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Session N 1

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theory for class (about 15 minutes)

Every thing in q.m. is described by the wave function $\Psi(x;t)$ which satisfies Schrödinger equation

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

Hamiltonian. if we now assume that

$\Psi(x;t) = e^{-i\omega t}\psi(x)$, substitution back gives us:

$\hbar\omega\, e^{-i\omega t}\psi(x) = e^{-i\omega t}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x)$; and thus we get time independent Schrödinger equation.

$\boxed{E\psi(x) = \hat{H}\psi(x)}$ i.e. $\psi(x)$ are eigenfunctions of Hamiltonian operator and E is corresponding eigenvalue. Wave function express probability distribution given by probability density $\boxed{\rho(x;t) = \Psi^*(x;t)\,\Psi(x;t)}$, thus

w.f. should be normalised in a proper way:

$\boxed{\int \Psi\Psi^* dx = 1;}$ Using this concept of probability we can finally define average of some operator $\hat{O}$

$\boxed{\langle\hat{O}\rangle = \int \Psi^*\,\hat{O}\,\Psi\, dx}$, where Ψ is already normalised.

Most of operator we deal with today are functons of $\hat{x}$ and $\hat{p}$ operator, which in x-representation, are written in the following form: $\boxed{\hat{x} = x;\ \hat{p} = -i\hbar\frac{\partial}{\partial x};}$ Now, using definition

of average and Schrodinger equation we are able to show that:

$$\frac{d}{dt}\langle\hat{O}\rangle = \frac{d}{dt}\int \Psi^*\,\hat{O}\,\Psi\, dx = \int\left\{\frac{\partial\Psi^*}{\partial t}\hat{O}\Psi + \Psi^*\hat{O}\frac{\partial\Psi}{\partial t}\right\}dx =$$

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

time evolution of averages is given by:

$\boxed{\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}\langle[\hat{H};\hat{O}]\rangle}$; here we have used hermiticity of H:

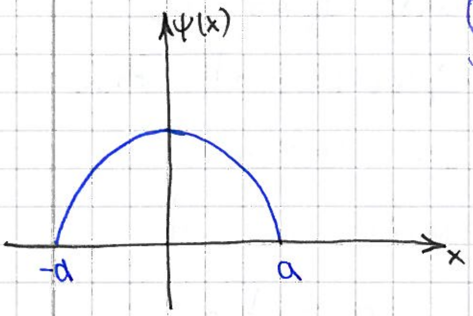
$\boxed{\int \Psi^*(\hat{H}\Psi)dx = \int(\hat{H}\Psi)^*\,\Psi\, dx;}$ - definition of hermiticity.

Problems

N1 Consider the wave function at $t=0$; $\Psi(x;0) = \psi(x)$ where

$$\psi(x) = \begin{cases} A(a^2-x^2) & ; |x|<a \\ 0 & ; |x|>a \end{cases}$$

ⓐ Find A in terms of a so that $\psi(x)$ is properly normalised



We should find such A that

$$\int \psi^*(x)\,\psi(x)\,dx = 1, \quad \text{or}$$

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

$$\int_{-a}^{a} (a^2-x^2)^2 dx = \int_{-a}^{a} (a^4 - 2a^2x^2 + x^4)dx =$$

$$= \left(a^4 x - \frac{2}{3}a^2x^3 + \frac{1}{5}x^5\right)\Big|_{-a}^{a} = 2a^5\left(1 - \frac{2}{3} + \frac{1}{5}\right) = \frac{16a^5}{15}, \text{ thus}$$

$\boxed{|A|^2 \cdot \frac{16a^5}{15} = 1}$ and $A = \sqrt{\frac{15}{16a^5}}$ – we have chosen A to be real.

ⓑ Find $\langle x \rangle$ and $\langle p \rangle$ in terms of a

$$\langle x \rangle \equiv A^2 \int dx\, \psi^* x\, \psi = A^2 \int_{-a}^{a} (a^2-x^2)\,x\,dx = 0$$

, because expression under integral is odd

$$\langle p \rangle \equiv A^2 \int dx\, (a^2-x^2)\, \hat{p}\, (a^2-x^2) = A^2 \int_{-a}^{a} dx\, (a^2-x^2)\left(-i\hbar\frac{\partial}{\partial x}\right)(a^2-x^2) =$$

$$= A^2 2i\hbar \int_{-a}^{a} dx\,(a^2-x^2)\,x = 0$$

Because of the same reason

$\langle x \rangle = 0$; $\langle p \rangle = 0$

ⓒ Find $\langle x^2 \rangle$ and $\langle p^2 \rangle$ in terms of a.

$$\langle x^2 \rangle \equiv \int dx\, x^2 \cdot |\psi(x)|^2 = A^2 \int_{-a}^{a} dx\, x^2 (a^2-x^2)^2 = A^2 \cdot 2 \int_{0}^{a} dx\,(a^4x^2 - 2a^2x^4 + x^6) =$$

$$= A^2 \cdot 2a^7 \left(\frac{1}{3} - \frac{2}{5} + \frac{1}{7}\right) = 2a^7 \cdot \frac{15}{16a^5} \cdot \frac{8}{15 \cdot 7} = \frac{a^2}{7}; \quad \langle x^2 \rangle = \frac{a^2}{7};$$

$$\langle p^2 \rangle \equiv \int dx\, \psi^*(x)\, \hat{p}^2\, \psi(x) = \int dx\, \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \psi(x) =$$

$$= -\hbar^2 A^2 \int_{-a}^{a} dx\,(a^2-x^2) \cdot \frac{\partial^2}{\partial x^2}(a^2-x^2) = +\hbar^2 A^2 \cdot 2 \int_{-a}^{a} dx\,(a^2-x^2) = 4a^3\hbar^2 A^2 \cdot \frac{2}{3}$$

$$\langle p^2\rangle = \frac{8}{3}a^3\hbar^2\cdot\frac{15}{16a^5} = \frac{5\hbar^2}{2a^2};$$

$$\boxed{\langle x^2\rangle = \frac{a^2}{7};\quad \langle p^2\rangle = \frac{5\hbar^2}{2a^2};}$$

d) Show that your results are consistent with Heisenberg uncertainty.

Heisenberg uncertainty is $(\Delta x)^2(\Delta p)^2 \geq \frac{\hbar^2}{4}$

where $(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$; $(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2$;

as in our case $\langle x\rangle = \langle p\rangle = 0$ we just get

$\langle x^2\rangle\langle p^2\rangle \geq \frac{\hbar^2}{4}$; $\frac{a^2}{7}\cdot\frac{5\hbar^2}{2a^2} \geq \frac{\hbar^2}{4} \Rightarrow \frac{5}{14}\hbar^2 \geq \frac{1}{4}\hbar^2$ – true

e) Suppose hamiltonian is

$H = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$, find $\langle E\rangle$;

$\langle E\rangle = \langle H\rangle = \frac{1}{2m}\langle p^2\rangle + \frac{1}{2}m\omega^2\langle x^2\rangle$. Now using result of part c) we get

$\langle E\rangle = \frac{1}{2m}\frac{5\hbar^2}{2a^2} + \frac{1}{2}m\omega^2\cdot\frac{a^2}{7}$; $\langle E\rangle = \boxed{\frac{5\hbar^2}{4ma^2} + \frac{m\omega^2a^2}{14};}$

f) What is $\langle E\rangle$ at a later time?

We can use formula from theoretical introduction.

$\frac{d}{dt}\langle E\rangle = \frac{i}{\hbar}\langle\underbrace{[\hat{H};\hat{H}]}_{0}\rangle = 0$, thus $\langle E\rangle$ is constant in time

4 N2

Compendium N1

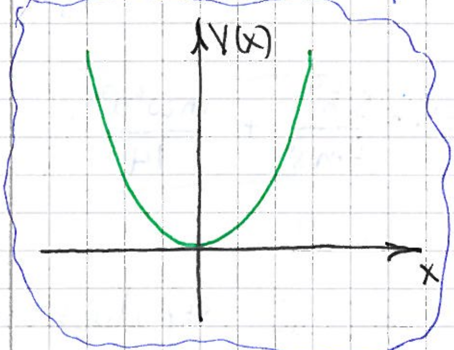
Consider a particle of mass m in a one dimensional potential $V(x) = \lambda x^4$ where λ is positive. Using the Heisenberg uncertainty relation ($\Delta x \Delta p \geqslant \frac{\hbar}{2}$), estimate the ground state energy of the particle as a function of $m, \hbar$, and λ;

Potential is simmetric under $x \to -x$, and usually in this case lowest energy state possess symmetric wave function i.e. $\psi(-x) = \psi(x)$, thus

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

$$= -\int_{-\infty}^{+\infty} \psi^*(x)\, x\, \psi(x)\, dx \Rightarrow \langle x \rangle = 0$$

, the same is valid for momentum operator $\langle p \rangle = 0$. Other way to



understand this is more physical. Obviously state with the lowest energ shouldn't "move" and should just oscillate ($\langle p \rangle = 0$) around $x = 0$ ($\langle x \rangle = 0$)

Average energy is given by $\langle E \rangle = \langle H \rangle = \frac{\langle p^2 \rangle}{2m} + \lambda \langle x^4 \rangle$

What should we do with $\langle x^4 \rangle$? let's write down

$$(\Delta x^2)^2 = \langle x^4 \rangle - \langle x^2 \rangle^2 \Rightarrow \langle x^4 \rangle = (\Delta x^2)^2 + \langle x^2 \rangle^2 \geqslant \langle x^2 \rangle^2$$, as $(\Delta x^2)^2 \geqslant 0$

$$\langle E \rangle \geqslant \frac{\langle p^2 \rangle}{2m} + \lambda \langle x^2 \rangle^2 = \frac{(\Delta p)^2}{2m} + \lambda (\Delta x)^4$$, using Heisenberg unc.

$$\langle E \rangle \geqslant \frac{\hbar^2}{8m(\Delta x)^2} + \lambda (\Delta x)^4$$. Now minimizing r.h.s with respect to $(\Delta x)^2$ we get: $\frac{\partial \langle E \rangle_{r.h.s}}{\partial (\Delta x)^2} = -\frac{\hbar^2}{8m(\Delta x)^4} + 2\lambda (\Delta x)^2 = 0$

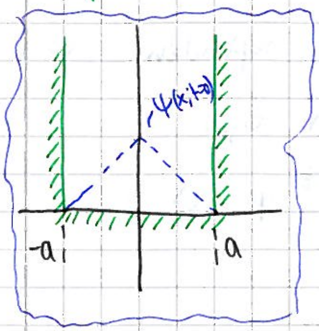
$$(\Delta x)^2 = \left(\frac{\hbar^2}{16 m \lambda}\right)^{\frac{1}{3}}$$

$$\langle E \rangle \geqslant \frac{\hbar^2}{8m}\left(\frac{16 m \lambda}{\hbar^2}\right)^{\frac{1}{3}} + \lambda \left(\frac{\hbar^2}{16 m \lambda}\right)^{\frac{2}{3}} = \left(\frac{\hbar^4 \lambda}{32 m^2}\right)^{\frac{1}{3}} + \left(\frac{\hbar^4 \lambda}{16 m^2}\right)^{\frac{1}{3}} =$$

$$= \left(\frac{\hbar^4 \lambda}{32 m^2}\right)^{\frac{1}{3}} \left(1 + \frac{1}{2}\right) \qquad \boxed{E_{min} = \frac{3}{2}\left(\frac{\hbar^4 \lambda}{32 m^2}\right)^{\frac{1}{3}}}$$

(5) (N3) Compendium N2

Consider a particle with mass m in 1^d infinite square well



$$V(x) = \begin{cases} \infty & ; |x|>a \\ 0 & ; |x|\leq a \end{cases}$$

At time $t=0$ w.f. for this particle is $\boxed{\psi(x) = A(a-|x|)}$

(a) find coefficient A that gives proper normalisation.

$$A^2\int_{-a}^{a} dx\, (a-|x|)^2 = 2A^2\int_0^a dx\,(a-x)^2 = 2A^2\left(a^2x - \frac{2}{2}ax^2 + \frac{1}{3}x^3\right)\Big|_0^a =$$

$$= 2A^2\cdot a^3\cdot\frac{1}{3} = 1 \Rightarrow \boxed{A = \sqrt{\frac{3}{2a^3}}}$$ - chosen to be real

(b) determine the time dependent w.f. $\Psi(x;t)$ (get infinite summ)

Let's first find eigenfunctions and values of Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ + boundary conditions $\psi(a) = \psi(-a) = 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) = E_n\psi_n(x)$$

$$\psi_n(x) = A_n\cos\left(\frac{\sqrt{2mE_n}}{\hbar}x\right) + B_n\sin\left(\frac{\sqrt{2mE_n}}{\hbar}x\right)$$ We take $B_n=0$ and

when $|x|\leq a$, when $|x|>a$ we get 0

out of boundary condition we get

$$\frac{\sqrt{2mE_n}\,a}{\hbar} = \frac{\pi}{2}(2n+1) \quad n\in\mathbb{Z}$$ - and from normalisation condition:

$$A_n^2\cdot\frac{2a}{2} = 1 \Rightarrow A_n = \frac{1}{\sqrt{a}}$$

$$\boxed{\begin{aligned}\psi_n(x) &= \frac{1}{\sqrt{a}}\cos\left[\frac{\pi x}{a}\left(n+\frac{1}{2}\right)\right]; \quad |x|\leq a \\ E_n &= \frac{1}{2m}\left(\frac{\pi\hbar}{2a}\right)^2(2n+1)^2;\end{aligned}}$$

Now we are able to expand any wave function over this basis $\psi(x) = \sum_{n=0}^{\infty} c_n\cdot\psi_n(x)$, where coefficients c_n are given by $\boxed{c_n = \int dx\, \psi_n^*(x)\psi(x)}$ in our case

$$c_n = \int_{-a}^{+a} dx\, \frac{1}{\sqrt{a}}\cos\left[\frac{\pi x}{a}\left(n+\frac{1}{2}\right)\right]\cdot\sqrt{\frac{3}{2a^3}}\,(a-|x|) =$$

$$= \frac{1}{a^2}\sqrt{\frac{3}{2}}\cdot 2\int_0^a dx\,\cos\left[\frac{\pi x}{a}\left(n+\frac{1}{2}\right)\right](a-x) = \frac{\sqrt{6}}{a^2}\left\{a\cdot\frac{a}{\pi(n+\frac{1}{2})}\sin\left(\frac{\pi x}{a}\left(n+\frac{1}{2}\right)\right)\Big|_0^a - \right.$$

⑥ $$-\frac{ax}{\pi(n+\frac{1}{2})}\sin\left[\pi(n+\tfrac{1}{2})\frac{x}{a}\right]\Big|_0^a + \frac{a}{\pi(n+\frac{1}{2})}\int_0^a dx\,\sin\left[\pi(n+\tfrac{1}{2})\frac{x}{a}\right]\Big\} =$$

$$= \sqrt{6}\left\{\frac{(-1)^n}{\pi(n+\frac{1}{2})} - \frac{(-1)^n}{\pi(n+\frac{1}{2})} + \frac{1}{\pi^2(n+\frac{1}{2})^2}\cos\left[\pi(n+\tfrac{1}{2})\frac{x}{a}\right]\Big|_0^a\right\} =$$

$$= \frac{\sqrt{6}}{\pi^2(n+\frac{1}{2})^2}; \quad \boxed{C_n = \frac{\sqrt{6}}{\pi^2(n+\frac{1}{2})^2};}$$ time-dependent w.f. is given by:

$$\Psi(x;t) = e^{-\frac{i}{\hbar}\hat{H}t}\cdot\Psi(x;t=0) = \sum_n C_n\cdot e^{-\frac{i}{\hbar}\hat{H}t}\varphi_n(x) =$$

$$= \sum_n C_n e^{-\frac{i}{\hbar}E_n t}\varphi_n(x)$$ or, in our case

$$\boxed{\Psi(x;t) = \sum_n \frac{\sqrt{6}}{\pi^2(n+\frac{1}{2})^2}\exp\left(-\frac{i}{2m\hbar}\left[\frac{\pi\hbar}{a}(n+\tfrac{1}{2})\right]^2 t\right)\frac{1}{\sqrt{a}}\cos\left((n+\tfrac{1}{2})\frac{\pi x}{a}\right)}$$

ⓒ What is the w.f. after a time $t = \frac{2ma^2}{\pi\hbar}$ has elapsed?

Let's write down exponents in a little bit more explicit way $$\exp\left(-\frac{i}{2m\hbar}\left[\frac{\pi\hbar}{a}(n+\tfrac{1}{2})\right]^2\cdot\frac{2ma^2}{\pi\hbar}\right) = \exp\left(-i\pi(n+\tfrac{1}{2})^2\right) =$$

$$= e^{-\frac{i\pi}{4}(2n+1)^2} = e^{-i\frac{\pi}{4}}$$ thus $$\Psi(x;t) = \sum_n C_n\varphi_n(x)\,e^{-\frac{i\pi}{4}} =$$

$$= e^{-i\frac{\pi}{4}}\Psi(x;t=0)$$

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

ⓓ Does this state have definite parity?

$\Psi(-x;t) = \Psi(x;t)$ so this w.f. has definite parity equals to $+1$;

(N4) Compendium N8

Consider particle of mass m in 1D harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2x^2$

ⓐ Show that $\psi(x) = Cx\cdot\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$ is a solution of the time independent Schrödinger equation. C is constant

Let's find $$\hat{H}\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi(x) =$$

⑦

$$= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right) C\cdot x\cdot \exp\left(-\frac{m\omega^2x^2}{2\hbar}\right) =$$

$$= C\cdot\left(-\frac{\hbar^2}{2m}\frac{d}{dx}\left\{1-\frac{m\omega^2x^2}{\hbar}\right\}\exp\left(-\frac{m\omega^2x^2}{2\hbar}\right) + \frac{1}{2}m\omega^2x^2\exp\left(-\frac{m\omega^2x^2}{2\hbar}\right)\right) =$$

$$= C\cdot\left(-\frac{\hbar^2}{2m}\left(1-\frac{m\omega^2x^2}{\hbar}\right)\left(-\frac{m\omega^2x}{\hbar}\right) + \frac{\hbar^2}{2m}\cdot\frac{2m\omega^2x}{\hbar} +\right.$$

$$\left. + \frac{1}{2}m\omega^2x^2\right)\exp\left(-\frac{m\omega^2x^2}{2\hbar}\right) = C\cdot\frac{3}{2}\hbar\omega\cdot x\exp\left(-\frac{m\omega^2x^2}{2\hbar}\right)$$

thus we get $\boxed{\hat{H}\psi(x) = \frac{3}{2}\hbar\omega\,\psi(x);}$

ⓑ Determine C such that the w.f. is properly normalized

$$\int|\psi(x)|^2dx = |C|^2\int_{-\infty}^{+\infty}x^2\exp\left(-\frac{m\omega x^2}{\hbar}\right)dx = 2|C|^2\int_0^{\infty}x^2e^{-ax^2}dx =$$

$$= 2|C|^2\cdot\frac{1}{4a}\sqrt{\frac{\pi}{a}} \Rightarrow \quad C=\left(\frac{4a^3}{\pi}\right)^{\frac{1}{4}}; \quad \boxed{C=\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{\frac{1}{4}}};$$

ⓒ Find the expectation value for x^2

$$\langle x^2\rangle = \int\psi^*(x)\cdot x^2\cdot\psi(x) = |C|^2\cdot\int_{-\infty}^{+\infty}x^4e^{-ax^2}dx = 2|C|^2\int_0^{\infty}x^4e^{-ax^2}dx =$$

$$= -2|C|^2\frac{d}{da}\int_0^{\infty}x^2e^{-ax^2}dx = 2|C|^2\cdot\frac{1}{4}\cdot\frac{3}{2}\frac{1}{a^2}\sqrt{\frac{\pi}{a}}$$

$$\langle x^2\rangle = 2\cdot 2a\cdot\sqrt{\frac{a}{\pi}}\cdot\frac{1}{2a^2}\sqrt{\frac{\pi}{a}}\cdot\frac{3}{4} = \frac{3}{2a}; \quad \boxed{\langle x^2\rangle = \frac{3\hbar}{2m\omega}};$$

ⓓ What is the inner product of $\psi(x)$ and $\psi_1(x) = Ax^2\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$?

We should calculate $\langle\psi_1(x),\psi(x)\rangle = \int dx\,\psi_1^*(x)\,\psi(x) =$

$= \int_{-\infty}^{+\infty}dx\,A\cdot C\cdot x^3\exp\left(-\frac{m\omega x^2}{\hbar}\right) = 0$ because of function under integral being odd. Another way to say it $\psi_1(x)$ is parity even $\psi(x)$ is odd thus they should be orthogonal.

⑧ N5

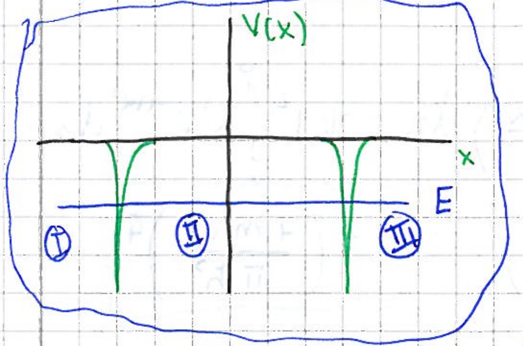
Compendium N5

Consider 1^d double δ-function potential

$V(x) = -\rho\,\delta(x+a) - \rho\,\delta(x-a)$, $\rho > 0$ the effect of δ-functions is to introduce a discontinuity in the derivatives of the wave function.

$$\lim_{\varepsilon\to 0}\left(-\frac{\hbar^2}{2m}\frac{d}{dx}\psi(x)\right)\Big|_{-a-\varepsilon}^{-a+\varepsilon} = \rho\,\psi(-a);\quad \lim_{\varepsilon\to 0}\left(-\frac{\hbar^2}{2m}\frac{d}{dx}\psi(x)\right)\Big|_{a-\varepsilon}^{a+\varepsilon} = \rho\,\psi(a)$$

ⓐ Find an equation for the energies of the bound state w.f. that are even under parity $(x \to -x)$



Let the energy of state be E $(E<0)$ Then S. equation is

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

+ boundary conditions for derivatives.

General solution looks like

$$\psi(x) = A e^{-\varkappa x} + B e^{\varkappa x}$$

where $\varkappa = \frac{\sqrt{-2mE}}{\hbar}$ If we write such solution for each region we get:

$$\begin{cases} \psi_I(x) = A_I e^{-\varkappa x} + B_I e^{\varkappa x} \\ \psi_{II}(x) = A_{II} e^{-\varkappa x} + B_{II} e^{\varkappa x} \\ \psi_{III}(x) = A_{III} e^{-\varkappa x} + B_{III} e^{\varkappa x} \end{cases}$$

We want $\psi(x) \xrightarrow[x\to\pm\infty]{} 0$ thus $A_I = B_{III} = 0$, and we get

$$\begin{cases} \psi_I(x) = A e^{\varkappa x} \\ \psi_{II}(x) = B(e^{\varkappa x} + e^{-\varkappa x}) \\ \psi_{III}(x) = A e^{-\varkappa x} \end{cases}$$

here we have taken only even parity w.f. as asked in problem (thus it should be $\psi(x) = \psi(-x)$)

Finally we should take boundary condition

$$\left\{\frac{d}{dx}\psi_{II}(x) - \frac{d}{dx}\psi_I(x)\right\}\Big|_{x=a} = \varkappa\cdot\left(Ae^{-a\varkappa} + B(e^{-a\varkappa} - e^{a\varkappa})\right) = \rho\, A e^{-a\varkappa}(a)\frac{2m}{\hbar^2}$$

(+) condition of continuity $\quad Ae^{-a\varkappa} = B(e^{-a\varkappa} + e^{a\varkappa})$

~~thus~~ $\cancel{A = B(1+e^{2a\varkappa})}$ $\quad \cancel{\varkappa B(1+e^{2a\varkappa}) \ldots = \varkappa B(e^{a}+e^{a})}$

~~this leads to equation~~ $\cancel{\varkappa =}$

(9) thus we get 2 equations

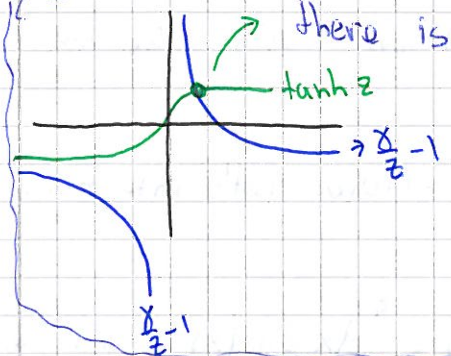
$A = 2B \cdot ch\, a\varkappa \cdot e^{a\varkappa}$ and

$\varkappa B\,(ch\, a\varkappa + sh\, a\varkappa) = B\gamma\, ch\, a\varkappa$ where $\gamma = \frac{2m\alpha}{\hbar^2}$

and we get equation:

$\boxed{\tanh z = \frac{\gamma}{z} - 1}$, where $z = a\varkappa$

show graphical solution how many solutions are there?



there is only 1 solution

(B) the same problem for odd solutions.

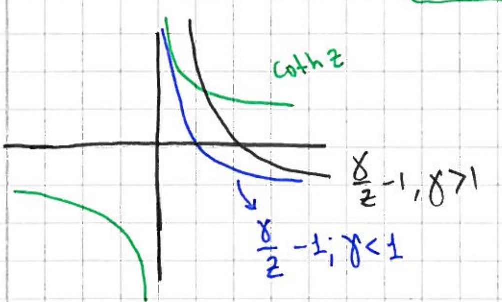
$$\begin{cases} \psi_I(x) = -A e^{\varkappa x} \\ \psi_{II}(x) = B\,(e^{\varkappa x} - e^{-\varkappa x}) \\ \psi_{III}(x) = A e^{-\varkappa x} \end{cases}$$

continuity and bound. conditions in $x = a$:

$A e^{-z} = 2B \cdot \sinh z$

$2B\, ch\, z + A e^{-z} = \frac{\gamma}{z} 2B \sinh z$

and we find $\boxed{\coth z = \frac{\gamma}{z} - 1;}$



How should we understand the fact that solutions exist only when $\gamma > 1$

$z \coth z = \gamma - z$, if we look on l.h.s and find it derivative we get

$(z \coth z)' = \coth z - \frac{z}{sh^2 z} = \frac{ch 2z - z}{sh^2 z} > 0$ alwas mean while

$(\gamma - z)' = -1 < 0$ always, thus if we want to obtain intersection point we should assume that

$\gamma > \lim\limits_{z \to 0} z \coth z = 1 \Rightarrow \gamma > 1$

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Some theoretical material on δ-functions (if it will be enough time)

The δ-function has following properties

$\delta(x)=0 \quad x\neq 0$

$\delta(x)=\infty \quad x=0$

$\int_a^b \delta(x)\,dx = \begin{cases} 1 & a<0,\ b>0 \\ 0 & \text{otherwise} \end{cases}$

and actually it is functional, not function:

$\int_a^b f(x)\,\delta(x)\,dx = f(0);$

where the condition for derivatives comes from?

Let's consider Schrödinger equation with only one δ-potential: $V=-g\delta(x)$;

$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - g\delta(x)\right)\psi(x) = E\psi(x)$. Now let's integrate this in thin shell $(-\varepsilon;\varepsilon)$:

$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon} dx\,\frac{d^2}{dx^2}\psi(x) - g\int_{-\varepsilon}^{\varepsilon}\delta(x)\,\psi(x)\,dx = \int_{-\varepsilon}^{\varepsilon} dx\,E\psi(x)$ and we then get:

$-\frac{\hbar^2}{2m}\psi'(x)\Big|_{-\varepsilon}^{\varepsilon} - g\psi(0) = E\,\psi(x)\Big|_{-\varepsilon}^{\varepsilon}$. r.h.s. is 0 due to continuity of w.f. and we get that w.f. derivatives appear to be discontinious

$$\boxed{-\frac{\hbar^2}{2m}\left(\psi'(\varepsilon)-\psi'(-\varepsilon)\right) = -g\psi(0);}$$

1

Session 2

Theory for class (about 15 min)

Previously we have worked with w.f. as some functions defined in space. Now we will introduce something more general then just w.f. We have already considered inner product during previous class.

$\langle\psi_1|\psi_2\rangle = \int \psi_1^* \psi_2 \, dx$; $\langle\psi_1|\psi_2\rangle^* = \langle\psi_2|\psi_1\rangle$. The inner product is bilinear, i.e.

$\langle\psi_1|a_2\psi_2 + a_3\psi_3\rangle = a_2\langle\psi_1|\psi_2\rangle + a_3\langle\psi_1|\psi_3\rangle$;

$\langle a_1\psi_1 + a_2\psi_2|\psi_3\rangle = a_1^*\langle\psi_1|\psi_3\rangle + a_2^*\langle\psi_2|\psi_3\rangle$; and inner product satisfy Schwarz inequality: $\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_1\rangle \leq \langle\psi_1|\psi_1\rangle\langle\psi_2|\psi_2\rangle$

All this let us consider quantum states as vectors defined in some abstract vector space

$\bar{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$ - vector; $\bar{u}^+ = (u_1^*, u_2^*, \dots, u_N^*)$ - dual vector; Inner product:

$\langle u|v\rangle \equiv u_1^* v_1 + u_2^* v_2 + \dots + u_N^* v_N$; Vector space where we define our states is called Hilbert space. and other usual notations $|v\rangle$ - ket $\langle u|$ - bra. We can also define linear operators in this Hilbert space

$O|\psi\rangle = |\chi\rangle$ it's linear i.e $O(|\psi_1\rangle + |\psi_2\rangle) = O|\psi_1\rangle + O|\psi_2\rangle$

For particle number of states, which is equal to dimension of Hilbert space, is infinite, but we can consider systems with finite number of states. The analog of operator $\hat{O}$ in finite dimensional Hilbert space is just matrix acting on column, which describe quantum states.

$$M|v\rangle \equiv \begin{pmatrix} M_{11} & M_{12} & \dots & M_{1N} \\ \vdots & & & \\ M_{N1} & M_{N2} & \dots & M_{NN} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} \equiv \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix} = |u\rangle;$$

Some words about probability and measurement

If we measure some value described by operator $\hat{A}$ w.f. collapse into one of the ~~basi~~ eigenfunction of $\hat{A}$ operator

② with probability $P_n = |\langle\psi_n|\psi\rangle|^2$; (i.e. we measure some concrete value of P;

Problems N1 (compendium N6)

$$|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}; \quad |2\rangle = \begin{pmatrix}0\\1\end{pmatrix}; \quad H = \alpha\begin{pmatrix}3 & -4i\\ 4i & -3\end{pmatrix}; \quad U = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$\alpha > 0$.

ⓐ Find eigenvalues of H.

How we usually do it?

$H\bar{h}_i = \lambda_i \bar{h}_i$ where $\bar{h}_i$ - eigenvector, λ_i - eigenvalue

$(H - \lambda I)\bar{h}_i = 0 \Rightarrow \det(H - \lambda I) = 0$ - equation which determin eigenvalues and then we solve equation $(H - \lambda I)\bar{h}_i = 0$ and determin eigenvectors.

$$\begin{Vmatrix} 3\alpha - \lambda & -4i\alpha \\ 4i\alpha & -3\alpha - \lambda \end{Vmatrix} = \lambda^2 - 9\alpha^2 - 16\alpha^2 = \lambda^2 - 25\alpha^2; \quad \boxed{\lambda = \pm 5\alpha}$$

now eigenvectors $\begin{bmatrix}a_i\\b_i\end{bmatrix}$ first $\lambda = 5\alpha$

$$\begin{bmatrix} -2\alpha & -4i\alpha \\ 4i\alpha & -8\alpha \end{bmatrix}\begin{bmatrix}a_1\\b_1\end{bmatrix} = 0 \qquad a_1 = -2ib_1 + \text{normalization condition } |a_1|^2 + |b_1|^2 = 0$$

finally we get

$h_+ = \begin{pmatrix}-2i\\1\end{pmatrix}\frac{1}{\sqrt{5}}$ or $|h_+\rangle = \frac{1}{\sqrt{5}}|2\rangle - \frac{2i}{\sqrt{5}}|1\rangle$ in ket notation

Now for $\lambda = -5\alpha$;

$$\begin{bmatrix} 8\alpha & -4i\alpha \\ 4i\alpha & 2\alpha \end{bmatrix}\begin{bmatrix}a_2\\b_2\end{bmatrix} = 0 \qquad b_2 = -2ia_2 + \text{same normalisation}$$

and we get $h_- = \begin{pmatrix}1\\-2i\end{pmatrix}\frac{1}{\sqrt{5}}$ or

$|h_-\rangle = \frac{1}{\sqrt{5}}|1\rangle - \frac{2i}{\sqrt{5}}|2\rangle$;

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

Lowest energy state is $\lambda = -5\alpha$ with corresponding eigenvector $|h_-\rangle$. Probability to find system in $+1$ state

(3) of U is given by

$P_+ = |\langle + | h_- \rangle|^2$ wher $U|+\rangle = |+\rangle$. Note now that $|1\rangle$ and $|2\rangle$ are eigenstates of U:

$U|1\rangle = |1\rangle$; $U|2\rangle = -|2\rangle$ whith eigenvalues ± 1.

thus $|+\rangle = |1\rangle$, so that

$P_{+1} = |\langle 1 | h_- \rangle|^2 = \left|(1\ 0)\begin{pmatrix}1\\-2i\end{pmatrix}\frac{1}{\sqrt{5}}\right|^2 = \frac{1}{5}$ probability is $\frac{1}{5}$ or just 20%

$\boxed{P_{u=+1} = \frac{1}{5}}$;

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

We again should work with the state $|h_-\rangle$. Expectation value is given by:

$\langle U \rangle = \langle h_- | U | h_- \rangle = \bar{h}_-^{+} U h_- = \frac{1}{5}(1\ 2i)\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}1\\-2i\end{pmatrix} =$

$= \frac{1}{5}(1-4) = -\frac{3}{5}$; $\boxed{\langle U \rangle = -\frac{3}{5}}$;

(N2) compendium N7

$|1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}$; $|2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$; $|3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$;

$H = \mathcal{L}\begin{pmatrix}1 & \frac{1}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}}\\ 0 & \frac{1}{\sqrt{2}} & 1\end{pmatrix}$, $\mathcal{L} > 0$

a) find 3 energy eigenvalues

we again should write $\det(H - \lambda I) = 0$ or

$\begin{Vmatrix}\mathcal{L}-\lambda & \frac{\mathcal{L}}{\sqrt{2}} & 0\\ \frac{\mathcal{L}}{\sqrt{2}} & \mathcal{L}-\lambda & \frac{\mathcal{L}}{\sqrt{2}}\\ 0 & \frac{\mathcal{L}}{\sqrt{2}} & \mathcal{L}-\lambda\end{Vmatrix} = 0 = (\mathcal{L}-\lambda)^3 - \frac{1}{2}\mathcal{L}^2(\mathcal{L}-\lambda) - \frac{1}{2}\mathcal{L}^2(\mathcal{L}-\lambda) =$

$= (\mathcal{L}-\lambda)(\mathcal{L}^2 - 2\mathcal{L}\lambda + \lambda^2 - \mathcal{L}^2) = (\lambda - \mathcal{L})(\lambda - 2\mathcal{L})\cdot\lambda = 0$

eigenvalues are

$\boxed{\lambda = 0 ; \lambda = \mathcal{L} ; \lambda = 2\mathcal{L} ;}$

④ ⓑ Find normalised energy eigenstates.

$\lambda = 0$

$$\begin{bmatrix} 1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ b_1 \\ c_1 \end{bmatrix} = 0$$

$b_1 = -\sqrt{2}\, a_1 = -\sqrt{2}\, c_1$ normalised eigenstate is

$$h_0 = \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} \cdot \frac{1}{2};$$

$\lambda = \alpha$

$$\begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} a_2 \\ b_2 \\ c_2 \end{bmatrix} = 0 \Rightarrow$$

$b_2 = 0;$ $c_2 = -a_2$, normalised eigenvector is

$$h_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix};$$

$\lambda = 2\alpha$

$$\begin{bmatrix} -1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -1 \end{bmatrix} \begin{bmatrix} a_3 \\ b_3 \\ c_3 \end{bmatrix} = 0 \Rightarrow$$

$b_3 = \sqrt{2}\, a_3 = \sqrt{2}\, c_3$

$$h_2 = \frac{1}{2} \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix};$$

ⓒ If the system is in ground state what is probability that it is in state $|1\rangle$

Probability as usually is given by inner product:

$$P = |\langle 1 | h_0 \rangle|^2 = \left| (1\ 0\ 0) \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \frac{1}{2} \right|^2 = \frac{1}{4} \qquad \boxed{P_1 = \frac{1}{4};} \text{ or } 25\%.$$

ⓓ 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 $t = \frac{\pi\hbar}{a}$?

To undestand how do state evolves we should expand it over the basis of Hamiltonians eigenstates $|n\rangle$ which evolve int time, as prescribed by Schrödinger equation, in the following way:

$|n, t\rangle = e^{-\frac{i}{\hbar}E_n t} |n, t=0\rangle$, where E_n is corresponding eigenvalue of Hamiltonian

$$|1\rangle = c_0 \cdot |h_0\rangle + c_1 |h_1\rangle + c_2 |h_2\rangle$$

(5) $C_0 = \langle h_0 | 1\rangle = \frac{1}{2}$; $C_1 = \langle h_1 | 1 \rangle = \frac{1}{\sqrt{2}}$; $C_2 = \langle h_2 | 1\rangle = \frac{1}{2}$;

$|\psi, t=0\rangle = |1\rangle = \frac{1}{2}|h_0\rangle + \frac{1}{\sqrt{2}}|h_1\rangle + \frac{1}{2}|h_2\rangle$ if we "turn on" time evolution we get

$$|\psi; t\rangle = e^{-\frac{i}{\hbar}Ht}|\psi, t=0\rangle = \frac{1}{2}|h_0\rangle + \frac{1}{\sqrt{2}}e^{-\frac{i}{\hbar}\lambda t}|h_1\rangle + \frac{1}{2}e^{-\frac{i}{\hbar}2\lambda t}|h_2\rangle$$

$$|\psi; t=\tfrac{\pi\hbar}{\lambda}\rangle = \frac{1}{2}|h_0\rangle - \frac{1}{\sqrt{2}}|h_1\rangle + \frac{1}{2}|h_2\rangle \doteq \frac{1}{2}\begin{bmatrix}1\\ \sqrt{2}\\ 1\end{bmatrix} \doteq |3\rangle$$

thus probability is jus 1 : $P_{31} = |\langle 3|3\rangle|^2 = 1$;

(N3)

Let's consider 4 states

$|\uparrow\uparrow\rangle$; $|\uparrow\downarrow\rangle$; $|\downarrow\uparrow\rangle$; $|\downarrow\downarrow\rangle$;

A_1 measure sign of first arrow.

A_2 ——‖—— second arrow.

$F_{1,(2)}$ flips 1 (2) arrow.

write down A_1, A_2, F_1, F_2 as 4x4 matrices.

Let's denote

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

Now let's look how this operators $(A_1; A_2; F_1; F_2)$ act on this states. For example F_1 that flips "spin" 1;

$$F_1|\uparrow\uparrow\rangle = |\downarrow\uparrow\rangle \Rightarrow F_1 \cdot \begin{bmatrix}1\\0\\0\\0\end{bmatrix} = \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \Rightarrow F_1 = \begin{bmatrix}0 & - & - & -\\ 0 & - & - & -\\ 1 & - & - & -\\ 0 & - & - & -\end{bmatrix}$$

$$F_1|\uparrow\downarrow\rangle = |\downarrow\downarrow\rangle = F_1 \cdot \begin{bmatrix}0\\1\\0\\0\end{bmatrix} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \Rightarrow F_1 = \begin{bmatrix}0 & 0 & - & -\\ 0 & 0 & - & -\\ 1 & 0 & - & -\\ 0 & 1 & - & -\end{bmatrix}$$

$F_1|\downarrow\uparrow\rangle = |\uparrow\uparrow\rangle$

$F_1|\downarrow\downarrow\rangle = |\uparrow\downarrow\rangle$

$$\Rightarrow F_1 = \begin{bmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\end{bmatrix}$$ in analogy

$F_2|\uparrow\uparrow\rangle = |\uparrow\downarrow\rangle$, $F_2|\downarrow\downarrow\rangle = |\downarrow\uparrow\rangle$

$F_2|\uparrow\downarrow\rangle = |\uparrow\uparrow\rangle$

$F_2|\downarrow\uparrow\rangle = |\downarrow\downarrow\rangle$

$$F_2 = \begin{bmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}$$

⑥ $A_1|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$; $A_2|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$;

$A_1|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle$; $A_2|\uparrow\downarrow\rangle = -|\uparrow\downarrow\rangle$;

$A_1|\downarrow\uparrow\rangle = -|\downarrow\uparrow\rangle$; $A_2|\downarrow\uparrow\rangle = |\downarrow\uparrow\rangle$;

$A_1|\downarrow\downarrow\rangle = -|\downarrow\downarrow\rangle$; $A_2|\downarrow\downarrow\rangle = -|\downarrow\downarrow\rangle$;

$$A_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} ; \quad A_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

ⓒ Find the eigenvalues and eigenstates of F_1F_2, are there any degeneracies?

$$F_1 \cdot F_2 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

let's find eigenvalues

$$\begin{Vmatrix} -\lambda & 0 & 0 & 1 \\ 0 & -\lambda & 1 & 0 \\ 0 & 1 & -\lambda & 0 \\ 1 & 0 & 0 & -\lambda \end{Vmatrix} = -\lambda \begin{Vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{Vmatrix} - 1 \begin{Vmatrix} 0 & -\lambda & 1 \\ 0 & 1 & -\lambda \\ 1 & 0 & 0 \end{Vmatrix} = -\lambda(-\lambda^3 + \lambda) - (\lambda^2 - 1) =$$

$$= (\lambda^2 - 1)^2$$

$\lambda = \pm 1$ - both eigenvalues are twice degenerate.

We cant define eigenvectors for degenerate case good enough but we can built orthoromal basis in the following way:

$$\lambda = +1 \quad \begin{bmatrix} -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \qquad \begin{matrix} a = d \\ b = c \end{matrix}$$

we choose

$$\boxed{f_{1+} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \frac{1}{\sqrt{2}} ; \quad f_{2+} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} ;}$$

actually any linear combination of this 2 vectors is eigenvector of F_1F_2

$$\lambda = -1 \quad \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \qquad \begin{matrix} a = -d \\ b = -c \end{matrix}$$

$$\boxed{f_{-1} = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \frac{1}{\sqrt{2}} ; \quad f_{-2} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} ;}$$

the same comment about linear combination as in previous case.

7 d) Wich eigenstates of F_1F_2 are not eigenstates of F_1 and F_2?

F_1 and F_2 obviously commute (as they act on different spins), thus we can take degeneracy of F_1 and F_2 eigenstates by looking for simultaneous eigenvector of F_1, F_2 and F_1F_2

eigenstates of F_1 are given by

$$\det\begin{bmatrix} -\lambda & 0 & 1 & 0 \\ 0 & -\lambda & 0 & 1 \\ 1 & 0 & -\lambda & 0 \\ 0 & 1 & 0 & -\lambda \end{bmatrix} = -\lambda\begin{Vmatrix} -\lambda & 0 & 1 \\ 0 & -\lambda & 0 \\ 1 & 0 & -\lambda \end{Vmatrix} + 1\begin{Vmatrix} 0 & 1 & 0 \\ -\lambda & 0 & 1 \\ 1 & 0 & -\lambda \end{Vmatrix} = -\lambda(-\lambda^3+\lambda) + 1 - \lambda^2 =$$

$$= \lambda^4 - 2\lambda^2 + 1 = (\lambda^2-1)^2 \quad ; \lambda = \pm 1 \text{ - double degenerate state}$$

corresponding eigenvectors:

$\lambda = +1$ $\begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow \begin{matrix} c = a \\ b = d \end{matrix}$ $\quad V_{+1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$; $V_{+2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$ and any linear comb. of them.

$\lambda = -1$ $\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow \begin{matrix} c = -a; \\ b = -d; \end{matrix}$ $\quad V_{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}$; $V_{-2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}$; ⊕ and any linear combin.

eigenstates of F_2 are given by:

$$\det\begin{bmatrix} -\lambda & 1 & 0 & 0 \\ 1 & -\lambda & 0 & 0 \\ 0 & 0 & -\lambda & 1 \\ 0 & 0 & 1 & -\lambda \end{bmatrix} = -\lambda\begin{Vmatrix} -\lambda & 0 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{Vmatrix} - 1\begin{Vmatrix} 1 & 0 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{Vmatrix} = -\lambda(-\lambda^3+\lambda) - \lambda^2 + 1 =$$

$= (\lambda^2-1)^2$; $\lambda = \pm 1$ - doble degenerate states, corresponding eigenvectors:

$\lambda = +1$: $\begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow$ $\quad U_{+1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$; $U_{+2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$ ⊕ any linear combination

$\lambda = -1$; $\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow$ $\quad U_{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}$; $U_{-2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix}$; ⊕ any linear combination

Now we can compare set of eigenvectors:

$F_1 \cdot F_2$: $\quad f_{+1} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}\frac{1}{\sqrt{2}}$; $f_{+2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$; $f_{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$; $f_{-2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix}$;

F_1: $\quad V_{+1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$; $V_{+2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$; $V_{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}$; $V_{-2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}$;

F_2: $\quad U_{+1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$; $U_{+2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$; $U_{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}$; $U_{-2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix}$

simultaneous eigenvectors and corresponding eigenvalues of F_1, F_2 and F_1F_2:

I) $\frac{1}{\sqrt{2}}(f_{+1} + f_{+2}) = \frac{1}{\sqrt{2}}(V_{+1} + V_{+2}) = \frac{1}{\sqrt{2}}(U_{+1} + U_{+2})$; $F_1F_2 = +1 = F_1 = F_2$;

⑧ II $\frac{1}{\sqrt{2}}(f_{+1}-f_{+2}) = \frac{1}{\sqrt{2}}(V_{-1}-V_{-2}) = \frac{1}{\sqrt{2}}(U_{-1}-U_{-2})$; $F_1F_2=+1$
$F_1=F_2=-1$

III $\frac{1}{\sqrt{2}}(f_{-1}+f_{-2}) = -\frac{1}{\sqrt{2}}(V_{-1}+V_{-2}) = \frac{1}{\sqrt{2}}(U_{+2}-U_{+1})$; $F_1F_2=-1$;
$F_1=-1$; $F_2=+1$;

IV $\frac{1}{\sqrt{2}}(f_{-1}-f_{-2}) = \frac{1}{\sqrt{2}}(V_{+2}-V_{+1}) = -\frac{1}{\sqrt{2}}(U_{-1}+U_{-2})$; $F_1F_2=-1$
$F_1=+1$; $F_2=-1$

Eventually we have 4 states that take degeneracy away

I $\frac{1}{2}\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$, $F_1F_2=F_1=F_2=+1$; II $\frac{1}{2}\begin{bmatrix}-1\\-1\\1\\1\end{bmatrix}$; $F_1F_2=+1$
$F_1=F_2=-1$;

III $\frac{1}{2}\begin{bmatrix}-1\\-1\\1\\1\end{bmatrix}$; $F_1F_2=-1$
$F_1=-1$; $F_2=+1$; ; IV $\frac{1}{2}\begin{bmatrix}-1\\1\\-1\\1\end{bmatrix}$ $F_1F_2=-1$
$F_1=1$; $F_2=-1$;

Degeneracy is away because now measuring F_1F_2, F_1 and F_2 at the same time gives us definite wave function (one of the wavefunctions written above).
But in problem we are asked to find opposite object: eigenfunction of F_1F_2 wich is not eigenfunction of F_1 and F_2 individually. There are a lot of such states, in fact any linear combinations of $f_{\pm1}$ and f_{+2}, or f_{-1} and f_{-2} different from 4 combinations written above. as example we can take

$f_{\pm1}$ and $f_{\pm2}$ wich in terms of spins are just

$$(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)\frac{1}{\sqrt{2}} \; ; \quad (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)\frac{1}{\sqrt{2}} \; ;$$

This result we were able to obtain from the very beginning just noting, that $f_{\pm1}$ and $f_{\pm2}$ are not eigenvectors of F_1 or F_2 individually.
This can be, in principle, understood from physical point of view (i.e. not going into matrix representation)

(9) because same states $\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)$ and $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$ can be found by hands after looking for states, wich don't go to itself after flipping of one spin, but go after flipping both of them.

(e) Describe what happens with eigenstates of F_1F_2 for measurement A_2 after measurement of A_1?

Let's take, for example, state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

if we make measurement with A_1 w.f. collapse

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \xrightarrow[\text{with } A_1]{\text{measurement}} \begin{cases} |\uparrow\downarrow\rangle \text{ with prob. } p=\frac{1}{2} \\ \text{or} \\ |\downarrow\uparrow\rangle \text{ with } p=\frac{1}{2} \end{cases}$$

and then when we measure with A_2 we get in result either $S=\uparrow$ or $S=\downarrow$ with $p=1$ (depends on the result of first measurement). This is simple example of EPR paradox.

№4 Generalized uncertainty

(a) Find an uncertainty relation between x^2 and p^2 for a general state.

generalised uncertainty relation is

$$(\Delta A)^2 (\Delta B)^2 \geq \left(\left\langle \frac{1}{2i} [\hat{A};\hat{B}] \right\rangle \right)^2$$

sketch of proof (if there will be enough time)

$$(\Delta A)^2 = \langle |(\hat{A} - \langle A \rangle)^2 | \rangle \; ; \; (\Delta B)^2 = \langle |(\hat{B} - \langle B \rangle)^2 | \rangle$$

here $|\rangle$ is any state over which we take average

let's define new states:

$|f\rangle \equiv (\hat{A} - \langle A \rangle) |\rangle \; ; |g\rangle \equiv (\hat{B} - \langle B \rangle) |\rangle$ thus

$(\Delta A)^2 = \langle f | f \rangle ; \; (\Delta B)^2 = \langle g | g \rangle$. Now we can use Schwarz inequality

$$\langle f|f\rangle \langle g|g\rangle \geq \langle f|g\rangle \langle g|f\rangle$$

to prove Schwarz inequality we should consider some other state $|f\rangle + \lambda |g\rangle$ and it's norm, which is positive definite

$$\langle f + \lambda g | f + \lambda g \rangle = \langle f|f\rangle + |\lambda|^2 \langle g|g\rangle + \lambda \langle f|g\rangle + \lambda^* \langle g|f\rangle \geq 0$$

now we choose $\lambda = -\frac{\langle g|f\rangle}{\langle g|g\rangle}$ then

$$\langle f|f\rangle + \langle g|f\rangle\langle f|g\rangle / \langle g|g\rangle - \frac{\langle g|f\rangle\langle f|g\rangle}{\langle g|g\rangle} -$$

$$- \frac{\langle f|g\rangle\langle g|f\rangle}{\langle g|g\rangle} \geq 0 \Rightarrow \boxed{\langle f|f\rangle \langle g|g\rangle \geq \langle f|g\rangle \langle g|f\rangle}$$

q.e.d.

now let's consider r.h.s of Schwarz inequality.

$$\langle f|g\rangle\langle g|f\rangle = (\mathrm{Re}\langle f|g\rangle)^2 + (\mathrm{Im}\langle f|g\rangle)^2 \geq (\mathrm{Im}\langle f|g\rangle)^2 =$$

$$= \left(\frac{1}{2i} (\langle f|g\rangle - \langle g|f\rangle)\right)^2 \quad \text{now}$$

$$\langle f|g\rangle - \langle g|f\rangle = \langle |(\hat{A} - \langle A \rangle)(\hat{B} - \langle B \rangle)| \rangle -$$

$$- \langle |(\hat{B} - \langle B \rangle)(\hat{A} - \langle A \rangle)| \rangle = \langle |[\hat{A}, \hat{B}]| \rangle$$, and finally we get

11) $(\Delta A)^2 (\Delta B)^2 \geqslant \left(\langle \frac{1}{2i}[\hat{A};\hat{B}]\rangle\right)^2$

so we should find following commutator:

$[x^2;p^2] = [x^2;p]\,p + p\,[x^2;p]$, now we will use two relations

$[f(x);p] = i\hbar \frac{\partial}{\partial x} f(x)$

$[x;p] = i\hbar$

and get

$[x^2;p^2] = 2i\hbar\,(xp+px) = 2i\hbar\,(2xp + [p;x]) = 2i\hbar\,(2xp - i\hbar)$

and we get the following

$$\boxed{(\Delta x^2)^2 (\Delta p^2)^2 \geqslant \left(\langle \hbar\,(2xp - i\hbar)\rangle\right)^2}$$

b) What is this relation for the ground state of harmonic oscillator?

W.f. of h.o. ground state is $\varphi_0(x) = \sqrt[4]{\frac{a}{\pi}}\, e^{-\frac{a}{2}x^2}$; $a = \frac{m\omega}{\hbar}$

now let's consider average $\langle xp\rangle$:

$\langle xp\rangle = \sqrt{\frac{a}{\pi}} \int_{-\infty}^{+\infty} dx\; e^{-\frac{a}{2}x^2}\, x\left(-i\hbar\frac{\partial}{\partial x}\right) e^{-\frac{a}{2}x^2} = \sqrt{\frac{a}{\pi}}\; i\hbar\, a \int x^2 e^{-ax^2}\, dx =$

$= \sqrt{\frac{a}{\pi}}\, i\hbar a \cdot \frac{1}{2a}\sqrt{\frac{\pi}{a}} = \frac{i\hbar}{2}$; $\langle xp\rangle = \frac{i\hbar}{2}$ thus

$2\langle xp\rangle - i\hbar = 0$ and

$(\Delta x^2)^2 (\Delta p^2)^2 \geqslant 0$

c) How does it compare to the square of uncertainty $\Delta x \Delta p$

$(\Delta x)^2(\Delta p)^2 \geqslant \left(\langle \frac{1}{2i}[x;p]\rangle\right)^2 = \frac{1}{4}\hbar^2 > 0$ this one is more strict.

Session 3 (oscillator, second quantisation)

Some theory on h.o.

Let's introduce Ladder operators

$$\hat a \equiv \frac{1}{\sqrt2}\left(\alpha\hat x + \frac{i}{\alpha\hbar}\hat p\right);\quad \hat a^+ \equiv \frac{1}{\sqrt2}\left(\alpha\hat x - \frac{i}{\alpha\hbar}\hat p\right);\qquad [\hat x;\hat p] = i\hbar$$

Suppose hamiltonian is

$$H = \frac12\hbar\omega(aa^+ + a^+a) = \frac12\hbar\omega\left(2\cdot\frac12\alpha^2\hat x^2 + 2\frac{1}{2\alpha^2\hbar^2}\hat p^2 - \frac{i}{2\hbar}[\hat x,\hat p] + \frac{i}{2\hbar}[\hat x;\hat p]\right) =$$

$= \frac{\omega}{2\alpha^2\hbar}\hat p^2 + \frac{\hbar\omega\alpha^2}{2}\hat x^2$, to get usual kinetik term we set $\frac{\omega}{2\alpha^2\hbar} = \frac{1}{2m} \Rightarrow \alpha = \sqrt{\frac{m\omega}{\hbar}}$ and we get usual h.o.

hamiltonian $\hat H = \frac{1}{2m}\hat p^2 + \frac12 m\omega^2\hat x^2$; commutation relation for ladder operators is $[a;a^+] = 1$, If we define $\hat N \equiv a^+a$ as operator of "number" we get $[N,a^n] = -na^n$; $[N,(a^+)^n] = n(a^+)^n$, and $H = \hbar\omega(\hat N + \frac12)$

Now if we define ground state $|0\rangle$ as

$a|0\rangle = 0$ (a annihilates $|0\rangle$) then $N|0\rangle = 0$ $H|0\rangle = \frac{\hbar\omega}{2}|0\rangle$ → ground state energy

Now we can define state $(a^+)^n|0\rangle$ and we get

$$H(a^+)^n|0\rangle = \hbar\omega(\hat N + \tfrac12)(a^+)^n|0\rangle = \frac{\hbar\omega}{2}(a^+)^n|0\rangle + \hbar\omega(a^+)^n\underbrace{\hat N|0\rangle}_{0} +$$

$+\hbar\omega[\hat N,(\hat a^+)^n]|0\rangle = \hbar\omega(n+\frac12)(a^+)^n|0\rangle$. So that acting with a^+ we create excited states. Now we can normalise this excited states $|n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n|0\rangle$; and this states are in fact orthonormal $\langle m|n\rangle = \delta_{mn}$;

If we want to know smth. about time evolution we should do what we usually do, i.e. expand in the basis of hamiltonian eigenfunctions:

$\Psi(x;t) = \sum_n c_n e^{-iE_nt/\hbar}|n\rangle$, where $c_n = \langle n|\Psi(x,t=0)\rangle$ and $E_n = \hbar\omega(n+\frac12)$;

one more important formula is

$$\hat x = \frac{1}{\sqrt2\,\alpha}(a+a^+);\quad \hat p = -\frac{i\alpha\hbar}{\sqrt2}(a-a^+);\quad \alpha = \sqrt{\frac{m\omega}{\hbar}};$$

②

Problems

N1 compendium N9

Suppose for oscillator at time $t=0$ the system is in state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + a^{+}|0\rangle)$

ⓐ Find time dependent $|\psi(t)\rangle$;

$$|\psi(t)\rangle = \sum_i c_n e^{-iE_n t/\hbar} |n\rangle$$

$|\psi; t=0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$; - the state at $t=0$

then at time t we get:

$$\boxed{|\psi; t\rangle = \frac{e^{-\frac{i\omega t}{2}}}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}e^{-3i\omega t/2}|1\rangle} \quad |\psi(t)\rangle = \frac{e^{-i\omega t/2}}{\sqrt{2}}(|0\rangle + e^{-i\omega t}|1\rangle)$$

ⓑ Find the expectation value for the energy of $|\psi(t)\rangle$

$$\langle\psi(t)|\hat{H}|\psi(t)\rangle = \frac{1}{2}(\langle 0| + e^{i\omega t}\langle 1|)\hbar\omega(\hat{N}+\tfrac{1}{2})(|0\rangle + e^{-i\omega t}|1\rangle) =$$

$$= \frac{\hbar\omega}{2}\left(\langle 0|\hat{N}+\tfrac{1}{2}|0\rangle + e^{-i\omega t}\underbrace{\langle 0|\hat{N}+\tfrac{1}{2}|1\rangle}_{0} + e^{i\omega t}\underbrace{\langle 1|\hat{N}+\tfrac{1}{2}|0\rangle}_{0} + \langle 1|\hat{N}+\tfrac{1}{2}|1\rangle\right) =$$

$$= \frac{\hbar\omega}{2}\left(\frac{1}{2} + \frac{3}{2}\right) = \hbar\omega$$

$$\langle E\rangle = \hbar\omega$$

ⓒ find expectation value of x

$$\langle x(t)\rangle = \langle\psi(t)|x|\psi(t)\rangle = \frac{1}{2}(\langle 0| + e^{+i\omega t}\langle 1|)\,x\,(|0\rangle + e^{-i\omega t}|1\rangle) =$$

$$= \frac{1}{2}(\langle 0| + e^{i\omega t}\langle 1|)\sqrt{\frac{\hbar}{2m\omega}}(a+a^{+})(|0\rangle + e^{-i\omega t}|1\rangle) =$$

terms $\langle 0|(a+a^{+})|0\rangle = 0$

$\langle 1|(a+a^{+})|1\rangle = 0$

$\langle 0|a+a^{+}|1\rangle = \langle 0|a|1\rangle = 1$

$\langle 1|a+a^{+}|0\rangle = 1 \Rightarrow \boxed{\langle x(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t}$

ⓓ Show that $\langle x(t)\rangle$ is a solution to the classical equations of motion of the harmonic oscillator with potential $V(x) = \frac{1}{2}m\omega^2 x^2$;

$F = m\ddot{x}$ - 2^{nd} Newton law $\quad F = -\nabla V = -m\omega^2 x$

$\ddot{x} + \omega^2 x = 0$ we have $\langle x(t)\rangle = C\cdot\cos\omega t$ which is, indeed solution of classical equation of motion.

③

N2 Compendium N10

ⓐ Find the expectation values $\langle x \rangle$ and $\langle p \rangle$ for the ground state and the first excited state.

We know that

$a|0\rangle = 0$; $a|1\rangle = |0\rangle$;

$a^+|0\rangle = |1\rangle$; $a^+|1\rangle = \sqrt{2}\,|2\rangle$;

$\langle 0|x|0\rangle = \frac{1}{\alpha\sqrt{2}} \langle 0|\, a + a^+ |0\rangle = 0$

$\langle 0|p|0\rangle = -i\frac{\alpha\hbar}{\sqrt{2}} \langle 0|\, a - a^+ |0\rangle = 0$, the same is valid for all othe excited states $|n\rangle$ including $|1\rangle$

ⓑ Same expectation values for $\langle x^2\rangle$; $\langle p^2 \rangle$;

$x^2 = \frac{1}{2\alpha^2}(a+a^+)(a+a^+) = \frac{1}{2\alpha^2}(a^2 + a^{+2} + a^+a + aa^+) =$

$= \frac{1}{2\alpha^2}\left(a^2 + (a^+)^2 + 2a^+a + 1\right)$

$p^2 = -\frac{\alpha^2\hbar^2}{2}(a-a^+)(a-a^+) = -\frac{\alpha^2\hbar^2}{2}\left(a^2 + (a^+)^2 - a^+a - aa^+\right) =$

$= -\frac{\alpha^2\hbar^2}{2}\left(a^2 + (a^+)^2 - 2a^+a - 1\right)$

$\langle n|a^2|n\rangle = \langle n|(a^+)^2|n\rangle = 0$ thus

$\langle x^2\rangle_n = \frac{1}{2\alpha^2}\langle n|\,2\hat{N}+1|n\rangle = \frac{1}{2\alpha^2}(2n+1)$ in particular for states $|0\rangle$ and $|1\rangle$ we get

$$\boxed{\langle 0|x^2|0\rangle = \frac{1}{2\alpha^2};\quad \langle 1|x^2|1\rangle = \frac{3}{2\alpha^2};\quad \langle n|x^2|n\rangle = \frac{1}{2\alpha^2}(2n+1);}$$

$\langle n|p^2|n\rangle = \frac{\alpha^2\hbar^2}{2}\langle n|\,2\hat{N}+1|n\rangle = \alpha^2\hbar^2\left(n+\frac{1}{2}\right)$

$$\boxed{\langle 0|p^2|0\rangle = \frac{\alpha^2\hbar^2}{2};\quad \langle 1|p^2|1\rangle = \frac{3\alpha^2\hbar^2}{2};\quad \langle n|p^2|n\rangle = \alpha^2\hbar^2\left(n+\frac{1}{2}\right);}$$

ⓒ Show that results from ⓐ and ⓑ are consistent with Heisenberg uncertainty.

Let's find deviation:

$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{1}{2\alpha^2}(2n+1)$; $(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2 = \alpha^2\hbar^2\left(n+\frac{1}{2}\right)$;

$(\Delta x)^2\cdot(\Delta p)^2 = \hbar^2\left(n+\frac{1}{2}\right)^2 \geq \frac{\hbar^2}{4}$. Note that uncertanty

4

becomes equality for $n=0$ (we say that it is saturated in this case, i.e. uncertainty is minimal)

N3 Compendium 10B

$H = \hbar\omega(a^\dagger a + \frac{1}{2})$; $[a, a^\dagger] = 1$; $a|0\rangle = 0$

"Coherent" state is defined by

$|A\rangle \equiv C \cdot \exp(A a^\dagger)|0\rangle$;

Other useful commutator is $[a, (a^\dagger)^n] = n(a^\dagger)^{n-1}$;

ⓐ Find $|A\rangle$ in terms of the normalized energy eigenstates

$\exp(A a^\dagger) = \sum_{n=0}^{\infty} \frac{A^n (a^\dagger)^n}{n!}$, thus $|A\rangle = C \sum_{n=0}^{\infty} \frac{A^n (a^\dagger)^n}{n!} |0\rangle =$

$= C \cdot \sum_{n=0}^{\infty} \frac{A^n}{\sqrt{n!}} |n\rangle$, because $\frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \equiv |n\rangle$;

$$\boxed{|A\rangle = C \cdot \sum_{n=0}^{\infty} \frac{A^n}{\sqrt{n!}} |n\rangle ;}$$

ⓑ Find normalisation factor C

$1 = \langle A|A\rangle = |C|^2 \sum_{n,m} \frac{A^n}{\sqrt{n!}} \frac{(A^*)^m}{\sqrt{m!}} \langle m|n\rangle = |C|^2 \sum_{n,m} \frac{A^n A^{*m}}{\sqrt{m!\,n!}} \delta_{m,n} =$

$= |C|^2 \cdot \sum_n \frac{(|A^*|)^{2n}}{n!} = |C|^2 \cdot \exp(+|A|^2)$ as C and A are real we get $C^2 \exp(A^2) = 1 \Rightarrow$ $\boxed{C = e^{-A^2/2} ;}$

ⓒ Show that $|A\rangle$ is an eigenstate of the annihilation operator a and find the eigenvalue.

$a|A\rangle = a\, C \sum_{n=0}^{\infty} \frac{A^n (a^\dagger)^n}{n!} |0\rangle = C \sum_{n=0}^{\infty} \frac{A^n}{n!} a (a^\dagger)^n |0\rangle$, now

$a(a^\dagger)^n|0\rangle = (a^\dagger)^n a|0\rangle + [a, (a^\dagger)^n]|0\rangle = n(a^\dagger)^{n-1}|0\rangle$

$a|A\rangle = C \sum_{n=1}^{\infty} A^n \cdot \frac{n (a^\dagger)^{n-1}}{n!} |0\rangle = CA \cdot \sum_{n=0}^{\infty} \frac{A^n (a^\dagger)^n}{n!} |0\rangle =$

$= A \cdot |A\rangle$

$$\boxed{a|A\rangle = A|A\rangle}$$

⑤ ⓐ Find expectation value $\langle A | H | A \rangle$;

$$\langle A | H | A \rangle = \langle A | \hbar\omega (a^+ a + \tfrac{1}{2}) | A \rangle = \hbar\omega \{ (\langle A | a^+)(a | A \rangle) +$$

$$+ \tfrac{1}{2} \langle A | A \rangle \} = \hbar\omega (A \cdot A + \tfrac{1}{2}) \underbrace{\langle A | A \rangle}_{1} = \hbar\omega (A^2 + \tfrac{1}{2})$$

$$\boxed{\langle A | H | A \rangle = \hbar\omega (A^2 + \tfrac{1}{2})}$$

№4 Consider "fermionic" oscillator

$$H = \frac{\hbar\omega}{2} (b^+ b - b b^+) \quad ; \quad \{b; b^+\} \equiv b b^+ + b^+ b = 1$$

$$\{b; b\} = \{b^+, b^+\} = 0;$$

Find normalised states and energies for this system, assuming that there is ground state $|0\rangle$ where $b|0\rangle = 0$

From anticommutation relations it follows that $(b^+)^2 = 0$ thus let's denote $b^+|0\rangle = |1\rangle$, and we get $b^+|1\rangle = b^+ b^+ |0\rangle = 0$ this will be only 2 states $|0\rangle$ and $|1\rangle$

$$\boxed{\begin{aligned} & b^+|0\rangle = |1\rangle \; ; \; b|0\rangle = 0; \\ & b^+|1\rangle = 0 \; ; \; b|1\rangle = |0\rangle; \end{aligned}}$$

Now let's define energies of this states

$$\hat{H} = \frac{\hbar\omega}{2}(b^+ b - b b^+) = \hbar\omega \left(b^+ b - \tfrac{1}{2} \right),$$ here $b^+ b = \hat{N}$ is "number" operator"

$$\hat{H}|0\rangle = \frac{\hbar\omega}{2}(2b^+ b - 1)|0\rangle = -\frac{\hbar\omega}{2}|0\rangle$$

$$\hat{H}|1\rangle = \frac{\hbar\omega}{2}(2b^+ b b^+ - b^+)|0\rangle = \frac{\hbar\omega}{2}(-2\underbrace{(b^+)^2}_{0} b + 2b^+ - b^+)|0\rangle =$$

$$= \frac{\hbar\omega}{2} b^+|0\rangle = \frac{\hbar\omega}{2}|1\rangle.$$ Thus we have 2 states

$$\boxed{\begin{aligned} & |0\rangle \; ; \; E_0 = -\frac{\hbar\omega}{2} \; ; \; b|0\rangle = 0 \; ; \; b^+|0\rangle = |1\rangle; \\ & |1\rangle \; ; \; E_1 = \frac{\hbar\omega}{2} \; ; \; b^+|1\rangle = 0 \; ; \; b|1\rangle = |0\rangle; \end{aligned}}$$

This is simple enough example of finite (2-dim)

⑥ Hilbert space. We can use matrix represantation in description of fermionic oscillator if we define $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

then

$$b^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \; ; \; b = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad H = \frac{\hbar\omega}{2}(2b^+b - 1) =$$

$$= \frac{\hbar\omega}{2}\left\{2\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right\} = \frac{\hbar\omega}{2}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix};$$

$$H = \frac{\hbar\omega}{2}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix};$$

1

Session 4

Theory

In classical mechanics $\bar{L} = \bar{r} \times \bar{p}$. In q.m. we just put operators instead or usual functions into this formula. (i.e. $\hat{L} = -i\hbar\, \bar{r} \times \bar{\nabla}$)

$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$; $\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$; $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$;

And we will often use $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$

We will sometimes use polar coordinates:

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\cdot\sin\varphi \\ z = r\cos\theta \end{cases} \quad \text{or} \quad \begin{cases} r = \sqrt{x^2+y^2+z^2}; \\ \tan\theta = \dfrac{\sqrt{x^2+y^2}}{z}; \\ \tan\varphi = \dfrac{y}{x}; \end{cases}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x}\frac{\partial}{\partial \varphi} = \frac{x}{r}\frac{\partial}{\partial r} + \cos^2\theta\cdot\frac{x}{z\sqrt{x^2+y^2}} +$$

$$+ \cos^2\varphi\left(-\frac{x}{y^2}\right)\partial_\varphi = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \cos^2\theta\cos\varphi\tan\theta\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta} -$$

$$- \frac{\sin\varphi}{r\sin\theta}\cdot\frac{\partial}{\partial\varphi};$$

$$\frac{\partial}{\partial y} = \frac{y}{r}\frac{\partial}{\partial r} + \cos^2\theta\frac{y}{z\sqrt{x^2+y^2}}\frac{\partial}{\partial\theta} + \cos^2\varphi\left(+\frac{1}{x}\right)\frac{\partial}{\partial\varphi} =$$

$$= \sin\theta\cdot\sin\varphi\frac{\partial}{\partial r} + \cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial z} = \cos^2\theta\frac{\partial}{\partial\theta}\cdot\left(-\frac{\sin\theta}{\cos^2\theta}\right) + \cos\theta\frac{\partial}{\partial r}$$

Now we can write down (omit calculations in class, just write down final result):

$$\boxed{\begin{aligned} \frac{\partial}{\partial x} &= \sin\theta\cos\varphi\frac{\partial}{\partial r} + \cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}; \\ \frac{\partial}{\partial y} &= \sin\theta\cdot\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}; \\ \frac{\partial}{\partial z} &= \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}; \end{aligned}}$$

$$\boxed{\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} - \operatorname{ctg}\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{L}_y &= -i\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right); \quad \hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}; \end{aligned}}$$

(2)

$$L_\pm = \hbar e^{\pm i\varphi}\left(\pm \frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\varphi}\right);$$

$$L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right);$$

commutation relations

$[L_x; L_y] = i\hbar L_z$; $[L_y; L_z] = i\hbar L_x$; $[L_z; L_x] = i\hbar L_y$;

$[L^2; L_i] = 0$; $[L_z; L_\pm] = \pm\hbar L_\pm$;

③ Problems

N1 Show that

$[L_z; x] = i\hbar y$; $[L_x; x] = [(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y), \hat{x}] =$

$[L_z; x] = [xp_y - yp_x; x] = [xp_y; x] - [yp_x; x] = x[\cancel{p_y; x}]_0 +$
$+ p_y[\cancel{x; x}]_0 - y[p_x; x] - [\cancel{y; x}]_0 p_x = i\hbar y$; $\boxed{[L_z; x] = i\hbar y}$;

We have used here that

$[AB, C] = ABC - CAB = A[B, C] + [A, C]B$, and $[p_i; x_j] = -i\hbar\delta_{ij}$;

did this before

$[L_z; y] = [xp_y - yp_x; y] = [xp_y; y] - [yp_x; y] = x[p_y; y] +$
$+ p_y[\cancel{x; y}]_0 - y[\cancel{p_x; y}]_0 - p_x[\cancel{y; y}]_0 = -i\hbar x$; $\boxed{[L_z; y] = -i\hbar x}$;

$[L_z; z] = [xp_y - yp_x; z] = 0$

$[L_z; p_x] = [xp_y; p_x] - [yp_x; p_x] = p_y[x; p_x] = i\hbar p_y$; $\boxed{[L_z; p_x] = i\hbar p_y}$;

$[L_z; p_y] = -p_x[y; p_y] = -i\hbar p_x$; $\boxed{[L_z; p_y] = -i\hbar p_x}$

$[L_z; p_z] = [xp_y; p_z] - [yp_x; p_z] = 0$; $\boxed{[L_z; p_z] = 0}$

N2 Consider potential $V(\bar{r})$

ⓐ If $V(\bar{r})$ is spherically symmetric show that $\frac{\partial}{\partial t}\langle L\rangle = 0$
(i.e. angular momentum is conserved)

$\frac{\partial}{\partial t}\langle \bar{L}\rangle = \langle -\frac{i}{\hbar}[\bar{L}; H]\rangle$, we take usual hamiltonian

$H = \frac{p_r^2}{2m} + \frac{\bar{L}^2}{2mr^2} + V(r)$; $[\bar{L}; \bar{L}^2] = 0$ (can check this is valid always) ; $[\bar{L}; \frac{p_r^2}{2m} + V(r)] = 0$ because L contains only angle derivatives and $\left(\frac{p_r^2}{2m} + V(r)\right)$ only radial coordinates and derivatives.

ⓑ For general $V(\bar{r})$, show that

$\frac{\partial}{\partial t}\langle \bar{L}\rangle = \langle \bar{T}\rangle$ where $\bar{T} = \bar{r} \times (-\bar{\nabla} V)$ is torque.

Let's find commutator $[H, \bar{L}] = [V(r); \bar{L}] = [V(\bar{r}); -i\hbar\bar{r}\times\bar{\nabla}]$;

Let's act on some w.f. with this commutator.

$[V(\bar{r}); -i\hbar\bar{r}\times\bar{\nabla}]\psi = (-i\hbar\cancel{\bar{r}\times\bar{\nabla}\psi})_0 \cdot V(\bar{r}) + (i\hbar\cancel{\bar{r}\times\bar{\nabla}}\psi)_0 V(r) + i\hbar\bar{r}\times\bar{\nabla}V(\bar{r}) =$

$= -i\hbar \bar{T}$, thus

$$\boxed{\frac{\partial}{\partial t}\langle \bar{L} \rangle = \langle \bar{T} \rangle}$$

(N3) - this problem is the same as one in problem set N5 and we will consider it later

(N4)

A particle of mass μ is constrained to move on a 2d sphere of radius R, but is otherwise free to move on the sphere. Assuming that the lowest energy state is 0, find the energies degeneracies of all states.

As usually we have Hamiltonian

$$H = \frac{P_r^2}{2\mu} + \frac{\bar{L}^2}{2\mu r^2} + V(r) \quad \text{in our case } V(r) = V_0 - \text{constant}$$

taken in such way that ground state will be $E=0$ (as demanded by the formulation of problem). It's constant on the sphere and infinite evrywhere else

$$V(r) = \begin{cases} V_0 & r \in [R-\Delta R; R+\Delta R] \\ \infty & \text{evrywher else} \end{cases} \quad \text{and we take limit } \Delta R \to 0$$

then we can neglect P_r^2 (there is no motion transverse to sphere) Thus we have Schrödinger equation

$$\frac{\hat{L}^2}{2\mu r^2} \cdot R_e(r)\, Y_{em}(\theta;\varphi) = (E - V_0)\, R_e(r)\, Y_{em}(\theta;\varphi)$$

Thus radial part can be anything we want (actually we should take it being constant on sphere and 0 evrywhere else)

as for angular part of w.f. we get

$\hat{L}^2 Y_{em}(\theta;\varphi) = \hbar^2 \ell(\ell+1)\, Y_{em}$, thus energy levels are

$\boxed{E_e = \frac{\hbar^2 \ell(\ell+1)}{2\mu R^2}}$ here we have substituted R instead of r because w.f. is "0" everywher but on the

⑤ sphere. As for degeneracies as usually we have m parameter (projection of angular momentum) which takes $(2\ell+1)$ values when "ℓ" is fixed. As energy doesn't depend on "m" we get $2\ell+1$ degeneracy of levels.

N5

Let's consider system with the hamiltonian

$$\hat{H} = \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + \frac{1}{2}\mu\omega^2(x^2+y^2+z^2)$$

a) Separating the variables, find the allowed energy levels and degeneracies for this system.

First let's separate w.f. in the following way

$\Psi(x;y;z) = X(x)\,Y(y)\,Z(z)$ we get 3 equations instead of one

$$\left\{\frac{\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2}{2m} + \frac{1}{2}\mu\omega^2(x^2+y^2+z^2)\right\} X(x)\,Y(y)\,Z(z) = E\,X(x)\,Y(y)\,Z(z)$$

$\Downarrow$

$$\begin{cases} \left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2}\mu\omega^2x^2\right)X(x) = E_x X(x) \\ \left(\frac{\hat{p}_y^2}{2m} + \frac{1}{2}\mu\omega^2y^2\right)Y(y) = E_y Y(y) \\ \left(\frac{\hat{p}_z^2}{2m} + \frac{1}{2}\mu\omega^2z^2\right)Z(z) = E_z Z(z) \end{cases}$$

and total energy then is given by

$E = E_x + E_y + E_z$;

to show this we can consider in more details

$$\left\{-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}\mu\omega^2(x^2+y^2+z^2)\right\} XYZ = E\,XYZ$$

$$\left(-\frac{\hbar^2}{2\mu}X'' + \frac{1}{2}\mu\omega^2 x X\right)YZ + \left(-\frac{\hbar^2}{2\mu}Y'' + \frac{1}{2}\mu\omega^2 y Y\right)XZ +$$

$$+\left(-\frac{\hbar^2}{2\mu}Z'' + \frac{1}{2}\mu\omega^2 z Z\right)XY = E\,XYZ$$ and we see that

we can reduce this equation to the system written above.

⑥ we know that all this equations are just equations for h.o. Their spectrum is known well enough

$$E_i = \hbar\omega\left(n_i + \frac{1}{2}\right) \quad ; \quad i = x, y, z.$$

$E = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right) ;= \hbar\omega\left(n + \frac{3}{2}\right)$ but what is degeneracy N of this level? Let n_z be free parameter

$$N = \sum_{n_x=0}^{n}\sum_{n_y=0}^{n-n_x} 1 = \sum_{n_x=0}^{n}(n - n_x + 1) = \sum_{n_x}^{n}(n+1) - \sum_{n_x=0}^{n} n_x =$$

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

We have summated over all possible n_x and n_y what fixes our n_z;

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

⑥ the same problem but separating system into radial coordinates.

$$H = \frac{p_r^2}{2\mu} + \frac{\mu\omega^2 r^2}{2} + \frac{\hat{L}^2}{2\mu r^2}$$ let's separate radial variables

$\Psi = R_{n_r}(r)\cdot Y_{em}(\theta;\varphi)$ as usually $\hat{L}^2 Y_{em}(\theta;\varphi) = \ell(\ell+1)\,Y_{em}(\theta;\varphi)$

and we get equation for radial part

$$\left[\frac{p_r^2}{2\mu} + \frac{\mu\omega^2 r^2}{2} + \frac{\ell(\ell+1)}{2\mu r^2}\right] R_{\tilde{n}_e}(r) = E_{\tilde{n}_e} R_{\tilde{n}_e}(r)$$

In general this is difficult problem involving special functions and it's a bit boring but at the moment we are interested only in case $\ell = 0$ which makes our life much simpler. We get

$$\cancel{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{\mu\omega^2 r^2}{2}} \quad \left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\mu\omega^2 r^2}{2}\right] R_{n_e}(r) = E_{ne} R_{ne}(r)$$

if we substitute $u_\ell(r) = r\cdot R_\ell(r)$ (this is usual trick) we get:

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\frac{1}{r}u_e(r) = \frac{1}{r^2}\frac{\partial}{\partial r}\frac{r^2}{r}u_e'(r) - \frac{1}{r^2}u_e'(r) = \frac{1}{r}u_e''(r)$$

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and thus

$$\boxed{\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\mu\omega^2 r^2}{2}\right]u_0(r)=E_n u_0(r)}$$ + condition $u_0(0)=0$

this is usual h.o. with energy

$\boxed{E_{\tilde{n}}=\hbar\omega\left(\tilde{n}+\frac{1}{2}\right)}$ $\tilde{n}$ - odd because otherwise we get $u_0(0)\neq 0$ as $\tilde{n}$-even w.f. of h.o. are symmetric.

if $\tilde{n}=1$ $E=\frac{3}{2}\hbar\omega$ wich correspond to $n=0$

$\tilde{n}=3$ $E=\frac{7}{2}\hbar\omega$ which correspond to $n=2$

if $n=1$ we get level $E=\frac{5}{2}\hbar\omega$ which is 3-degenerate it is not contained in the spectrum of $\tilde{n}$ because it should correspond to $\tilde{n}=2$, but $\tilde{n}$ are all should be odd, thus we have $l=1$ for first excited level (which agree with 3-degeneracy)

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 $\psi(x,t) = e^{-iEt/\hbar}\psi(x)$ we obtain stationary Schr. eq.: $\hat{H}\psi = E\psi$ → thus ψ 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 $\hat{H}$:

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

* 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 $V = V_0 = const$, then Schr. eq. reads

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

** 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)

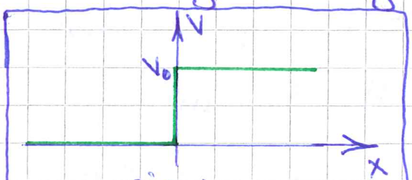
Suppose an electron hits a potential step with height $V_0 = 5eV$. Find the reflection and transmission coefficients, R and T when electon energy is:

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

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:

Ⓘ: $x<0$ and Ⓘⅈ $x>0$;

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 Ⓘ 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 Ⓘⅈ 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 $x=0$

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

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

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:

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

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

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

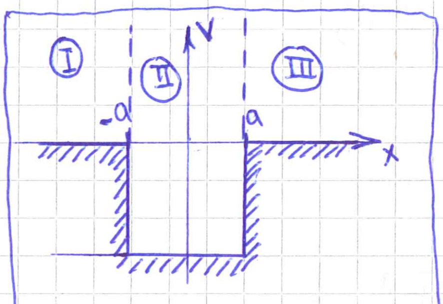
$\underline{R = 0{,}071;\quad T = 1-R = 0{,}929\,eV;}$

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:

$$\begin{cases} \psi_I = Ae^{\varkappa x}; & x<-a; \\ \psi_{II} = B\sin kx + C\cdot\cos kx; & -a<x<a; \\ \psi_{III} = De^{-\varkappa x}; & x>a; \end{cases}$$

where $\varkappa = \frac{\sqrt{-2mE}}{\hbar}$; $k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$;

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.:

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

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

$\Rightarrow C=0$. 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:

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

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

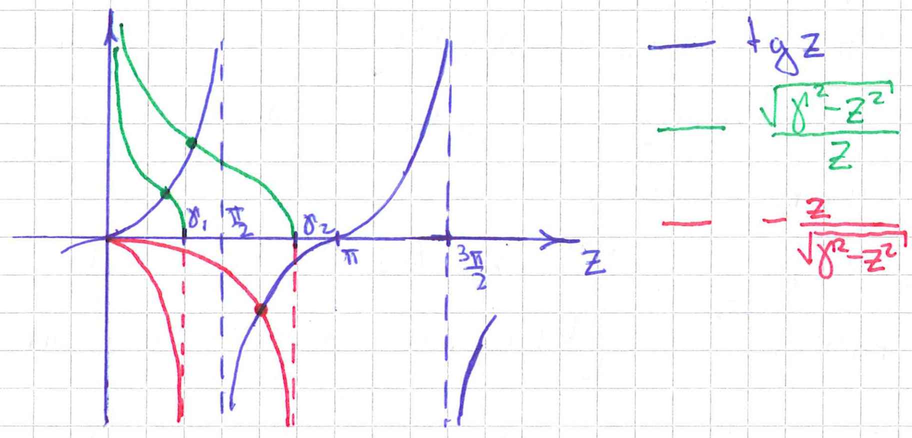
To draw graphical solution we shold draw $\frac{\sqrt{\gamma^2 - z^2}}{z}$ and $-\frac{z}{\sqrt{\gamma^2 - z^2}}$ functions. But as we should do it only qualitavly it's enough to know theirs asymptotes:

** $\frac{\sqrt{\gamma^2 - z^2}}{z} \to +\infty$ 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

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

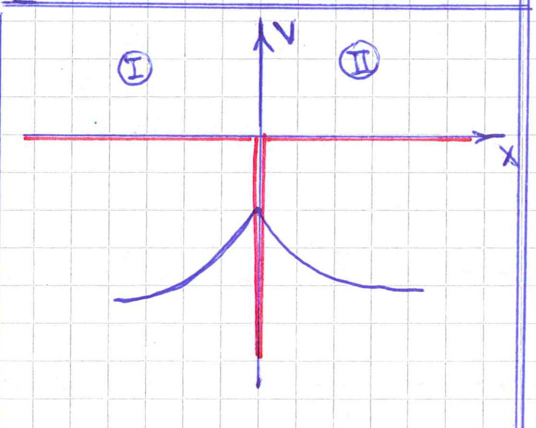
* We now have seen that odd solutions exist only if $\gamma>\frac{\pi}{2} \Rightarrow \boxed{V_0 a^2 \geq \frac{\pi^2\hbar^2}{8m}}$

Problem III (Delta function potential)

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

$\psi_{I} = A e^{\varkappa x}$ — here we have ommited unnormalizable

$\psi_{II} = B e^{-\varkappa x}$ exponent already.

* 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 $x=0$:

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

substituting ψ_I and ψ_{II} we obtain:

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

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

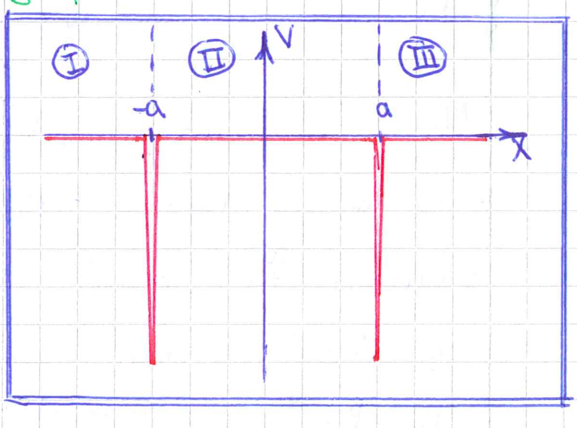
$$\boxed{\psi(x) = \sqrt{\varkappa}\, e^{-\varkappa|x|}; \quad \varkappa = \frac{\sqrt{-2mE}}{\hbar}; \quad E = -\frac{m\alpha^2}{2\hbar^2};}$$

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

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

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

And substitution into eq. (III) gives:

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

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

$$D = \frac{(Ae^{-ika} + Be^{ika})e^{-ika}}{1 - \left(\frac{2}{\lambda}+1\right)e^{-4ika}}$$; and substitute this into eq. (VI) we get:

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

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

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

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

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

So we get:

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

thus

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

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

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

Reflection coefficient is then given by:

(11)

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

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:

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

(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

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

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

$$\left. + \cancel{B^*Ae^{2ikx}} - \cancel{BA^*e^{-2ikx}} - |A|^2 + |B|^2 + \cancel{A^*Be^{-2ikx}} - \cancel{B^*Ae^{2ikx}}\right) \Rightarrow$$

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

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

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

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

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

so that $\left(A^* \; D^*\right)\left(S^+S - \mathbb{1}\right)\begin{pmatrix} A \\ D \end{pmatrix} = 0$ 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:

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

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

① Session 6 (hydrogen atom)

Theory

We take usual Coulomb potential for description of motion of electrons $V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$, and we get following equation $\mu = \frac{mM_n}{m+M_n}$ - electron reduced mass

$$H = \frac{1}{2\mu} p_r^2 + \frac{\bar{L}^2}{2\mu r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r} \; ; \; \psi(r,\theta,\varphi) = R_e(r) Y_{em}(\theta;\varphi)$$

then as usally we get: Schrödinger equation

$$\left[\frac{p_r^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right] R_e(r) = E R_e(r) \; ; \quad R_e(r) = \frac{u_e(r)}{r} \; + u(0) = 0$$

We want to find negative energy solutions $E<0$ thus $u(\infty)=0$ $u(0)=0$ we get equation.

$$-\frac{\hbar^2}{2\mu} u_e''(r) + V_{eff}(r) u_e(r) = E u_e(r)$$

, We introduce $\rho = \varkappa r$, where $\varkappa = \sqrt{-\frac{2\mu E}{\hbar^2}}$; $u_e(r) \approx A e^{-\rho}$ when $\rho \gg 1$; $\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$; $\lambda = Z\alpha\sqrt{-\frac{\mu c^2}{2E}}$;

Full ansatz is then $u_e(r) = \rho^{l+1} e^{-\rho} g_e(\rho)$

$$\rho g_e''(\rho) + 2(l+1-\rho) g_e'(\rho) + 2(\lambda - l - 1) g_e(\rho) = 0 \; ;$$

$g_e(\rho) = \sum_{k=0}^{\infty} c_k \rho^k = c_0 + c_1\rho + \dots c_{k_r}\rho^{k_r}$, substituting this back we get following relation $c_{k+1} = \frac{2(k+l+1-\lambda)}{(k+1)(k+2l+2)} c_k$; $c_{k+1} = 0$ when $\lambda = k+l+1$, λ is integer n, $n \geq l+1$, if $n=1$ $l=0$, $n=2$, $l=0,1$; $n=3$, $l=0,1,2$, etc. Solutions are

$R_{nl}(r) = \rho^l e^{-\rho} g_{nl}(\rho)$ where $g_{nl}(\rho)$ Laguerre polynomials.

degenerasy of atom "n" level is $\sum_{l=0}^{n-1} (2l+1) = \frac{1}{2} n \cdot (1 + 2n - 1) = n^2$ (degeneracy of each l wavefunction is $(2l+1)$ and we have such levels going from $l=0$ till $n-1$)

$E_n = -\frac{Z^2}{2n^2} \frac{e^2}{4\pi\varepsilon_0 a_\mu}$; $a_\mu = \frac{\hbar}{\alpha c \mu}$. One very usefull formula on this session is

$$\int_0^\infty t^n e^{-t} = \lim_{\alpha\to 1} \frac{d^n}{d\alpha^n} \int_0^\infty e^{-\alpha t} = \lim_{\alpha \to 1} \frac{d^n}{d\alpha^n} \frac{1}{\alpha} = (-1)^n n!$$

②

Problems

N1 compendium N 14

$$\psi_{100}(r,\theta,\varphi) = \frac{2}{\sqrt{4\pi}}\left(\frac{1}{a_\mu}\right)^{3/2}\exp\left(-\frac{r}{a_\mu}\right);$$ - this is $n=1$ level of hydrogen atom.

ⓐ find expectation value for x^2 for this state.

$$\langle x^2\rangle = \int d^3x\; x^2 \frac{1}{\pi}\frac{1}{a_\mu^3}\exp\left(-\frac{2r}{a_\mu}\right) = \int d\cos\theta\, d\varphi\, dr \frac{r^2}{\pi a_\mu^3} r^2\cos^2\varphi\sin^2\theta \times$$

$$\times\exp\left(-\frac{2r}{a_\mu}\right) = \frac{1}{\pi a_\mu^3}\cdot\frac{1}{2}\cdot 2\pi\cdot\left(\cos\theta - \frac{1}{3}\cos^3\theta\right)\Big|_{-1}^{1}\cdot\int_0^\infty dr\; r^4 e^{-\frac{2r}{a_\mu}} =$$

$$= \frac{4}{2^5\cdot 3}a_\mu^2\int_0^\infty dt\, t^4 e^{-t};$$ best way to evaluate

this integral $\int_0^\infty dt\, t^4 e^{-t} = \lim_{\alpha\to 1}\frac{d^4}{d\alpha^4}\int_0^\infty dt\, e^{-\alpha t} = \lim_{\alpha\to 1}\frac{d^4}{d\alpha^4}\frac{1}{\alpha} =$

$= \lim_{\alpha\to 1}\frac{4!}{\alpha^5} = 4!$, then initial integral is

$$\langle x^2\rangle = \frac{2^5}{2^5}\cdot\frac{3}{3}a_\mu^2 = a_\mu^2 \quad ; \quad \boxed{\langle x^2\rangle = a_\mu^2}$$

ⓑ Find expectation value for p_x^2 for this state.

$$\langle p_x^2\rangle = -\frac{\hbar^2}{\pi a_\mu^3}\int d^3x\,\exp\left(-\frac{r}{a_\mu}\right)\frac{d^2}{dx^2}\exp\left(-\frac{r}{a_\mu}\right)$$

let's now show that $\langle x^2\rangle = \langle y^2\rangle = \langle z^2\rangle$ and $\langle p_x^2\rangle = \langle p_y^2\rangle = \langle p_z^2\rangle$

First of all it is understandable because of spherical symmetry of problem - there is no special direction, and this is in fact enough for us (it may be shown explicitely but we won't do this here)

thus $\langle x^2\rangle = \langle y^2\rangle = \langle z^2\rangle = \frac{1}{3}\langle r^2\rangle$; $\langle p_x^2\rangle = \langle p_y^2\rangle = \langle p_z^2\rangle = \frac{1}{3}\langle p_r^2\rangle$

$$\langle p_r^2\rangle = -\frac{\hbar^2}{\pi a_\mu^3}\int d^3x\,\exp\left(-\frac{r}{a_\mu}\right)\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\exp\left(-\frac{r}{a_\mu}\right) =$$

$$= -\frac{\hbar^2 4}{a_\mu^3}\int r^2 dr\,\exp\left(-\frac{2r}{a_\mu}\right)\left(\frac{1}{a_\mu^2} + \frac{2}{r a_\mu}\right) = -\frac{4\hbar^2}{a_\mu^2}\int dr\left(\left(\frac{r}{a_\mu}\right)^2 + 2\frac{r}{a_\mu}\right)\exp\left(-\frac{2r}{a_\mu}\right)$$

(3) $= -\frac{4\hbar^2}{a_\mu^2}\cdot\frac{1}{2}\int_0^\infty dt\,\left(\frac{t^2}{4}-t\right)e^{-t} = -\frac{\hbar^2}{2a_\mu^2}\int_0^\infty dt\,(t^2-4t)\,e^{-t} =$

$= -\frac{\hbar^2}{2a_\mu^2}\left(+\frac{d^2}{d\lambda^2}+4\frac{d}{d\lambda}\right)\int dt\, e^{-\lambda t}\Big|_{\lambda\to 1} = -\frac{\hbar^2}{2a_\mu^2}(2-4) = \frac{\hbar^2}{a_\mu^2}$

and thus as $\langle p_r^2\rangle = \frac{\hbar^2}{a_\mu^2}$; $\langle p_x^2\rangle = \frac{1}{3}\langle p_r^2\rangle$

$$\boxed{\langle p_x^2\rangle = \frac{\hbar^2}{3a_\mu^2};}$$

(c) $(\Delta x\Delta p_x)^2 = \langle p_x^2\rangle\langle x^2\rangle$ because $\langle x\rangle = \langle p_x\rangle = 0$ because of the same rotational invariance and abscent preferable direction. (But this of course can be obtained by direct calculation) thus

$(\Delta x)^2(\Delta p_x)^2 = \frac{\hbar^2}{3}$ wich is larger then $\frac{\hbar^2}{4}$ thus

Heisenberg uncertainty is ok.

(N2) compendium N15

$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$; as usually we have hydrogen atom

$R_{10}(r) = 2\left(\frac{Z}{a_\mu}\right)^{3/2}\exp\left(-\frac{Zr}{a_\mu}\right)$; $R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_\mu}\right)^{3/2}\left(\frac{Zr}{a_\mu}\right)\exp\left(-\frac{Zr}{2a_\mu}\right)$;

(a) compute the expectation value $\langle 1s|r|1s\rangle$

In principle we should calculate

$\langle r\rangle_{1s} = \int d^3\vec{r}\; r\cdot R_{10}^2\cdot|Y_{00}|^2$ but as r doesn't depend on angles we have $\int d\Omega\,|Y_{00}|^2 = 1$ and thus we should calculate:

$\langle r_{1s}\rangle = \int_0^\infty dr\, r^3\cdot R_{10}^2 = \int_0^\infty dr\cdot r^3\cdot\frac{4Z^3}{a_\mu^3}e^{-\frac{2Zr}{a_\mu}} = \frac{4Z^3}{a_\mu^3}\cdot\frac{a_\mu^4}{2^4Z^4}\int_0^\infty dt\cdot t^3e^{-t} =$

$= \frac{4a_\mu}{2^4 Z}\cdot 3! = \frac{3}{2}\frac{a_\mu}{Z}$; $\boxed{\langle r_{1s}\rangle = \frac{3}{2}\frac{a_\mu}{Z};}$

(b) compute the expectation value $\langle 2p|r|2p\rangle$

$\langle r_{2p}\rangle = \int_0^\infty dr\cdot r^3\cdot R_{21}^2 = \int_0^\infty dr\cdot r^3\cdot r^2\cdot\frac{Z^5}{3\cdot 8\cdot a_\mu^5}\exp\left(-\frac{Zr}{a_\mu}\right) =$

④ $= \frac{a_\mu}{24Z_0}\int_0^\infty dt \cdot t^5 e^{-t} = \frac{a_\mu}{24 \cdot \cdot Z} \cdot 5! = 5\frac{a_\mu}{Z}$

$$\boxed{\langle r \rangle_{2p} = 5\frac{a_\mu}{Z};}$$

© assume that there is small perturbative correction to the Hamiltonian, $H' = \lambda r$. Compute the first order correction to the energies of the 1s and 2p states.

This is theme of next session but already here we can understand what is first order correction.

Assume that w.f. doesn't change thus energy corrections for levels can be estimated by just looking for the average of hamiltonian operator.

$$\langle H' \rangle_{1s} = \lambda \langle r \rangle_{1s} = \frac{3}{2}\lambda \frac{a_\mu}{Z}$$

$$\langle H \rangle_{2p} = \lambda \langle r \rangle_{2p} = 5\lambda \frac{a_\mu}{Z}$$

N3 Compendium N16

Let's take w.f. from previous problem

$$R_{10}(r) = 2\left(\frac{Z}{a_\mu}\right)^{3/2} \exp\left(-\frac{Zr}{a_\mu}\right); \quad R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_\mu}\right)^{3/2}\left(\frac{Zr}{a_\mu}\right)\exp\left(-\frac{Zr}{2a_\mu}\right)$$

W.f. of ground state for tritium and helium

is $\psi^Z_{100} = R^Z_{10}(r)\, Y_{00}(\theta;\varphi)$

for tritium we take $Z=1$; for Helium $Z=2$

Probability to go from 1s state of T to 1s state of Helium is given by following inner product

$$P(1s \to 1s) = |\langle \psi^{Z=1}_{100} | \psi^{Z=2}_{100} \rangle|^2 = \left|\int dr \cdot r^2 \cdot 4\, \frac{2^{3/2}}{a_\mu^3} \cdot \exp\left(-\frac{3r}{a_\mu}\right)\right|^2$$

Let's calculate integral

(5) $$\frac{1}{a_\mu^3}\int_0^\infty dr\cdot r^2 \exp\left(-\frac{3r}{a_\mu}\right) = \frac{1}{27}\int_0^\infty dt\cdot t^2 e^{-t} = \frac{2}{27}$$

total probability is.

$$P = 4^2\cdot 2^3\cdot \frac{4}{(27)^2} = \frac{2^9}{3^6} \qquad P = 2^3\left(\frac{2}{3}\right)^6 = \frac{512}{729};$$

(6) Now let's calculate probability to go to 2p state of Helium³. it is given by following inner product

$P(1s\to 2p) = |\langle R_{10}Y_{00}|R_{21}Y_{1m}\rangle|^2$ but

$\langle Y_{00}|Y_{1m}\rangle = 0$ thus probability goes to 0.

(N4) Find the probability that an electron in the ground state is inside the proton in a hydrogen atom. Assume that the proton radius $b \ll a_\mu$ take $b = 10^{-15}$ m, $a = 0{,}5\cdot 10^{-10}$ m.

Probability will be given by

$$P = \int_0^b dr\cdot r^2 (R_{10}(r))^2$$ wher R_{10} is the same as in previous problem

$$P = \int_0^b dr\cdot r^2\cdot \frac{4}{a_\mu^3}\exp\left(-\frac{2r}{a_\mu}\right);$$ we can integrate by parts or use usual trick

$$\int_0^b dr\cdot r^2 e^{-\lambda r} = \frac{d^2}{d\lambda^2}\int_0^b dr\, e^{-\lambda r} = \frac{d}{d\lambda^2}\left(e^{-\lambda b}-1\right)\cdot\frac{1}{\lambda} =$$

$$= \frac{d}{d\lambda}\left(-be^{-\lambda b}\frac{1}{\lambda} - \frac{1}{\lambda^2}\left(e^{-\lambda b}-1\right)\right) =$$ [and so on] actually answer will be big and ugly. We should use $a \gg b$ and write down $\exp\left(-\frac{2r}{a_\mu}\right)\approx 1$

$$P = \int_0^b dr\cdot r^2\frac{4}{a_\mu^3} = \left(\frac{4}{3}\right)\left(\frac{b}{a_\mu}\right)^3; \quad P = \frac{4}{3}\cdot\left(\frac{2\cdot 10^{-15}}{10^{-10}}\right)^3 = \frac{4\cdot 8\cdot 10^{-15}}{3} \approx 10^{-14}$$

(6) Now we can find the same probability for ψ_{210} state, this time however

$$P = \int_0^b dr\, r^2 \cdot R_{21}^2(r) = \int_0^b dr \cdot r^4 \, \frac{1}{3} \frac{1}{8a_\mu^3} \frac{1}{a_\mu^2} \exp\left(-\frac{r}{2a_\mu}\right), \text{ again}$$

we can neglect exponent and get

$$P = \frac{1}{24 \cdot 5} \cdot \left(\frac{b}{a_\mu}\right)^5 \quad \text{numerical value is} \quad P = \frac{2^5}{2^3 \cdot 15} \cdot 10^{-25} = \frac{4}{15} 10^{-25}$$

(N5) Consider the hydrogen atom wave function $\psi = \frac{1}{\sqrt{2}} \psi_{211} + \frac{1}{\sqrt{2}} \psi_{21-1}$ Find the expectation values $\langle x^2 \rangle, \langle y^2 \rangle$ and $\langle z^2 \rangle$ for this state.

ψ wave function is given by:

$$\psi = \frac{1}{\sqrt{2}} R_{21}(r) \left(Y_{11} + Y_{1-1}\right) = \frac{1}{\sqrt{2}} R_{21}(r) \sqrt{\frac{3}{8\pi}} \sin\theta \left(-e^{+i\varphi} + e^{-i\varphi}\right) =$$

$$\psi = -i\sqrt{\frac{3}{4\pi}} R_{21}(r) \sin\theta \sin\varphi \quad ; \quad R_{21} = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_\mu}\right)^{3/2} \frac{Zr}{a_\mu} e^{-Zr/2a_\mu};$$

remind you that in spherical coordinates

$$\begin{cases} x = r\sin\theta \cdot \cos\varphi \\ y = r\sin\theta \sin\varphi \\ z = r\cos\theta \end{cases}$$

$$\langle x^2 \rangle = \int dV\, |\psi|^2 r^2 \sin^2\theta \cos^2\varphi = \underbrace{\int_{-1}^{1} d\cos\theta \sin^4\theta}_{A} \cdot \underbrace{\int_0^\infty dr \cdot r^4 |R_{21}|^2}_{B} \underbrace{\int_0^{2\pi} d\varphi \sin^2\varphi \cos^2\varphi \frac{3}{4\pi}}_{C}$$

$$\langle x^2 \rangle = \frac{3}{4\pi} A \cdot B \cdot C$$

$$\langle y^2 \rangle = \int dV\, |\psi|^2 r^2 \sin^2\theta \sin^2\varphi = \underbrace{\int_{-1}^{1} d\cos\theta \cdot \sin^4\theta}_{A} \underbrace{\int_0^\infty dr \cdot r^4 |R_{21}|^2}_{B} \cdot \underbrace{\int_0^{2\pi} d\varphi \sin^4\varphi}_{D} \cdot \frac{3}{4\pi}$$

$$\langle y^2 \rangle = \frac{3}{4\pi} A \cdot B \cdot D$$

$$\langle z^2 \rangle = \frac{3}{4\pi} \underbrace{\int_{-1}^{1} d\cos\theta \cdot \cos^2\theta \sin^2\theta}_{E} \underbrace{\int_0^\infty dr \cdot r^4 |R_{21}|^2}_{B} \underbrace{\int_0^{2\pi} d\varphi \sin^2\varphi}_{F}$$

$$\langle z^2 \rangle = \frac{3}{4\pi} E \cdot B \cdot F$$

Here we have denoted:

⑦ $A = \int_{-1}^{1} d\cos\theta \cdot \sin^4\theta = \int_{-1}^{1} dt\, (1-t^2)^2 = \left(t - \frac{2}{3}t^3 + \frac{1}{5}t^5\right)\Big|_{-1}^{1} = \frac{16}{15}$; $A = \frac{16}{15}$

$B = \int_0^\infty dr \cdot r^4 \, |R_{21}|^2 = \frac{1}{3} \frac{Z^3}{8a_\mu^3} \frac{Z^2}{a_\mu^2} \int_0^\infty dr\, r^6\, e^{-\frac{Zr}{a_\mu}} =$

$= \frac{1}{24} \left(\frac{a_\mu}{Z}\right)^2 \int_0^\infty dt \cdot t^6 e^{-t} = \frac{1}{24} \cdot 6! \left(\frac{a_\mu}{Z}\right)^2 = 30\left(\frac{a_\mu}{Z}\right)^2$; $B = 30\left(\frac{a_\mu}{Z}\right)^2$

$C = \int_0^{2\pi} d\varphi \cdot \sin^2\varphi \cos^2\varphi = \int_0^{2\pi} d\varphi \frac{1}{4} \sin^2 2\varphi = \int_0^{2\pi} d\varphi\, \frac{1}{8}(1-\cos 4\varphi) = \frac{\pi}{4}$; $C = \frac{\pi}{4}$

$D = \int_0^{2\pi} d\varphi \sin^4\varphi = \int_0^{2\pi} d\varphi\, \frac{1}{4}(1-\cos 2\varphi)^2 = \int_0^{2\pi} d\varphi \left(\frac{1}{4} - \underbrace{\frac{1}{2}\cos 2\varphi}_{0} + \frac{1}{8} + \underbrace{\frac{1}{8}\cos 4\varphi}_{0}\right) = \frac{3}{8} 2\pi$

$D = \frac{3\pi}{4}$;

$E = \int_{-1}^{1} d\cos\theta\, \cos^2\theta \cdot \sin^2\theta = \int_{-1}^{1} dt\, (t^2 - t^4) = 2\cdot\left(\frac{1}{3} - \frac{1}{5}\right) = \frac{4}{15}$; $E = \frac{4}{15}$

$F = \int_0^{2\pi} d\varphi \sin^2\varphi = \pi$; $F = \pi$

Taking all obtained results together we get:

$\langle x^2 \rangle = \frac{3}{4\pi} \cdot \frac{16}{15} \cdot \frac{\pi}{4} \cdot 30\left(\frac{a_\mu}{Z}\right)^2 = 6\left(\frac{a_\mu}{Z}\right)^2 = \frac{1}{5}\langle r^2 \rangle$ as $\langle r^2 \rangle = B = \int dr \cdot r^4 |R_{21}|^2$

$\langle y^2 \rangle = \frac{3}{4\pi} \cdot \frac{16}{15} \cdot 30\left(\frac{a_\mu}{Z}\right)^2 \cdot \frac{3\pi}{4} = 18\left(\frac{a_\mu}{Z}\right)^2 = \frac{3}{5}\langle r^2 \rangle$;

$\langle z^2 \rangle = \frac{3}{4\pi} \cdot 30\left(\frac{a_\mu}{Z}\right)^2 \cdot \pi \cdot \frac{4}{15} = 6\left(\frac{a_\mu}{Z}\right)^2 = \frac{1}{5}\langle r^2 \rangle$;

$$\boxed{\begin{aligned} \langle x^2 \rangle &= 6\left(\frac{a_\mu}{Z}\right)^2 = \frac{1}{5}\langle r^2 \rangle; \\ \langle y^2 \rangle &= 18\left(\frac{a_\mu}{Z}\right)^2 = \frac{3}{5}\langle r^2 \rangle; \\ \langle z^2 \rangle &= 6\left(\frac{a_\mu}{Z}\right)^2 = \frac{1}{5}\langle r^2 \rangle; \end{aligned}}$$

1

Session 7 Perturbation theory

Assume we know eigenfunctions and eigenvalues of the Hamiltonian of some system H : $H_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$; Then we add some small term H' to this hamiltonian and get $H = H_0 + H'$ what are new eigenstates and eigenvalues.

$H|\psi_n\rangle = E_n|\psi_n\rangle$. Let's first assume that spectrum is nondegenerate. i.e. $E_n \neq E_m$ for $n \neq m$. Now we can introduce small parameter ε : $H' \to \varepsilon H'$ and expand E_n and ψ_n in series of this parameter: $|\psi_n\rangle = \sum_{k=0}^{\infty} \varepsilon^k |\psi_n^{(k)}\rangle$; $E_n = \sum_{k=0}^{\infty} \varepsilon^k E_n^{(k)}$;

Then we get in orders of ε:

ε^0: $H_0|\psi_n^{(0)}\rangle = E_n|\psi_n^{(0)}\rangle$ - no surprise we get Schrödinger equation.

ε^1: $H_0|\psi_n^{(1)}\rangle + H'|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}|\psi_n^{(0)}\rangle$;

ε^2: $H_0|\psi_n^{(2)}\rangle + H'|\psi_n^{(1)}\rangle = E_n^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)}|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle$; now if we multiply with Bra $\langle\psi_n^{(0)}|$ from the right we get

$$\langle\psi_m^{(0)}|H_0|\psi_n^{(1)}\rangle + \langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle = E_n^{(0)}\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}\underbrace{\langle\psi_m^{(0)}|\psi_n^{(0)}\rangle}_{\delta_{mn}};$$

if $m=n$: $\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle = E_n^{(1)}$ thus $\boxed{E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle}$

if $m \neq n$ we get

$\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle = (E_n^{(0)} - E_m^{(0)})\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle$; now we can expand $|\psi_n^{(1)}\rangle$ over complete basis of $|\psi_n^{(0)}\rangle$: $|\psi_n^{(1)}\rangle = \sum_{k\neq n} C_{nk}^{(1)}|\psi_k^{(0)}\rangle$

$C_{nk}^{(1)} = \dfrac{\langle\psi_k^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$ thus $\boxed{|\psi_n^{(1)}\rangle = \sum_{k\neq n} \dfrac{\langle\psi_k^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle}$;

The case of degenerate spectrum is a little bit different. The leading order now is not 1 state anymore but linear combination of degenerate states $|\psi_n^{(0)}\rangle$; then we have $|\psi\rangle = \sum_{n'} b_{n'n}|\psi_{n'}^{(0)}\rangle + \sum_{k=1}^{\infty}\varepsilon^k|\psi^{(k)}\rangle$ if we define $|\chi_n^{(0)}\rangle = \sum_{n'} b_{n'n}|\psi_{n'}^{(0)}\rangle$ substituting this into Schrodinger equation we get

$$\langle\psi_{n'}^{(0)}|H'|\chi_n^{(0)}\rangle = E_n^{(1)}\langle\psi_{n'}^{(0)}|\chi_n^{(0)}\rangle \Rightarrow \boxed{\sum_{n''} H'_{n'n''} b_{n''n} = \Delta E_n b_{n'n}};$$

So, we are just looking for solutions of eigenvalue equation with determines coefficients $b_{n'n}$ and first order energy corrections

②

Problems

N1 Compendium N17

Consider the four state system with states given by

$$|1\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix};\quad |2\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix};\quad |3\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix};\quad |4\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix};$$

and Hamiltonian $H = H_0 + H_1$

$$H_0 = \mathcal{L}\begin{bmatrix}0&1&0&0\\1&0&0&0\\0&0&0&0\\0&0&0&3\end{bmatrix};\quad H_1 = \lambda\begin{bmatrix}2&-1&0&-1\\-1&2&-1&0\\0&-1&2&-1\\-1&0&-1&2\end{bmatrix};\quad \mathcal{L} \gg \lambda$$

ⓐ find eigenvalues and normalized eigenstates of H_0.

$$\begin{Vmatrix}-\lambda & \mathcal{L} & 0 & 0\\ \mathcal{L} & -\lambda & 0 & 0\\ 0 & 0 & -\lambda & 0\\ 0&0&0&3\mathcal{L}-\lambda\end{Vmatrix} = \lambda^3(\lambda-3) + (3\mathcal{L}-\lambda)\cdot\lambda\mathcal{L}^2 = (\lambda-3\mathcal{L})\lambda(\lambda-\mathcal{L})(\lambda+\mathcal{L})$$

we have 4 roots for eigenvalues equation

$\lambda = -\mathcal{L}$; $\lambda = \mathcal{L}$; $\lambda = 0$; $\lambda = 3\mathcal{L}$. Now let's find normalised eigenstates.

① $\lambda = -\mathcal{L}$

$$\begin{bmatrix}1&1&0&0\\1&1&0&0\\0&0&1&0\\0&0&0&4\end{bmatrix}\begin{bmatrix}a\\b\\c\\d\end{bmatrix} = 0 \qquad a=-b,\quad c=d=0 \qquad \Psi_{-1} = \begin{pmatrix}1\\-1\\0\\0\end{pmatrix}\frac{1}{\sqrt{2}} = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

② $\lambda = 0$

$$\begin{bmatrix}0&1&0&0\\1&0&0&0\\0&0&0&0\\0&0&0&3\end{bmatrix}\begin{bmatrix}a\\b\\c\\d\end{bmatrix} = 0 \Rightarrow \quad b=a=d=0,\ c - \text{any} \qquad |\psi_0\rangle = |3\rangle$$

③ $\lambda = \mathcal{L}$

$$\begin{bmatrix}-1&1&0&0\\1&-1&0&0\\0&0&-1&0\\0&0&0&2\end{bmatrix}\begin{bmatrix}a\\b\\c\\d\end{bmatrix} = 0 \Rightarrow \quad a=b;\ c=d=0 \qquad |\psi_{+1}\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$$

④ $\lambda = 3\mathcal{L}$

$$\begin{bmatrix}-3&1&0&0\\1&-3&0&0\\0&0&-3&0\\0&0&0&0\end{bmatrix}\begin{bmatrix}a\\b\\c\\d\end{bmatrix} = 0 \Rightarrow \quad b=3a;\ c=0;\ d - \text{any} \qquad |\psi_{+3}\rangle = |4\rangle$$

ⓑ treating H_1 as a perturbation of H_0, find the correction to the energy of the ground state up to second order in perturbation theory.

(3) First one more theoretical tip.

In case of nondegenerate perturbation theory second order correction can be found from equation

$$H_0|\psi_n^{(2)}\rangle + H'|\psi_n^{(1)}\rangle = E_n^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)}|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle$$

multplying with $\langle\psi_n^{(0)}|$ from left we get

$$E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle + \langle\psi_n^{(0)}|H'|\psi_n^{(1)}\rangle = E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle + \underbrace{E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle}_{0} +$$

$+ E_n^{(2)}\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle$ now if we use our previous results for lower order terms of perturbation series we get

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\langle\psi_n^{(0)}|H'|\psi_k^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

- in 2^{nd} order we can see repulsion of levels (consider cases when $E_n < E_k$ or vice versa)

this is second-order correction for energy levels.

now back to solving problem

to find corrections to ground state $E = -\alpha$; $|\psi_{-1}\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$

We should find matrix elements

$\langle\psi_{-1}|H_1|\psi_m\rangle$ where $m = 0, 1, 3; -1$.

$$\langle\psi_{-1}|H_1|\psi_{-1}\rangle = \frac{\lambda}{2}(1\ {-1}\ 0\ 0)\begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix} = \frac{\lambda}{2}(1\ {-1}\ 0\ 0)\begin{pmatrix} 3 \\ -3 \\ 1 \\ -1 \end{pmatrix} = 3\lambda$$

$\boxed{E_{-1}^{(1)} = 3\lambda;}$ Now it will be usefull to use $H_1|\psi_{-1}\rangle =$

$= \frac{\lambda}{\sqrt{2}}\begin{bmatrix} 3 \\ -3 \\ 1 \\ -1 \end{bmatrix}$; then

$$\langle\psi_0|H_1|\psi_{-1}\rangle = \frac{\lambda}{\sqrt{2}}[0\ 0\ 1\ 0]\begin{bmatrix} 3 \\ -3 \\ 1 \\ -1 \end{bmatrix} = \frac{\lambda}{\sqrt{2}}; \quad \langle\psi_2|H_1|\psi_{-1}\rangle = \frac{\lambda}{2}[1\ 1\ 0\ 0]\begin{bmatrix} 3 \\ -3 \\ 1 \\ -1 \end{bmatrix} = 0$$

$$\langle\psi_3|H_1|\psi_{-1}\rangle = \frac{\lambda}{\sqrt{2}}[0\ 0\ 0\ 1]\begin{bmatrix} 3 \\ -3 \\ 1 \\ -1 \end{bmatrix} = -\frac{\lambda}{\sqrt{2}}$$

then we get second order correction

$$E_{-1}^{(2)} = -\frac{\lambda^2}{2}\cdot\left\{\frac{1}{\alpha} + \frac{1}{4\alpha}\right\} = -\frac{5}{8}\frac{\lambda^2}{\alpha};$$

$$\boxed{E_{-1} = -\alpha + 3\lambda - \frac{5}{8}\frac{\lambda^2}{\alpha};}$$

4

№2 Compendium N 18

Consider hamiltonian $H = H_0 + H_1$, where

$H_0 = \frac{\hbar\omega}{2}(a^+a + aa^+)$; $H_1 = \lambda(a^+ + a)^4$; $[a, a^+] = 1$, a and a^+ are as usually creation and annihilation operators.

Find energy ground state to second order.

We know that grand state is given by $|0\rangle$ which can be annihilated by a:

$a|0\rangle = 0$ Excited states are given by $\frac{(a^+)^n}{\sqrt{n!}}|0\rangle = |n\rangle$

in first order we need to find

$$E_0^{(1)} = \langle 0|\lambda(a^+ + a)^4|0\rangle$$

$$(a^+ + a)^4 = ((a^+)^2 + a^+a + aa^+ + a^2)^2 = ((a^+)^4 + a^+aa^+a + a^4 + aa^+aa^+ +$$
$$+ (a^+)^3a + (a^+)^2aa^+ + (a^+)^2a^2 + a^+a(a^+)^2 + a(a^+)^3 + a^2(a^+)^2 +$$
$$+ a^+a^2a^+ + a^+a^3 + a(a^+)^2a + aa^+a^2 + a^2a^+a + a^3a^+$$

Now let's consider state $H_1|0\rangle$ all terms that contain a standing to the right of everything else go away

$$H_1|0\rangle = (a^+)^4 + (a^+)^2aa^+ + a(a^+)^3 + a^2(a^+)^2 + a^+a^2a^+ + a^3a^+$$

now let's use commutation relations to bring a in all terms to the right: $aa^+aa^+ \Rightarrow aa^+a^+a + aa^+ \Rightarrow 1$

$(a^+)^2aa^+ = (a^+)^3a + (a^+)^2 \to (a^+)^2$; $a(a^+)^3 = (a^+)^3a + 3(a^+)^2 \to 3(a^+)^2$;

$a^2(a^+)^2 = a(a^+)^2a + 2aa^+ = a(a^+)^2a + 2a^+a + 2 \to 2$; $a^+a(a^+)^2 = 2(a^+)^2 + (a^+)^3a$

$a^+a^2a^+ = a^+aa^+a + a^+a \to 0$; $a^3a^+ = a^2a^+a + a^2 \to 0$

thus we get $H_1|0\rangle = \lambda\left((a^+)^4 + 3(a^+)^2 + 3(a^+)^2 + 3\right)|0\rangle =$

$= \lambda\left((a^+)^4 + 6(a^+)^2 + 3\right)|0\rangle = \lambda\left(\sqrt{4!}\,|4\rangle + 6\sqrt{2}\,|2\rangle + 3|0\rangle\right)$

thus in first order of perturbation theory we get:

$$E_0^{(1)} = \langle 0|\lambda(a^+ + a)^4|0\rangle = \lambda \cdot 3.$$

Second order is given by matrix elements

$\langle 2|H_1|0\rangle = \lambda 6\sqrt{2}$ and $\langle 4|H_1|0\rangle = \lambda\sqrt{24}$

$$E_0^{(2)} = \frac{|\langle 2|H_1|0\rangle|^2}{E_0^{(0)} - E_2^{(0)}} + \frac{|\langle 4|H_1|0\rangle|^2}{E_0^{(0)} - E_4^{(0)}} = -\lambda^2\left(\frac{(6\sqrt{2})^2}{2} + \frac{(2\sqrt{6})^2}{4}\right)\frac{1}{\hbar\omega};$$

⑤ $E_0^{(2)} = -\frac{\lambda^2}{\hbar\omega}\cdot 42$; full energy is

$$\boxed{E_0 = \frac{\hbar\omega}{2} + 3\lambda - 42\frac{\lambda^2}{\hbar\omega} + O(\lambda^3)};$$

N3 Compendium N19.

Particle of mass m in 1^d potential $V(x) = V_0(x) + V_1(x)$

$V_0(x) = \frac{1}{2}m\omega^2x^2$;

$V_1(x) = \lambda|x|$;

ⓐ Assuming that $V_1(x)$ is a small perturbation to $V_0(x)$, compute the first order correction to the energy of the ground state.

Wave function for harmonic oscillator is given by

$$\psi_n^{(0)}(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}}\frac{1}{\sqrt{2^n n!}}H_n(\alpha x)e^{-\frac{\alpha^2x^2}{2}}, \text{ where } \alpha = \sqrt{\frac{m\omega}{\hbar}} \text{ and}$$

$H_n(\alpha x)$ are Hermite polynomials. We need $\psi_1(x)$ and $\psi_0(x)$

$$\psi_0^{(0)}(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}}e^{-\alpha^2x^2/2}; \quad \psi_1^{(0)}(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}}\sqrt{2}\alpha x\cdot e^{-\alpha^2x^2/2};$$

$$E_0^{(1)} = \langle\psi_0^{(0)}|V_1(x)|\psi_0^{(0)}\rangle = \lambda\int_{-\infty}^{+\infty}dx\,\frac{\alpha}{\sqrt{\pi}}e^{-\alpha^2x^2}|x| = 2\frac{\alpha}{\sqrt{\pi}}\lambda\int_0^{\infty}dx\,xe^{-\alpha^2x^2} =$$

$= 2\frac{\alpha}{\sqrt{\pi}}\cdot\frac{\lambda}{2\alpha^2}\Gamma(1)$ here and in next calculation it will be usefull to know $\int_0^\infty dx\,x^{z-1}e^{-x} = \Gamma(z)$

$$\boxed{E_0^{(1)} = \frac{\lambda}{\alpha\sqrt{\pi}}}$$

ⓑ Now compute 1 order correction to the excited state.

$$E_1^{(1)} = \langle\psi_1^{(0)}|V_1|\psi_1^{(0)}\rangle = \lambda\int_{-\infty}^{+\infty}dx\cdot\frac{\alpha}{\sqrt{\pi}}2\alpha^2x^2e^{-\alpha^2x^2}|x| =$$

$$= \frac{2\alpha^3\lambda}{\sqrt{\pi}}\cdot 2\int_0^\infty dx\,x^3e^{-\alpha^2x^2} = \frac{2\alpha^3\lambda}{\sqrt{\pi}}\int_0^\infty dt\cdot te^{-t}\cdot\frac{1}{\alpha^4} = \frac{2\alpha^3\lambda}{\sqrt{\pi}\alpha^4}\cdot\Gamma(2)$$

$$\boxed{E_1^{(1)} = \frac{2\lambda}{\alpha\sqrt{\pi}}};$$

(6) (N4) compendium N20

Let's consider hyperfine splitting of $l=0$ energy levels of a hydrogen atom. Let $\bar{I}$ be the spin of nucleus, and $\bar{S}$ - spin of electron. We consider corrections to the ground state of atom, i.e. $\psi_{100}(r) = \frac{2}{\sqrt{4\pi}}\left(\frac{Z}{a_\mu}\right)^{3/2}\exp\left(-\frac{Zr}{a_\mu}\right)$;

Perturbative correction to the Hamiltonian is given by $H' = \lambda\, \bar{S}\cdot\bar{I}\, \delta^{(3)}(\bar{r})$; Let's rewrite it in the following form:

$\bar{S}\cdot\bar{I} = \frac{1}{2}\left(\bar{J}^2 - \bar{S}^2 - \bar{I}^2\right)$; $\bar{J} = \bar{S} + \bar{I}$; $I - \frac{1}{2} < j < \frac{1}{2} + I$

thus $j = \begin{cases} I + \frac{1}{2} \\ I - \frac{1}{2} \end{cases}$

$$H' \cdot |1s\rangle = \lambda \delta^{(3)}(\bar{r})\, \bar{S}\cdot\bar{I}\, |1s\rangle = \frac{\hbar^2}{2}\lambda\, \delta^{(3)}(\bar{r})\left(j(j+1) - s(s+1) - I(I+1)\right)|1s\rangle =$$

$$= \frac{\hbar^2}{2}\lambda\, \delta^{(3)}(\bar{r}) \cdot \left(\left(I \pm \tfrac{1}{2}\right)\left(I \pm \tfrac{1}{2} + 1\right) - \frac{3}{4} - I(I+1)\right)|1s\rangle =$$

$$= \frac{\hbar^2}{2}\lambda\, \delta^{(3)}(\bar{r}) \begin{cases} I, & \text{if } j = \frac{1}{2} + I ; \\ -(I+1), & \text{if } j = I - \frac{1}{2} ; \end{cases}$$

Now we can find 1^{st} order correction in both cases.

$$\Delta E_{\pm}^{(1)} = \frac{\hbar^2 \lambda}{2}\begin{Bmatrix} I \\ -(I+1) \end{Bmatrix} \cdot \langle 1s | \delta^{(3)}(\bar{r}) | 1s \rangle =$$

$$= \frac{\hbar^2\lambda}{2}\begin{Bmatrix} I \\ -(1+I) \end{Bmatrix} \int d^3\bar{r}\, \delta^{(3)}(\bar{r})\, |\psi_{100}(\bar{r})|^2 = \frac{\hbar^2\lambda}{2} \cdot |\psi_{100}(0)|^2 \cdot \begin{Bmatrix} I \\ -(1+I) \end{Bmatrix} =$$

$$= \frac{\hbar^2\lambda}{2} \cdot \frac{1}{\pi}\left(\frac{Z}{a_\mu}\right)^3 \begin{Bmatrix} I \\ -(I+1) \end{Bmatrix}$$ in fact we are asked to find difference between this two energies

$$\Delta E = \Delta E_+ - \Delta E_- = \frac{\hbar^2\lambda}{2\pi}\left(\frac{Z}{a_\mu}\right)^3 (2I+1);$$

$$\boxed{\Delta E = \frac{\hbar^2\lambda}{2\pi}\left(\frac{Z}{a_\mu}\right)^3 (2I+1);}$$

7

N5 compendium 20

Consider case of 2 "coupled" h.o.

$$H = H_0 + H'$$

$$H_0 = \frac{\hbar\omega_1}{2}(aa^+ + a^+a) + \frac{\hbar\omega_2}{2}(bb^+ + b^+b)$$

$H' = \lambda\left((a^+)^2 b^2 + (b^+)^2 a^2\right)$; $[a,a^+]=1$; $[b,b^+]=1$; $[a,b]=[a,b^+]=0$

ground state $a|0,0\rangle = b|0,0\rangle = 0$, assume $\omega_1 \neq \omega_2$ - i.e. there are no degeneracies.

Find energy of the normalised state $|2,0\rangle = \frac{1}{\sqrt{2}}(a^+)^2|0\rangle$;

Energy on non perturbed system is given by

$\mathcal{E} = \frac{\hbar\omega_1}{2}(2n_1+1) + \frac{\hbar\omega_2}{2}(2n_2+1)$ in our case we have.

$n_1 = 2$; $n_2 = 0$; $\mathcal{E}_{2,0} = \frac{5\hbar\omega_1}{2} + \frac{1}{2}\hbar\omega_2$;

Now let's find $H'|2,0\rangle$ state

$H'|2,0\rangle = \lambda\left(\underbrace{(a^+)^2 b^2}_{0} + (b^+)^2 a^2\right)|2,0\rangle = \lambda (b^+)^2 a^2|2,0\rangle = 2\lambda|0,2\rangle$

only nonzero matrix element of perturbation is

$\langle 0,2|H'|2,0\rangle = 2\lambda$, then we conclud

1st order correction is

$$\Delta E^{(1)}_{2,0} = \langle 2,0|H'|2,0\rangle = 0$$

2nd order correction is $\Delta E^{(2)}_{2,0} = \sum_{\substack{n\neq m \\ n\neq 2 \\ m\neq 0}} \frac{|\langle n,m|H'|2,0\rangle|^2}{E_{2,0} - E_{n,m}}$

only contribution comes from

$n=0$, $m=2$ $E_{0,2} = \frac{5\hbar\omega_2}{2} + \frac{\hbar\omega_1}{2}$; $E_{20} - E_{02} = 2\hbar(\omega_1 - \omega_2)$

$$\Delta E^{(2)}_{2,0} = \frac{|\langle 0,2|H'|2,0\rangle|^2}{2\hbar(\omega_1-\omega_2)} = \frac{2\lambda^2}{\hbar(\omega_1-\omega_2)}$$

$$\boxed{E_{2,0} = \frac{\hbar}{2}(5\omega_1 + \omega_2) + \frac{2\lambda^2}{\hbar(\omega_1-\omega_2)};}$$

(1) # Session 8 (real hydrogen atom)

Hydrogen-like atom levels are highly degenerate. On this session we will consider corrections to this energy levels and use degenerate perturbation theory.

Note exclude deg. perturbation theory from previous session and include it here.

In difference with non degenerate perturbation theory here zero order w.f. is not 1 state anymore but rather linear combination of wave functions. $|\psi_n^{(0)}\rangle$, thus we have $|\psi\rangle = \sum_{n'} b_{n'n} |\psi_{n'}^{(0)}\rangle + \sum_{k=1}^{\infty} \varepsilon^k |\psi^{(k)}\rangle$. First question coming is how should we determine $b_{n'n}$ coefficients? Let's introduce $|\chi_n^{(0)}\rangle = \sum_{n'} b_{n'n} |\psi_{n'}^{(0)}\rangle$ substituting into Schrodinger equation we get $\langle\psi_{n'}^{(0)}| H' |\chi_n^{(0)}\rangle = E_n^{(1)} \langle\psi_{n'}^{(0)}|\chi_n^{(0)}\rangle; \Rightarrow$

$$\boxed{\sum_{n''} H'_{n'n''} b_{n''n} = \Delta E_n b_{n'n}}$$

and thus we are just solving eigenvalues and eigenfunctions equation.

Problem N1

Consider a spin-orbit type coupling applied to the harmonic oscillator

$$H_{so} = \frac{1}{2m^2c^2} \bar{S} \cdot \bar{L} \cdot \frac{1}{r} \frac{dV(r)}{dr}; \text{ where } V(r) = \frac{1}{2} m^2\omega^2 r^2.$$

Compute the changes to the energies of the harmonic operator states from H_{so}.

First remind that energy spectrum of 3 dimensional h.o. is given by $E_n^{(0)} = \hbar\omega(n+\frac{3}{2})$ with degeneracy $\frac{(n+1)(n+2)}{2}$

Let's rewrite hamiltonian in the following form

$\frac{1}{r}\frac{d}{dr} V(r) = \frac{1}{r} m^2\omega^2 r = m^2\omega^2$; $\quad \bar{S}\cdot\bar{L} = \frac{1}{2}(\bar{J}^2 - \bar{L}^2 - \bar{S}^2)$; thus

$$H_{so} = \frac{\omega^2}{2c^2} \frac{1}{2}(\bar{J}^2 - \bar{L}^2 - \bar{S}^2) \Rightarrow H_{so} = \frac{\omega^2}{4c^2}(\bar{J}^2 - \bar{L}^2 - \bar{S}^2);$$

Now we should calculate matrix elements of H_{so} in

(1) some basis. The question is how should we choose this basis? The best way is to choose it in such way that H_{so} would be diagonal already this is in our case $|j, m; l, s\rangle$ in this case we get

$$\bar{S}\cdot\bar{L}\,|j,m;l,s\rangle = \frac{1}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)\hbar^2\,|j,m;l,s\rangle$$

there are 2 cases possible $j = l \pm \frac{1}{2}$; thus

$$\bar{S}\cdot\bar{L}\,|j,m;l,s\rangle = \begin{cases} \frac{\hbar^2}{2}\left((l+\frac{1}{2})(l+\frac{3}{2}) - l(l+1) - \frac{3}{4}\right)|j,m;l,s\rangle \\ \frac{\hbar^2}{2}\left((l-\frac{1}{2})(l+\frac{1}{2}) - l(l+1) - \frac{3}{4}\right)|j,m;l,s\rangle \end{cases} =$$

$$= \begin{cases} \frac{\hbar^2}{2}l\,|j,m;l,s\rangle \,; & j = l+\frac{1}{2}; \\ -\frac{\hbar^2}{2}(l+1)\,|j,m;l,s\rangle \,; & j = l-\frac{1}{2}; \end{cases}$$ thus energy corrections

are given by

$$E^{(1)}_{j=l+\frac{1}{2}} = \langle l+\tfrac{1}{2}, l\,|\,H_{so}\,|\,l+\tfrac{1}{2}, l\rangle = \frac{\hbar^2\omega^2 l}{4mc^2};$$

$$E^{(1)}_{j=l-\frac{1}{2}} = \langle l-\tfrac{1}{2}, l\,|\,H_{so}\,|\,l-\tfrac{1}{2}, l\rangle = -\frac{\hbar^2\omega^2(l+1)}{4mc^2};$$

Now for 3d h.o. we know that $l = n - 2k_r$ $k_r \in \mathbb{N}$ thus for n^{th} level of spherical h.o. we get $E^{(0)} = \hbar\omega(n+\frac{3}{2})$ and set of corrections for each value of l wich is ranged as

$l = n, n-2, \dots, 2, 0$ if n is even

$l = n, n-1, n-3, \dots, 1$ if n is odd

③ Problem 2 (Stark effect)

$H_S = e\bar{r}\cdot\bar{E} = eEr\cos\theta$ - this is our correction hamiltonian of hydrogen atom in external electric field.

ⓐ Using H_s as a perturbation, show that there is no correction to the ground-state energy to first order in perturbation theory.

Ground state w.f. for hydrogen atom is given by:

$\psi_{100}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_B}\right)^{3/2} e^{-r/a_B}$; Correction for energy is given by:

$$E^{(1)}_{100} = \langle \psi_{100} | H_s | \psi_{100}\rangle = \int_0^\infty dr\, r^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi\, \psi^*_{100}(r,\theta,\varphi) H_s \psi_{100}(r,\theta,\varphi) =$$

$$= \frac{eE}{\pi (a_B)^3}\int_0^\infty dr\cdot r^2 \cdot \int_0^\pi d\theta\cdot\sin\theta \int_0^{2\pi} d\varphi\, r\cos\theta\, e^{-2r/a_B} \Rightarrow$$ if we consider

integral over θ angle we get $\int_0^\pi d\theta\cdot \frac{1}{2}\sin 2\theta = -\frac{1}{2}\cos 2\theta\Big|_0^\pi = 0$

thus $E^{(1)}_{100} = 0$; Note that this is nondegenerate perturbation theory because our states are non-degenerat, but if we proceed further to the higher levels we get degenerate perturbation theory.

ⓑ First excited state is four-fold degenerate with states $|2,0,0\rangle$; $|2,1,1\rangle$, $|2,1,0\rangle$ and $|2,1,-1\rangle$. Find the lowest order corrections to the energy using degenerate perturbation theory.

In general for hydrogen atom we have $\psi_{n\ell m} = R_{n\ell}(r) Y_{\ell m}(\theta,\varphi)$

thus in our case

$$|2,0,0\rangle = R_{20} Y_{00} = R_{20}\frac{1}{\sqrt{4\pi}};$$

$$|2,1,\pm1\rangle = R_{21} Y_{1\pm1} = R_{21}(r)\cdot\left\{\mp\sqrt{\frac{3}{8\pi}}\, e^{\pm i\varphi}\sin\theta\right\};$$

$$|2,1,0\rangle = R_{21} Y_{10} = R_{21}(r)\cdot\sqrt{\frac{3}{4\pi}}\cos\theta;$$

$$R_{20} = \frac{2}{a_B^{3/2}}\exp\left(-\frac{r}{a}\right);\ R_{20} = \frac{1}{\sqrt{2}} a_B^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a_B}\right)\exp\left(-\frac{r}{2a_B}\right);$$

(4) $R_{21} = \frac{1}{\sqrt{24}} a_B^{-3/2} \frac{r}{a_B} \exp\left(-\frac{r}{2a_B}\right)$; (table 4.7 in Griffiths)

now we should calculate all matrix elements of form $\langle 2l'm'|H_s|2lm\rangle = \int d^3\bar{r} \cdot \Psi^*_{2l'm'} \Psi_{2lm} eE \cdot r\cos\theta$

First let's consider integration over azimuthal angle φ

We know that $\Psi_{nlm} \sim e^{im\varphi}$ thus

$$\int_0^{2\pi} d\varphi\, e^{i(m-m')\varphi} = \begin{cases} 0 & \text{if } m' \neq m; \\ 2\pi & \text{if } m' = m; \end{cases}$$

thus we are interested only in $m' = m$ case

Now if we consider integral over θ angle, we can show directly that all element's $\langle l'm|Z|lm\rangle = 0$ if $l' = l$.

$$\langle 200|H_s|200\rangle \propto \int_0^\pi d\theta \cos\theta \sin\theta = 0$$

$$\langle 21\pm1|H_s|21\pm1\rangle \sim \int_0^\pi d\theta \cdot \sin^3\theta \cos\theta = 0$$

$$\langle 210|H_s|210\rangle \sim \int_0^\pi d\theta \cdot \sin\theta \cos^3\theta = 0$$

the only nonzero element is thus given by $\langle 200|H_s|210\rangle$ let's evaluate it:

$$2\pi \int_0^\infty \int_{-1}^1 dr\, d\cos\theta\; r^2 \cdot R_{20}(r) \cdot R_{21}(r) \cdot \frac{\sqrt{3}}{4\pi} \cos\theta \cdot eEr\cos\theta =$$

$$= \frac{\sqrt{3}eE}{2} \left(\int_{-1}^1 d\cos\theta \cos^2\theta\right)\left(\int_0^\infty dr \cdot r^3 \cdot \frac{1}{\sqrt{24}} a_B^{-3/2} \cdot \frac{r}{a_B} \exp\left(-\frac{r}{2a_B}\right) \times\right.$$

$$\left.\times \frac{1}{\sqrt{2}} a_B^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a_B}\right) \exp\left(-\frac{r}{2a_B}\right)\right); \quad \int_{-1}^1 d\cos\theta \cos^2\theta = \frac{2}{3}$$

$$\int dr\, r^3 \cdot a_B^{-3} \frac{r}{a_B}\left(1 - \frac{1}{2}\frac{r}{a_B}\right) \exp\left(-\frac{r}{a_B}\right) = a_B \int_0^\infty dt\, t^4 \left(1 - \frac{1}{2}t\right) \exp(-t);$$

Now we use our formula $\int_0^\infty dt\, t^n e^{-t} = n!$ wich gives us

$a_B \cdot \left(4! - \frac{1}{2} 5!\right) = a_B(24 - 60) = -36 a_B$; taking all terms together we get

$$\langle 200|H_s|210\rangle = \frac{\sqrt{3}eE}{2} \cdot \frac{2}{3} \cdot \frac{1}{4\sqrt{3}} \cdot (-36a_B) = -3eEa_B$$

⑤ thus matrix of perturbative part of Hamiltonian is given by.

$$\langle 2 l' m' | H_s | 2 l m \rangle = \begin{bmatrix} 0 & 0 & -3eEa_B & 0 \\ 0 & 0 & 0 & 0 \\ -3eEa_B & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Now to find first order corrections for energy we should calculate eigen values of this matrix:

$\lambda^4 - (3ea_BE)^2\lambda^2 = 0 \Rightarrow \lambda = 0$ or $\lambda = \pm 3eEa_B$;

thus $\boxed{E^{(1)}_{(2)} = 0;\ E^{(1)}_2 = \pm 3ea_BE;}$ $\Rightarrow$ after turning electric field on on 4-fold degenerate level splits into 3 levels.

(c) Find the basis where the first-order matrix elements for the first excited states are diagonalized.

here we should just find eigenvectors of perturbation matrix corresponding to it's eigenvalues.

(I) $E^{(1)}_2 = -3ea_BE$ we get matrix

$$\begin{bmatrix} +1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \qquad \begin{matrix} a = c \\ b = d = 0 \end{matrix} \qquad |\psi_-\rangle = \frac{1}{\sqrt{2}}(|\psi_{200}\rangle + |\psi_{210}\rangle)$$

(II) $E^{(1)}_2 = 3ea_BE$

$$\begin{bmatrix} -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0 \Rightarrow \begin{matrix} a = -c \\ b = d = 0 \end{matrix} \qquad |\psi_+\rangle = \frac{1}{\sqrt{2}}(|\psi_{200}\rangle - |\psi_{210}\rangle)$$

(III) $E^{(1)}_2 = 0$

$$\begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0$$

$a = c = 0$ $|\psi_0\rangle$ is any normalised linear combination of $|\psi_{211}\rangle$ and $|\psi_{21-1}\rangle$;

(d) In this diagonal basis, compute the expectation value for the electric dipole moment $\bar{p} = -e\bar{r}$ for this states. Show that this and your results in (b) are consistent with an electric dipole in the presence of a constant

⑥ electric field.

We should calculate here elements

$\langle \psi_\pm | \bar{r} | \psi_\pm \rangle$, note that both $|\psi_+\rangle$ and $|\psi_-\rangle$

contain only states whith $m=0$. Let's consider elements

$$\langle 2l'0|x|2l0\rangle = \langle 2l'0|r\cos\varphi\sin\theta|2l0\rangle \sim \int_0^{2\pi} d\varphi \cos\varphi = 0$$

$$\langle 2l'0|y|2l0\rangle = \langle 2l'0|r\sin\varphi\sin\theta|2l0\rangle \propto \int_0^{2\pi} d\varphi \sin\varphi = 0$$

thus only nonzero elements are given by z:

$$\langle 2l'0|z|2l0\rangle \Rightarrow \langle 2l'0|\bar{p}|2l0\rangle = \left[0 \;\; 0 \;\; \langle 2l'0|H_s|2l0\rangle\left(-\frac{1}{E}\right)\right]^T$$

Now we know that

$H_s|\psi_\pm\rangle = \pm 3eEa_B|\psi_\pm\rangle$ and thus $\langle\psi_\pm|H_s|\psi_\pm\rangle =$

$= \pm 3eEa_B$ and finally if we consider states

with $l=0, m=0$, and $l=\pm1, m=\pm1$ we get

$$\langle 200|x|200\rangle \text{ (and } \langle 200|y|200\rangle) \sim \int_0^{2\pi} d\varphi \cos\varphi \text{ (or } \sin\varphi) = 0$$

$$\langle 21\pm1|x|21\pm1\rangle \approx \int d\varphi \cos\varphi = 0 \qquad \langle 21\pm1|x|21\mp1\rangle \sim \int d\varphi \cos\varphi \cdot e^{-2i\varphi} = 0$$

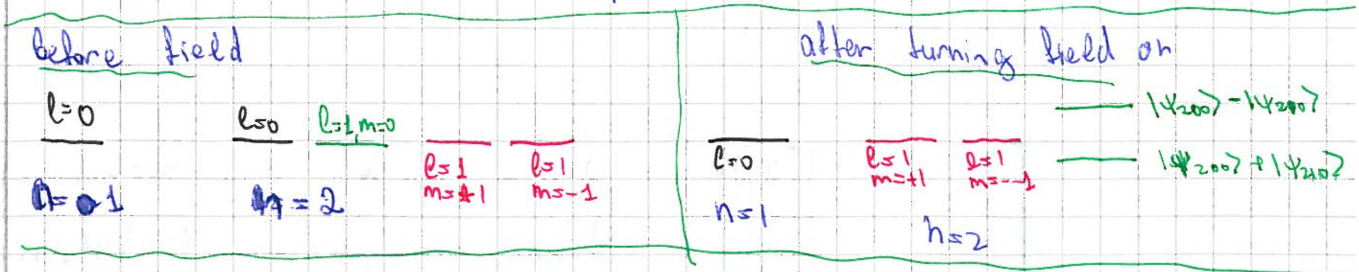
$$\langle 21\pm1|y|21\pm1\rangle \sim \int d\varphi \sin\varphi = 0 \qquad \langle 21\pm1|y|21\mp1\rangle \approx \int d\varphi \sin\varphi\, e^{2i\varphi} = 0$$

and we left again with z-component which is

proportional to H_s, while we know that

$\hat{H}_s|\psi_{21\pm1}\rangle = 0$

Thus, let's conclyd this problem:



When we turn field on state $|100\rangle$ doesn't change but second 4-degenerate level splits into 3 levels: levels whith $|21\pm1\rangle$ stay at the same energy (this level is double degenerate) and states $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|200\rangle \pm |210\rangle)$ correspond to dipole moment $\langle \bar{p}\rangle = \begin{bmatrix} 0 \\ 0 \\ \pm 3ea_B \end{bmatrix}$ and energy shift $\Delta E = -\bar{E}\langle\bar{p}\rangle$ which coinsides whit our intuition.

① Session 9

Now we move to the systems of several particles. We assume that total wave function is given by

$\psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = \psi_{K_1}(\bar{r}_1)\psi_{K_2}(\bar{r}_2)\cdots\psi_{K_N}(\bar{r}_N)$;

Now we can introduce operator P_{ij} that interchange 2 particles i and j. If particles are really identical probability distribution shouldn't change thus, for example

$P_{12}\psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) = \psi(\bar{r}_2; \bar{r}_1, \dots, \bar{r}_N) = e^{i\alpha}\psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N) \Rightarrow$

wave function can change only overall phase, ~~thus~~ if we change position of particles twice we obtain same position again, thus $P_{12}^2 = 1$;

there are 2 kind of particles in nature

bosons are symmetric under interchange of particles

fermions are antisymmetric. As the simpiest example we will further consider just 2 particles:

$\psi(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_1(\bar{r}_1)\psi_2(\bar{r}_2) \pm \psi_2(\bar{r}_1)\psi_1(\bar{r}_2)\right)$, here

upper sign correspond to bosons and the lower one - to fermions. From here we can easy see that two fermions can't be placed at the same point - this is Pauli exclusion principle. (to see this put $\bar{r}_1 = \bar{r}_2$) But if we introduce spin we can put 2 particles in 1 point. For example let's consider 2 fermions with spins $\frac{1}{2}$. We should overal w. function that is product of space wave function and spin part:

$$\psi_{S=0}(\bar{r}_1; \bar{r}_2) = \frac{1}{\sqrt{2}}\underbrace{\left(\psi_1(\bar{r}_1)\psi_2(\bar{r}_2) + \psi_2(\bar{r}_1)\psi_1(\bar{r}_2)\right)}_{\text{Symm.}}\underbrace{\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)}_{\text{antisymmetric.}}$$

$$\psi_{S=1}(\bar{r}_1; \bar{r}_2) = \frac{1}{\sqrt{2}}\underbrace{\left(\psi_1(\bar{r}_1)\psi_2(\bar{r}_2) - \psi_1(\bar{r}_2)\psi_2(\bar{r}_1)\right)}_{\text{antisymmetric.}}\underbrace{\left\{\begin{array}{l}|\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right) \\ |\downarrow\downarrow\rangle\end{array}\right.}_{\text{antisymmetric.}}$$

② (N1) compendium 24

N noninteracting spinless particles with mass m in the two dimensional potential $V(x;y)$, where:

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

For the following you may use known results for a single particle on this potential.

ⓐ Assuming that the particles are unidentical, find the ground state energy.

If particles are unidentical they can be placed on the same p level

Energy of 2d oscillator is given by

$$E = \hbar\omega\left(n_x + \frac{1}{2} + n_y + \frac{1}{2}\right) = \hbar\omega\left(n_x + n_y + 1\right)$$

Degeneracy of each level is given by $\sum_{n_x=0}^{n} 1 = n$

Because given n_x fixes n_y at the same time.

Thus on each n^{th} level we can place n fermions (we don't take spin into account yet) and any number of bosons

thus all unidentical particles and all identical bosons will be placed on the lowest level which energy

$E = \hbar\omega$; thus for unidentical particals or identical bosons we get energy being equal. $\boxed{E = N\hbar\omega;}$

For fermions everything is a little bit more complicated.

We should find maximal occupation number;

$$N = \sum_{n>0}^{n_{max}} n = \frac{n_{max}(n_{max}+1)}{2} \approx \frac{n_{max}^2}{2} \text{ (assuming } N \gg 1) \qquad n_{max} = \sqrt{2N};$$

Now total energy will be given by:

$$E = \sum_{n>0}^{n_{max}} n \cdot \hbar\omega n \approx \int_0^{n_{max}} \omega\hbar (x^2+x)\, dx \approx \frac{1}{3}\hbar\omega\, n_{max}^3 = \frac{1}{3}\hbar\omega (2N)^{3/2};$$

$$\boxed{E = \frac{1}{3}\hbar\omega (2N)^{3/2};}$$

③ (N2) compendium 25

Consider 3 identical particles with mass m and spin $\frac{1}{2}$ in 3-dimensional potential $V(r) = \frac{1}{2} m\omega^2 r^2$;

ⓐ Assuming that the particles are fermions, find the ground state energy.

For this problem it will be useful to remind some facts about 3 dimensional oscillator

Energy of n^{th} level of 3d h.o. is given by

$\mathcal{E}_n = \hbar\omega\left(n + \frac{3}{2}\right)$; degeneracy is $N = \frac{(n+1)(n+2)}{2}$

If we assume now that we have 3 fermions

We assume they have spin $s=\frac{1}{2}$ thus 2 fermions can be placed on the lowest level $n=0$ and 1 will be placed on the level $n=1$ and we get: Thus lowest energy is given by:

$\mathcal{E}_0 = 2 \cdot \frac{3}{2}\hbar\omega + \frac{5}{2}\hbar\omega = \frac{11}{2}\hbar\omega$; $\quad \mathcal{E}_0 = \frac{11}{2}\hbar\omega$;

ⓑ What is degeneracy of the lowest energy level?

two fermions are placed on the level $n=0$ and there is no degeneracy, but third one is on level $n=1$ which is triple degenerate. The over all degeneracy is the same.

$\boxed{N=3 \text{ degeneracy.}}$

ⓒ What is orbital momentum of the state.

We shoud remind here the result of problem 5 from set 4 where we have found that lowest state have $l=0$ and 1^{st} excited state - $l=1$ thus $L=1$ Two fermions on level $n=0$ should be in singlet state $s=0$, thus over all spin is $S=\frac{1}{2}$ and momentum take values $j = l \pm \frac{1}{2} = \frac{1}{2}, \frac{3}{2}$;

$\boxed{L=1, \quad J=\frac{1}{2}, \frac{3}{2};}$

(4) (N3)

2s and 2p states of hydrogen atom are degenerate but 2s is filled before 2p. Consider lithium which has $Z=3$ and 2 electrons in the 1s shell. Inner electrons screen nucleus; so the last electron sees $Z=1$;

(a) find expectation value $\langle r^2 \rangle$ for the 2s and 2p states, assuming $Z=1$;

r^2 doesn't depend on angles so that we integrate only over radial coordinates while looking for average, and we are interested only in $R_{nl}(r)$ function. From table 4.7. in Griffiths we find:

$$R_{20}(r) = 2\left(\frac{Z}{2a_B}\right)^{3/2}\left(1-\frac{Zr}{2a_B}\right)e^{-\frac{Zr}{2a_B}};$$

$$R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_B}\right)^{3/2}\left(\frac{Zr}{a_B}\right)e^{-\frac{Zr}{2a_B}};$$

$$\langle r^2\rangle_{2s} = \int_0^\infty dr\, r^2 R_{20}^*(r)\, r^2 R_{20}(r) = \int_0^\infty dr\, r^4\, 4\frac{Z^3}{8a_B^3}\left(1-\frac{Zr}{2a_B}\right)^2 e^{-\frac{Zr}{a_B}} =$$

$$= \frac{1}{2}\frac{a_B^2}{Z^2}\int_0^\infty dt\, t^4\left(1-\frac{t}{2}\right)^2 e^{-t} = \frac{1}{2}\frac{a_B^2}{Z^2}\int dt\left(t^4 - t^5 + \frac{1}{4}t^6\right)e^{-t} =$$

$$= \frac{1}{2}\frac{a_B^2}{Z^2}\left(4! - 5! + \frac{1}{4}6!\right) = \frac{1}{2}\frac{a_B^2}{Z^2}(24-120+180) = 42\left(\frac{a_B}{Z}\right)^2$$

$$\langle r^2\rangle_{2p} = \int_0^\infty dr\, r^4 (R_{21}(r))^2 = \int_0^\infty dr\, r^4\, \frac{1}{3}\left(\frac{Z}{2a_B}\right)^3 \frac{Z^2r^2}{a_B^2} e^{-\frac{Zr}{a_B}} =$$

$$= \int_0^\infty dt\, t^6 e^{-t}\cdot\frac{1}{3\cdot 8}\left(\frac{a_B}{Z}\right)^2 = \frac{6!}{24}\left(\frac{a_B}{Z}\right)^2 = 30\left(\frac{a_B}{Z}\right)^2$$

$$\boxed{\langle r^2\rangle_{2s} = 42\left(\frac{a_B}{Z}\right)^2; \quad \langle r^2\rangle_{2p} = 30\left(\frac{a_B}{Z}\right)^2;}$$

(b) Find the probability that the 2s and 2p states are inside the rms radius for a 1s state with $Z=3$. Argue why your result means that the 2s state in lithium has less energy then the 2p state.

(5) i. The radius of 1s orbital is $\frac{a_B}{\sqrt{Z^2}} = \frac{a_B}{\sqrt{3^2}} = r_{1s}$

thus the probability of 2s and 2p states are inside rms radius of 1s state whith $Z=3$ is given by

$$P_{2s} = \int_0^{r_{1s}} \frac{1}{2} \frac{Z^3}{a_B^3} \left(1 - \frac{Zr}{2a_B}\right)^2 e^{-\frac{Zr}{a_B}} r^2 dr = \frac{1}{2}\int_0^{\sqrt{3}} dt\, t^2\left(1-\frac{t}{2}\right)^2 e^{-t}$$

$$\int_0^x dt\left(t^2 - t^3 + \frac{1}{4}t^4\right)e^{-t} = \left(-t^2 + \cancel{t^3} - \frac{1}{4}t^4 - 2t + 3\cancel{t^2} - \cancel{t^3} - 2 + 6t - 3\cancel{t^2} + 6 - \right.$$
$$\left. - 6t - 6\right) e^{-t}\Big|_0^x = \left(-\frac{1}{4}t^4 - t^2 - 2t - 2\right)e^{-t}\Big|_0^x =$$

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

$$P_{2s} = \frac{1}{2}\left\{2 - \left(\frac{1}{4}\frac{1}{9} + \frac{1}{3} + 2\sqrt{3} + 2\right)e^{-\sqrt{3}}\right\} = 0{,}013$$; probability is

1,3%

$$P_{2p} = \int_0^{r_{\cdot}} dr \frac{r^2}{3} \cdot \frac{Z^3}{8a_B^3} \frac{Z^2 r^2}{a_B^2} e^{-\frac{Zr}{a_B}} = \frac{1}{24}\int_0^{\sqrt{3}} dt\, t^4 e^{-t} =$$

$$= -\frac{1}{24}\left(t^4 + 4t^3 + 12t^2 + 24t + 24\right)e^{-t}\Big|_0^{\sqrt{3}} \approx 3{,}3 \cdot 10^{-4}$$ probability is

0,03% thus 2 orders smaller than probability for 2s state

Note here that $\langle r^2\rangle_{2s} > \langle r^2\rangle_{2p}$ nevertheless

Thus 2s can be effected by bare nucleus whith higher probability and thus it has smaller energy.

⑥ N4

Consider two electrons in a p-orbital.

(a) ignoring spins, write down all 9 states, using a basis where they are either symmetric or antisymmetric.

Both electrons are on p-orbital thus we have $l_{1,2} = 1$, $m_{1,2} = \pm 1, 0$;

as usually we start with the highest weight state $|2,2\rangle = |1,1\rangle$ (here on l.h.s we write $|j,m\rangle$ state and on r.h.s. $|m_1, m_2\rangle$ state) Acting as usually with lowering operator we get

$|2,1\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$; $\quad |1,1\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$ comes from orthogonality condition

$|2,0\rangle = \frac{1}{\sqrt{6}}(|1\,-1\rangle + |-1\,1\rangle + 2|0\,0\rangle)$;

$|2\,-1\rangle = \frac{1}{\sqrt{2}}(|0\,-1\rangle + |-1\,0\rangle)$; $\quad |1,0\rangle = \frac{1}{\sqrt{2}}(|1\,-1\rangle - |-1\,1\rangle)$

$|2\,-2\rangle = |-1\,-1\rangle$; $\quad |1\,-1\rangle = \frac{1}{\sqrt{2}}(|0\,-1\rangle - |-1\,0\rangle)$

and finally $|0\,0\rangle$ state can be found from orthogonality condition.

$|0\,0\rangle = \frac{1}{\sqrt{6}}(|1\,-1\rangle + |-1\,1\rangle - 2|0\,0\rangle)$

note that states white $l=2$ and $l=0$ are even under interchange of particles, while $l=1$ states are odd.

(b) we have done all construction explicitely but just to check that $|1,1\rangle$ is really the state that corresponds to $l=1$ we should act with L_+ generator:

$L_+ |1,1\rangle = (L_{1+} + L_{2+}) \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle) = \frac{1}{\sqrt{2}}(|11\rangle - |11\rangle) = 0$

thus here $m = 1 = m_1 + m_2$ and $j = m$ (we have shown just

⑦ how that this is highest weight state)

(c) This can be done using Slater determinant.

$$|AS\rangle = \frac{1}{\sqrt{6}} \begin{vmatrix} |1\rangle_1 & |0\rangle_1 & |-1\rangle_1 \\ |1\rangle_2 & |0\rangle_2 & |-1\rangle_2 \\ |1\rangle_3 & |0\rangle_3 & |-1\rangle_3 \end{vmatrix} = \frac{1}{\sqrt{6}} \big(|1\,0\,{-1}\rangle + |0\,{-1}\,1\rangle +$$

$$+ |{-1}\,1\,0\rangle - |{-1}\,0\,1\rangle - |0\,1\,{-1}\rangle - |1\,{-1}\,0\rangle \big);$$

this corresponds to the projection $m=0$, let's act with L_+ operator we get.

$$L_+|AS\rangle = \frac{1}{\sqrt{3}} \big(|1\,1\,{-1}\rangle + |1\,0\,0\rangle + |1\,{-1}\,1\rangle + |0\,0\,1\rangle + |{-1}\,1\,1\rangle +$$

$$+ |0\,1\,0\rangle - |{-1}\,1\,1\rangle - |0\,0\,1\rangle - |1\,1\,{-1}\rangle - |0\,1\,0\rangle - |1\,0\,0\rangle - |1\,{-1}\,1\rangle \big) = 0$$

as $L_+|AS\rangle = 0$ we get $L = m = 0$;

another way to find L value is to find out how does L^2 acting on $|AS\rangle$ state. Here we shoul use.

$$L^2 = L_1^2 + L_2^2 + 2\vec{L}_1\vec{L}_2 = L_1^2 + L_2^2 + 2L_{1z}L_{2z} + L_{1+}L_{2-} + L_{1-}L_{2+};$$

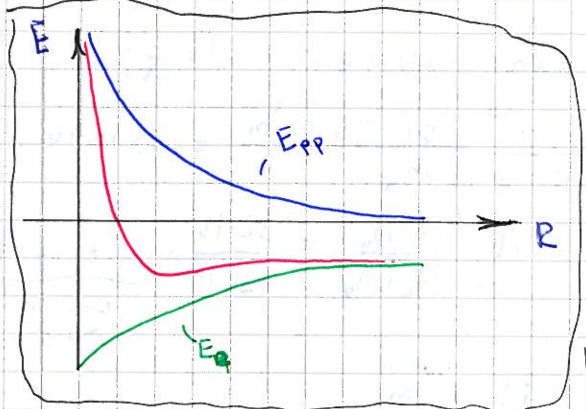
the same but for 3 particles but this is too long and boring. Described way of derivation is much more convinient.

(4)

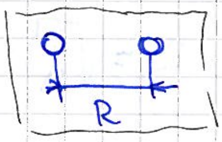
Session 10

Some small amount of theory

Assume we have system consisting of 2 nucleus and electron. Assume electron is in atomic groung state $E_H = -\frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 a_\mu} = -\frac{1}{2}\frac{\hbar^2}{\mu a_\mu^2}$; if $R \gg a_\mu$; now if we take $R=0$ this is just like single nucleus with charge $+2e$ and electron energy is lowered to $4E_H$; $E_{pp}(R) = \frac{e^2}{4\pi\varepsilon_0 R}$ is energy of nucleus interaction. and overall energy get some minimum value where overall force goes to 0



So in equilibrium position nucleus are separated by some distance R which give us the minimum of overall energy



Now we assume that there are som vibrations about this equilibrium position. to find it we expand $V(R) = V(R_0) + \frac{1}{2}(R-R_0)^2 \frac{d^2V}{dR^2}\Big|_{R=R_0} + O((R-R_0)^3)$; the full hamiltonian is then given by:

$$H_{diatom} = -\frac{\hbar^2}{2M}\frac{d^2}{dR^2} + \frac{\ell(\ell+1)\hbar^2}{2MR^2} + V(R) \quad \text{or}$$

$$H_{diatom} = H_{vib} + H_{rot} + V(R_0); \quad H_{vib} \approx -\frac{\hbar^2}{2M}\cdot\frac{d^2}{dR^2} + \frac{1}{2}k(R-R_0)^2;$$

$H_{rot} = \frac{\ell(\ell+1)\hbar^2}{2MR^2}$; for vibrational part we know that

$E_{vib} = \hbar\omega(n+\frac{1}{2})$; where $\omega^2 = \frac{k}{M}$. Now the question comes what is k? $V(R_0) \sim E_H$, $R_0 \sim a_\mu$ $\quad k \sim \frac{|E_H|}{a_\mu^2}$

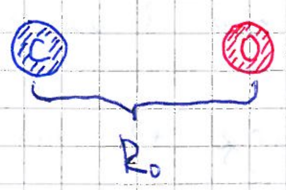
Frequencies are given by $h\nu_{vib} = \hbar\omega(n+\frac{1}{2})\Big|_{n=0}^{n=1} = \hbar\omega$

$$h\nu_{rot} = \frac{\hbar^2}{2MR^2}\ell(\ell+1)\Big|_{\ell=0}^{\ell=1} = \frac{\hbar^2}{MR_0^2}$$

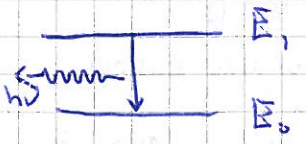
②

Problem 1

Carbon monoxide (CO) has an absorption line at 2,60 nm in transition from the molecular $l=1$ to the $l=0$ state. Find moment of inertia and mean separation.



$$E_{rot} = \frac{l(l+1)\hbar^2}{2MR_0^2}$$ rotational frequencies are given by energy difference between levels



$$h\nu = E_{rot}\Big|^{\text{before}}_{\text{after}} = E_{rot}^{l=1} - E_{rot}^{l=0} = \frac{\hbar^2}{MR_0^2}$$

if we consider molecule as rod with two balls on the ends we can write $\nu = \frac{c}{\lambda}$; $h = 2\pi\hbar$

$$I = MR_0^2 = \frac{\hbar^2}{h\nu} = \frac{\hbar\lambda}{2\pi c} = \frac{1{,}054\cdot10^{-34}\,J\cdot s\cdot 2{,}6\cdot10^{-3}\,m}{2\cdot\pi\cdot 3\cdot10^{8}\,m/s} = 1{,}45\cdot10^{-46}\,kg\,m^2$$

now we can estimate R_0. $M = \frac{M_c M_o}{M_c + M_o} = \frac{12\cdot16}{12+16}\cdot\underbrace{1{,}67\cdot10^{-27}kg}_{\text{proton mass}}$

$M = 1{,}14\cdot10^{-26}\,kg$; $R_0 = \sqrt{\frac{I}{M}} = 1{,}13\cdot10^{-10}\,m$

Problem 2

Hydrogen fluoride (HF) has it's lowest rotational frequency mode at 651,1 GHz and a vibrational mode at 12400 GHz. Find mean separation between the two nuclei and the spring constant k.

Lowest vibrational mode is given by

$h\nu_{rot} = \frac{\hbar^2}{MR_0^2} = \frac{\hbar^2}{I}$; $M = \frac{M_H \cdot M_F}{M_H + M_F} = \frac{19}{20}\cdot 1{,}66\cdot10^{-27}\,kg = 1{,}59\cdot10^{-27}\,kg$;

$\nu_{vib} = \frac{\omega}{2\pi}$; $\omega = \sqrt{\frac{k}{M}}$; thus we get

$$R_0 = \sqrt{\frac{\hbar^2}{Mh\nu}} = \sqrt{\frac{\hbar}{2\pi M\nu}} = \left[\frac{1{,}05\cdot10^{-34}\,J\cdot s}{2\cdot3{,}14\cdot1{,}6\cdot10^{-27}\,kg\cdot 651{,}1\cdot10^{9}\,s^{-1}}\right] = 1{,}27\cdot10^{-10}\,m$$

$$k = 4\pi^2\nu_{vib}^2\cdot M = 1{,}6\cdot10^{-27}\cdot(1{,}24\cdot10^{13}\,s^{-1})^2\cdot 4\cdot10 \approx 9{,}65\cdot N/m;$$

(3)

Problem 3

Suppose that the electron in the H_2^+ molecule were replace by a muon, which has the same charge as electron but weights 207 times more than electron. Estimate the nuclear separation and binding energy of the molecule.

We know (see long derivation in hand out) that nucleus separation is given by

$E_{Bind} \sim E_H$, $R \sim a_\mu$, here a_μ is Bohr radius and coefficients are complicated but we are not interested in this coefficients right now. $\left(E_H = -\frac{\hbar^2}{2\mu a_\mu^2};\ a_\mu = \frac{\hbar^2 \cdot 4\pi\varepsilon_0}{e^2 \mu}\right)$

$$\frac{E_{Bind}^{(\mu)}}{E_{Bind}^{(e)}} = \frac{E_H^{(\mu)}}{E_H^{(e)}} = \frac{m_e a_e^2}{m_\mu a_\mu^2} = \frac{m_\mu}{m_e} = 207$$

$$E_{Bind}^{(\mu)} = 207\, E_H = 207\,(-2{,}8\,eV) = -580\,eV;$$

taken from lecture

$$\frac{R_H^{(\mu)}}{R_{H_2^+}} = \frac{a_\mu}{a_e} = \frac{m_e}{m_\mu} = \frac{1}{207};\quad R_H^{(\mu)} = \frac{R_{H_2^+}}{207};\quad R_H^{(\mu)} = \frac{1{,}06\,\mathring{A}}{207} = 5\cdot 10^{-3}\,\mathring{A};$$

Problem 4

The rotational part of the diatomic Hamiltonian is usually treated at fixed R_0. Assuming the rotational energies ~~[illegible]~~ are much smaller than the vibrational modes as a function of l by assuming the rotational part of the Hamiltonian is $H_{rot} = \frac{l(l+1)\hbar^2}{2MR^2}$. In other words, don't treat R as a constant. You should be able to express your answer in terms of ν_{vib} and ν_{rot}, where ν_{rot} is the frequency coming from the $l=1$ to $l=0$ transition

Let's take rotational hamiltonian in the following form

$$H_{rot} = \frac{l(l+1)\hbar^2}{2M(R^*+R_0)^2} = \frac{l(l+1)\hbar^2}{2M}\left\{\frac{1}{R_0^2} - \frac{2}{R_0^3}(R-R_0) + \frac{1}{2!}\frac{6}{R_0^4}(R-R_0)^2 + \dots\right\}$$

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Substituting this back to hamiltonian we get

$$H_{diatom} = \frac{l(l+1)}{2M}\hbar^2\left(\frac{1}{R_0^2} - \frac{2}{R_0^3}(R-R_0) + \frac{3}{R_0^4}(R-R_0)^2 + \dots\right) -$$

$$- \frac{\hbar^2}{2M}\frac{d^2}{dR^2} + \frac{1}{2}k(R-R_0)^2 + V(R_0)$$

$$H_{diatom} = -\frac{\hbar^2}{2M}\frac{d^2}{dR^2} + \frac{1}{2}\underbrace{\left(k + \frac{3l(l+1)\hbar^2}{2MR_0^4}\right)}_{k'}(R-R_0)^2 + \frac{l(l+1)\hbar^2}{2MR_0^2}\left(1 - \frac{2}{R_0}(R-R_0)\right) +$$

$$+ V(R_0)$$

$$h\nu'_{vib} = \hbar\sqrt{\frac{k'}{M}} = \frac{\hbar}{\sqrt{M}}\sqrt{k + \frac{3l(l+1)\hbar^2}{2MR_0^4}}$$

Now we use $4\pi^2\nu_{vib}^2 = \frac{k}{M} \Rightarrow k = 4\pi^2\nu_{vib}^2 M$

$h\nu_{rot} = \frac{\hbar^2}{MR_0^2}$ $\quad R_0^2 = \frac{\hbar}{2\pi M\nu_{rot}}$ thus we get:

$$\hbar\nu'_{vib} = \frac{\hbar}{\sqrt{M}}\sqrt{4\pi^2\nu_{vib}^2 M + \frac{3l(l+1)\hbar^2}{2M}\frac{4\pi^2M^2\nu_{rot}^2}{\hbar^2}} \Rightarrow$$

$$\Rightarrow \nu'_{vib} = 2\pi\nu_{vib}\sqrt{1 + \frac{3}{2}l(l+1)\cdot\frac{\nu_{rot}^2}{\nu_{vib}^2}}$$ as $\nu_{rot} \ll \nu_{vib}$ we get:

$$\boxed{\nu'_{vib} = \nu_{vib}\left(1 + \frac{3}{4}l(l+1)\frac{\nu_{rot}^2}{\nu_{vib}^2}\right)}$$