrow \sqrt{E+V_0} \approx \sqrt{V_0}$ so that $E \approx 0$;
Thus kinetic energy of electron is given by:
$T = V_0$ and thus

$v_n = \sqrt{\frac{2V_0}{m}}$ here v_n is velocity of electron on the highest level. So for $\sqrt{\frac{2V_0}{m}} > c$ electron will surpass speed of light. "Critical" V_0 is given by:

$$\boxed{V_0 = \frac{1}{2}mc^2 = 0,25\,\text{MeV} = 4 \cdot 10^{-14}\,\text{J};}$$

Problem III (A shallow finite square well)

Consider a particle with mass m in a finite square well with potential:

$$V(x) = \begin{cases} -V_0, & -a < x < a; \\ 0, & x < -a \text{ or } x > +a; \end{cases}$$

and suppose that the well is shallow in the sense that $\frac{mV_0a^2}{\hbar^2} \ll 1$;

(a) Find an estimate for the energy of the one bound state in terms of $V_0, m, a, \hbar$.

From graphical solution we see that even for shallow well ther exists one even solution which satisfies equation

$$z \cdot tg\,z = \sqrt{\gamma^2 - z^2} \quad ; \quad z = ka; \quad \gamma = \sqrt{2mV_0}\,\frac{a}{\hbar}; \quad \varkappa a = \sqrt{\gamma^2 - z^2};$$

(note that here width of well is twice bigger then one in problem I and is $2a$)

As well is shallow and condition $\frac{mV_0a^2}{\hbar^2} \ll 1$ is satisfied we conclude that $\gamma^2 \ll 1$ and as $z < \gamma$ for

⑥ bound states ($E+V_0<V_0$ as $E<0$ - condition for the bound state). So as z is small we can expand in Taylor series $\operatorname{tg} z$: $\operatorname{tg} z \approx z$ so we get approximate equation:

$$z^2 = \sqrt{\gamma^2 - z^2} \Rightarrow z^4 + z^2 - \gamma^2 = 0 \Rightarrow z^2 = -\frac{1}{2} \pm \frac{1}{2}\sqrt{1+4\gamma^2};$$

We are interested of course in positive answer $z>0$:

$z^2 = \frac{1}{2}\left(\sqrt{1+4\gamma^2} - 1\right)$ expanding square root we get:

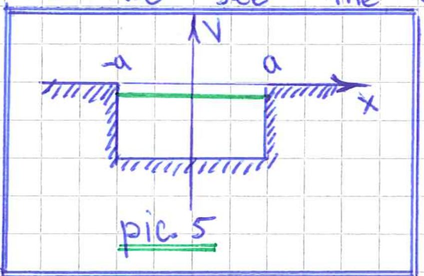
$z^2 = \frac{1}{2}\left(\frac{1}{2}\cdot 4\gamma^2 - \frac{1}{8}(4\gamma^2)^2\right) = \gamma^2 - \gamma^4$. So we've got:

$z^2 = \gamma^2 - \gamma^4$; then:

$$\frac{2m(E+V_0)a^2}{\hbar^2} = \frac{2mV_0a^2}{\hbar^2} - \frac{4m^2V_0^2a^4}{\hbar^4} \Rightarrow$$

$\Rightarrow \boxed{E = -\frac{2ma^2}{\hbar^2}V_0^2}$ this is the answer we were looking for.

As we see the level is near the edge of well $E \approx 0$. (pic5)



pic. 5

ⓑ Estimate the probability that the particle is outside the well for bound state.

In classical theory particle is bounded to be inside well. In quantum mechanics there exists nonzero probability that particle will be found outside the box. This probability is given by:

$$P = \left(\int_{-\infty}^{-a} + \int_{a}^{+\infty}\right)|\psi(x)|^2 = 2\int_a^{+\infty} dx\,|A|^2 e^{-2\varkappa x}$$

To find probability we should find "A". For this let's normalize w.f. we use. As we know from the begining bounded state is necessarily even so that

$\psi_I = Ae^{\varkappa x}$, $x<a$

$\psi_{II} = B\cos kx$, $-a<x<a$

$\psi_{III} = Ae^{-\varkappa x}$, $x>a$

Normalization condition is

$$1 = \int_{-\infty}^{+\infty} |\psi|^2 = 2\int_0^a dx\,|B|^2\cos^2 kx + 2\int_a^{\infty} dx\,|A|^2 e^{-2\varkappa x};$$ so that

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$$|B|^2\left(a+\frac{1}{2k}\sin 2ka\right)+\frac{|A|^2}{\varkappa}e^{-2\varkappa a}=1;$$

To find $|A|^2$ we will use relation coming from continuity condition at $x=a$ point:

$\psi_{II}(a)=\psi_{III}(a) \Rightarrow B\cos ka = Ae^{-\varkappa a}$ so that

$B=\dfrac{e^{-\varkappa a}}{\cos ka}A$; Substituting this into equation above we get:

$$|A|^2 e^{-2\varkappa a}\left(\frac{1}{\cos^2 ka}\left(a+\frac{1}{2k}\sin 2ka\right)+\frac{1}{\varkappa}\right)=1;$$

Now it will be usefull to remember equation defining position of even level:

$k\,tg\,ka=\varkappa$, so that $\dfrac{1}{\cos^2 ka}=1+tg^2 ka = 1+\dfrac{\varkappa^2}{k^2}$; and

$\dfrac{\sin 2ka}{2\cos^2 ka}=tg\,ka=\dfrac{\varkappa}{k}$; Then we get:

$$|A|^2 e^{-2\varkappa a}\left(a\frac{k_0^2}{k^2}+\frac{\varkappa}{k^2}+\frac{1}{\varkappa}\right)=1$$ where we have denoted

$k_0^2=k^2+\varkappa^2=\dfrac{2mV_0}{\hbar^2}$. Finally we get

$$|A|^2 e^{-2\varkappa a}=\left(a\frac{k_0^2}{k^2}+\frac{k_0^2}{\varkappa k^2}\right)^{-1}=\frac{k^2}{k_0^2}\frac{\varkappa}{1+a\varkappa};$$

Finally we can estimate probability:

$$P=2\int_a^{+\infty}dx\,|A|^2e^{-2\varkappa x}=\frac{1}{\varkappa}|A|^2e^{-2\varkappa a}=\frac{k^2}{k_0^2}\frac{1}{1+a\varkappa}$$, so we get

$$\boxed{P=\frac{k^2}{k_0^2}\frac{1}{1+a\varkappa};}$$ Note that this is general formula in which we don't do any approximations.

Now let's try to substitute our particular solution.

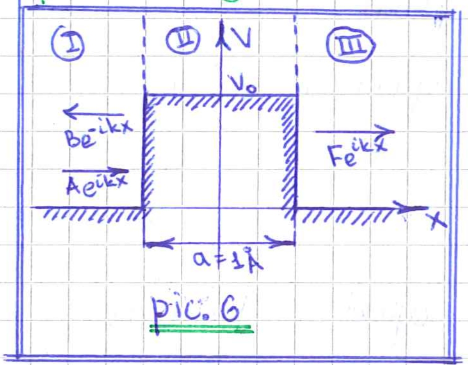
$k^2=\dfrac{2m(E+V_0)}{\hbar^2}=\dfrac{2m}{\hbar^2}V_0\left(1-\dfrac{2ma^2}{\hbar^2}V_0\right)=k_0^2-k_0^2(\varkappa a)$ as

$\varkappa=\dfrac{\sqrt{-2mE}}{\hbar}=\dfrac{2maV_0}{\hbar^2}$, so we get:

$P=\dfrac{1-\varkappa a}{1+\varkappa a}\approx 1-(\varkappa a)^2 \Rightarrow$ $\boxed{P\approx 1-\dfrac{4m^2a^4V_0^2}{\hbar^4}}$. As we see the result is contr intuitive - probability for particle to be outside the well is almost 1!

(8) Problem II (Tunneling with numbers)

An electron with 1eV of kinetic energy encounters a square barrier that is 2eV high and 1Å wide. Compute the probability for the electron to tunnel through barrier.



pic. 6

Short reminder of tunneling. To solve the problem we

* Devide space into 3 regions as shown on pic.6
* Write down general solution in each of this regions:

$$\psi_I = A e^{ikx} + B e^{-ikx}; \quad k = \frac{\sqrt{2mE}}{\hbar}; \quad \varkappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar};$$

$$\psi_{II} = C e^{\varkappa x} + D e^{-\varkappa x};$$

$$\psi_{III} = F e^{ikx};$$

* apply continuity conditions at $x = a_1, a_2$ (a_1 and a_2 being end points of the potential step)

$$\psi_I(a_1) = \psi_{II}(a_1); \quad \left.\frac{d\psi_I}{dx}\right|_{x=a_1} = \left.\frac{d\psi_{II}}{dx}\right|_{x=a_1}; \text{ and similar for } x = a_2;$$

* From set of continuity equations we are able to extract transmission coefficient

$$T = 1 - \frac{|B|^2}{|A|^2} = \frac{|F|^2}{|A|^2}$$

which gives the probability for the particle to go through the potential step. In particular we get:

$$\boxed{T = \frac{E(V_0 - E)}{E(V_0 - E) + V_0^2 \sinh^2 \varkappa L}; \quad T \approx \frac{4E(V_0 - E)}{V_0^2} e^{-2\varkappa L};}$$

and if $\varkappa L \gg 1$ we get: (see the second formula in the box)

* For potential V(x) of arbitrary form this tunneling coefficient can be modified into:

$$\boxed{T \sim \exp\left(-\frac{2}{\hbar} \int_{x_i}^{x_f} \sqrt{2m(V(x) - E)}\, dx\right)}$$

where $V(x_{i,f}) = E$, $x_{i,f}$ are called turning points.

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Let's estimate T for our problem.

$$\varkappa L = \frac{\sqrt{2m(V_0-E)}}{\hbar} L$$

$V_0 = 2\,eV$; $E = 1\,eV$; $L = 10^{-10}\,m$; $\hbar = 4{,}13\cdot10^{-15}\,eV\cdot s$;

$m_e \approx 0{,}5\cdot10^{6}\,eV/c^2$. Then we get

$$\varkappa L = \frac{\sqrt{10^6\cdot 1}\,eV\cdot10^{-10}\,m}{4{,}13\cdot10^{-15}\,eV\cdot s\cdot 3\cdot10^{8}\,\frac{m}{s}} = \frac{1}{12{,}4} = 0{,}08 \ll 1$$

So $\sinh^2\varkappa L \approx (\varkappa L)^2 \approx 6{,}4\cdot10^{-3}$ and

$$T = \frac{1}{1+\frac{V_0^2}{E(V_0-E)}\sinh^2\varkappa L} = \frac{1}{1+4\cdot\sinh^2\varkappa L} \approx 1 - 2{,}5\cdot10^{-2} \text{ so:}$$

$$\boxed{T = 1 - 2{,}5\cdot10^{-2};}$$

As we can, despite potential is larger then kinetic energy of electron twice, due to the parameters of the potential tunneling probability is almost 1

Problem IV The density of states

In statistical mechanics we are often interested in the "density of states". The density of states $\rho(E)$ is defined such that $\int_{E_1}^{E_2}\rho(E)\,dE$ is the number of quantum states with energies between E_1 and E_2.

a) Find $\rho(E)$ for a particle of mass m in a 1d box of size L. You should assume that the box is very wide so that the spacing in energy between the different energy levels is small so that you can approximate sums by integrals. Your answer should be in terms of $E, m, \hbar$ and L.

Let's consider integral $\int_{E_1}^{E_2}\rho(E)\,dE$ and write it down assuming that $E = E(n)$ and n is the number of levels: $\int_{E_1}^{E_2}\rho(E)\,dE = \sum_{E(n_1)}^{E(n_2)} \rho(E_n)\frac{dE}{dn}$ so we want:

10 $\sum_{n_1}^{n_2} \rho(E_n) \frac{dE_n}{dn} = n_2 - n_1 \Rightarrow \rho(E_n) \frac{dE_n}{dn} = 1$ and we

finally can define $\boxed{\rho(E_n) = \frac{dn}{dE}}$

In particular if we substitute our expression for energy levels: $E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}$ we get:

$$n = \sqrt{2mE_n}\,\frac{L}{\pi\hbar} \Rightarrow \boxed{\rho(E) = \frac{dn}{dE} = \sqrt{\frac{m}{2E}}\,\frac{L}{\pi\hbar}}$$ pic.7

pic. 7

b) What is the density of states per unit length?

Per unit length we get:

$$\boxed{\frac{1}{L}\rho(E) = \sqrt{\frac{m}{2E}}\,\frac{1}{\pi\hbar}}$$

As we see density of states decreases with levels which is reasonable since levels are growing as n^2 and become less and less frequent while increasing energy.

(1) Seminar 9 (Harmonic oscillator)

Theoretical reminder

* Usual Hamiltonian for harmonic oscillator is

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$;

* If we now introduce ladder operators

$\hat{a} = \frac{1}{\sqrt{2}}\left(\alpha\hat{x} + \frac{i}{\alpha\hbar}\hat{p}\right)$; $\hat{a}^{+} = \frac{1}{\sqrt{2}}\left(\alpha\hat{x} - \frac{i}{\alpha\hbar}\hat{p}\right)$; with

$\alpha = \sqrt{\frac{m\omega}{\hbar}}$ this standart Hamiltonian can be rewritten in the following form:

$H = \frac{1}{2}\hbar\omega(aa^{+} + a^{+}a)$

* from fundamental commutation relation $[\hat{x},\hat{p}] = i\hbar$ we can easily derive commutation relations for ladder operators: $\boxed{[a,a^{+}] = 1;\ [a,a] = [a^{+},a^{+}] = 0;}$

* Using this commutation relations we can rewrite Hamiltonian in the following form:

$\boxed{\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})}$ where $\boxed{\hat{N} = \hat{a}^{+}a}$ is number operator (we will see later why)

Useful relations for number operator

$[\hat{N}, \hat{a}^n] = -n\hat{a}^n$; $\Rightarrow$ $[\hat{H}, \hat{a}^n] = -n\hbar\omega\hat{a}^n$;

$[\hat{N}, (\hat{a}^{+})^n] = n(\hat{a}^{+})^n$; $\Rightarrow$ $[\hat{H}, (\hat{a}^{+})^n] = n\hbar\omega(\hat{a}^{+})^n$;

Proof Let's proove for one of the identities:

- we start with $n=1$. Then:

$$[\hat{N}, \hat{a}] = [\hat{a}^{+}\hat{a}, \hat{a}] = \hat{a}^{+}\underbrace{[\hat{a},\hat{a}]}_{0} + [\hat{a}^{+},\hat{a}]\hat{a} = -\hat{a}$$

- Now we can go for higher powers of $\hat{a}$ using as usually derivation property of commutator:

$[\hat{N}, \hat{a}^n] = [\hat{N},\hat{a}]\hat{a}^{n-1} + \hat{a}[\hat{N},\hat{a}]\hat{a}^{n-2} + \ldots + \hat{a}^{n-1}[\hat{N},\hat{a}] =$

$= -n\hat{a}^n$; q.e.d. For other commutators proof is similar.

(2) * Hamiltonian eigenspectrum

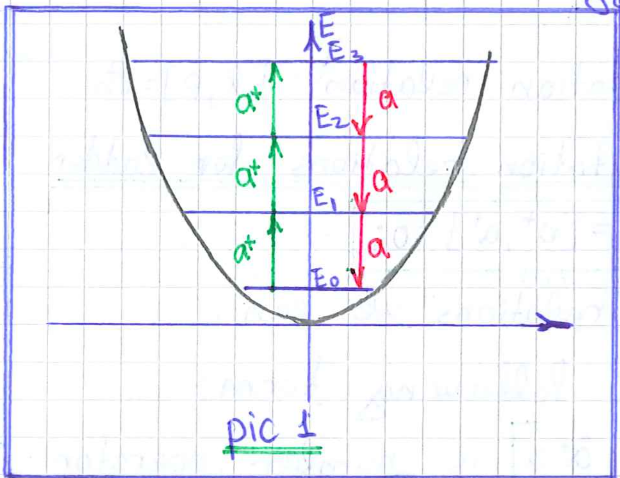
- Let's assume $|\psi\rangle$ is Hamiltonian eigenstate: $\hat{H}|\psi\rangle = E|\psi\rangle$, and consider states $a^+|\psi\rangle$ and $a|\psi\rangle$

This are eigenstates of $\hat{H}$ too:

$$\hat{H}\hat{a}^+|\psi\rangle = \underbrace{[\hat{H},\hat{a}^+]|\psi\rangle}_{\hbar\omega\, a^+|\psi\rangle} + \hat{a}^+\underbrace{\hat{H}|\psi\rangle}_{E|\psi\rangle} = (E+\hbar\omega)\hat{a}^+|\psi\rangle;$$

$$\hat{H}\hat{a}|\psi\rangle = \underbrace{[\hat{H},\hat{a}]|\psi\rangle}_{-\hbar\omega\,\hat{a}|\psi\rangle} + \underbrace{\hat{a}\hat{H}|\psi\rangle}_{E\hat{a}|\psi\rangle} = (E-\hbar\omega)\hat{a}|\psi\rangle;$$

So that $\hat{a}^+$ increase energy by $\hbar\omega$ ("raising" operator) and $\hat{a}$ decreases energy by $\hbar\omega$ ("lowering" operator) (see pic.1)



pic 1

As energy can't go to negative values (potential is $\frac{1}{2}m\omega^2x^2 > 0$) There thus should be lowest energy state (ground state) annihilated by $\hat{a}$: $\hat{a}|0\rangle = 0$

- Starting with $|0\rangle$ and acting with $\hat{a}^+$ we can build full tower of excited states: $\boxed{|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle}$ $\boxed{E_n = \hbar\omega(n+\frac{1}{2})}$

This states are orthonormal already: $\langle m|n\rangle = \delta_{mn}$;

* Finally one more useful formula is expression of $\hat{x}$ and $\hat{p}$ through ladder operators:

$$\boxed{\begin{aligned} &\hat{x} = \frac{1}{\sqrt{2}\alpha}(\hat{a}+\hat{a}^+); \qquad \alpha = \sqrt{\frac{m\omega}{\hbar}}; \\ &\hat{p} = -\frac{i\alpha\hbar}{\sqrt{2}}(\hat{a}-\hat{a}^+); \end{aligned}}$$

③ Problem I (Compendium 9)

Consider the 1d h.o. with Hamiltonian

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{a}\hat{a}^+ + \hat{a}^+\hat{a})$$

In terms of the creation and annihilation operators, the position operator is given by

$$\hat{x} = \frac{1}{\sqrt{2}\alpha}(\hat{a} + \hat{a}^+) \; ; \; \alpha^2 = \frac{m\omega}{\hbar} ;$$

Suppose at time $t=0$, the system is in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + a^+|0\rangle)$$

ⓐ Find the time-dependent wave function $|\psi(t)\rangle$;

Usually to find time dependent w.f. we:

- Expand $|\psi, t=0\rangle$ in series of $\hat{H}$ eigenstates:

$$|\psi, t=0\rangle = \sum_n c_n |\psi_n\rangle \; ; \; c_n = \langle\psi_n|\psi, t=0\rangle;$$

- Act with time evolution operator:

$$|\psi, t\rangle \equiv e^{-i\hat{H}t/\hbar}|\psi, t=0\rangle = \sum_n c_n e^{-i\hat{H}t/\hbar}|\psi_n\rangle = \sum_n c_n e^{-iE_n t/\hbar}|\psi_n\rangle$$

Here first step is already done for us, as w.f. is already expressed through eigenstates $|n\rangle$ of Hamiltonian.

$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and we can directly apply time evolution operator:

$$|\psi, t\rangle \equiv e^{-i\hat{H}t/\hbar}|\psi, t=0\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\hat{H}t/\hbar}|0\rangle + e^{-i\hat{H}t/\hbar}|1\rangle\right) =$$

$$= \frac{1}{\sqrt{2}}\left(e^{-i\hbar\omega t/2\hbar}|0\rangle + e^{-i3\hbar\omega t/2\hbar}|1\rangle\right) = \frac{1}{\sqrt{2}}e^{-i\omega t/2}(|0\rangle + e^{-i\omega t}|1\rangle)$$

so $\boxed{|\psi, t\rangle = \frac{1}{\sqrt{2}}e^{-i\omega t/2}(|0\rangle + e^{-i\omega t}|1\rangle);}$

ⓑ Find the expectation value for the energy of $|\psi, t\rangle$

There are 2 ways to find this expectation value:

* First way is streightforward:

$$\langle\psi, t|\hat{H}|\psi, t\rangle = \frac{\hbar\omega}{2}e^{i\omega t/2}(\langle 0| + e^{i\omega t}\langle 1|)(\hat{N} + \tfrac{1}{2})(|0\rangle + e^{-i\omega t}|1\rangle)e^{-i\omega t/2} =$$

4

$= \frac{\hbar\omega}{2} \left(\langle 0|\hat{N}+\frac{1}{2}|0\rangle + e^{i\omega t}\langle 1|\hat{N}+\frac{1}{2}|0\rangle + e^{-i\omega t}\langle 0|\hat{N}+\frac{1}{2}|1\rangle + \right.$

$\left. + \langle 1|\hat{N}+\frac{1}{2}|1\rangle \right)$. As $\hat{N}|n\rangle = n|n\rangle$ we get

$\langle m|\hat{N}|n\rangle = n\,\delta_{m,n}$. In particular:

$\langle 0|\hat{N}+\frac{1}{2}|0\rangle = \frac{1}{2}$; $\langle 1|\hat{N}+\frac{1}{2}|1\rangle = \frac{3}{2}$; $\langle 0|\hat{N}+\frac{1}{2}|1\rangle = (\langle 1|\hat{N}+\frac{1}{2}|0\rangle) = 0$;

So, we eventually get:

$\langle\psi(t)|\hat{H}|\psi(t)\rangle = \frac{\hbar\omega}{2}\left(\frac{1}{2}+\frac{3}{2}\right) = \hbar\omega$; $\boxed{\langle E\rangle = \hbar\omega}$

* Second way is even easier:

Remember Heisenberg equation describing time evolution of expectation values

$\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{O}]\rangle$. In particular for the energy we get: $\frac{d}{dt}\langle\hat{H}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{H}]\rangle = 0$ so $\langle\hat{H}\rangle$ is conserved in time.

Thus we can calculate $\langle E\rangle$ at $t=0$ which is much easier:

$\langle E\rangle = \frac{\hbar\omega}{2}(\langle 0| + \langle 1|)(\hat{N}+\frac{1}{2})(|0\rangle + |1\rangle) = \frac{\hbar\omega}{2}\left(\langle 0|\hat{N}+\frac{1}{2}|0\rangle + \right.$

$\left. + \langle 1|\hat{N}+\frac{1}{2}|1\rangle + \langle 0|\hat{N}+\frac{1}{2}|1\rangle + \langle 1|\hat{N}+\frac{1}{2}|0\rangle\right) = \frac{\hbar\omega}{2}\left(\frac{1}{2}+\frac{3}{2}\right) = \hbar\omega$;

$\boxed{\langle E\rangle = \hbar\omega;}$

c) Find $\langle x(t)\rangle$, the time dependent expectation value for the position x.

By definition:

$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{2}(\langle 0| + e^{i\omega t}\langle 1|)\left(\frac{1}{\alpha\sqrt{2}}(\hat{a}^+ + \hat{a})\right)(|0\rangle + e^{-i\omega t}|1\rangle) =$

$= \frac{1}{2\sqrt{2}\alpha}\left(\langle 0|\hat{a}^+ + \hat{a}|0\rangle + \langle 1|\hat{a}^+ + \hat{a}|1\rangle + e^{i\omega t}\langle 1|\hat{a}^+ + \hat{a}|0\rangle + \right.$

$\left. + e^{-i\omega t}\langle 0|\hat{a}^+ + \hat{a}|1\rangle\right) = \begin{bmatrix}\text{as } \hat{a}|0\rangle = 0 \\ \text{and } \langle 0|\hat{a}^+ = 0\end{bmatrix} = \frac{1}{2\sqrt{2}\alpha}\left(\langle 1|\hat{a}^+|1\rangle + \langle 1|\hat{a}|1\rangle + \right.$

$\left. + e^{i\omega t}\langle 0|0\rangle + e^{-i\omega t}\langle 0|0\rangle\right)$

as $\langle 0|\hat{a}^+|0\rangle = \langle 1|\hat{a}^+|1\rangle = \langle 1|\hat{a}|1\rangle = 0$

This always happen for expectation values of the form:

$\langle n|\hat{a}^+|m\rangle = 0$ if $n=m$ (or even more - if $n \neq m+1$)

⑤

So we finally get

$$\boxed{\langle x(t)\rangle = \frac{1}{\alpha\sqrt{2}}\cos\omega t = \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t}$$

ⓓ Show that $\langle x(t)\rangle$ is a solution to the classical equations of motion of the harmonic oscillator with potential $V(x) = \frac{1}{2}m\omega^2 x^2$;

Classical equations of motion are just given by Newtons law: $F = m\ddot{x} = -\frac{dV}{dx} = -m\omega^2 x$, so $\ddot{x} = -\omega^2 x$. Let's now substitute $\langle x(t)\rangle$ instead of x into this equation:

$$\frac{d^2}{dt^2}\langle x(t)\rangle = -\omega^2\langle x(t)\rangle; \quad \frac{d^2}{dt^2}\langle x(t)\rangle = -\omega^2\frac{1}{\alpha\sqrt{2}}\cos\omega t = -\omega^2\langle x(t)\rangle;$$

So we see that indeed $\langle x(t)\rangle$ satisfies classical equations of motion as it should be due to Ehrenfest correspondence principle.

Problem II (Compendium 10)

Consider the Hamiltonian: $H = \frac{\hbar\omega}{2}(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+)$;

where $\hat{a}^+$ and $\hat{a}$ are the h.o. creation and annihilation operators which satisfy the relation

$$[\hat{a}, \hat{a}^+] = 1.$$

Operators $\hat{x}$ and $\hat{p}$ are given by

$$\hat{x} = \frac{1}{\alpha\sqrt{2}}(\hat{a} + \hat{a}^+); \quad \hat{p} = -i\frac{\alpha\hbar}{\sqrt{2}}(\hat{a} - \hat{a}^+); \quad \alpha = \sqrt{\frac{m\omega}{\hbar}};$$

ⓐ Find the expectation values $\langle x\rangle$ and $\langle p\rangle$ for ground and the first excited states.

Let's solve this problem more generally - for any state $|n\rangle$

$$\langle n|\hat{x}|n\rangle = \frac{1}{\sqrt{2}\alpha}\langle n|\hat{a} + \hat{a}^+|n\rangle = 0$$ Because as we have noticed $\langle n|(\hat{a}^+)^i(\hat{a})^j|n\rangle = 0$ if $i \neq j$.

⑥ This can be understood without calculation:
if $i \neq j$ we act with raising operator more times then lowering (if $i>j$) or vice versa (if $i<j$) and end up with state $|m\rangle \neq |n\rangle$ (up to coefficient that we don't care about). Due to orthogonality of states we get: $\langle n|(\hat{a}^+)^i(\hat{a})^j|n\rangle = \langle n|m\rangle = 0$ as $|m\rangle \neq |n\rangle$.

So $\boxed{\langle n|\hat{x}|n\rangle = 0 \text{ for any } n}$

In the same way for $\hat{p}$:

$$\langle n|\hat{p}|n\rangle = i\frac{\alpha\hbar}{\sqrt{2}}\langle n|\hat{a}^+ - \hat{a}|n\rangle = 0\text{, i.e.}$$

$$\boxed{\langle n|\hat{p}|n\rangle = 0 \text{ for any } n;}$$

ⓑ Find the expectation values $\langle\hat{x}^2\rangle$ and $\langle\hat{p}^2\rangle$ for the ground state and first excited state.

* First let's write down $\hat{x}^2$ and $\hat{p}^2$ operators:

$$\hat{x}^2 = \frac{1}{2\alpha^2}(\hat{a}+\hat{a}^+)(\hat{a}+\hat{a}^+) = \frac{1}{2\alpha^2}(\hat{a}^2+(\hat{a}^+)^2+\hat{a}^+\hat{a}+\hat{a}\hat{a}^+);$$

$$\hat{p}^2 = -\frac{\alpha^2\hbar^2}{2}(\hat{a}-\hat{a}^+)(\hat{a}-\hat{a}^+) = -\frac{\alpha^2\hbar^2}{2}(\hat{a}^2+(\hat{a}^+)^2-\hat{a}\hat{a}^+-\hat{a}^+\hat{a});$$

* Now let's go for expectation values for general state $|n\rangle$;

$$\langle n|\hat{x}^2|n\rangle = \frac{1}{2\alpha^2}(\langle n|\hat{a}^2|n\rangle + \langle n|(\hat{a}^+)^2|n\rangle + \langle n|\hat{a}^+a+\hat{a}\hat{a}^+|n\rangle)$$

As we have mentioned above $\langle n|\hat{a}^2|n\rangle = \langle n|(\hat{a}^+)^2|n\rangle = 0$;

and $\langle n|\underbrace{\hat{a}^+\hat{a}+\hat{a}\hat{a}^+}_{2\hat{a}^+\hat{a}+1}|n\rangle = \langle n|2\hat{N}+1|n\rangle = 2n+1$.

So $\langle n|\hat{x}^2|n\rangle = \frac{1}{2\alpha^2}(2n+1)$ in particular:

$$\boxed{\langle 0|\hat{x}^2|0\rangle = \frac{1}{2\alpha^2};\quad \langle 1|\hat{x}^2|1\rangle = \frac{3}{2\alpha^2};}$$

In the same way we do for $\hat{p}^2$ expectation value:

$$\langle n|\hat{p}^2|n\rangle = -\frac{\alpha^2\hbar^2}{2}(\langle n|\hat{a}^2|n\rangle + \langle n|(\hat{a}^+)^2|n\rangle - \langle n|\hat{a}^+\hat{a}+\hat{a}\hat{a}^+|n\rangle) =$$

$$= \frac{\alpha^2\hbar^2}{2}(2n+1)$$

⑦ In particular:

$$\boxed{\langle 0|\hat{p}^2|0\rangle = \frac{\alpha^2\hbar^2}{2}\ ;\ \langle 1|\hat{p}^2|1\rangle = \frac{3\alpha^2\hbar^2}{2}\ ;}$$

ⓒ Show that your results from ⓐ and ⓑ are consistent with Heisenberg uncertainty.

Let's find uncertainties for $\hat{p}$ and $\hat{x}$ in $|n\rangle$ state.

$$\sigma_p = \sqrt{\langle n|\hat{p}^2|n\rangle - \langle n|\hat{p}|n\rangle^2} = \frac{\alpha\hbar}{\sqrt{2}}\sqrt{2n+1}$$

$$\sigma_x = \sqrt{\langle n|\hat{x}^2|n\rangle - \langle n|\hat{x}|n\rangle^2} = \frac{1}{\sqrt{2}\alpha}\sqrt{2n+1}$$

so that: $\boxed{\sigma_x \cdot \sigma_p = \frac{\hbar}{2}(2n+1).}$

From here we see:

- Heisenberg identity is saturated for $n=0$ (ground state), i.e. $\sigma_x \cdot \sigma_p = \frac{\hbar}{2}$
- For all excited states $|n\rangle$ (including $|1\rangle$) $\sigma_x \sigma_p > \frac{\hbar}{2}$;

Problem III (Compendium 10 B)

Consider the 1d h.o. with the Hamiltonian

$$\hat{H} = \hbar\omega(\hat{a}^+\hat{a} + \tfrac{1}{2})$$

where $[\hat{a}, \hat{a}^+] = 1$, $\hat{a}|0\rangle = 0$

A "coherent" state $|A\rangle$ is defined by:

$$|A\rangle \equiv C \cdot \exp(A\hat{a}^+)|0\rangle,$$

where C is normalization factor and A is a real number.

Hints: $\exp(A\hat{a}^+) = \sum_{n=0}^{\infty} \frac{A^n(\hat{a}^+)^n}{n!}$; $[\hat{a}, (\hat{a}^+)^n] = n(\hat{a}^+)^{n-1}$;

ⓐ Find $|A\rangle$ in terms of the normalized energy eigenstates.

We should consider any function with operator being it's argument as series, for example:

$\exp(A\hat{a}^+) = \sum_{n=0}^{\infty} \frac{A^n(\hat{a}^+)^n}{n!}$ so that

$|A\rangle = C \sum_{n=0}^{\infty} \frac{A^n(\hat{a}^+)^n}{n!}|0\rangle$ as $|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$ we get:

⑧

$$\boxed{|A\rangle = C\sum_{n=0}^{\infty} \frac{A^n}{\sqrt{n!}}|n\rangle;}$$

ⓑ Find the normalization factor C. This will contain summ that should be expressed as exponent.

Normalisation condition is as usually:

$$1 \equiv \langle A|A\rangle = |C|^2 \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{A^{*m}}{\sqrt{m!}} \frac{A^n}{\sqrt{n!}} \underbrace{\langle m|n\rangle}_{\delta_{mn}} = |C|^2 \sum_n \frac{|A|^{2n}}{n!} = |C|^2 e^{|A|^2}, \text{ so}$$

that $\boxed{|C| = e^{-|A|^2/2};}$

ⓒ Show that $|A\rangle$ is an eigenstate of the annihilation operator $\hat{a}$ and find the eigenvalue.

Let's find $\hat{a}|A\rangle$:

$$\hat{a}|A\rangle = C\sum_{n=0}^{\infty} \frac{A^n}{n!} \hat{a}(\hat{a}^+)^n|0\rangle \quad \text{, now:}$$

$$\hat{a}(\hat{a}^+)^n|0\rangle = \left(\hat{a}(\hat{a}^+)^n - (\hat{a}^+)^n\hat{a} + (\hat{a}^+)^n\hat{a}\right)|0\rangle = \underbrace{[\hat{a},(\hat{a}^+)^n]}_{n(\hat{a}^+)^{n-1}}|0\rangle +$$

$$+ (\hat{a}^+)^n \underbrace{\hat{a}|0\rangle}_{0} = n(\hat{a}^+)^{n-1}|0\rangle$$

Note We have used here commutator $[\hat{a},(\hat{a}^+)^n] = n(\hat{a}^+)^{n-1}$

To prove this it's convinient to use derivation property of commutator:

$$[\hat{a},(\hat{a}^+)^n] = [\hat{a},(\hat{a}^+)](\hat{a}^+)^{n-1} + \hat{a}^+[\hat{a},(\hat{a}^+)](\hat{a}^+)^{n-2} + (\hat{a}^+)^2[\hat{a},\hat{a}^+](\hat{a}^+)^{n-3} + \dots$$

$$+ (\hat{a}^+)^{n-1}[\hat{a},\hat{a}^+] = n(\hat{a}^+)^{n-1}, \text{ q.e.d.}$$

So we can proceed:

$$\hat{a}|A\rangle = C\sum_{n=1}^{\infty} \frac{A^n}{n!} n(\hat{a}^+)^{n-1}|0\rangle = C\cdot A\sum_{n=0}^{\infty} \frac{(\hat{a}^+)^n}{n!}|0\rangle = A|A\rangle$$

here we first thrown away $n=0$ term in series, as it is automatically 0, and then used $\frac{n!}{n} = (n-1)!$ and shifted $n \to (n-1)$ in series. So indeed state $|A\rangle$ is eigenstate of $\hat{a}$ with "A" eigenvalue:

$$\boxed{\hat{a}|A\rangle = A|A\rangle;}$$

ⓓ Find expectation value for the energy $\langle A|H|A\rangle$

⑨ By defenition of h.o. Hamiltonian $\hat{H} = \hbar\omega(\hat{a}^+\hat{a} + \frac{1}{2})$

$\langle A|\hat{H}|A\rangle = \langle A|\hbar\omega(\hat{a}^+\hat{a}+\frac{1}{2})|A\rangle = \hbar\omega(\langle A|\hat{a}^+\hat{a}|A\rangle + \frac{1}{2}\underbrace{\langle A|A\rangle}_{1}) =$

$= \hbar\omega((\langle A|\hat{a}^+)(\hat{a}|A\rangle) + \frac{1}{2})$

Now usung result of ©:

$\hat{a}|A\rangle = A|A\rangle$; $\langle A|\hat{a}^+ = (\hat{a}|A\rangle)^+ = \langle A|A^+$

we get: $\langle A|a^+a|A\rangle = |A|^2\langle A|A\rangle = |A|^2$ and finally:

$$\boxed{\langle A|\hat{H}|A\rangle = \hbar\omega(|A|^2 + \frac{1}{2});}$$

Problem V Consider the "fermionic harmonic oscillator" with Hamiltonian $H = \frac{\hbar\omega}{2}(\hat{b}^+\hat{b} - \hat{b}\hat{b}^+)$ where $\hat{b}$ and $\hat{b}^+$ satisfy the "anticommutation relations"

$\{\hat{b}, \hat{b}^+\} \equiv \hat{b}\hat{b}^+ + \hat{b}^+\hat{b} = 1$; $\{\hat{b}, \hat{b}\} = \{\hat{b}^+, \hat{b}^+\} = 0$;

Find the normalised states and energies for the system, assuming that there is a ground state $|0\rangle$ where $\hat{b}|0\rangle = 0$;

* Let's start with our ground state $|0\rangle$ and act with creation operator on it:

$\hat{b}^+|0\rangle = |1\rangle$

From anticommutation relations it follows that

$\hat{b}^+\hat{b}^+ + \hat{b}^+\hat{b}^+ = 2\hat{b}^+\hat{b}^+ = 0$ so that $\hat{b}^+\hat{b}^+ = 0$.

Thus $\hat{b}^+|1\rangle = \hat{b}^+\hat{b}^+|0\rangle = 0$; while

$b|1\rangle = |0\rangle$

* Normalization

Assuming $\langle 0|$ is normalized for $|1\rangle$ we get:

$\langle 1|1\rangle = \langle 0|\hat{b}\hat{b}^+|0\rangle = \langle 0|1 - \hat{b}^+\hat{b}|0\rangle = \langle 0|0\rangle = 1$

So we see that $|1\rangle$ is normalized too.

So we has got following 2 states:

$$\boxed{\begin{array}{l} |0\rangle;\ |1\rangle = \hat{b}^+|0\rangle;\ \text{which satisfy:} \\ \hat{b}^+|1\rangle = 0;\quad \hat{b}|1\rangle = |0\rangle; \end{array}}$$

⑩

* Now let's define energies of this states.

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{b}^+\hat{b} - \hat{b}^+\hat{b}) = \hbar\omega(\hat{b}^+\hat{b} - \tfrac{1}{2})$$, here $\hat{b}^+\hat{b} = \hat{N}$ is "number operator" as usually.

$$\hat{H}|0\rangle = \frac{\hbar\omega}{2}(2\hat{b}^+\hat{b} - 1)|0\rangle = -\frac{\hbar\omega}{2}|0\rangle$$

$$\hat{H}|1\rangle = \frac{\hbar\omega}{2}(2\hat{b}^+\hat{b}\hat{b}^+ - \hat{b}^+)|0\rangle = \frac{\hbar\omega}{2}(-2\underbrace{\hat{b}^+\hat{b}^+\hat{b}}_{0} + 2\hat{b}^+ - \hat{b}^+)|0\rangle = \frac{\hbar\omega}{2}|1\rangle$$

So we get finally

$$\boxed{\begin{array}{llll} |0\rangle: & E_0 = -\frac{\hbar\omega}{2}; & \hat{b}|0\rangle = 0; & \hat{b}^+|0\rangle = |1\rangle; \\ |1\rangle: & E_1 = \frac{\hbar\omega}{2}; & \hat{b}|1\rangle = |0\rangle; & \hat{b}^+|1\rangle = 0; \end{array}}$$

* Note that the problem we have considered is an example of 2-dimensional Hilbert space

Let's consider $|0\rangle$ and $|1\rangle$ as basis:

$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$; $|1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$; then only nonzero element of $\hat{b}$ matrix is

$\langle 0|\hat{b}|1\rangle = \langle 0|0\rangle = 1$ thus $\hat{b} = \begin{bmatrix}0 & 1\\0 & 0\end{bmatrix} \Rightarrow \hat{b}^2 = \begin{bmatrix}0 & 0\\0 & 0\end{bmatrix} = 0$

Analogously only nonzero element of $\hat{b}^+$ is

$\langle 1|\hat{b}^+|0\rangle = 1$ so that $\hat{b}^+ = \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix} \Rightarrow (\hat{b}^+)^2 = \begin{bmatrix}0 & 0\\0 & 0\end{bmatrix} = 0;$

Then Hamiltonian in this basis is given by:

$$\hat{H} = \frac{\hbar\omega}{2}(2\hat{b}^+\hat{b} - 1) = \frac{\hbar\omega}{2}\left\{2\begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\cdot\begin{bmatrix}0 & 1\\0 & 0\end{bmatrix} - \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\right\} =$$

$$= \frac{\hbar\omega}{2}\left\{2\begin{bmatrix}0 & 0\\0 & 1\end{bmatrix} - \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\right\} = \frac{\hbar\omega}{2}\begin{bmatrix}-1 & 0\\0 & 1\end{bmatrix}; \quad \hat{H} = \frac{\hbar\omega}{2}\begin{bmatrix}-1 & 0\\0 & 1\end{bmatrix};$$

From here we can see that:

$$\hat{H}|0\rangle = \frac{\hbar\omega}{2}\begin{bmatrix}-1 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = -\frac{\hbar\omega}{2}\begin{bmatrix}1\\0\end{bmatrix} = -\frac{\hbar\omega}{2}|0\rangle;$$

$$\hat{H}|1\rangle = \frac{\hbar\omega}{2}\begin{bmatrix}-1 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \frac{\hbar\omega}{2}\begin{bmatrix}0\\1\end{bmatrix} = \frac{\hbar\omega}{2}|1\rangle;$$

So we have reproduced all previous results using matrix formalism.

(1) Seminar 10 (3D Schrödinger equation)

Theory: In 1 dimension Schrodinger equation reads:

$$E\psi(x) = -\frac{\hbar^2}{2\mu}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x); \quad \text{where}$$

$-\hbar^2\frac{\partial^2}{\partial x^2} = \left(-i\hbar\frac{\partial}{\partial x}\right)^2 = \hat{p}_x^2$ is square of momentum operator.

Generalization to 3 dimensions is quite streight forward:

$\hat{p}_x^2 \to \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$, where we, in analogy with x-direction, introduced operators corresponding to momentum in y and z-directions: $\hat{p}_y = -i\hbar\frac{\partial}{\partial y}$; $\hat{p}_z = -i\hbar\frac{\partial}{\partial z}$;

So that Schrödinger equation for stationary levels reads:

$$\boxed{E\psi(\bar{r}) = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(\bar{r}) + V(\bar{r})\psi(\bar{r});}$$

Depending on the geometry of your problem you should apply separation of variables either in Cartesian, Cylindrical, Spherical coordinates.

(I) Separation of variables in Cartesian coordinates (problems I and II)

If potential is of the form $V(x,y,z) = V_1(x) + V_2(y) + V_3(z)$, then we can look for ansatz $\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$;

Substituting this ansatz into Sch. eq. we get:

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 X}{\partial x^2}Y\cdot Z - \frac{\hbar^2}{2\mu}\frac{\partial^2 Y}{\partial y^2}X\cdot Z - \frac{\hbar^2}{2\mu}\frac{\partial^2 Z}{\partial z^2}YX + (V_1+V_2+V_3)X\cdot Y\cdot Z =$$

$= EXYZ$. Deviding this by $X\cdot Y\cdot Z$ and recombining terms we get:

$$\underbrace{\left(-\frac{\hbar^2}{2\mu}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + V_1(x)X(x)\right)}_{x\text{-dependent}} + \underbrace{\left(-\frac{\hbar^2}{2\mu}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + V_2(y)Y(y)\right)}_{y\text{-dependent}} +$$

$$+\underbrace{\left(-\frac{\hbar^2}{2\mu}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} + V_3(z)Z(z)\right)}_{z\text{-dependent}} = E$$

②

As 3 parts of equations depend on different variables each of them should be constant:

$$-\frac{\hbar^2}{2\mu}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + V_1(x) = E_1;$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + V_2(y) = E_2;$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} + V_3(z) = E_3; \quad E = E_1 + E_2 + E_3;$$

So we have reduced our 3d problem to 3 1d problems which are much easier to solve.

Problem I Consider 3d box whose sides have lengths L_1, L_2, and L_3.

ⓐ Find the energy levels and corresponding normalized w.f.

We will reduce this 3d problem to 1d problems in the following way.

• Just as in the case of infinite square well we assume that w.f. $\psi(\bar{r})$ is zero everywhere, where potential is infinite:

$$V(\bar{r}) = \begin{cases} 0, & 0<x<L_1;\ 0<y<L_2;\ 0<z<L_3; \\ \infty, & \text{otherwise} \end{cases}$$ so that

$\psi(\bar{r}) = 0$, if $0<x<L_1$, $0<y<L_2$, $0<z<L_3$; and even more, we get boundary condition:

$$\psi(L_1, y, z) = \psi(x, L_2, z) = \psi(x, y, L_3) = \psi(0, y, z) = \psi(x, 0, z) = \psi(x, y, 0) = 0;$$

Schrödinger equation inside box is:

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 X}{\partial x^2} Y\cdot Z - \frac{\hbar^2}{2\mu}\frac{\partial^2 Y}{\partial y^2} X\cdot Z - \frac{\hbar^2}{2\mu}\frac{\partial^2 Z}{\partial z^2} Y\cdot X = E\, XYZ \,\Big|\cdot \frac{1}{XYZ};$$

$$\underbrace{-\frac{\hbar^2}{2\mu}\frac{1}{X}\frac{\partial^2 X}{\partial x^2}}_{x\text{-depend.}} \underbrace{-\frac{\hbar^2}{2\mu}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}}_{y\text{-depend.}} \underbrace{-\frac{\hbar^2}{2\mu}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}}_{z\text{-depend.}} = E$$

here we have used ansatz $\psi(x,y,z) = X(x)Y(y) \times Z(z)$;

③ As 3 parts of summ depend on different variables all of them are just constant:

$$\text{equations}\begin{cases} -\frac{\hbar^2}{2\mu}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = E_1; & X(L_1)=X(0)=0; \\ -\frac{\hbar^2}{2\mu}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = E_2; & Y(L_2)=Y(0)=0; \\ -\frac{\hbar^2}{2\mu}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = E_3; & Z(L_3)=Z(0)=0; \end{cases}\text{boundary conditions}$$

So we see that we have reduced our "box" problem to 3 infinite square well problems for which we already know solutions.

* $X''(x) = -k_1^2 X(x)$, where $k_1 = \frac{\sqrt{2\mu E_1}}{\hbar}$

• general solution of this is:

$$X(x) = A\cos k_1 x + B\sin k_1 x$$

• Boundary conditions give

$$X(0)=0 \Rightarrow A=0;$$

$X(L_1)=0 \Rightarrow \sin(k_1 L_1)=0$, so that $k_1 L_1 = \pi n \Rightarrow k_1 = \frac{\pi n}{L_1}$ and

$$\boxed{E_1 = \frac{\hbar^2 k_1^2}{2\mu} = \frac{\hbar^2\pi^2 n^2}{2\mu L_1^2};}$$

• Normalization condition reads

$$\int_{-\infty}^{+\infty} dx\,|X(x)|^2 = |A|^2\int_0^{L_1} dx\,\sin^2 k_1 x = |A|^2\int_0^{L_1} dx\left(\frac{1}{2}-\frac{1}{2}\cos 2k_1 x\right) = \frac{|A|^2 L_1}{2};$$

so that $|A| = \sqrt{\frac{2}{L_1}}$ and final solution is:

$$\boxed{X(x) = \sqrt{\frac{2}{L_1}}\sin\left(\frac{\pi n_1 x}{L_1}\right);\ E_1 = \frac{\pi^2\hbar^2 n_1^2}{2\mu L_1^2};}$$

and in analogy we can get the same solutions for $Y(y)$ and $Z(z)$;

$$\boxed{\begin{array}{l} * \ Y(y) = \sqrt{\frac{2}{L_2}}\cdot\sin\left(\frac{\pi n_2 y}{L_2}\right);\ E_2 = \frac{\pi^2\hbar^2 n_2^2}{2\mu L_2^2}; \\ * \ Z(z) = \sqrt{\frac{2}{L_3}}\cdot\sin\left(\frac{\pi n_3 z}{L_3}\right);\ E_3 = \frac{\pi^2\hbar^2 n_3^2}{2\mu L_3^2}; \end{array}}$$

④ So final solution we get is:

$$\boxed{\psi(x,y,z) = \sqrt{\frac{8}{L_1 L_2 L_3}}\ \sin\left(\frac{\pi n_1 x}{L_1}\right)\sin\left(\frac{\pi n_2 y}{L_2}\right)\cdot\sin\left(\frac{\pi n_3 z}{L_3}\right);}$$

with energy equal to

$$\boxed{E = E_1 + E_2 + E_3 = \frac{\pi^2\hbar^2}{2\mu}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right);}$$

ⓑ Discuss the degeneracies of the energy levels if $L_1 = L_2 = L_3 = L$;

First of all let's remember what is the definition of degeneracy: We say that energy level is degenerated if it corresponds to 2 different states (2 w.f.'s)

For the case of $L_1 = L_2 = L_3 = L$ we get energy
$E = \frac{\pi^2\hbar^2}{2\mu L^2}(n_1^2 + n_2^2 + n_3^2)$; with the corresponding w.f.:

$$\psi(x,y,z) = \sqrt{\frac{8}{L^3}}\ \sin\left(\frac{\pi n_1 x}{L}\right)\sin\left(\frac{\pi n_2 y}{L}\right)\sin\left(\frac{\pi n_3 z}{L}\right);$$

That is we have different combinations of n_1, n_2, n_3 which give the same energy $E \sim (n_1^2 + n_2^2 + n_3^2)$; Let's consider particular examples of (n_1, n_2, n_3) combinations:

	n_1	n_2	n_3	$n_1^2+n_2^2+n_3^2$	
E_1:	1	1	1	3	→ degeneracy 1;
E_2:	1	1	2		
	1	2	1	6	→ degeneracy 3;
	2	1	1		
E_3:	1	2	2		
	2	2	1	9	→ degeneracy 3;
	2	1	2		
E_4:	1	1	3		
	1	3	1	11	→ degeneracy 3;
	3	1	1		

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E_5 : 2 2 2 12 $\rightarrow$ degeneracy 1;

E_6 :

$$\left\{\begin{matrix} 1 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 1 & 3 \\ 2 & 3 & 1 \\ 3 & 1 & 2 \\ 3 & 2 & 1 \end{matrix}\right\}$$

14 $\rightarrow$ degeneracy 6.

Problem II Consider the 3d harmonic oscillator with potential

$$V(x,y,z) = \frac{1}{2}\mu\omega_1^2 x^2 + \frac{1}{2}\mu\omega_2^2 y^2 + \frac{1}{2}\mu\omega_3^2 z^2;$$

(a) Find energy levels and eigenstates in terms of ladder operators.

- Let's use separation of variables in Cartesian coordinates:

$$-\frac{\hbar^2}{2\mu}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + V_1(x) = E_1; \qquad \psi(x,y,z) = X(x)Y(y)Z(z);$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + V_2(y) = E_2;$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} + V_3(z) = E_3; \qquad E = E_1 + E_2 + E_3;$$

in our case $V_1(x) = \frac{1}{2}\mu\omega_1^2 x^2$; $V_2(y) = \frac{1}{2}\mu\omega_2 y^2$; $V_3(z) = \frac{1}{2}\mu\omega_3 z^2$;

So we get 3 similar equations:

$$-\frac{\hbar^2}{2\mu}\frac{d^2X}{dx^2} + \frac{1}{2}\mu\omega_1^2 x^2 X = E_1 X;$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2Y}{dy^2} + \frac{1}{2}\mu\omega_2^2 y^2 Y = E_2 Y;$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2Z}{dz^2} + \frac{1}{2}\mu\omega_3^2 z^2 Z = E_3 Z;$$

so we have reduced 3d harmonic oscillator to 3 1d ones.

- We already know how to solve 1d h.o. using ladder operators.

For example, let's consider equation for $X(x)$:

$$-\frac{\hbar}{2\mu}\frac{d^2X}{dx^2} + \frac{1}{2}\mu\omega_1^2 x^2 X(x) = E_1 X$$

Hamiltonian corresponding to this stationary Schrödinger