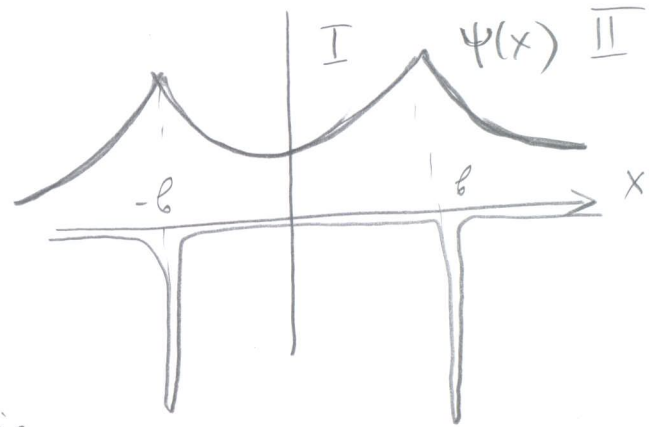


①  $V(x)$  is an even function. Therefore the eigenfunction of the Hamiltonian have definite parity. In fact, the ground state has to be even. Since  $\alpha$  is positive the bound state energy(ies) are negative,  $E < 0$ .

Since  $V=0$  everywhere except  $x = \pm b$ , the Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi, \quad x \neq \pm b$$



In region II the solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}, \quad \kappa = \sqrt{\frac{-2mE}{\hbar^2}}$$

We have to impose the square integrability of the wave function. That yields  $B=0$

In region I the solution is

$$\psi(x) = Ce^{-\kappa x} + De^{\kappa x} = F \cosh(\kappa x) + G \sinh(\kappa x)$$

Since  $\psi(x) = \psi(-x)$  we get  $G=0$ . Hence,

$$\psi(x) = \begin{cases} Ae^{-\kappa x}, & x > b \\ F \cosh(\kappa x), & 0 \leq x \leq b \end{cases}$$

The continuity of  $\psi$  at  $x=b$  requires that

$$Ae^{-\kappa b} = F \cosh(\kappa b)$$

Therefore

$$\psi(x) = \begin{cases} Fe^{\kappa b} \cosh(\kappa b) e^{-\kappa x}, & x > b \\ F \cosh(\kappa x), & 0 \leq x \leq b \end{cases}$$

Now, constant  $F$  can be obtained from the normalization condition:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1 \quad \text{or} \quad \int_0^{\infty} |\psi(x)|^2 dx = \frac{1}{2}$$

With that we get

$$\begin{aligned} \frac{1}{2} &= F^2 \left[ \int_0^b \cosh^2(kx) dx + e^{2kb} \cosh^2(kb) \int_b^\infty e^{-2kx} dx \right] = \\ &= F^2 \left[ \frac{1}{4} \int_0^b (e^{2kx} + 2 + e^{-2kx}) dx + e^{2kb} \cosh^2(kb) \frac{e^{-2kb}}{2k} \right] = \\ &= F^2 \left[ \frac{1}{4} \left( \frac{e^{2kb} - 1}{2k} + 2b + \frac{1 - e^{-2kb}}{2k} \right) + \frac{1}{8k} (e^{2kb} + 2 + e^{-2kb}) \right] = \\ &= F^2 \left[ \frac{1}{4k} e^{2kb} + \frac{b}{2} + \frac{1}{4k} \right] \Rightarrow F = \left( \frac{e^{2kb} + 1}{2k} + b \right)^{-1/2} \end{aligned}$$

At point  $x=b$  the wave function derivative has discontinuity, which follows from integrating the Schrödinger equation over an infinitely small interval  $[b-\epsilon, b+\epsilon]$ .

$$\psi'(b+\epsilon) - \psi'(b-\epsilon) = -\frac{2m\alpha}{\hbar^2} \psi(b)$$

This yields:

$$-k e^{kb} \cosh(kb) e^{-kb} - k \sinh(kb) = -\frac{2m\alpha}{\hbar^2} \cosh(kb)$$

or

$$k(1 + \tanh(kb)) = \frac{2m\alpha}{\hbar^2}$$

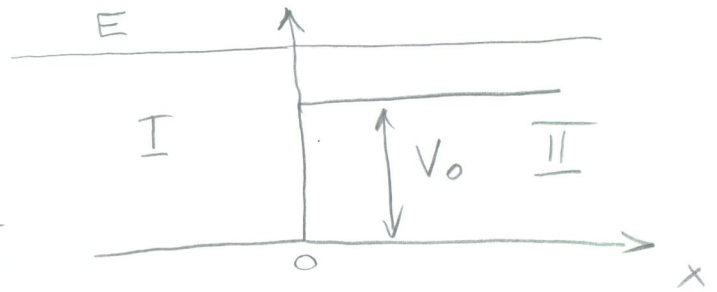
The latter transcendental equation gives  $k$  and  $E$ .

In the limit  $b \rightarrow 0$  it reduces to

$$k = \frac{2m\alpha}{\hbar^2} \quad \text{or} \quad E = -\frac{2m\alpha^2}{\hbar^2}$$

which is a familiar result for a single delta function potential

② Here we consider the Schrödinger equation in two regions - I and II



$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\psi_I'' + k\psi_I = 0$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_I = Ae^{ikx} + Be^{-ikx}$$

$$\psi_{II}'' + \alpha\psi_{II} = 0$$

$$\alpha = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$\psi_{II} = Fe^{i\alpha x} + Ge^{-i\alpha x}$$

$G=0$  (no incident wave coming from the right)

The continuity of  $\psi$  at  $x=0$  gives:

$$A+B=F$$

The continuity of  $\psi'$  at  $x=0$  gives:

$$ik(A-B) = i\alpha F$$

Hence

$$A+B = \frac{k}{\alpha}(A-B) \quad \text{or} \quad A\left(1 - \frac{k}{\alpha}\right) = -B\left(1 + \frac{k}{\alpha}\right)$$

The reflection coefficient is

$$R = \left|\frac{B}{A}\right|^2 = \frac{\left(1 - \frac{k}{\alpha}\right)^2}{\left(1 + \frac{k}{\alpha}\right)^2} = \frac{(\alpha - k)^2}{(\alpha + k)^2} = \frac{(\alpha - k)^4}{(\alpha^2 - k^2)^2} =$$

$$= \frac{(\sqrt{E} - \sqrt{E-V_0})^4}{V_0^2}$$

3. According to lecture #5 (or textbook chapter 2.3.1)

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + \frac{i\hat{p}}{\sqrt{2m\hbar\omega}} \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - \frac{i\hat{p}}{\sqrt{2m\hbar\omega}}$$

and

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

$\hat{x}$  and  $\hat{p}$  in terms of  $\hat{a}$  and  $\hat{a}^\dagger$  are:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}) \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^\dagger - \hat{a})$$

We also know that

$$a|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad \text{where } |n\rangle \equiv |\psi_n\rangle$$

With that matrix elements of  $\hat{x}$  are:

$$\langle n|\hat{x}|k\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n|(\hat{a}^\dagger + \hat{a})|k\rangle$$

Since both  $a$  or  $a^\dagger$  when acting on  $|n\rangle$  produce an eigenstate of  $\hat{H}$  (which are orthogonal to all other eigenstates) we can immediately write

$$\begin{aligned} \langle n|\hat{x}|k\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \left[ \sqrt{k+1} \langle n|k+1\rangle + \sqrt{k} \langle n|k-1\rangle \right] = \sqrt{\frac{\hbar}{2m\omega}} \left[ \sqrt{k+1} \delta_{n,k+1} + \sqrt{k} \delta_{n,k-1} \right] \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left[ \sqrt{k+1} \delta_{n,k+1} + \sqrt{n+1} \delta_{n+1,k} \right] \end{aligned}$$

In matrix form this looks as follow (remember that the index begins with 0 for our case):

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}$$

Similarly, for  $\hat{p}$  we have  $\langle n|\hat{p}|k\rangle = i\sqrt{\frac{m\hbar\omega}{2}} \langle n|(\hat{a}^\dagger - \hat{a})|k\rangle =$   
 $= i\sqrt{\frac{m\hbar\omega}{2}} \left( \sqrt{k+1} \langle n|k+1\rangle - \sqrt{k} \langle n|k-1\rangle \right) = i\sqrt{\frac{m\hbar\omega}{2}} \left[ \sqrt{k+1} \delta_{n,k+1} - \sqrt{n+1} \delta_{n+1,k} \right]$

$$\hat{p} = \sqrt{\frac{m\hbar\omega}{2}} \begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & \dots \\ 0 & 0 & i\sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Lastly, for  $\hat{H}$  we have:

$$\langle n | \hat{H} | k \rangle = E_k \langle n | k \rangle = E_k \delta_{nk} = \hbar\omega \left(k + \frac{1}{2}\right) \delta_{nk}$$

$$\hat{H} = \hbar\omega \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & \dots \\ 0 & \frac{3}{2} & 0 & 0 & \dots \\ 0 & 0 & \frac{5}{2} & 0 & \dots \\ 0 & 0 & 0 & \frac{7}{2} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The matrix of any operator is diagonal when computed in the basis of this operator's eigenstates (with eigenvalues on the diagonal)

④ First, let us compute some auxiliary commutators:

$$[x, H]f = [x, \frac{p^2}{2m}]f = -\frac{\hbar^2}{2m} [x, \frac{d^2}{dx^2}]f = -\frac{\hbar^2}{2m} (xf'' - \frac{d}{dx}(f + xf')) =$$

$$= -\frac{\hbar^2}{2m} (xf'' - f' - f' - xf'') = -\frac{\hbar^2}{m} f' \quad \text{So } [x, H] = \frac{i\hbar}{m} p$$

$$[p, H]f = [p, \frac{m\omega^2 x^2}{2}]f = (-i\hbar) \frac{m\omega^2}{2} [\frac{d}{dx}, x^2]f = -i\hbar \frac{m\omega^2}{2} (\frac{d}{dx}(x^2 f) - x^2 f'')$$

$$= -i\hbar \frac{m\omega^2}{2} (2xf' + x^2 f'' - x^2 f'') = -i\hbar m\omega^2 x f, \quad \text{So } [p, H] = -i\hbar m\omega^2 x$$

a)  $[X, H] = [x, H] \cos \omega t - [p, H] \frac{\sin \omega t}{m\omega} =$

$$= \frac{i\hbar}{m} p \cos \omega t + i\hbar \omega x \sin \omega t = \frac{i\hbar}{m} P \neq 0$$

$$[P, H] = [x, H] m\omega \sin \omega t + [p, H] \cos \omega t =$$

$$= i\hbar \omega p \sin \omega t - i\hbar m\omega^2 x \cos \omega t = -i\hbar m\omega^2 X$$

Hence, neither  $X$  nor  $P$  commute with  $H$

b) For  $X$  we have:

$$\frac{d}{dt} \langle X \rangle = \frac{1}{i\hbar} \langle [X, H] \rangle + \left\langle \frac{\partial X}{\partial t} \right\rangle = \frac{1}{i\hbar} \left( \frac{i\hbar}{m} \langle p \rangle \cos \omega t + i\hbar \omega \langle x \rangle \sin \omega t \right) -$$

$$- \langle x \rangle \omega \sin \omega t - \frac{1}{m} \langle p \rangle \cos \omega t = 0$$

Similarly, for  $P$  we have

$$\frac{d}{dt} \langle P \rangle = \frac{1}{i\hbar} \langle [P, H] \rangle + \left\langle \frac{\partial P}{\partial t} \right\rangle = \frac{1}{i\hbar} \left( i\hbar \omega \langle p \rangle \sin \omega t - i\hbar m\omega^2 \langle x \rangle \cos \omega t \right) +$$

$$+ \langle x \rangle m\omega^2 \cos \omega t - \langle p \rangle \omega \sin \omega t = 0$$

Hence, expectation values  $\langle X \rangle$  and  $\langle P \rangle$  are constant in time, i.e.  $X$  and  $P$  are conserved quantities

c) We may often hear that conservation requires commutativity with the Hamiltonian. Non-commutativity of  $X$  and  $P$  with  $H$  does not exclude them being conserved, however. This is because  $X$  and  $P$  contain explicit dependence on  $t$ .

⑤ a) Both terms in  $\psi$  contain spherical harmonics corresponding to  $l=1$ . Hence

$$L^2 = 2\hbar^2 \quad \text{and} \quad P(\text{probability}) = 1$$

b) First term has  $m_l=0$ , so  $L_z = 0$   $P = \left| \frac{1}{\sqrt{3}} \right|^2 = \frac{1}{3}$

Second term has  $m_l=1$ , so  $L_z = \hbar$   $P = \left| -i\frac{\sqrt{2}}{3} \right|^2 = \frac{2}{3}$

c)  $S^2 = \frac{1}{2}(\frac{1}{2}+1)\hbar^2 = \frac{3}{4}\hbar^2$   $P = 1$

d) First term has  $m_s = +\frac{1}{2}$ , so  $S_z = \frac{\hbar}{2}$   $P = \frac{1}{3}$

Second term has  $m_s = -\frac{1}{2}$ , so  $S_z = -\frac{\hbar}{2}$   $P = \frac{2}{3}$

e) Here we add two angular momenta:  $l=1$  and  $s = \frac{1}{2}$ . Possible outcomes are obviously  $j = \frac{3}{2}$  and  $\frac{1}{2}$ . In order to compute the probabilities of each we need Clebsch-Gordan coefficients for the expansions of  $|LM_L\rangle|SM_S\rangle$  in terms of  $|JM_J\rangle$ . These can be taken from the tables:

$$\begin{array}{ccc} l m_l & s m_s & j m_j \\ |1,0\rangle | \frac{1}{2}, \frac{1}{2} \rangle & = & \sqrt{\frac{2}{3}} | \frac{3}{2}, \frac{1}{2} \rangle - \frac{1}{\sqrt{3}} | \frac{1}{2}, \frac{1}{2} \rangle \\ |1,1\rangle | \frac{1}{2}, -\frac{1}{2} \rangle & = & \sqrt{\frac{1}{3}} | \frac{3}{2}, \frac{1}{2} \rangle + \sqrt{\frac{2}{3}} | \frac{1}{2}, \frac{1}{2} \rangle \end{array}$$

Then in the coupled representation

$$\psi = R_{21}(r) \left[ \frac{1}{\sqrt{3}} \left( \frac{\sqrt{2}}{\sqrt{3}} | \frac{3}{2}, \frac{1}{2} \rangle - \frac{1}{\sqrt{3}} | \frac{1}{2}, \frac{1}{2} \rangle \right) - i \frac{\sqrt{2}}{\sqrt{3}} \left( \frac{1}{\sqrt{3}} | \frac{3}{2}, \frac{1}{2} \rangle + \sqrt{\frac{2}{3}} | \frac{1}{2}, \frac{1}{2} \rangle \right) \right]$$

$$= R_{21}(r) \left[ (1-i) \frac{\sqrt{2}}{3} | \frac{3}{2}, \frac{1}{2} \rangle - \frac{1+2i}{3} | \frac{1}{2}, \frac{1}{2} \rangle \right]$$

Hence for  $j = \frac{3}{2}$   $P = \left| (1-i) \frac{\sqrt{2}}{3} \right|^2 = \frac{4}{9}$   $J^2 = \frac{15}{4} \hbar^2$

for  $j = \frac{1}{2}$   $P = \left| \frac{1+2i}{3} \right|^2 = \frac{5}{9}$   $J^2 = \frac{3}{4} \hbar^2$

$$f) \quad J_z = \frac{1}{2} \hbar \quad (\text{there is only one possibility}) \quad P = 1$$

$$g) \quad \rho(\vec{r}) = \psi^\dagger \psi = |R_{21}|^2 \cdot \begin{pmatrix} \frac{1}{\sqrt{3}} Y_1^0 \\ i \frac{\sqrt{2}}{\sqrt{3}} Y_1^1 \end{pmatrix}^* \begin{pmatrix} \frac{1}{\sqrt{3}} Y_1^0 \\ -i \frac{\sqrt{2}}{\sqrt{3}} Y_1^1 \end{pmatrix} =$$

$$= |R_{21}(r)|^2 \left[ \frac{1}{3} |Y_1^0(\theta, \phi)|^2 + \frac{2}{3} |Y_1^1(\theta, \phi)|^2 \right] = \frac{1}{3} \frac{1}{24} \frac{1}{a^3} \frac{r^2}{a^2} e^{-\frac{r}{a}} \left[ \frac{3}{4\pi} \cos^2 \theta + \right.$$

$$\left. + 2 \frac{3}{8\pi} \sin^2 \theta \right] = \frac{1}{96\pi a^5} r^2 e^{-\frac{r}{a}}$$

$$h) \quad \rho_{\uparrow}(r) = \int |R_{21}(r)|^2 \frac{1}{3} |Y_1^0(\theta, \phi)|^2 \sin \theta d\theta d\phi =$$

$$= \frac{1}{3} |R_{21}(r)|^2 = \frac{1}{3} \frac{1}{24a^3} \left(\frac{r}{a}\right)^2 e^{-\frac{r}{a}} = \frac{1}{72a^5} r^2 e^{-\frac{r}{a}}$$



(6) a) No translational degrees of freedom are involved since electron's speed is parallel to the magnetic field. Thus, the Hamiltonian includes only the interaction of electron's spin with  $\vec{B}$ :

$$H = -\vec{\mu} \cdot \vec{B} = \frac{e}{m} \vec{B} \cdot \vec{S} = \frac{e}{m} B S_y = \frac{eB}{2m\hbar} \hbar \sigma_y = \frac{\hbar\omega}{2} \sigma_y$$

where  $\omega = \frac{eB}{m\hbar}$        $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

The energies are obviously  $E_{\pm} = \pm \frac{\hbar\omega}{2}$  since the eigenvalues of  $\sigma_y = \pm 1$

The eigenvectors of  $\sigma_y$  are

$\eta_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix}$  ← corresponds to  $E_+$  and the positive projection of spin on the y-axis

$\eta_- = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix}$  ← corresponds to  $E_-$  and the negative projection of spin of the y-axis

Since  $H$  is time-independent, the general solution of the time-dependent Schrödinger equation can be written as

$$\chi(t) = a \eta_+ e^{-i\omega t} + b \eta_- e^{+i\omega t} \quad |a|^2 + |b|^2 = 1$$

At time  $t=0$  we have

$$\chi(0) = |S_z = -\frac{\hbar}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

This can be expanded in terms of  $\eta_+$  and  $\eta_-$ :

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = a \eta_+ + b \eta_- = \frac{1}{\sqrt{2}} \eta_+ + \frac{1}{\sqrt{2}} \eta_-$$

Thus

$$\begin{aligned} \chi(t) &= \frac{1}{\sqrt{2}} \eta_+ e^{-i\omega t} + \frac{1}{\sqrt{2}} \eta_- e^{+i\omega t} = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix} e^{-i\omega t} + \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} e^{+i\omega t} \\ &= \begin{pmatrix} -\sin\omega t \\ \cos\omega t \end{pmatrix} \end{aligned}$$

$$\begin{aligned} b) \quad \langle S_x \rangle &= \chi^\dagger(t) S_x \chi(t) = (-\sin\omega t \quad \cos\omega t) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -\sin\omega t \\ \cos\omega t \end{pmatrix} = \\ &= \frac{\hbar}{2} 2 \sin\omega t \cos\omega t = \hbar \sin(2\omega t) \end{aligned}$$

$$\begin{aligned} \langle S_y \rangle &= \chi^\dagger(t) S_y \chi(t) = (-\sin\omega t \quad \cos\omega t) \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} -\sin\omega t \\ \cos\omega t \end{pmatrix} = \\ &= 0 \end{aligned}$$

$$\begin{aligned} \langle S_z \rangle &= \chi^\dagger(t) S_z \chi(t) = (-\sin\omega t \quad \cos\omega t) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -\sin\omega t \\ \cos\omega t \end{pmatrix} = \\ &= \frac{\hbar}{2} (\sin^2\omega t - \cos^2\omega t) = -\frac{\hbar}{2} \cos 2\omega t \end{aligned}$$