question QA

<u>Solution:</u> $\sin(k_0 x) = \frac{1}{2i}\left(e^{ik_0x} - e^{-ik_0x}\right)$

(a) $\psi(x,t) = \dfrac{e^{-\frac{i\hbar k_0^2}{2m}t}}{2i}\left(e^{ik_0x} - e^{-ik_0x}\right)$

(b) $\dfrac{\hbar k_0}{2}\left(\delta_{k,k_0} - \delta_{k,-k_0}\right)$

(c) $\psi(k,t) = \frac{1}{i}\, e^{-\frac{i\hbar k_0^2}{2m}t}\, e^{ik_0x}$

question QB

Solution

1. For a 1D box, the normalized wavefunctions and the energy levels are

$$\varphi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}, \text{ and } E_n = n^2\frac{\pi^2\hbar^2}{2mL^2}$$

(a) Therefore, for a 3D box

$$\varphi^i{}_{111} = \frac{2}{L}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L}, \text{ and } E^i{}_{111} = (1+1+1)\frac{\pi^2\hbar^2}{2mL^2} = \frac{3\pi^2\hbar^2}{2mL^2}$$

(b) When x=L → x=4L,

$$\varphi^f{}_{111} = \frac{2}{L}\sqrt{\frac{2}{4L}}\sin\frac{\pi x}{4L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L} = \frac{2}{L}\sqrt{\frac{1}{2L}}\sin\frac{\pi x}{4L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L}$$

$$E^f{}_{111} = \frac{\pi^2\hbar^2}{2m(4L)^2} + 2\frac{\pi^2\hbar^2}{2mL^2} = \frac{33\pi^2\hbar^2}{32mL^2}$$

For the first exited state

$$\varphi^f{}_{211} = \frac{2}{L}\sqrt{\frac{2}{4L}}\sin\frac{2\pi x}{4L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L} = \frac{2}{L}\sqrt{\frac{1}{2L}}\sin\frac{\pi x}{2L}\sin\frac{\pi y}{L}\sin\frac{\pi z}{L}$$

$$E^f{}_{211} = 2^2\frac{\pi^2\hbar^2}{2m(4L)^2} + 2\frac{\pi^2\hbar^2}{2mL^2} = \frac{9\pi^2\hbar^2}{8mL^2}$$

(c)

$$\langle\varphi^f{}_{111}|\varphi^i{}_{111}\rangle = \int_0^L dx\int_0^L dy\int_0^L dz\,\varphi^f{}_{111}\varphi^i{}_{111}$$

$$= \int_0^L \sqrt{\frac{1}{2L}}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{4L}\sin\frac{\pi x}{L}dx$$

$$= \frac{1}{L}\int_0^L \frac{1}{2}\left(\cos\frac{3\pi x}{4L} - \cos\frac{5\pi x}{4L}\right)dx$$

$$= \frac{1}{2L}\left[\frac{4L}{3\pi}\sin\frac{3\pi x}{4L} - \frac{4L}{5\pi}\sin\frac{5\pi x}{4L}\right]_0^L$$

$$= \frac{8}{15\pi}$$

Therefore,

$$P = \left|\langle\varphi^f{}_{111}|\varphi^i{}_{111}\rangle\right|^2 = \left(\frac{8}{15\pi}\right)^2$$

question QC1

Prove the virial theorem (average kinetic energy = average potential energy) for the nth eigenstate of the simple harmonic oscillator

Solution: Total energy $E_n = \hbar\omega_0 (n + \frac{1}{2})$

$$X = \frac{(\hat{a} + \hat{a}^\dagger)}{\sqrt{2}\,\beta} \qquad \beta = \sqrt{\frac{m\omega_0}{\hbar}}$$

$$\langle V \rangle = \frac{1}{2}K\langle X^2 \rangle = \frac{K}{4\beta^2}\langle n|(a+a^\dagger)^2|n\rangle$$

$$= \frac{K}{4\beta^2}\langle n|a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2}|n\rangle$$

$[a, a^\dagger] = 1$

$\omega = \sqrt{K/m}$

$\frac{1}{2}kx$

$$= \frac{K}{4\beta^2}(0 + n + (n+1) + 0)$$

$\omega_0 =$

$$= \frac{K}{4\beta^2}(2n+1)$$

$\frac{\hbar K}{4m\omega_0} \quad \omega_0^2$

$$= \frac{\hbar\omega_0}{4}(2n+1) = \frac{\hbar\omega_0}{2}(n+\tfrac{1}{2})$$

$$\langle V \rangle = \tfrac{1}{2}E_n$$

So

$$\langle T \rangle = \tfrac{1}{2}E_n = \langle V \rangle$$

question QC2

Solution

1. (a)

A substitution

$$\psi_{n_r l m}(\mathbf{r}) = \frac{\phi_{n_r l}(r)}{r} Y_{lm}(\theta, \varphi),$$

where $Y_{lm}(\theta, \varphi)$ are spherical harmonics, reduces the 3d Shrödinger equation to its 1d version

$$\hat{H}\phi_{n_r l} = E_{n_r l}\phi_{n_r l}, \tag{1}$$

where

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)$$

and $\phi_{n_r l}(0) = 0$ (infinite well at $r = 0$). Now treating l in the Hamiltonian as a continuous parameter and using

$$\frac{\partial E_{n_r l}}{\partial l} = \left\langle n_r l \left| \frac{\partial \hat{H}}{\partial l} \right| n_r l \right\rangle = \left\langle n_r l \left| \frac{\hbar^2(2l+1)}{2mr^2} \right| n_r l \right\rangle > 0,$$

we see that $\partial E_{n_r l}/\partial l > 0$, i.e. $E_{n_r l}$ grows with l.

(b) and (c)

Bound states have energies $-V_0 \le E \le 0$. Here and below we drop indices n_r and l for the energy and wave functions.

The Schrödinger equation (1) for $l = 0$ reads

$$\phi_1'' = -k^2\phi_1 \quad \text{for} \quad r < a, \quad \phi_2'' = \kappa^2\phi_2 \quad \text{for} \quad r > a,$$

where

$$k^2 = \frac{2m}{\hbar^2}(E + V_0), \quad \kappa^2 = -\frac{2mE}{\hbar^2} = \frac{2m|E|}{\hbar^2} \quad (k > 0, \kappa > 0). \tag{2}$$

The solution that satisfies boundary conditions $\phi_1(0) = 0$ and $\phi_2(r) \to 0$ as $r \to +\infty$ is

$$\phi_1(r) = A\sin kr, \quad \phi_2(r) = Be^{-\kappa r}$$

The wave function and its derivative should be continuous at $r = a$. It follows that

$$\frac{\phi_1'(a)}{\phi_1(a)} = \frac{\phi_2'(a)}{\phi_2(a)}$$

We obtain

$$ka\cot ka = -\kappa a \tag{3}$$

Denote $u = ka$ and $v = \kappa a$ and note that Eqs. (2) and (3) imply

$$v = -u\cot u, \quad u^2 + v^2 = \frac{2mV_0 a^2}{\hbar^2} \equiv R^2, \quad u > 0, v > 0 \tag{4}$$

The number of bound states is the number of times a circle of radius R intersects the function $-u\cot u$ in the upper right quadrangle of the uv plane.

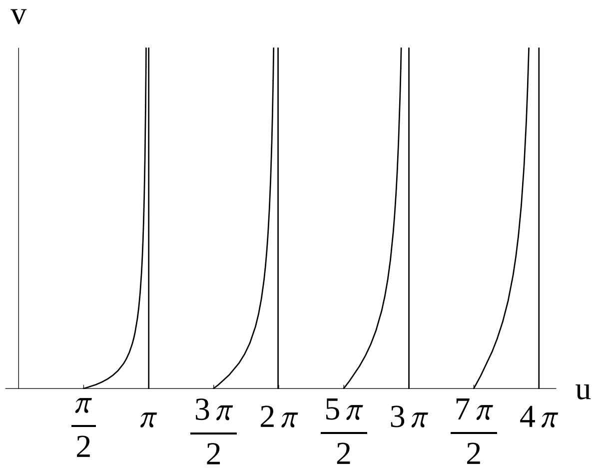


Figure 1: The graph of $v = -u \cot u$

We see from Fig. 1 that the number of bound states is $N = 0$ for $R < \pi/2$, $N = 1$ for $\pi/2 \leq R < 3\pi/2$, $N = 2$ for $3\pi/2 \leq R < 5\pi/2$ etc. In other words,

$$N = \left[\frac{R}{\pi} + \frac{1}{2}\right] = \left[\sqrt{\frac{2mV_0a^2}{\pi^2\hbar^2}} + \frac{1}{2}\right], \tag{5}$$

where $[x]$ denotes the integer part of x – the largest integer smaller or equal to x.

According to part a) the ground state must have $l = 0$. Then, it follows from Eq. (5) that there is at least one bound state when

$$\frac{2mV_0a^2}{\pi^2\hbar^2} \geq \frac{1}{4}$$

or equivalently

$$V_0 \geq \frac{\hbar^2\pi^2}{8ma^2}.$$

question QD1

2. The full Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2} - d\mathcal{E}\cos\phi$$

In a strong electric field the potential energy $V(\phi) = -d\mathcal{E}\cos\phi$ has a deep minimum at $\phi = 0$ and the wave functions of low lying levels are localized in a region of small ϕ. Approximating

$$V(\phi) \approx -d\mathcal{E} + d\mathcal{E}\phi^2/2,$$

we obtain a harmonic oscillator Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2} + \frac{d\mathcal{E}\phi^2}{2} - d\mathcal{E} \tag{4}$$

with frequency

$$\omega = \sqrt{\frac{d\mathcal{E}}{I}}.$$

The energies and eigenfunctions in this approximation are

$$E_n^{(0)} = -d\mathcal{E} + \hbar\sqrt{\frac{d\mathcal{E}}{I}}\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots \tag{5}$$

$$\psi_n^{(0)} = C\exp\left(-\frac{\phi^2}{2\phi_0^2}\right)H_n\left(\frac{\phi}{\phi_0}\right), \tag{6}$$

where

$$\phi_0 = \left(\frac{\hbar^2}{Id\mathcal{E}}\right)^{1/4}$$

and $H_n(x)$ are Hermite polynomials.

This approximation is applicable as long as the eigenfunctions are small for $|\phi| \sim 1$. Since the wave functions differ from zero appreciably only in the region of ϕ accessible to a classical rotator

$$-d\mathcal{E} + d\mathcal{E}\phi^2/2 \lesssim E_n^{(0)}, \quad \text{or} \quad \phi^2 \lesssim \phi_0^2(n + 1/2),$$

the condition of applicability takes the form

$$\mathcal{E} \gg \frac{\hbar^2(n + 1/2)^2}{dI}.$$

Higher orders can be obtained by keeping more terms in the expansion of $\cos\phi$ in ϕ^2 and treating them in standard perturbation theory for which Eqs. (4), (5), and (6) provide the *zeroth* approximation.

$\boxed{QD2}$

a) $n=2,\ l=1 \Rightarrow$

$-l \le m \le l$, integer $\Rightarrow$ $m = -1, 0, 1$

b) $J_{z\,max} = m_{max} + \frac{1}{2} = 1 + \frac{1}{2} = \frac{3}{2}$

$\Rightarrow j = \frac{3}{2};\ m_j = +\frac{3}{2}, +\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$

$j = \frac{1}{2};\ m_j = +\frac{1}{2}, -\frac{1}{2}$

c) $J_z|2,1,j,m_j\rangle = \hbar m_j|2,1,j,m_j\rangle$

$J_z|2,1,\frac{3}{2},\frac{3}{2}\rangle = (L_z+S_z)|2,1,1,\uparrow\rangle = \hbar(1+\frac{1}{2})|2,1,1,\uparrow\rangle$

so $|2,1,\frac{3}{2},\frac{3}{2}\rangle = |2,1,1,\uparrow\rangle$

$J_-|2,1,\frac{3}{2},\frac{3}{2}\rangle = \hbar\sqrt{(\frac{3}{2})(\frac{5}{2}) - (\frac{3}{2})(\frac{1}{2})}\,|2,1,\frac{3}{2},\frac{1}{2}\rangle$
$= \hbar\sqrt{3}\,|2,1,\frac{3}{2},\frac{1}{2}\rangle$

but $J_-|2,1,\frac{3}{2},\frac{3}{2}\rangle = (L_- + S_-)|2,1,1\uparrow\rangle$
$= L_-|2,1,1,\uparrow\rangle + S_-|2,1,1,\uparrow\rangle$
$= \sqrt{2}\hbar|2,1,0,\uparrow\rangle + \hbar|2,1,1,\downarrow\rangle$

$\Rightarrow\ |2,1,\frac{3}{2},\frac{1}{2}\rangle = \sqrt{\frac{2}{3}}|2,1,0,\uparrow\rangle + \frac{1}{\sqrt{3}}|2,1,1,\downarrow\rangle$

Now $|2,1,\frac{3}{2},-\frac{3}{2}\rangle = |2,1,-1,\downarrow\rangle$

$J_+|2,1,\frac{3}{2},-\frac{3}{2}\rangle = \sqrt{3}\hbar|2,1,\frac{3}{2},-\frac{1}{2}\rangle = \sqrt{2}\hbar|2,1,0,\downarrow\rangle + \hbar|2,1,-1,\uparrow\rangle$

QD2 - cont

So $|2,1,\frac{3}{2},\frac{3}{2}\rangle = |2,1,1,\uparrow\rangle$

$|\ \ ,\frac{3}{2},\frac{1}{2}\rangle = \sqrt{3/2}\,|2,1,0,\uparrow\rangle + \frac{1}{\sqrt{3}}|2,1,1\downarrow\rangle$

$|\ \ ,\frac{3}{2},-\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|2,1,-1\uparrow\rangle + \sqrt{\frac{3}{2}}|2,1,0,\uparrow\rangle$

$|\ \ ,\frac{3}{2},-\frac{3}{2}\rangle = |2,1,-1,\downarrow\rangle$

From orthogonality we get

$|2,1,\frac{1}{2},\frac{1}{2}\rangle = -\frac{1}{\sqrt{3}}|2,1,0,\uparrow\rangle + \sqrt{\frac{2}{3}}|2,1,1,\downarrow\rangle$

$|2,1,\frac{1}{2},-\frac{1}{2}\rangle = -\sqrt{\frac{2}{3}}|2,1,-1,\uparrow\rangle + \frac{1}{\sqrt{3}}|2,1,0,\downarrow\rangle$

(d) Linear polarized light $\Rightarrow \hat{\epsilon} = \hat{z} \Rightarrow \vec{\epsilon}\cdot\hat{r} = \vec{z}\cdot\hat{r} = r\cos\theta$

now $\cos\theta = P_1(\cos\theta) = \sqrt{\frac{3}{4\pi}}\, Y^0(\theta,\phi)$

so here terms such as: $\langle\downarrow|A^* R_{32}(r)\, Y_2^{*m'}(\theta\phi)\,|r\cos\theta|\,A R_{2,1}(r)\, Y_1^m(\theta,\phi)|\downarrow\rangle$

go into M_{fi}

write this as $A^*A\langle\downarrow|\downarrow\rangle\langle R_{32}|r|R_{21}\rangle\langle Y_2^{m'}|\sqrt{\frac{3}{4\pi}}\,Y_0^0\,|Y_1^m\rangle$

Last term is $\propto$ to $\int Y_2^{*m'}(\theta,\phi)\,Y_1^0(\theta,\phi)\,Y_1^m(\theta,\phi)\,d\Omega$

which is only nonzero for $\boxed{m'=m}$ and $\boxed{l_f = l_i+1}$ as we have here.

e) Circularly polarized light: $\hat{\epsilon} = \frac{1}{\sqrt{2}}(\hat{x}\pm i\hat{y}) \Rightarrow \hat{\epsilon}\cdot\hat{r} = \frac{1}{\sqrt{2}}(\hat{x}\cdot\hat{r} \pm i\,\hat{y}\cdot\hat{r})$

$\hat{x}\cdot\hat{r} = \sin\theta\cos\phi$, $\hat{y}\cdot\hat{r} = \sin\theta\sin\phi \Rightarrow \hat{\epsilon}\cdot\hat{r} = \frac{1}{\sqrt{2}}\sin\theta(\cos\phi \pm i\sin\phi) = \frac{1}{\sqrt{2}}\sin\theta\, e^{\pm i\phi}$

so $\hat{\epsilon}\cdot\hat{r} \propto Y_1^{\pm 1}(\theta,\phi)$

We then have terms that go as $\int Y_2^{*m'}\, Y_1^{\pm 1}\, Y_1^m\, d\Omega$

which are only nonzero for $l_f = l_i \pm 1$ and $m' = m_i \pm 1$

(we have (+) here.)

~~QD 2~~-cont.

Now, consider integrals.

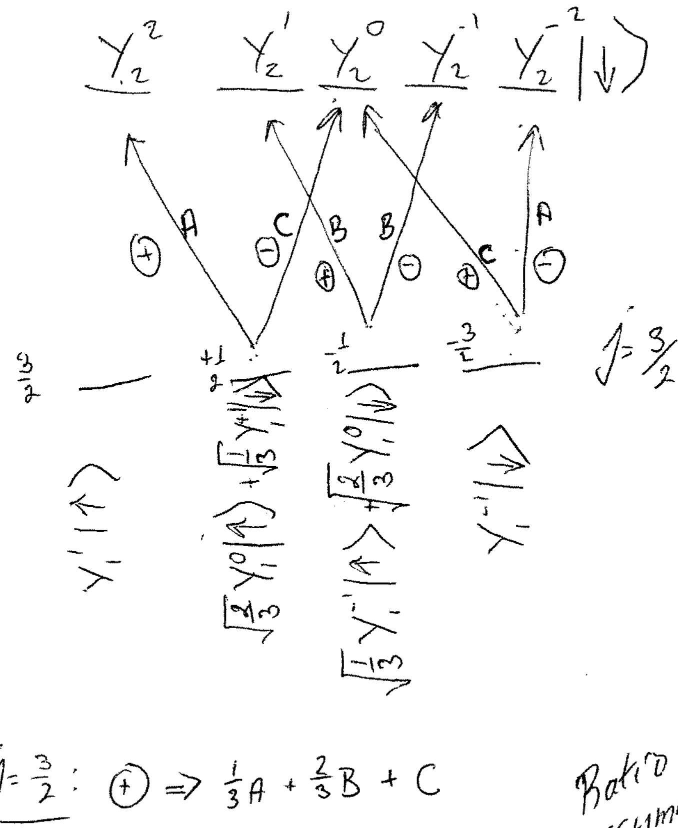
note that $\left|\int Y_2^{*m+1} Y_1^{1} Y_1^{m} \, d\Omega\right|^2 = \left|\int Y_2^{*(-(m+1))} Y_1^{-1} Y_1^{-m} \, d\Omega\right|^2$

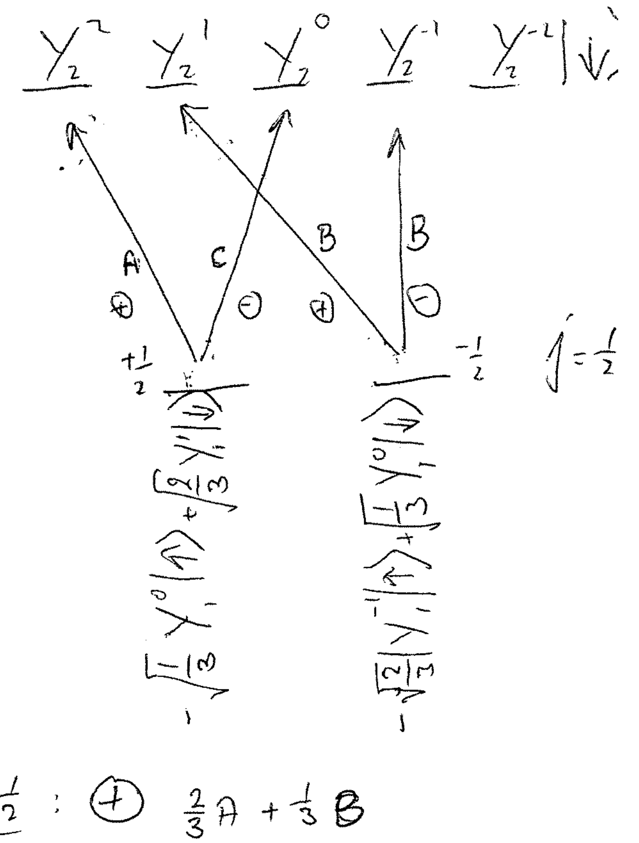
but differs for $m=0$ and $m=1$

So let $\left|\int Y_2^{\pm(m+1)*} Y_1^{\pm 1} Y_1^{\pm m} \, d\Omega\right|^2 = \begin{cases} A & \text{for } m=1 \\ B & \text{for } m=0 \end{cases}$

and $\left|\int Y_2^{0*} Y_1^{\pm 1} Y_1^{\mp 1} \, d\Omega\right|^2 = C$

Possible transitions where $\oplus + \ominus \Rightarrow e^{\pm i\phi} = l + r$ circular pol.





$j = \frac{3}{2}$: $\oplus \Rightarrow \frac{1}{3}A + \frac{2}{3}B + C$

$\ominus \Rightarrow A + \frac{2}{3}B + \frac{1}{3}C$

$\Rightarrow \boxed{\oplus - \ominus = -\frac{2}{3}A + \frac{2}{3}C}$ $j = \frac{3}{2}$

Ratio of assymmetry

$$\boxed{\frac{(\oplus - \ominus)_{\frac{3}{2}}}{(\oplus - \ominus)_{\frac{1}{2}}} = -1}$$

$j = \frac{1}{2}$: $\oplus$ $\frac{2}{3}A + \frac{1}{3}B$

$\ominus$ $\frac{2}{3}C + \frac{1}{3}B$

$\Rightarrow \boxed{\oplus - \ominus = \frac{2}{3}A - \frac{2}{3}C}$