Physics 215B- Quantum Mechanics, Winter 2014

Problem Set 4, due Tuesday February 18

[1.] Consider the quantum harmonic oscillator, and perturbation

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}\, m\omega_0^2\, \hat{x}^2 \qquad\qquad \hat{V} = \delta\, \hat{x}^2$$

Compute the first and second order shifts in the energy levels of $\hat{H}_0$ due to $\hat{V}$. If you have time, solve the problem exactly and expand your result in a Taylor series in δ to check the perturbation calculation. You may find the identity $\hat{x} = \sqrt{\hbar/(2m\omega_0)}\,(a\ + a^\dagger)$ useful.

[2.] *Qualifier Problem!* Solve for and the sketch the perturbed energy levels of the $n = 2$ level of hydrogen in the presence of both a uniform electric and a uniform magnetic field. Neglect the spin of the electron and consider only orbital degrees of freedom. Do this for two cases:
(a) The $\vec{E}$ and $\vec{B}$ fields are parallel in orientation.
(b) The $\vec{E}$ and $\vec{B}$ fields are at right angles to each other.
You may find the following relations useful: $\langle 2s|x|2p, m = \pm 1\rangle = (3/\sqrt{2})a_0$, and $\langle 2s|z|2p, m = 0\rangle = 3a_0$, *Note:* We may need to review how to put a magnetic field $\vec{B}$ into a quantum mechanical Hamiltonian. What you do is replace $\hat{p}$ by $\hat{p} - (e/c)\vec{A}$ where A is the vector potential which produces the desired $\vec{B} = \nabla \times \vec{A}$.

[3.] *Qualifier Problem!* Consider an atom in a crystal with two eigenstates ψ_1 and ψ_2 with energies $E_{1,0}, E_{2,0}$. As the crystal is compressed, the crystalline field varies and the eigenstates are perturbed. The matrix of the perturbation in the basis of ψ_1 and ψ_2 is

$$\hat{H} = \begin{pmatrix} 0 & 3\epsilon \\ 3\epsilon & 4\epsilon \end{pmatrix}$$

(a) What are the first and second order corrections to the energies of the states if $E_{1,0} \neq E_{2,0}$?
(b) What are the lowest order corrections to the energies if $E_{1,0} = E_{2,0}$?
(c) Sketch the energies of the two states as a function of the compression parameter ϵ.

[4.] Consider the three dimensional infinite cubical well, $V_0(x, y, z) = 0$ if $0 < x, y, z < a$ and $V_0(x, y, z) = \infty$ otherwise. Add a perturbation $V(x, y, z) = W$, if $0 < x, y < a/2$ and $V(x, y, z) = 0$ otherwise. Compute the shifted eigenenergies and eigenstates of the ground state and first excited states.

[5.] Compute, to first order, the correction to the ground state energy of a Hydrogen atom due to the finite spatial extent of the nucleus. For simplicity, assume the nucleus is spherical, of radius R, and that its charge e is uniformly distributed throughout its volume.

[6.] Compute, to first order, the changes to the energy levels of a Hydrogen-like atom (ie one with nuclear charge Ze) produced by a unit increase $Z \to Z + 1$ (due, for example, to β decay). Using the exact energies, discuss the validity of the approximation.

Problem Set 4 Solutions

Physics 215B

Winter 2014

1. $\hat{H} = \hat{P}^2/2m + 1/2\, m\omega_0^2 \hat{x}^2 + \delta \hat{x}^2$

Exact soln: $V(x) = 1/2\, m(\omega_0^2 + 2\delta/m)\hat{x}^2$

$$\omega^2 = \left(\omega_0^2 + 2\delta/m\right)$$

$$\omega = \left(\omega_0^2 + 2\delta/m\right)^{1/2}$$

$$E_n = \hbar\left(\omega_0^2 + 2\delta/m\right)^{1/2}(n+1/2)$$

$$\downarrow$$

Expanding $\omega_0\left(1 + 2\delta/m\omega_0^2\right)^{1/2}$

$$= \omega_0\left(1 + \delta/m\omega_0^2 - 1/2\left(\delta/m\omega_0^2\right)^2 + \ldots\right)$$

So 1st order $\hbar\dfrac{\delta}{m\omega_0}(n+1/2)$

2nd order $-\hbar\dfrac{\delta^2}{2m^2\omega_0^3}(n+1/2)$

Now do perturbation theory

$$\hat{x}^2 = \frac{\hbar}{2m\omega_0}(a+a^\dagger)^2 = \frac{\hbar}{2m\omega_0}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$$

1-2

$$E_{n1} = \langle n|\delta\hat{x}^2|n\rangle$$

$$= \frac{\hbar\delta}{2m\omega_0}\left\{\phi + (n+1) + n + \phi\right\} = \frac{\hbar\delta}{m\omega_0}(n+1/2) \quad \checkmark$$

$$E_{n2} = \sum_{m\neq n} |\langle n|\delta\hat{x}^2|m\rangle|^2 / E_{n0} - E_{m0}$$

$$= \delta^2\left(\frac{\hbar}{2m\omega_0}\right)^2\left\{\frac{(n+2)(n+1)}{-2\hbar\omega_0} + \frac{(n-1)n}{+2\hbar\omega_0}\right.$$

$m = n+2$ connected to n by aa

$m = n-2$ connected to n by a^+a^+

$$= -\delta^2\frac{\hbar}{8m^2\omega_0^3}\left\{n^2 + 3n + 2 - n^2 + n\right\}$$

$$4n+2 = 4(n+1/2)$$

$$= -\delta^2\hbar/2m^2\omega_0^3\ (n+1/2) \quad \checkmark\checkmark$$

2. a) $\vec{E} = E\hat{z}$

$\vec{B} = B\hat{z}$ $\qquad \vec{A} = -\frac{1}{2}By\hat{x} + \frac{1}{2}Bx\hat{y}$

$$\hat{H} = \frac{1}{2m}\left(\hat{p} - \frac{e}{c}\vec{A}\right)^2 - e^2/r + e\phi_E$$

$$= \underbrace{\hat{p}^2/2m - e^2/r}_{\hat{H}_0} + \underbrace{\frac{eB}{mc}(yp_x - xp_y) - eEz}_{\hat{V}\ \text{(ignore } B^2 \text{ term)}}$$

Note: $\hat{L}_z = x\hat{p}_y - y\hat{p}_x$ so

$$\hat{V} = -eB/mc\,\hat{L}_z - eEz.$$

The four $n=2$ levels are <u>degenerate</u>. We need to diagonalize the matrix $\langle \phi_{2\ell m} | \hat{V} | \phi_{2\ell' m'} \rangle$

$\ell = 1 \quad m = -1, 0, 1$

$\ell = 0 \quad m = 0$

Using the clue in the problems, and letting $w_0 = eB/mc$

$$\hat{V} = \begin{array}{c} \\ 1\,1 \\ 1\,-1 \\ 1\,0 \\ 0\,0 \end{array} \begin{array}{c} \begin{array}{cccc} 1\,1 & 1\,-1 & 1\,0 & 0\,0 \end{array} \\ \begin{pmatrix} -\hbar w_0 & \phi & \phi & \phi \\ \phi & +\hbar w_0 & \phi & \phi \\ \phi & \phi & \phi & -3a_0Ee \\ \phi & \phi & -3a_0Ee & \phi \end{pmatrix} \end{array}$$

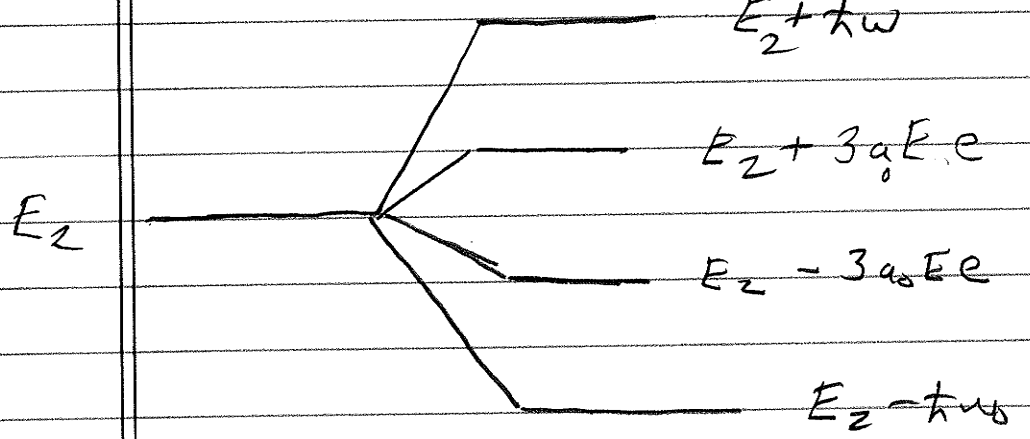
To construct this $\hat{V}$ we noticed the $-\omega_0 \hat{L}_z$ term is already diagonal in the H atom wavefunctions and also symmetries like $[z, L_z] = 0$ which tell us

$$0 = \langle lm | z \hat{L}_z - \hat{L}_z z | l'm' \rangle$$

$$= \langle lm | z | l'm' \rangle \hbar (m - m')$$

We also know $\langle lm | z | lm \rangle = 0$ by parity.

Our conclusion for this case is the picture



NB if E or B were a much larger perturbation than the other, one might try treating them separately.

(b) We leave $\vec{B} = B\hat{z}$ but choose $\vec{E} = E\hat{x}$

We have $\langle \ell m | \hat{x} | \ell m \rangle = 0$ by parity

and are given $\langle 2\,0\,0 | \hat{x} | 2\,1\,\pm 1 \rangle = {}^{3}/_{\sqrt{2}}\, a_0$

$2s$ $\quad$ $2p\ m = \pm 1$

So it seems as if our $\hat{V}$ matrix looks like

$$\hat{V} = \begin{array}{c} \\ |1\,1\rangle \\ |1\,-1\rangle \\ |1\,0\rangle \\ |0\,0\rangle \end{array} \begin{array}{c} \begin{array}{cccc} |1\,1\rangle & |1\,-1\rangle & |1\,0\rangle & |0\,0\rangle \end{array} \\ \begin{pmatrix} -\hbar\omega_0 & ? & ? & {}^{3}/_{\sqrt{2}}\, a_0 E \\ ? & +\hbar\omega_0 & ? & {}^{3}/_{\sqrt{2}}\, a_0 E \\ ? & ? & 0 & ? \\ {}^{3}/_{\sqrt{2}}\, a_0 E & {}^{3}/_{\sqrt{2}}\, a_0 E & ? & 0 \end{pmatrix} \end{array}$$

Do we know the ? values like $\langle 1\,1 | \hat{x} | 1\,0 \rangle$

and $\langle 1\,0 | \hat{x} | 0\,0 \rangle$. Since qual exam did not

give me might assume they vanish. But

let's check it out!

First see why $\langle 00 | \hat{x} | 1 \pm 1 \rangle$ are non vanishing

Y_{00} $\quad$ $\sin\theta\cos\phi$ $\quad$ $\sin\theta\, e^{\pm i\phi}$

get integral like $\int_0^\pi \sin\theta\, d\theta\, \sin^2\theta \int_0^{2\pi} d\phi \cos\phi (\cos\phi \pm i\sin\phi)$

nonzero since $\sin\theta > 0$ throughout $(0,\pi)$ $\quad$ $2\pi(\frac{1}{2})$

So this checks out. Let's examine others

$\langle 10 | \hat{x} | 00 \rangle \sim \int_0^{2\pi} d\phi \cos\phi$

$\cos\theta$ $\quad$ $\sin\theta\cos\phi$ $\quad$ Y_{00} $\quad$ vanishes

$\langle 11 | \hat{x} | 10 \rangle \sim \int_0^\pi \sin\theta d\theta \sin^2\theta\cos\theta \int_0^{2\pi} d\phi \cos\phi(\cos\phi \pm i\sin\phi)$

$\sin\theta\, e^{\pm i\phi}$ $\quad$ $\sin\theta\cos\phi$ $\quad$ $\cos\theta$ $\quad$ $2\pi(\frac{1}{2})$

$\frac{\sin^4\theta}{4}\Big|_0^\pi \to 0.$

So likely all other matrix elements do vanish

ie $\hat{x}$ connects only $m = \pm 1$ to $m = 0$ for

different ℓ.

2-5

Need eigenvalues then of the 4×4 matrix

$$\begin{pmatrix} -\hbar\omega_0 & 0 & 0 & \epsilon \\ 0 & \hbar\omega_0 & 0 & \epsilon \\ 0 & 0 & 0 & 0 \\ \epsilon & \epsilon & 0 & 0 \end{pmatrix} \qquad \text{with } \epsilon \equiv \frac{3}{\sqrt{2}} \mathcal{E}_0 e$$

$$(-\hbar\omega_0 - \lambda)\left[(\hbar\omega_0 - \lambda)\lambda^2 + \epsilon(0 + \lambda\epsilon)\right]$$

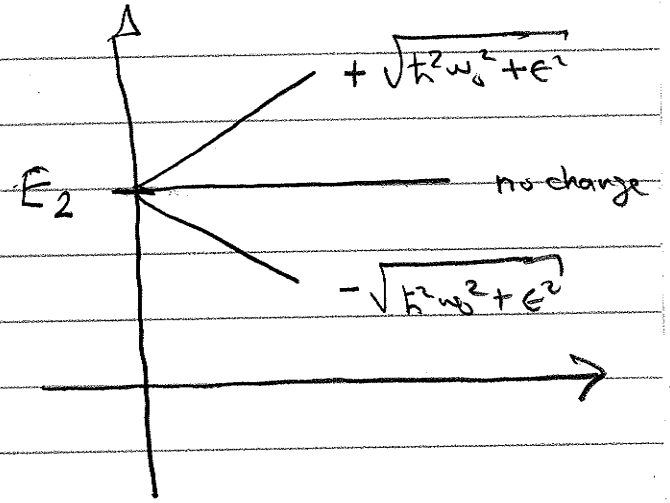
$$-\epsilon\left[(-\hbar\omega_0)(0 + \epsilon\lambda)\right]$$

$$= -(\lambda^2 - \hbar^2\omega_0^2)\lambda^2 - \epsilon^2\lambda(\lambda + \hbar\omega_0) + \epsilon^2\lambda\hbar\omega_0$$

$$= \lambda^2(\lambda^2 - \hbar^2\omega_0^2 - \epsilon^2)$$

$\lambda = 0$ (twice)

$\lambda = \pm\sqrt{\hbar^2\omega_0^2 + \epsilon^2}$

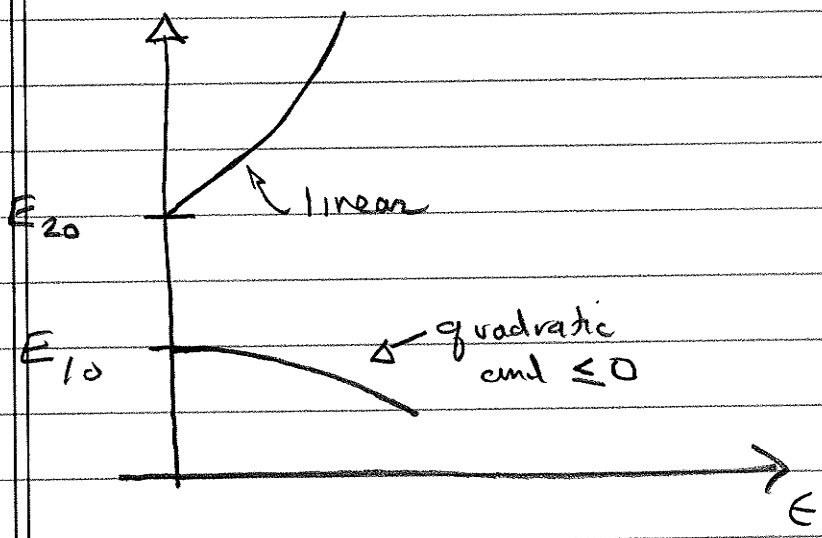


3 a) $E_{11} = (1\ 0)\begin{pmatrix} 0 & 3\epsilon \\ 3\epsilon & 4\epsilon \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \phi$

$$E_{21} = (0\ 1)\begin{pmatrix} 0 & 3\epsilon \\ 3\epsilon & 4\epsilon \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 4\epsilon$$

$$E_{12} = \frac{\left|(1\ 0)\begin{pmatrix} 0 & 3\epsilon \\ 3\epsilon & 4\epsilon \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right|^2}{E_{10} - E_{20}} = \frac{9\epsilon^2}{E_{10} - E_{20}} < 0$$

$$E_{22} = 9\epsilon^2 / E_{20} - E_{10} = -E_{12} > 0$$



b) Must diagonalize perturbation in degenerate subspace (Here entire 2 dim Hilbert space!)

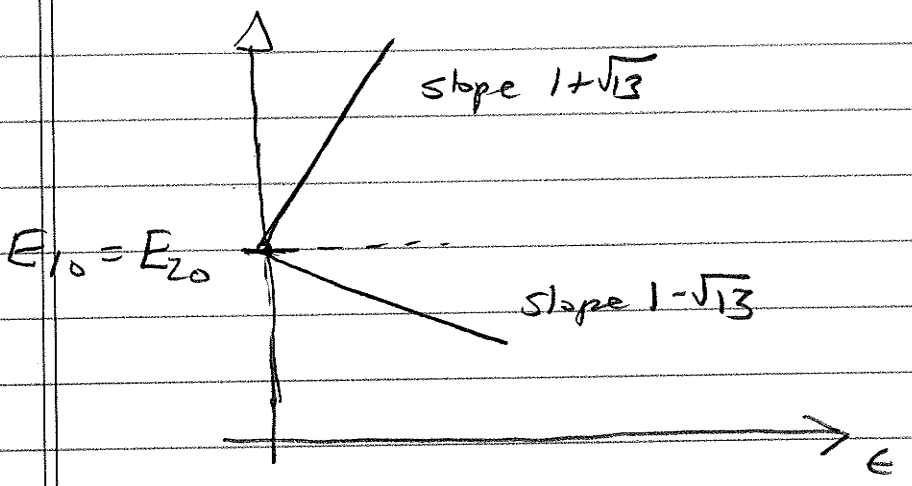
$$0 = -\lambda(4\epsilon - \lambda) - 9\epsilon^2 = \lambda^2 - 4\epsilon\lambda - 9\epsilon^2$$

3-2

$$\lambda = \frac{1}{2}\left\{4\epsilon \pm \sqrt{16\epsilon^2 + 36\epsilon^2}\right\}$$

$$= \frac{1}{2}\left\{2\epsilon \pm \epsilon 2\sqrt{13}\right\}$$

$$\lambda = \epsilon\left(1 \pm \sqrt{13}\right)$$



4 For the ground state (I am using L for a)

$$\phi_{111} = \left(2/L\right)^{3/2} \sin\frac{\pi x}{L} \sin \pi y/L \sin \pi z/L$$

The first order shift is

$$E_{111,1} = \int_0^L dz \int_0^{L/2} dx \int_0^{L/2} dy \; W |\phi_{111}|^2$$

$$= W\left(2/L\right)^3 \frac{L}{2} \left(\int_0^{L/2} dx \sin^2 \frac{\pi x}{L}\right)\left(\quad\right)$$

$\frac{L}{2}$: Z integration; $\int_0^{L/2} dx \sin^2 \frac{\pi x}{L}$: $L/4$; $(\quad)$: Y same as X

$$= W\left(2/L\right)^2 \left(L/4\right)^2 = W/4$$

This is sort of obvious — perturbation is spatially indep and particle spends 1/4 of its time in $0 < x, y < L/2$

I expect same answer for 1st excited state,

5-1

5 The electric field at distance r from the center of a uniform sphere of charge e is given by Gauss' law:

$$4\pi r^2 E = \left[\frac{4}{3}\pi r^3 \Big/ \frac{4}{3}\pi R^3\right] e \quad 4\pi$$

CGS: $\Phi_E = 4\pi Q_{enc}$

$$E = er/R^3$$

The potential at r is given by the potential at R plus the extra work to get to r

$$V(r) = e/R + \int_r^R er'/R^3\, dr'$$

$$= e/R + er'^2/2R^3 \Big|_r^R = e/R + e/2R - er^2/2R^3$$

$$V(r) = 3e/2R - er^2/2R^3$$

The perturbation is the difference between this potential energy and the usual point nucleus one

$$\hat{V} = -e\left\{\frac{3e}{2R} - \frac{er^2}{2R^3} - \frac{e}{r}\right\} \qquad 0 < r < R$$

According to first order perturbation theory

$$E_{11} = \int \phi_{100} V \phi_{100} \, d^3r$$

with $\phi_{100} = 1/\sqrt{\pi a^3} \, e^{-r/a}$ $\quad a = \hbar^2/me^2$

I will set $e^{-r/a} = 1$ because R, the nucleon radius, is much less than a, and we are only integrating out to $r = R$

$$E_{11} = 1/\pi a^3 \int_0^R -e^2 \left\{ \frac{3}{2R} - \frac{r^2}{2R^3} + \frac{e^2}{r} \right\} 4\pi r^2 \, dr$$

$$= \frac{-e^2 4\pi}{\pi a^3} \left\{ \frac{r^3}{2R} - \frac{r^5}{10R^3} - \frac{r^2}{2} \right\}_0^R$$

$$R^2 \{ 1/2 - 1/10 - 1/2 \}$$

$$E_{11} = +\frac{2}{5} e^2 R^2/a^3$$

Noticing $E_{10} = -me^4/2\hbar^2$

$$E_{10} + E_{11} = -me^4/2\hbar^2 \left\{ 1 - \frac{4}{5}\left(\frac{R}{a}\right)^2 \right\}$$

[6] The exact energy levels of a hydrogen-like atom with nuclear charge Ze instead of e are

$$E_n = -\frac{me^4}{2\hbar^2} Z^2/n^2$$

So the exact shift from $Z \to Z+1$ is

$$\Delta E_n^{exact} = -\frac{me^4}{2\hbar^2}\left((Z+1)^2 - Z^2\right) 1/n^2$$

$$= -me^4/2\hbar^2 \,(2Z+1)\, 1/n^2$$

The perturbation is $\hat{V} = -e^2/r$ if $Z \to Z+1$

and so the first order shift is

$$E_{n1} = -\int \phi_{nem}(r)\, \frac{e^2}{r}\, \phi_{nem}\, d^3r$$

A useful result for hydrogen like atoms is

$$\langle 1/r \rangle = 1/n^2\, 1/a \qquad a = \hbar^2/Zme^2$$

Thus $E_{n1} = -e^2/a\, 1/n^2 = -me^4 Z/\hbar^2\, 1/n^2$

This agrees with the exact result for $Z \gg 1$

which is reasonable.