Phys 522

Homework #3

Solution Set

3.1 C-T H_{XI}.1

1. $V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{else} \end{cases}$ $\qquad \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$

$W(x) = a\omega_0 \, \delta(x - a/2)$

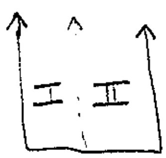
a. Calculate to first order, the change in energy

$$\varepsilon_1 = \int_0^a \psi_n^*(x)\, W(x)\, \psi_n(x)\, dx = \frac{2}{a} a\omega_0 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) \delta(x - a/2)$$

$$= 2\omega_0 \sin^2(n\pi/2) = 2\omega_0 \quad \text{for } n \text{ odd}$$

$E_n^{(1)} = \frac{\hbar^2 n^2 \pi^2}{2ma^2} + 2\omega_0$	n odd	$E_n^{(1)} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$	n even

b. Solve exactly



$K = \sqrt{\frac{2mE}{\hbar^2}}$

From the boundary conditions

$\psi_I(0) = 0 \qquad \psi_{II}(a) = 0$

we know the wavefunctions have the form

$\psi_I(x) = A \sin kx \qquad \psi_{II}(x) = B \sin(k(x-a))$

at $X = a/2$, we have

$$\boxed{\psi_I(a/2) = \psi_{II}(a/2)} \quad ①$$

& for derivative $\quad H\psi = E\psi \Rightarrow \int -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \int a w_0 \delta(x - a/2)\psi = \int E\psi$

$$\boxed{-\frac{\hbar^2}{2m}\left(\frac{d\psi_{II}}{dx} - \frac{d\psi_I}{dx}\right)\Bigg|_{X=a/2} + a w_0 \psi(a/2) = 0} \quad ②$$

↳ choose either ψ_I or ψ_{II}

From symmetry, we will have both even and odd solutions.

For odd solution $\psi_I(a/2) = \psi_{II}(a/2) = 0$

$$\Rightarrow \boxed{\sin ka/2 = 0}$$

For even ① $\Rightarrow A \sin ka/2 = B \sin(-ka/2) \Rightarrow A = -B$

② $\Rightarrow -\frac{\hbar^2}{2m}\left(BK \cos ka/2 - AK \cos ka/2\right) = -a w_0 A \sin ka/2$

$$\Rightarrow \frac{\hbar^2}{2m} 2AK \cos ka/2 = -a w_0 A \sin ka/2 \Rightarrow \boxed{\tan ka/2 = -\frac{\hbar^2 K}{m a w_0}}$$

The solution to these transcendental eqns will give the energy eigen values

Discuss as $\omega_0 \to 0$

for $\omega \to \infty$ $\tan ka/2 = 0 \Rightarrow ka/2 = n\pi \Rightarrow K = \frac{2\pi n}{a}$, $K = \sqrt{\frac{2mE}{\hbar^2}}$ ..

$$\Rightarrow E = \frac{2\pi^2 n^2 \hbar^2}{m a^2}$$

for $\omega \to 0$ $\tan ka/2 = \infty \Rightarrow ka/2 = n\pi/2 \Rightarrow K = n\pi/a \Rightarrow E = \frac{\pi^2 n^2 \hbar^2}{2ma^2}$

so the original energy is recovered

We see as ω_0 goes from 0 to ∞, the energy eigenvalues quadruple

3.2 CT H_{XI}-4

2-D Rotator:

a. $M = \frac{\hbar}{i}\frac{d}{d\alpha}$ is M hermitian?

$\langle\psi|M|\psi\rangle \overset{?}{=} \langle\psi|M^{+}|\psi\rangle$

$$\langle\psi|M|\psi\rangle = \int_0^{2\pi} d\alpha\ \psi^*(\alpha)\frac{\hbar}{i}\frac{d\psi}{d\alpha} = \cancel{\frac{\hbar}{i}|\psi|^2\Big|_0^{2\pi}} - \int \frac{\hbar}{i}\psi(\alpha)\frac{d\psi^*}{d\alpha}$$

→ continuity of wavefunction

Integrate by parts

$= \langle\psi|M|\psi\rangle^* = \langle\psi|M^{+}|\psi\rangle$ ∴ M is hermitian

Calculate Eigenvalues

$$\frac{\hbar}{i}\frac{d\psi(\alpha)}{d\alpha} = m\psi(\alpha) \Rightarrow \psi(\alpha) = Ce^{\frac{im\alpha}{\hbar}}$$

↳ Eigenvalue

but $\psi(\alpha+2\pi) = \psi(\alpha) \Rightarrow e^{\frac{im(\alpha+2\pi)}{\hbar}} = e^{\frac{im\alpha}{\hbar}} \Rightarrow e^{i\frac{2\pi m}{\hbar}} = 1$

$\Rightarrow m = n\hbar \quad n = 0, \pm1, \pm2, \ldots$

$$\int_0^{2\pi}|\psi(\alpha)|^2 d\alpha = 1 = \int_0^{2\pi} d\alpha\ |C|^2 = 2\pi|C|^2 \Rightarrow C = \frac{1}{\sqrt{2\pi}}$$

∴ $\psi_n(\alpha) = \sqrt{\frac{1}{2\pi}}\,e^{in\alpha}$ w/ eigenvalues $n\hbar$ $\quad n = 0, \pm1, \pm2, \ldots$

M has the physical meaning of being the angular momentum i.e. L_z

b. $H_0 = \frac{M^2}{2\mu\rho^2}$ calc eigenvalues & functions of H_0

$[H_0, M] = 0 \Rightarrow$ common eigenstates

$$H_0 \psi_n(\alpha) = \frac{-\hbar^2}{2\mu\rho^2}\frac{d^2}{d\alpha^2}\left(\sqrt{\frac{1}{2\pi}}\, e^{in\alpha}\right) = \frac{(\hbar n)^2}{2\mu\rho^2}\psi_n(\alpha)$$

Eigenfunction $\psi_n(\alpha) = \frac{1}{\sqrt{2\pi}} e^{in\alpha}$ w/ eigenvalues $\frac{(n\hbar)^2}{2\mu\rho^2}$

The energies are doubly degenerate from when n is equal & opposite

c. At $t=0$ $\psi(\alpha,0) = N\cos^2\alpha$. Discuss localization at time t

$$\psi(\alpha,t) = e^{-iH_0t/\hbar}\psi(\alpha,0) \qquad \psi(\alpha,0) = N\cos^2\alpha = \frac{N}{2}(1+\cos 2\alpha)$$

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

$$\Rightarrow \psi(\alpha,0) = \frac{N\sqrt{2\pi}}{4}\left(2\psi_0(\alpha) + \psi_2(\alpha) + \psi_{-2}(\alpha)\right)$$

$$\therefore e^{-iH_0t/\hbar}\psi(\alpha,0) = \frac{N\sqrt{2\pi}}{4}\left(2\psi_0(\alpha) + e^{-it/\hbar\cdot\frac{4\hbar^2}{2\mu g^2}}\psi_2(\alpha) + e^{-it/\hbar\frac{4\hbar^2}{2\mu g^2}}\psi_{-2}(\alpha)\right)$$

$$= \frac{N\sqrt{2\pi}}{4}\left(2\psi_0(\alpha) + e^{-\frac{2t\hbar}{\mu g^2}}\psi_2(\alpha) + e^{-\frac{2t\hbar}{\mu g^2}}\psi_{-2}(\alpha)\right)$$

$$= \frac{N}{4}\left(2 + 2e^{-2t\hbar i/\mu g^2}\cos 2\alpha\right) = \frac{N}{2}\left(1 + e^{-2t\hbar i/\mu g^2}\cos 2\alpha\right)$$

$$\boxed{\psi(\alpha,t) = \frac{N}{2}\left(1 + e^{-2t\hbar i/\mu g^2}\cos 2\alpha\right)}$$

when $\frac{2t\hbar}{\mu g^2} = 2\pi n$ we have our orginal wave function back

Also Note $\langle\psi|\alpha|\psi\rangle = \frac{N^2}{4}\int \alpha\left(1 + \cos^2 2\alpha + 2\cos\left(\frac{2t\hbar}{2\mu g^2}\right)\cos 2\alpha\right)$

$$\int \alpha \cos 2\alpha \, d\alpha = 0$$

$= \frac{N^2}{4}\int \alpha(1+\cos^2\alpha)\,d\alpha \Rightarrow \langle\psi|\alpha|\psi\rangle$ IS CONSTANT IN TIME.

d. $W = -q\mathcal{E}\rho \cos\alpha$

Calculate new wave function of the ground state to first order.

GS $\Rightarrow n=0 \Rightarrow$ No Degeneracy

$$|\psi_n^{(1)}\rangle = |\phi_n\rangle + \sum_{p\neq n} \frac{\langle\phi_p|W|\phi_n\rangle}{E_n^{(0)} - E_p^{(0)}} |\phi_p\rangle \qquad E_m^{(0)} = \frac{(\hbar m)^2}{2\mu\rho^2}$$

$n=0$

$$\langle\phi_p|W|\phi_0\rangle = \int_0^{2\pi} \frac{1}{2\pi} e^{ip\alpha}(-q\mathcal{E}\rho\cos\alpha)\,1\, d\alpha = \frac{-q\mathcal{E}\rho}{2\pi}\int_0^{2\pi} d\alpha\, e^{ip\alpha}\cos\alpha$$

$$= \frac{-q\mathcal{E}\rho}{2\pi}\int_0^{2\pi} \frac{1}{2}\left(e^{i(p\alpha+\alpha)} + e^{i(p\alpha-\alpha)}\right) d\alpha =$$

$$= \frac{-q\mathcal{E}\rho}{2\pi}\,\frac{2\pi}{2}\left(\delta_{p+1} + \delta_{p-1}\right) = \frac{-q\mathcal{E}\rho}{2}\left(\delta_{p,-1} + \delta_{p,1}\right)$$

$$\Rightarrow |\psi_0^{(1)}\rangle = |\psi_0\rangle + \frac{-q\mathcal{E}\rho}{2}\left(|\psi_{-1}\rangle + |\psi_1\rangle\right)\cdot\frac{-2\mu\rho^2}{\hbar^2}$$

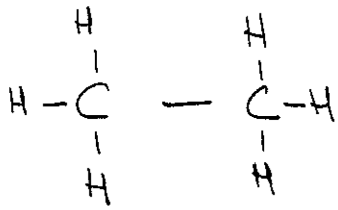
$$\Rightarrow \psi^{(1)}(\alpha) = \frac{1}{\sqrt{2\pi}}\left(1 + \frac{q\mathcal{E}\mu\rho^3}{\hbar^2}\left(e^{i\alpha} + e^{-i\alpha}\right)\right)$$

$$\boxed{\psi^{(1)}(\alpha) = \frac{1}{\sqrt{2\pi}}\left(1+\frac{2q\mathcal{E}\mu\rho^3}{\hbar^2}\cos\alpha\right)}$$

Dipole moment in X is $q\rho\cos\alpha = qX$ $\quad \langle qX\rangle = \frac{q\rho}{2\pi}\int_0^{2\pi}\left(1+\frac{2q\mathcal{E}\mu\rho^3}{\hbar^2}\cos\alpha\right)^2\cos\alpha\,d\alpha$

$$= \frac{q\rho}{2\pi}\int_0^{2\pi}\frac{4q\mathcal{E}\mu\rho^3}{\hbar^2}\cos^2\alpha = \frac{2q^2\mathcal{E}\mu\rho^4}{\hbar^2} \quad \Rightarrow \quad \boxed{\chi = \frac{2q^2\mu\rho^4}{\hbar^2}}$$

e.



$W = b\cos 3\alpha$

Give a physical justification for the α-dependence of W.

As we rotate, the 3 hyrogens' locations will vary, changing the interaction strength. The symmetry of the molecule suggests a periodic potential. Thus, an angular dependence of 3α

Calc. energy & wave function of the new ground state (to first order in b for wavefnct. to 2nd order in Energy)

$$E_0^{(1)} = \langle \psi_0 | W | \psi_0 \rangle = \frac{1}{2\pi}\int_0^{2\pi} b\cos 3\alpha = 0$$

$$E_0^{(2)} = \sum_{p\neq 0} \frac{|\langle \psi_p | W | \psi_0\rangle|^2}{E_0 - E_p} = \sum_{p\neq 0} \frac{|\langle \psi_p | W | \psi_0\rangle|^2}{-\frac{\hbar^2 p^2}{\lambda I}} = -\frac{\lambda I}{\hbar^2}\sum_{p\neq 0}\frac{|\langle \psi_p | W | \psi_0\rangle|^2}{p^2}$$

$$\langle \psi_p | W | \psi_0\rangle = \frac{b}{2\pi}\int_0^{2\pi} e^{ip\alpha}\cos 3\alpha = \frac{b}{2\pi}\,\frac{1}{2}\int_0^{2\pi} d\alpha \left[e^{i\alpha(p+3)} + e^{i\alpha(p-3)}\right]$$

$$= \frac{b}{2}\left(\delta_{p,-3} + \delta_{p,3}\right)$$

$$\Rightarrow E_0^{(2)} = -\frac{\lambda I}{\hbar^2}\,\frac{b^2}{4}\left(\frac{1}{9}+\frac{1}{9}\right) \qquad \boxed{E_0^{(2)} = -\frac{\lambda I b^2}{18\hbar^2}}$$

$$|\psi_0^{(1)}\rangle = \frac{-\lambda I}{\hbar^2}\left(\frac{b}{2\cdot 9}|\psi_{-3}\rangle + \frac{b}{2\cdot 9}|\psi_3\rangle\right) + |\psi_0\rangle$$

$$\boxed{\psi_0^{(1)}(\alpha) = \frac{1}{\sqrt{2\pi}}\left(1 - \frac{\lambda I}{9\hbar^2}\cos 3\alpha\right)}$$

We see that the Electro interaction lowers the GS energy making the molecule more stable.

3.3 CT H_{XI}-8

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{else} \end{cases}$$

$$W = q\mathcal{E}\,(X - a/2) \qquad \psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi x}{a}\right) \qquad E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

a) ε_1 & ε_2 = 1st/2nd order energy corrections to $\psi_1(x)$

$$\varepsilon_1 = \langle \psi_1 | W | \psi_1 \rangle = \frac{2}{a}\int_0^a dx \; q\mathcal{E}\,(X - a/2)\,\sin^2\frac{\pi x}{a} = \frac{2q\mathcal{E}}{a}\int_0^a dx\, X \sin^2\left(\frac{\pi x}{a}\right) - q\mathcal{E}\int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx$$

$$= q\mathcal{E}\left[\frac{2}{a}\int_0^a X\, d\left(\frac{X}{2} - \frac{a}{4\pi}\sin\frac{2\pi x}{a}\right) - \frac{X}{2} + \frac{a}{4\pi}\sin\frac{2\pi x}{a}\Big|_0^a\right]$$

$$= q\mathcal{E}\left[\frac{2}{a}\left(\frac{X^2}{2} - \frac{aX}{4\pi}\sin\frac{2\pi x}{a}\right)\Big|_0^a - \frac{2}{a}\int_0^a\left(\frac{X}{2} - \frac{a}{4\pi}\sin\frac{2\pi x}{a}\right)dx - a/2\right]$$

$$= q\mathcal{E}\left[a - a/2 - a/2\right] = 0$$

$$\varepsilon_2 = \sum_{p \ne 1} \frac{|\langle \psi_p | W | \psi_1 \rangle|^2}{E_1 - E_p} \qquad E_1 - E_p = \frac{\pi^2\hbar^2}{2ma^2}(1 - p^2)$$

$$\langle \psi_p | W | \psi_1 \rangle = \frac{2}{a} \int dx \, \sin\left(\frac{p\pi x}{a}\right) \, q\mathcal{E}\,(x - a/2) \sin\frac{\pi x}{a} = q\mathcal{E}\,\frac{2}{a}\int_0^a (x - a/2) \sin\frac{p\pi x}{a} \sin\frac{\pi x}{a}\, d$$

when $p = 2n$ we have $\langle \psi_{2n} | W | \psi_1 \rangle = -q\mathcal{E}\,\frac{16na}{\pi^2}\,\frac{1}{(1-4n^2)^2}$

when p is odd, it is easily seen that $\langle \psi_p | W | \psi_1 \rangle = 0$ from the integrand being odd over $(0,a)$.

$$\therefore \quad \mathcal{E}_2 = \sum_{n=1}^{\infty} q^2 \mathcal{E}^2 \frac{256 n^2 a^2}{\pi^4} \frac{1}{(1-4n^2)^4} \cdot \frac{2ma^2}{\pi^2\hbar^2} \frac{1}{(1-4n^2)}$$

$$\boxed{\mathcal{E}_2 = \frac{512\, q^2 \mathcal{E}^2 m a^4}{\pi^6 \hbar^2} \sum_{n=1}^{\infty} \frac{n^2}{(1-4n^2)^5}}$$

LOWER BOUND $\Rightarrow n = 1$ $\quad \mathcal{E}_2 \approx \frac{512\, q^2 \mathcal{E}^2 m a^4}{\pi^6 \hbar^2} \frac{1}{(-3)^5} = \frac{-512\, q^2 \mathcal{E}^2 m a^4}{243\, \pi^6 \hbar^2}$

UPPER BOUND IS GIVEN BY CHAPT XI B-21

$$e_2 \le \frac{1}{\Delta E} (\Delta W)^2 \qquad \Delta W^2 = \langle \psi_n | W^2 | \psi_n \rangle - \langle \psi_n | W | \psi_n \rangle$$

$$\langle \psi_n | W^2 | \psi_n \rangle = \frac{2}{a} \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) q^2 \mathcal{E}^2 (x - a/2)^2$$

$$= \frac{2q^2\mathcal{E}^2}{a} \int_0^a \sin^2\left(\frac{n\pi x}{a}\right)(x^2 - xa + a^2/4) = \frac{2q^2\mathcal{E}^2}{a}\left[\int_0^a dx\, x^2 \sin^2 \frac{n\pi x}{a} - xa \sin^2 \frac{n\pi x}{a} + \frac{a^2}{4} \sin^2 \frac{n\pi x}{a}\right.$$

$$\int_0^a x^2 \sin^2 \frac{n\pi x}{a} dx = \frac{a^3}{6} + \frac{a^3}{4n^2\pi^2}$$

$$\int_0^a x \sin^2 \frac{n\pi x}{a} = a^2/4$$

$$\int_0^a \sin^2 \frac{n\pi x}{a} = a/2$$

$$\langle \psi_n | W^2 | \psi_n \rangle = \frac{2q^2\mathcal{E}^2}{a}\left(\frac{a^3}{6} + \frac{a^3}{4n^2\pi^2}\right) - 2q^2\mathcal{E}^2 \frac{a^2}{4} + \frac{q^2\mathcal{E}^2 a}{2} \cdot \frac{a}{2}$$

$$= \frac{q^2\mathcal{E}^2 a^2}{3} + \frac{q^2\mathcal{E}^2 a^2}{2n^2\pi^2} - \frac{q^2\mathcal{E}^2 a^2}{2} + \frac{q^2\mathcal{E}^2 a^2}{4} = q^2\mathcal{E}^2 a^2\left(\frac{1}{12} - \frac{1}{4n^2\pi^2}\right)$$

$$= \frac{q^2\mathcal{E}^2 a^2}{4}\left(\frac{1}{3} - \frac{1}{n^2\pi^2}\right)$$

$$\langle \psi_n | W | \psi_n \rangle = \frac{2}{a} \int_0^a \sin^2 \frac{n\pi x}{a}\, q\mathcal{E} (x - a/2) = 0$$

$$\mathcal{E}_2 \le \frac{q^2\mathcal{E}^2a^2}{4}\left(\frac{1}{3}-\frac{1}{n^2\pi^2}\right)\cdot\frac{2ma^2}{\pi^2\hbar^2}\,\frac{1}{(1-n^2)} = \frac{q^2\mathcal{E}^2a^4m}{2\pi^2\hbar^2}\underbrace{\left(\frac{1}{3}-\frac{1}{n^2\pi^2}\right)\frac{1}{(1-n^2)}}_{\text{This is smallest when } n=2}$$

$$\mathcal{E}_2 \le \frac{q^2\mathcal{E}^2a^4m}{\hbar^2}\,\frac{-1}{6\pi^2}\left(\frac{1}{3}-\frac{1}{4\pi^2}\right) = \frac{q^2\mathcal{E}^2a^4m}{\hbar^2}\,\frac{(4\pi^2-3)}{72\pi^4}$$

$$\therefore\ \Delta\mathcal{E} = \frac{q^2\mathcal{E}^2a^4m}{\hbar^2}\left[\frac{(4\pi^2-3)}{72\pi^4}+\frac{512}{243\pi^6}\right] \approx \frac{q^2\mathcal{E}^2a^4m}{\hbar^2}(.007)$$

2. VARIATIONAL Calc.

$$\mathcal{H} = \frac{p^2}{2m} + q\mathcal{E}(x - a/2) = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + q\mathcal{E}(x - a/2)$$

$\langle \mathcal{H} \rangle = \langle \psi | H | \psi \rangle$

$$H\psi(x) = \left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + q\mathcal{E}(x-a/2)\right]\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2))$$

$$\frac{d\psi}{dx} = \frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2)) + \sin\frac{\pi x}{a}\,\alpha q\mathcal{E}$$

$$\frac{d^2\psi}{dx^2} = -\frac{\pi^2}{a^2}\sin\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2)) + \frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right)\alpha q\mathcal{E} + \frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right)\alpha q\mathcal{E}$$

$$= \frac{-\pi^2}{a^2}\sin\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2)) + \frac{2\pi}{a}\alpha q\mathcal{E}\cos\frac{\pi x}{a}$$

$$\langle \mathcal{H} \rangle = \frac{2}{a}\int_0^a \frac{+\pi^2\hbar^2}{a^2 2m}\sin^2\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2))^2 + -\frac{2\pi\hbar^2}{a\,2m}\alpha q\mathcal{E}\cos\frac{\pi x}{a}\sin\frac{\pi x}{a}(1+\alpha q\mathcal{E}(x-a/2))$$

$$+ q\mathcal{E}\sin^2\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2))^2(x-a/2) \quad dx$$

$$= \frac{+\hbar\pi^2}{ma^3}\int_0^a dx\,\sin^2\left(\frac{\pi x}{a}\right)(1+\alpha q\mathcal{E}(x-a/2))^2 - \frac{\hbar^2 2\pi}{ma^2}\alpha q\mathcal{E}\int_0^a dx\cos\frac{\pi x}{a}\sin\frac{\pi x}{a}(1+\alpha q\mathcal{E}(x-a/2))$$

$$+ \frac{2q\mathcal{E}}{a}\int_0^a dx\,\sin^2\frac{\pi x}{a}(x-a/2)(1+\alpha q\mathcal{E}(x-a/2))^2$$

$$\int_0^a dx \sin^2\frac{\pi x}{a}\left(1+\alpha q\mathcal{E}(x-a/2)\right)^2 = \int_0^a dx \sin^2\frac{\pi x}{a}\left(1+2\alpha q\mathcal{E}(x-a/2)+\alpha^2q^2\mathcal{E}^2(x-a/2)^2\right)$$

$$\int_0^a \sin^2\frac{\pi x}{a} = a/2 \qquad \int_0^a (x-a/2)\sin^2\frac{\pi x}{a} = 0 \qquad \int_0^a \sin^2\frac{\pi x}{a}(x-a/2)^2 = \frac{a^3}{4}\left(\frac{1}{6}-\frac{1}{\pi^2}\right)$$

$$= \frac{a}{2} + 0 + \frac{a^3}{4}\left(\frac{1}{6}-\frac{1}{\pi^2}\right)\alpha^2q^2\mathcal{E}^2 = \frac{a}{2} + \frac{a^3}{4}\left(\frac{1}{6}-\frac{1}{\pi^2}\right)\alpha^2q^2\mathcal{E}^2$$

$$\int_0^a dx \cos\frac{\pi x}{a}\sin\frac{\pi x}{a}\left(1+\alpha q\mathcal{E}(x-a/2)\right) = \int dx \cos\frac{\pi x}{a}\sin\frac{\pi x}{a} + \alpha q\mathcal{E}\int dx\cos\frac{\pi x}{a}\sin\frac{\pi x}{a}(x-a/2)$$

$$\int \cos\frac{\pi x}{a}\sin\frac{\pi x}{a}dx = 0 \qquad \int\cos\frac{\pi x}{a}\sin\frac{\pi x}{a}(x-a/2)dx = \frac{-a^2}{4\pi}$$

$$= -\alpha q\mathcal{E}\frac{a^2}{4\pi}$$

$$\int_0^a dx \sin^2\frac{\pi x}{a}(x-a/2)\left(1+\alpha q\mathcal{E}(x-a/2)\right)^2 = \int dx \sin^2\frac{\pi x}{a}(x-a/2)\left(1+2\alpha q\mathcal{E}(x-a/2) + \alpha^2q^2\mathcal{E}^2(x-a/2)^2\right)$$

$$= \int dx \sin^2\frac{\pi x}{a}(x-a/2) + 2\alpha q\mathcal{E}\int dx \sin^2\frac{\pi x}{a}(x-a/2)^2 + \alpha^2q^2\mathcal{E}^2\int dx^2 \sin^2\frac{\pi x}{a}(x-\tfrac{a}{2})^3$$

$$= 0 + 2\alpha q\mathcal{E}\frac{a^3}{4}\left(\frac{1}{6}-\frac{1}{\pi^2}\right) + 0$$

$$\therefore \langle H\rangle = +\frac{\hbar^2\pi^2}{ma^3}\left(\frac{a}{2}+\alpha^2q^2\mathcal{E}^2\frac{a^3}{4}\left(\frac{1}{6}-\frac{1}{\pi^2}\right)\right) - \frac{\hbar^2\alpha\pi}{ma^2}\alpha q\mathcal{E}\left(-\alpha q\mathcal{E}\frac{a^2}{4\pi}\right)$$

$$-\frac{2q\mathcal{E}}{a}\left(2\alpha q\mathcal{E}\,a^3\left(\frac{1}{6}-\frac{1}{\pi^2}\right)\right)$$

$$\langle H\rangle = \frac{\hbar^2\pi^2}{2ma^2} + \alpha^2 \frac{g^2\varepsilon^2\hbar^2\pi^2}{4m}\left(\frac{1}{6}-\frac{1}{\pi^2}\right) + \alpha^2\frac{g^2\varepsilon^2\hbar^2}{2m}$$

$$+ \alpha\, g^2\varepsilon^2 a^2\left(\frac{1}{6}-\frac{1}{\pi^2}\right)$$

$$\langle H\rangle = \frac{\hbar^2\pi^2}{2ma^2} + \alpha^2\left(\frac{g^2\varepsilon^2\hbar^2\pi^2}{24m} - \frac{g^2\varepsilon^2\hbar^2}{4m} + \frac{g^2\varepsilon^2\hbar^2}{2m}\right) + \alpha g^2\varepsilon^2 a^2\left(\frac{1}{6}-\frac{1}{\pi^2}\right)$$

$$= \frac{\hbar^2\pi^2}{2ma^2} + \alpha^2\left(\frac{g^2\varepsilon^2\hbar^2\pi^2}{24m} + \frac{g^2\varepsilon^2\hbar^2}{4m}\right) + \alpha g^2\varepsilon^2 a^2\left(\frac{1}{6}-\frac{1}{\pi^2}\right)$$

$$\frac{\partial\langle H\rangle}{\partial\alpha} = 0 = 2\alpha\left(g^2\frac{\varepsilon^2\hbar^2\pi^2}{24m} + g^2\frac{\varepsilon^2\hbar^2}{4m}\right) + g^2\varepsilon^2 a^2\left(\frac{1}{6}-\frac{1}{\pi^2}\right)$$

$$\Rightarrow \frac{g^2\varepsilon^2\hbar^2}{2m}\alpha\left(\frac{\pi^2}{6}+1\right) + g^2\varepsilon^2 a^2\left(\frac{1}{6}-\frac{1}{\pi^2}\right) = 0$$

$$\alpha_{min} = \frac{a^2\left(\frac{1}{\pi^2}-\frac{1}{6}\right)}{\frac{\hbar^2}{2m}\left(\frac{\pi^2}{6}+1\right)} = \frac{\frac{a^2}{6\pi^2}\left(6-\pi^2\right)}{\frac{\hbar^2}{2m6}\left(\pi^2+6\right)} = \frac{2a^2m}{\hbar^2\pi^2}\frac{(6-\pi^2)}{(6+\pi^2)}$$

$$\langle H \rangle_{min} = \frac{\hbar^2 \pi^2}{2ma^2} + \frac{g^2 \varepsilon^2 \hbar^2}{24m}(\pi^2+6) \cdot \frac{4a^4 m^2}{\hbar^4 \pi^4}\frac{(6-\pi^2)^2}{(6+\pi^2)^2} + \frac{g^2\varepsilon^2 a^2}{6\pi^2}(\pi^2-6) \cdot \frac{2a^2 m}{\hbar^2\pi^2}\frac{(6-\pi^2)}{(6+\pi^2)}$$

$$= \frac{\hbar^2\pi^2}{2ma^2} + \frac{g^2\varepsilon^2 a^4 m}{6\hbar^2\pi^4}\frac{(6-\pi^2)^2}{(6+\pi^2)} + \frac{g^2\varepsilon^2 a^4 m}{3\hbar^2\pi^4}\frac{(6-\pi^2)^2}{(6+\pi^2)}$$

$$\boxed{= \frac{\hbar^2\pi^2}{2ma^2} + \frac{g^2\varepsilon^2 a^4 m}{2\hbar^2\pi^4}\frac{(\pi^2-6)^2}{(\pi^2+6)} = \langle H \rangle_{MIN}}$$

$$\Delta E_2 = \frac{g^2\varepsilon^2 a^4 m}{\hbar^2}\left[\frac{(\pi^2-6)^2}{2\pi^4(\pi^2+6)}\right] \approx \frac{g^2\varepsilon^2 a^4 m}{\hbar^2}(.005)$$

SO, THE VARIATIONAL CALCULATION GIVES A SIMILARLY ACCURATE VALUE.

3.4. C-T H_{XI}.7

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial^2 u}{\partial y \partial z} = \frac{\partial^2 u}{\partial z \partial x} = 0$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$$

$$H_0 = \frac{qQ}{2I(2I-1)\hbar^2}\left(a_x I_x^2 + a_y I_y^2 + a_z I_z^2\right)$$

$$a_x = \left(\frac{\partial^2 u}{\partial x^2}\right)_0, \quad a_y = \left(\frac{\partial^2 u}{\partial y^2}\right)_0, \quad a_z = \left(\frac{\partial^2 u}{\partial z^2}\right)_0$$

$$a_x + a_y + a_z = 0$$

Generally

$$a_x I_x^2 + a_y I_y^2 + a_z I_z^2 = \frac{1}{2}\overbrace{(a_x + a_y)}^{-a_z}\overbrace{(I_x^2 + I_y^2)}^{\vec{I}^2 - I_z^2}$$

$$\frac{1}{2}(a_x - a_y)\underbrace{(I_x^2 - I_y^2)}_{\frac{1}{2}(I_+^2 + I_-^2)}$$

$$+ a_z I_z^2$$

$$= \frac{1}{2}a_z\left(3I_z^2 - \vec{I}^2\right) + \frac{1}{4}(a_x - a_y)\left(I_+^2 + I_-^2\right)$$

$\vec{I}^2$ = $I(I+1)\hbar^2$ in this ang mom subspace

$$\boxed{\begin{aligned} H_0 &= \underbrace{\frac{qQ}{2I(2I-1)\hbar^2}\frac{1}{2}a_z}_{A}\left(3I_z^2 - I(I+1)\hbar^2\right) \\ &+ \underbrace{\frac{qQ}{2I(2I-1)\hbar^2}\frac{1}{4}(a_x - a_y)}_{B}\left(I_+^2 + I_-^2\right) \end{aligned}}$$

a. $\mathcal{U}$ cylindrically symmetric $\Longrightarrow a_x = a_y$

$$H_0 = A\left(3I_z^2 - \frac{15}{4}\hbar^2\right)$$

H_0 commutes w/ $\vec{I}^2$ and I_z, so eigenstates of H_0 are $|Im\rangle = |m\rangle$.

State	Eigenvalue
$\left\lvert\frac{3}{2}\frac{3}{2}\right\rangle$	$3A\hbar^2$
$\left\lvert\frac{3}{2}\frac{1}{2}\right\rangle$	$-3A\hbar^2$
$\left\lvert\frac{3}{2}, -\frac{1}{2}\right\rangle$	$-3A\hbar^2$
$\left\lvert\frac{3}{2}, -\frac{3}{2}\right\rangle$	$3A\hbar^2$

b. Nonzero matrix elements of $I_\pm^2$ are

$$\left\langle -\tfrac{3}{2}\right| I_-^2 \left|\tfrac{1}{2}\right\rangle = \left\langle \tfrac{1}{2}\right| I_+^2 \left| -\tfrac{3}{2}\right\rangle = \underbrace{C_+\left(\tfrac{3}{2}, -\tfrac{3}{2}\right)}_{\sqrt{3}} \underbrace{C_+\left(\tfrac{3}{2}, -\tfrac{1}{2}\right)}_{2} \hbar^2 = 2\sqrt{3}\hbar^2$$

$$\left\langle -\tfrac{1}{2}\right| I_-^2 \left|\tfrac{3}{2}\right\rangle = \left\langle \tfrac{3}{2}\right| I_+^2 \left| -\tfrac{1}{2}\right\rangle = C_-\left(\tfrac{3}{2}, +\tfrac{3}{2}\right) C_-\left(\tfrac{3}{2}, \tfrac{1}{2}\right)\hbar^2 = 2\sqrt{3}\hbar^2$$

$$H_0 \longrightarrow \begin{array}{c c} & \begin{array}{cccc} \tfrac{3}{2} & -\tfrac{1}{2} & -\tfrac{3}{2} & \tfrac{1}{2} \end{array} \\ \begin{array}{c} \tfrac{3}{2} \\ -\tfrac{1}{2} \\ -\tfrac{3}{2} \\ \tfrac{1}{2} \end{array} & \hbar^2 \begin{pmatrix} 3A & 2\sqrt{3}B & 0 & 0 \\ 2\sqrt{3}B & -3A & 0 & 0 \\ 0 & 0 & 3A & 2\sqrt{3}B \\ 0 & 0 & 2\sqrt{3}B & -3A \end{pmatrix} \end{array}$$

$$\boxed{\begin{array}{l} C_+\left(\tfrac{3}{2}, -\tfrac{3}{2}\right) = C_-\left(\tfrac{3}{2}, \tfrac{3}{2}\right) = C_+\left(\tfrac{3}{2}, \tfrac{1}{2}\right) = C_-\left(\tfrac{3}{2}, -\tfrac{1}{2}\right) = \sqrt{3} \\ C_+\left(\tfrac{3}{2}, -\tfrac{1}{2}\right) = C_-\left(\tfrac{3}{2}, \tfrac{1}{2}\right) = 2 \end{array}}$$

In each 2-d subspace we want to diagonalize

$$\begin{pmatrix} 3A & 2\sqrt{3}B \\ 2\sqrt{3}B & -3A \end{pmatrix} = 3A\sigma_3 + 2\sqrt{3}B\sigma_1$$
$$= \sqrt{3}\left(2B\sigma_1 + \sqrt{3}A\sigma_3\right)$$

$$\alpha = (3A^2 + 4B^2)^{1/2}$$
$$n_1 = \frac{2B}{\alpha} = \sin\theta, \quad n_3 = \frac{\sqrt{3}A}{\alpha} = \cos\theta$$

$$\cos(\theta/2) = \frac{1}{\sqrt{2}}\sqrt{1+\cos\theta}$$

$$\begin{pmatrix} 3A & 2\sqrt{3}B \\ 2\sqrt{3}B & -3A \end{pmatrix} = \sqrt{3}\alpha\left(n_1\sigma_1 + n_3\sigma_3\right)$$

Eigenvalues	Eigenvectors
$+\sqrt{3}\alpha\hbar^2$	$\cos\frac{\theta}{2}\begin{pmatrix}1\\0\end{pmatrix} + \sin\frac{\theta}{2}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\sqrt{1+\frac{\sqrt{3}A}{\alpha}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\sqrt{1-\frac{\sqrt{3}A}{\alpha}}\begin{pmatrix}0\\1\end{pmatrix}$
$-\sqrt{3}\alpha\hbar^2$	$\sin\frac{\theta}{2}\begin{pmatrix}1\\0\end{pmatrix} - \cos\frac{\theta}{2}\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\sqrt{1-\frac{\sqrt{3}A}{\alpha}}\begin{pmatrix}1\\0\end{pmatrix} - \frac{1}{\sqrt{2}}\sqrt{1+\frac{\sqrt{3}A}{\alpha}}\begin{pmatrix}0\\1\end{pmatrix}$

In real life

$$+\sqrt{3}\alpha\hbar^2 \qquad \cos(\theta/2)\left|\tfrac{3}{2}\right\rangle + \sin(\theta/2)\left|-\tfrac{1}{2}\right\rangle \equiv |\psi_1\rangle$$
$$-\sqrt{3}\alpha\hbar^2 \qquad \sin(\theta/2)\left|\tfrac{3}{2}\right\rangle - \cos(\theta/2)\left|-\tfrac{1}{2}\right\rangle \equiv |\psi_2\rangle$$
$$+\sqrt{3}\alpha\hbar^2 \qquad \cos(\theta/2)\left|-\tfrac{3}{2}\right\rangle + \sin(\theta/2)\left|\tfrac{1}{2}\right\rangle \equiv |\phi_1\rangle$$
$$-\sqrt{3}\alpha\hbar^2 \qquad \sin(\theta/2)\left|-\tfrac{3}{2}\right\rangle - \cos(\theta/2)\left|\tfrac{1}{2}\right\rangle \equiv |\phi_2\rangle$$

c. $\vec{M} = \gamma \vec{I}$, $\vec{B}_0 = B_0 \vec{u}$

$$\boxed{W = -\vec{M}\cdot\vec{B}_0 = \underbrace{-\gamma B_0}_{\omega_0} \vec{I}\cdot\vec{u} = \omega_0 \vec{I}\cdot\vec{u}}$$

$$W = \omega_0 \big(\underbrace{I_x u_x + I_y u_y}_{\frac{1}{2}(u_x - iu_y) I_+ + \frac{1}{2}(u_x + iu_y) I_-} + I_z u_z \big) = \frac{1}{2}\omega_0 (u_x - iu_y) I_+ + \frac{1}{2}\omega_0 (u_x + iu_y) I_- + \omega_0 u_z I_z$$

To get the 1st order energy corrections, we must diagonalize W in the 2 degenerate subspaces. Notice that I_z couples m to m, $I_\pm$ couples m to $m \pm 1$.

$|\psi_1\rangle, |\phi_1\rangle$ subspace:

$$\langle \psi_1 | W | \psi_1 \rangle = \cos^2(\theta/2) \underbrace{\langle \tfrac{3}{2} | W | \tfrac{3}{2} \rangle}_{= \omega_0 u_z \langle \frac{3}{2} | I_z | \frac{3}{2} \rangle = \frac{3}{2}\hbar\omega_0 u_z} + \sin^2(\theta/2) \underbrace{\langle -\tfrac{1}{2} | W | -\tfrac{1}{2} \rangle}_{-\frac{1}{2}\hbar\omega_0 u_z}$$

$$= \frac{1}{2}\hbar\omega_0 u_z \big(\underbrace{3\cos^2(\theta/2) - \sin^2(\theta/2)}_{} \big)$$

$$= \frac{3}{2}(1+\cos\theta) - \frac{1}{2}(1-\cos\theta)$$

$$= 1 + 2\cos\theta$$

$$= 1 + 2\sqrt{3}A/\alpha$$

$$\langle \psi_1 | W | \psi_1 \rangle = \frac{1}{2}\hbar\omega_0 u_z (1 + 2\sqrt{3}A/\alpha)$$

$$\langle \phi_1 | W | \phi_1 \rangle = \cos^2(\theta/2) \langle -\tfrac{3}{2} | W | -\tfrac{3}{2} \rangle + \sin^2(\theta/2) \langle \tfrac{1}{2} | W | \tfrac{1}{2} \rangle$$

negative of $\langle \psi_1 | W | \psi_1 \rangle$

$$= -\tfrac{1}{2} \hbar\omega_0 u_z (1 + 2\sqrt{3} A/\alpha)$$

$$\langle \psi_1 | W | \phi_1 \rangle = \overbrace{\cos(\theta/2)\sin(\theta/2)}^{\frac{1}{2}\sin\theta} \langle \tfrac{3}{2} | W | \tfrac{1}{2} \rangle + \overbrace{\cos(\theta/2)\sin(\theta/2)}^{\frac{1}{2}\sin\theta} \langle -\tfrac{1}{2} | W | -\tfrac{3}{2} \rangle$$

$$+ \sin^2(\theta/2) \langle -\tfrac{1}{2} | W | \tfrac{1}{2} \rangle$$

$$= \tfrac{1}{2}\omega_0 (u_x - i u_y) \underbrace{\langle \tfrac{3}{2} | I_+ | \tfrac{1}{2} \rangle}_{C_+(\frac{3}{2},\frac{1}{2})\hbar = \sqrt{3}\hbar} = \tfrac{\sqrt{3}}{2} \hbar\omega_0 (u_x - i u_y)$$

$$= \tfrac{1}{2}\omega_0 (u_x - i u_y) \underbrace{\langle -\tfrac{1}{2} | W | -\tfrac{3}{2} \rangle}_{C_+(\frac{3}{2},-\frac{3}{2})\hbar = \sqrt{3}\hbar} = \tfrac{\sqrt{3}}{2} \hbar\omega_0 (u_x - i u_y)$$

$$= \tfrac{1}{2}\omega_0 (u_x + i u_y) \underbrace{\langle -\tfrac{1}{2} | I_- | \tfrac{1}{2} \rangle}_{C_-(\frac{3}{2},\frac{1}{2})\hbar = 2\hbar}$$

$$= \hbar\omega_0 (u_x + i u_y)$$

$$\langle \psi_1 | W | \phi_1 \rangle = \sin\theta \, \tfrac{\sqrt{3}}{2} \hbar\omega_0 (u_x - i u_y) + \tfrac{1}{2}(1 - \cos\theta) \hbar\omega_0 (u_x + i u_y)$$

$$= \tfrac{1}{2}\hbar\omega_0 \Big(u_x (\sqrt{3}\sin\theta + 1 - \cos\theta) + i u_y \big(\underbrace{-\sqrt{3}\sin\theta + 1 - \cos\theta}_{1 - \frac{\sqrt{3}(A+2B)}{\alpha}}\big) \Big)$$

$$\frac{2\sqrt{3}B}{\alpha} + 1 - \frac{\sqrt{3}A}{\alpha} = 1 - \frac{\sqrt{3}(A-2B)}{\alpha}$$

$$\langle \psi_1 | W | \phi_1 \rangle = \tfrac{1}{2}\hbar\omega_0 \left(u_x \left(1 - \frac{\sqrt{3}(A-2B)}{\alpha} \right) + i u_y \left(1 - \frac{\sqrt{3}(A+2B)}{\alpha} \right) \right)$$

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$$W \longrightarrow \begin{array}{c|c} & |\psi_1'\rangle \qquad\qquad\qquad |\phi_1\rangle \\ \begin{array}{c} |\psi_1'\rangle \\ |\phi_1\rangle \end{array} & \frac{1}{2}\hbar\omega_0 \begin{pmatrix} u_z\left(1+\frac{2\sqrt{3}A}{\alpha}\right) & u_x\left(1-\frac{\sqrt{3}(A-2B)}{\alpha}\right)+iu_y\left(1-\frac{\sqrt{3}(A+2B)}{\alpha}\right) \\ u_x\left(1-\frac{\sqrt{3}(A-2B)}{\alpha}\right)-iu_y\left(1-\frac{\sqrt{3}(A+2B)}{\alpha}\right) & -u_z\left(1+\frac{2\sqrt{3}A}{\alpha}\right) \end{pmatrix} \end{array}$$

$$= \frac{1}{2}\hbar\omega_0\left(u_z\left(1+\frac{2\sqrt{3}A}{\alpha}\right)\sigma_z + u_x\left(1-\frac{\sqrt{3}(A-2B)}{\alpha}\right)\sigma_x - u_y\left(1-\frac{\sqrt{3}(A+2B)}{\alpha}\right)\sigma_y \right)$$

Eigenvalues (1st order energy corrections) are

$$\pm\frac{1}{2}\hbar\omega_0\left(u_z^2\left(1+\frac{2\sqrt{3}A}{\alpha}\right)^2 + u_x^2\left(1-\frac{\sqrt{3}(A-2B)}{\alpha}\right)^2 + u_y^2\left(1-\frac{\sqrt{3}(A+2B)}{\alpha}\right)^2\right)^{1/2}$$

Total energy is $+\sqrt{3}\,\alpha\hbar^2 \pm$ (same thing)

$|\psi_2\rangle, |\phi_2\rangle$ subspace: Notice that under the change

$\theta \to \theta' = \theta - \pi$

$\cos(\theta/2) \longrightarrow \sin(\theta/2)$

$\sin(\theta/2) \longrightarrow -\cos(\theta/2)$

$\cos\theta \longrightarrow -\cos\theta$

$\sin\theta \longrightarrow -\sin\theta$

$\Rightarrow$ $A \to -A$, $B \to -B$

$|\psi_1\rangle \longrightarrow |\psi_2\rangle$

$|\phi_1\rangle \longrightarrow |\phi_2\rangle$

180° rotation on the 2 Bloch spheres

Eigenvalues (1st order energy corrections) are

$$\pm \frac{1}{2}\hbar\omega_0 \left(u_z^2\left(1-\frac{2\sqrt{3}A}{\alpha}\right)^2 + u_x^2\left(1+\frac{\sqrt{3}(A-2B)}{\alpha}\right)^2 + u_y^2\left(1+\frac{\sqrt{3}(A+2B)}{\alpha}\right)^2 \right)^{1/2}$$

Total energy is $-\sqrt{3}\alpha\hbar^2 \pm$ (same thing)

d. $\vec{B}_0 = B_0\vec{e}_z$ $\begin{pmatrix} u_x = u_y = 0 \\ u_z = 1 \end{pmatrix}$

Notice that in this case, the 2x2 perturbation matrices found in (c) are already diagonal, but with equal and opposite elements on the diagonal. The perturbation lifts the degeneracy but leaves the unperturbed eigenstates alone.

0-order eigenstates	1st order energies
$\vert\psi_1\rangle$	$\sqrt{3}\alpha\hbar^2 + \frac{1}{2}\hbar\omega_0(1+2\sqrt{3}A/\alpha)$
$\vert\phi_1\rangle$	$\sqrt{3}\alpha\hbar^2 - \frac{1}{2}\hbar\omega_0(1+2\sqrt{3}A/\alpha)$
$\vert\psi_2\rangle$	$-\sqrt{3}\alpha\hbar^2 + \frac{1}{2}\hbar\omega_0(1-2\sqrt{3}A/\alpha)$
$\vert\phi_2\rangle$	$-\sqrt{3}\alpha\hbar^2 - \frac{1}{2}\hbar\omega_0(1-2\sqrt{3}A/\alpha)$

Bohr frequencies of $I_x = \frac{1}{2}(I_+ + I_-)$?

Which energy eigenstates are coupled by I_x:

$\langle \psi_1 | I_x | \psi_2 \rangle = \langle \phi_1 | I_x | \phi_2 \rangle = 0$

$\Delta m = 0, \pm 2$ $\Delta m = 0, \pm 2$

no Bohr frequencies

$\pm(E_{\psi_1} - E_{\psi_2})/\hbar$

or

$\pm(E_{\phi_1} - E_{\phi_2})/\hbar$

$\langle \psi_1 | I_x | \phi_1 \rangle \neq 0$

$\Delta m = 3, \pm 1$

Bohr frequencies $\pm(E_{\psi_1} - E_{\phi_1})/\hbar$

$$\boxed{\pm \omega_0 (1 + 2\sqrt{3} A/\alpha)}$$

$\langle \psi_1 | I_x | \phi_2 \rangle \neq 0$

$\Delta m = 3, \pm 1$

Bohr frequencies $\pm(E_{\psi_1} - E_{\phi_2})/\hbar$

$$\boxed{\pm(2\sqrt{3}\alpha\hbar + \omega_0)}$$

$\langle \phi_1 | I_x | \psi_2 \rangle \neq 0$

$\Delta m = -3, \pm 1$

Bohr frequencies $\pm(E_{\phi_1} - E_{\psi_2})/\hbar$

$$\boxed{\pm(2\sqrt{3}\alpha\hbar - \omega_0)}$$

$\langle \psi_2 | I_x | \phi_2 \rangle \neq 0$

$\Delta m = 3, \pm 1$

Bohr frequencies $\pm(E_{\psi_2} - E_{\phi_2})/\hbar$

$$\boxed{\pm \omega_0 (1 - 2\sqrt{3} A/\hbar)}$$

RF field $\vec{B}_1 = B_1 \cos\omega_{RF} t\, \vec{e}_x$ gives rise to a term in the Hamiltonian:

$$-\vec{M}\cdot\vec{B}_1 = -\gamma B_1 \cos\omega_{RF} t\, I_x$$

The NMR spectrum will be nonzero when ω_{RF} is resonant with a transition driven by I_x (i.e, nonzero matrix element of I_x):