Finite Spatial Extent of the Nucleus

(a) The first step is to find $V(r)$ for our Hamiltonian.

$$V(r) = -\int_0^\infty eEdr' = -\int_r^R eE_{in}dr' - \int_R^\infty eE_{out}dr \tag{1}$$

Where E_{in} is the field inside the proton and and E_{out} is the field outside. Treating the proton as a sphere of uniform charge density ρ, we have

$$E_{in} = \frac{Q_{enc}}{r^2} = \rho\frac{4\pi r^3}{3r^2} = \rho\frac{4\pi r}{3}. \tag{2}$$

where ρ is

$$\rho = \frac{3Ze}{4\pi R^3}. \tag{3}$$

Thus the field becomes

$$E_{in} = \frac{Zer}{R^3}. \tag{4}$$

The first integral in equation 1 is then

$$\begin{aligned} -\int_r^R eE_{in}dr' &= -\int_r^R \frac{Ze^2r'}{R^3}dr' \\ &= -\frac{Ze^2}{2R^3}(R^2 - r^2) \\ &= -\frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{1}{2}\right). \end{aligned} \tag{5}$$

And because we know that $E_{out} = Ze/r^2$, the second integral becomes

$$-\int_R^\infty eE_{out}dr = -\int_R^\infty \frac{Ze^2}{r^2}dr = -\frac{Ze^2}{R}. \tag{6}$$

Plugging equations 5 and 6 into equation 1, we have

$$V(r) = \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right). \tag{7}$$

(b) We can break up the full Hamiltonian $\hat{H}_a$ into a two parts

$$\hat{H}_1 = \hat{H}_0 + \hat{V} \tag{8}$$

Where $\hat{H}_0$ is the Hamiltonian for a hydrogen atom with a point nucleus and $\hat{V}$ is the perturbation resulting from the potential we derived above. $hatV$ is simply the difference between $V(r)$ and the potential for a point nucleus.

$$\hat{V} = V(r) - (-\frac{Ze^2}{r}) = \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2} + \frac{R}{r}\right). \tag{9}$$

The perturbation $\hat{V}$ is only effective within the radius of the proton, that is

$$\hat{V} = \begin{cases} \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2} + \frac{R}{r}\right) & \text{for } 0 \leq r \leq R \\ 0 & \text{for } r < R \end{cases} \tag{10}$$

And the full Hamiltonian is

$$\hat{H} = \begin{cases} \frac{\hat{p}^2}{2m} + \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2}\right) & \text{for } 0 \leq r \leq R \\ \frac{\hat{p}^2}{2m} + \frac{Ze^2}{r} & \text{for } r < R \end{cases} \tag{11}$$

(c) The ground state wave function for hydrogen is

$$\psi_{100} = R_{10}Y_{00} = \frac{1}{\sqrt{4\pi}} 2a_0^{-3/2} e^{-r/a_0} \tag{12}$$

Because we know $R \ll a_0$, we can assume that the exponential term in the integral goes to 1, and we have

$$\psi_{100} \approx \frac{1}{\sqrt{4\pi}} 2a_0^{-3/2} \tag{13}$$

The first order correction to the ground state energy level is thus given by

$$\begin{aligned} \langle\psi_{100}|\hat{V}|\psi_{100}\rangle &= \int_0^R \frac{1}{4\pi} 2a_0^{-3} \frac{Ze^2}{R}\left(\frac{r^2}{2R^2} - \frac{3}{2} + \frac{R}{r}\right) 4\pi r^2 dr \\ &= \frac{2ZeR^2}{5a_0^3}. \end{aligned} \tag{14}$$

Meanwhile, the ground state energy for a hydrogen atom with a point nucleus is

$$E_{100}^{(0)} = \frac{e^2}{2a_0}. \tag{15}$$

Given that

$$a_0 = 5.3 * 10^{-11}\text{m} \quad \text{and} \quad R = 1.2 \times 10^{-15}\text{m} \tag{16}$$

the ratio between the unperturbed level and the first order correction is

$$\frac{E_{100}^{(1)}}{E_{100}^{(0)}} = \frac{4}{5}\frac{R}{a_0}^2 \approx 4.1 \times 10^{-10}, \tag{17}$$

a very small pertubation. We can compare this to hyperfine splitting

$$\frac{E_{hf}}{E_{100}^{(0)}} = \frac{5.9 \times 10^{-6}}{13.6} \approx 4.3 \times 10^{-7} \tag{18}$$

Prob. 10.9.12 *(solution by Michael Fisher)*

a

We can denote the spin states as + for spin up and − for spin down. We have

$$\hat{H}_o = \frac{\hbar w}{2}\hat{\sigma}_z + \hbar w(\hat{a}\hat{a}^\dagger + \frac{1}{2})$$

so

$$\hat{H}_o \left|n-\right\rangle = -\frac{\hbar w}{2} + \hbar w(n + \frac{1}{2}) = n\hbar w$$
$$\hat{H}_o \left|n+\right\rangle = \frac{\hbar w}{2} + \hbar w(n + \frac{1}{2}) = (n+1)\hbar w$$

b

The ground state is $|0-\rangle$ with energy

$$\hat{H}_o \left|0-\right\rangle = (-\frac{\hbar w}{2} + \frac{\hbar w}{2}) \left|0-\right\rangle = 0$$

The first excited states are $|0+\rangle$ and $|1-\rangle$ with energies

$$\hat{H}_o \left|0+\right\rangle = \hbar w \left|0+\right\rangle$$
$$\hat{H}_o \left|1-\right\rangle = \hbar w \left|1-\right\rangle$$

c

First we apply $\hat{H}_1$ to arbitrary states

$$\hat{H}_1 \left|n+\right\rangle = \frac{\hbar\Omega}{2}\hat{a}^\dagger \left|n-\right\rangle = \frac{\hbar\Omega}{2}\sqrt{n+1} \left|(n+1)-\right\rangle$$
$$\hat{H}_1 \left|n-\right\rangle = \frac{\hbar\Omega}{2}\sqrt{n} \left|(n-1)-\right\rangle$$

So for the ground and first excited states we get

$$\hat{H}_1 |0-\rangle = 0$$
$$\hat{H}_1 |0+\rangle = \frac{\hbar\Omega}{2} |1-\rangle$$
$$\hat{H}_1 |1-\rangle = \frac{\hbar\Omega}{2} |0+\rangle$$

We can write the the ground and first excited states as a vector

$$\begin{pmatrix} |0-\rangle \\ |0+\rangle \\ |1-\rangle \end{pmatrix}$$

Then, with this representation we get

$$\hat{H} = \hat{H}_o + \hat{H}_1 = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & w & \frac{\Omega}{2} \\ 0 & \frac{\Omega}{2} & w \end{pmatrix}$$

d

For the nondegenerate ground level, $E_o = 0$ and $\langle 0-| \hat{H}_1 |0-\rangle = 0$ so the total energy to first order is $E = 0$.

For the degenerate first excited state, we consider the vector

$$\begin{pmatrix} |0+\rangle \\ |1-\rangle \end{pmatrix}$$

and write the subspace matrix in this representation as

$$\frac{\hbar\Omega}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The eigenvalues of this matrix are

$$\pm\frac{\hbar\Omega}{2}$$

So the energy to first order of the excited state is

$$E = \hbar w \pm \frac{\hbar\Omega}{2}$$

In other words, the perturbation gets rid of the degeneracy of the first excited state.

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Physics 113
Boccio 10.9.18.

In this problem we supposed that the Hamiltonian of a rigid rotator in a magnetic field is of the form $\hat{H} = A\vec{L}^2 + B\hat{L}_z + C\hat{L}_y$. We assume that $A, B >> C$, which means that $C\hat{L}_y$ is the perturbation of the system. We want to use perturbation theory to lowest nonvanishing order to get approxiamate energy eigenvalues.

First, without the perturbation, we have that the energy values are $E_n = A\hbar^2 l(l+1) + Bm\hbar$.

When adding the perturbation, we remember that $\hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-$. We also remember that $L_\pm|lm\rangle = \sqrt{(l \mp m)(l \pm m + 1)}\hbar|l, m \pm 1\rangle$.

We can see that the first order corrections vanish. For example, $\langle 10|C\hat{L}_y|10\rangle = 0$. Therefore, we must look at the second order corrections.

For the second order corrections we have that

$$\begin{aligned}
E_n^{(2)} &= C^2 \sum_{m'} \frac{|\langle l'm'|\frac{1}{2i}(\hat{L}_+ - \hat{L}_-)|lm\rangle|^2}{E_{lm}^{(0)} - E_{l'm'}^{(0)}} \quad \text{l' must equal l} \\
&= \frac{C^2\hbar^2(l-m)(l+m+1)}{-4B\hbar} + \frac{C^2\hbar^2(l+m)(l-m+1)}{4B\hbar} \\
&= \frac{C^2\hbar^2}{4B}[(-l^2 - l + m^2 + m) + l^2 + l - m^2 + m] \\
&= \frac{C^2\hbar^2}{4B}(2m) \\
&= \frac{C^2\hbar m}{2B}.
\end{aligned}$$

Therefore, we have that using perturbation theory, we have that the new expression for the energy is given by $E_n = A\hbar^2 l(l+1) + Bm\hbar + \frac{C^2\hbar m}{2B}$.

Given $\hat{H} = \hat{H}_0 + \frac{1}{2}m\omega^2 x^2 + \lambda \sin kx$ and $\hat{H}_0 = \hbar\omega(\hat{a}\hat{a}^+ + \frac{1}{2})$.

We know

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}kx^2 \qquad \text{where } k = m\omega^2$$
$$\hat{V} = \lambda \sin kx \to \hat{W} = \sin kx = e^{ik\hat{x}} = e^{ik(\hat{a}^+ + \hat{a})}$$

Then we can find the perturbed ground state

$$|0'\rangle = |0\rangle - \frac{\lambda}{\hbar\omega}\sum_{n=1}^{\infty} \frac{\langle n|e^{ik(\hat{a}^+ + \hat{a})}|0\rangle}{|n\rangle}$$

$$= \hbar\omega(n+\tfrac{1}{2})\,|n\rangle - \frac{\lambda}{\hbar\omega}\sum_{n=1}^{\infty} e^{-\frac{1}{4}\frac{\hbar}{m\omega_0}k^2} \frac{\langle n|e^{ik\sqrt{\frac{\hbar}{2m\omega_0}}}|0\rangle}{|n\rangle}$$

$$= \hbar\omega(n+\tfrac{1}{2})\,|n\rangle - \frac{\lambda}{\hbar\omega}e^{-\frac{1}{4}\frac{\hbar}{m\omega_0}k^2}\sum_{n=odd}^{\infty} \frac{\langle n|(ik\sqrt{\frac{\hbar}{2m\omega_0}})^n|n\rangle}{n\sqrt{n!}}$$

$$|0'\rangle = \hbar\omega(n+\tfrac{1}{2})\,|n\rangle - \frac{\lambda}{\hbar\omega}e^{-\frac{1}{4}\frac{\hbar}{m\omega_0}k^2}\sum_{n=odd}^{\infty} \frac{(ik\sqrt{\frac{\hbar}{2m\omega_0}})^n}{n\sqrt{n!}}$$

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In this problem we have a paricle of mass m that moves in a one dimensional potential box:

$$V(x) = \begin{cases} \infty & \text{for} \quad |x| > 3a \\ 0 & \text{for} \quad a < x < 3a \\ 0 & \text{for} \quad -3a < x < -a \\ V_0 & \text{for} \quad |x| < a \end{cases}$$

We want to use first order perturbation theory to calculate the new energy of the ground state. So, first, we have that the energies without the perturbation are $E_n = \frac{\hbar^2\pi^2n^2}{72ma^2}$. Thus, with the perturbation of V_0, we have that the energies are $E_n = \frac{\hbar^2\pi^2n^2}{72ma^2} + E_n^{(1)}$.

Then, for the first order correction we have,

$$\begin{aligned} E_n^{(1)} &= \langle\psi_n|V_0|\psi_n\rangle \\ &= \frac{1}{3a}\int_{-a}^{a} \sin^2(\frac{n\pi x}{6a})V_0 dx \\ &= \frac{V_0}{3a}\int_{-a}^{a} \sin^2(\frac{n\pi x}{6a})dx \\ &= \frac{V_0}{3} - \frac{V_0 n\pi}{36a^2}\sin(\frac{n\pi}{6}). \end{aligned}$$

Therefore, the new energy expression is $E_n = \frac{\hbar^2\pi^2n^2}{72ma^2} + \frac{V_0}{3} - \frac{V_0n\pi}{36a^2}\sin(\frac{n\pi}{6})$. Thus, the new ground state energy is $E_1 = \frac{\hbar^2\pi^2}{72ma^2} + \frac{V_0}{3} - \frac{V_0\pi}{36a^2}\sin(\frac{\pi}{6}) = \frac{\hbar^2\pi^2 - mV_0\pi}{72ma^2} + \frac{V_0}{3}$.

Perturbing the 2-dimensional Infinite Square Well

Consider a particle in a 2-dimensional infinite square well given by

$$V(x,y) = \begin{cases} 0 & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ \infty & \text{otherwise} \end{cases}$$

(a) What are the energy eigenvalues and eigenkets for the three lowest levels?

(b) We now add a perturbation given by

$$V(x,y) = \begin{cases} \lambda xy & \text{for } 0 \le x \le a \text{ and } 0 \le y \le a \\ 0 & \text{otherwise} \end{cases}$$

Determine the first order energy shifts for the three lowest levels for $\lambda \ll 1$

(c) Draw an energy diagram with and without the perturbation for the three energy states. Make sure to specify which unperturbed state is connected to which perturbed state.

Solution

(a) We know that the energy levels for an unperturbed, 2-dimensional, infinite square well are given by

$$\epsilon_{n_x n_y} = \frac{\hbar^2 \pi}{2ma^2}(n_x^2 + n_y^2) \tag{1}$$

From this equation, we can determine the first three energy levels

$$\epsilon_{11} = \frac{\hbar^2\pi^2}{2ma^2} \qquad \epsilon_{12} = \epsilon_{21} = \frac{5\hbar^2\pi^2}{2ma^2} \qquad \epsilon_{22} = \frac{4\hbar^2\pi^2}{ma^2} \tag{2}$$

Where the first excited energy is two-fold degenerate. We also know that the corresponding wave functions are

$$\begin{aligned} \psi_{11} &= \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{\pi x}{a} & \psi_{12} &= \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} \\ \psi_{21} &= \frac{2}{a}\sin\frac{2\pi x}{a}\sin\frac{\pi x}{a} & \psi_{12} &= \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} \end{aligned} \tag{3}$$

(b) For the two non-degenerate states, the first order corrections are given by

$$E_{11}^{(1)} = \langle 11|V_1|11\rangle = \int_0^a \int_0^a \frac{4}{a^2} \sin^2\left(\frac{\pi x}{a}\right) \sin^2\left(\frac{\pi x}{a}\right) xydxdy = \frac{\lambda a^2}{4} \tag{4}$$

and

$$E_{22}^{(1)} = \langle 22|V_1|22\rangle = \int_0^a \int_0^a \frac{4}{a^2} \sin^2\left(\frac{2\pi x}{a}\right) \sin^2\left(\frac{2\pi x}{a}\right) xydxdy = \frac{\lambda a^2}{4}. \tag{5}$$

For the degenerate states, we need to find the eigenvalues of the matrix representation of V_1 in the degenerate basis. We have

$$V_1 = \begin{pmatrix} \langle 12|V_1|12\rangle & \langle 12|V_1|21\rangle \\ \langle 21|V_1|12\rangle & \langle 21|V_1|21\rangle \end{pmatrix} = \lambda a^2 \begin{pmatrix} \frac{1}{4} & \frac{256}{81\pi^4} \\ \frac{256}{81\pi^4} & \frac{1}{4} \end{pmatrix} \tag{6}$$

which has eigenvalues

$$E_{12}^{(1)} = \frac{81\pi^2 + 1024}{324\pi^2} \quad \text{and} \quad E_{21}^{(1)} = \frac{81\pi^2 - 1024}{324\pi^2} \tag{7}$$

where I have arbitrarily assigned each eigenvalue to a first order correction to the degenerate energy levels.

A mass m is attached by a massless rod of length L to a pivot P and swings in a vertical plane under the influence of gravity.

(a) We can use the small angle approximation to find the quantum mechanical energy levels. First, we know

$$\hat{H} = \frac{\hat{p}^2}{2mL^2} + mgL(1 - \cos\phi)$$

We can assume $x << L$ therefore $\phi \approx \frac{x}{L}$ and small angle approximation lets us estimate $\cos\phi \approx 1 - \frac{\psi^2}{2}$.

$$\hat{H} = \frac{\hat{p}^2}{2mL^2} + mgL(\frac{x^2}{2L^2})$$
$$\hat{H} \approx \frac{\hat{p}^2}{2mL^2} + \frac{mgx^2}{2L})$$

Also,

$$E_n = \hbar\omega(n + \tfrac{1}{2}) = \hbar\sqrt{\tfrac{g}{l}}(n + \tfrac{1}{2})$$

(b) We can also find he lowest order correction to the ground state energy resulting from the inaccurracy of the small angle approximation by looking at the next term of the taylor expansion.

$$\hat{H} = \frac{\hat{p}^2}{2mL^2} + mgL(1 - \cos\phi)$$
$$E_n^{(1)} = \langle n| \frac{x_0^4}{4L^4}(\hat{a}^2 + 2\hat{a}\hat{a}^+ + \hat{a^+}^2)^2 |n\rangle$$
$$= 6n^2 + 6n + 3$$

a only

We can write

$$\hat{H} = \hat{H}_o + \hat{V} = \frac{1}{2}mw^2x^2 + (\alpha x^3 + \beta x^4)$$

Let

$$c = \sqrt{\frac{2\hbar}{mw}}$$

Then

$$x^3 = \frac{c^3}{8}(\hat{a} + \hat{a}^\dagger)^3$$
$$x^4 = \frac{c^4}{16}(\hat{a} + \hat{a}^\dagger)^4$$

Since $\hat{H}_o$ is the harmonic oscillator, the eigenvalues and eigenvectors are those of the harmonic oscillator. The first order perturbation term is given by

$$\langle n| \hat{V} |n\rangle$$

In order for this to not equal zero, an equal number of $\hat{a}$ and $\hat{a}^\dagger$ must be applied. Therefore, the x^3 term cannot contribute. This leaves just the x^4 term with only the terms that have exactly two each of $\hat{a}$ and $\hat{a}^\dagger$. So, we can compute

$$\langle n| \hat{V} |n\rangle = \beta\frac{c^4}{16} \langle n| (\hat{a}^2\hat{a}^{\dagger^2} + \hat{a}^{\dagger^2}\hat{a}^2 + \hat{a}\hat{a}^{\dagger^2}\hat{a} + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}^2\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}) |n\rangle$$

$$= \beta\frac{c^4}{16}((n+1)(n+2) + n(n-1) + n(n+1) + (n+1)^2 + n(n+1) + n^2) = \beta\frac{c^4}{16}(6n^2 + 6n + 3)$$

So the energy to first order is

$$E_n = \hbar w(n + \frac{1}{2}) + \beta\frac{c^4}{16}(6n^2 + 6n + 3)$$

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Physics 113
Boccio 10.9.8.

In this problem we have a particle of mass m moves in a 1-dimensional oscillator potential $V(x) = \frac{1}{2}m\omega^2 x^2$. In the non-relativistic limit, where the kinetic energy and the momentum are related by $T = \frac{p^2}{2m}$. Here the ground state energy is $E_0 = \frac{\hbar}{2}$.

Relativistically, the kinetic energy and the momentum are related by $T = E - mc^2 = \sqrt{m^2c^4 + p^2c^2} - mc^2$. For part (a) we want to find the lowest order correction to the kinetic energy. So, we have that $T = \sqrt{m^2c^4 + p^2c^2} - mc^2$. To get the nonrelativistic relation of $T = \frac{p^2}{2m}$, we using the binomial approxiamation, but only take the p^2 term. For the relativistic correction, we then take the next term in the approxiamation, which is p^4. Thus, the lowest order correction to the kinetic energy is:

$$\begin{aligned}
T &= \sqrt{m^2c^4 + p^2c^2} - mc^2 \\
&= mc^2\sqrt{1 + \frac{p^2}{m^2c^2}} - mc^2 \\
&= mc^2(1 + \frac{1}{2}\frac{p^2}{m^2c^2} + \frac{3}{2}\frac{p^4}{m^4c^4}) - mc^2 \\
&= mc^2 + \frac{p^2}{2m} + \frac{3p^4}{2m^3c^2} - mc^2 \\
&= \frac{p^2}{2m} + \frac{3p^4}{2m^3c^2}.
\end{aligned}$$

For part (b), we want to use this new correction and consider it the perturbation. With this perturbation, we want to compute the relativistic correction to the ground state energy. So, we have

$$\begin{aligned}
E_n^{(1)} &= \langle n|\hat{V}|n\rangle \\
&= \langle n|\frac{3}{2}\frac{p^4}{m^3c^2}|n\rangle \\
&= \langle n|\frac{3}{2m^3c^2}(\hat{a} - \hat{a}^\dagger)^4|n\rangle \\
&= \langle n|\frac{3}{2m^3c^2}(\hat{a}^2\hat{a}^{\dagger^2} + \hat{a}^{\dagger^2}\hat{a}^2 + \hat{a}\hat{a}^{\dagger^2}\hat{a} + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}^2\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{3}{2m^3c^2}[(n+1)(n+2) + n(n-1) + n(n+1) + (n+1)^2 + n(n+1) + n^2] \\
&= \frac{9}{2m^3c^2}(2n^2 + 2n + 1).
\end{aligned}$$

Prob. 10.9.3 *(solution by Alexandra Werth)*

Given the spin Hamiltonian for a system of spin = 1

$$\hat{H} = A\hat{S}_z^2 + B(\hat{S}_x^2 - \hat{S}_y^2), \qquad B << A$$

(a) We can solve the unperturbed problem for $\hat{H}_0 = A\hat{S}_z^2$.

$$\hat{H}_0 = A\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Therefore,

$$E_1 = 0 \qquad E_2 = E_3 = A\hbar^2$$

$$\langle\phi_1| = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \langle\phi_2| = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \langle\phi_3| = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

(b) We can solve for the perturbed energy levels to the first order.

$$\hat{H}_p = B(\hat{S}_x^2 - \hat{S}_y^2) = \tfrac{1}{2}B(\hat{S}_+ + \hat{S}_-)$$

$$E_0 = 0$$

$$E_2 = E_3 = A\hbar^2 + B\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$E_2 = A\hbar^2 + B\hbar^2$$

$$E_3 = A\hbar^2 - B\hbar^2$$

(c) We can also solve the problem exactly by diagonalizing the Hamiltonian matrix in some basis.

$$\hat{H}_p = B(\hat{S}_x^2 - \hat{S}_y^2) = B\hbar^2 \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$E_1 = 0$$

$$E_2 = A\hbar^2 + B\hbar^2$$

$$E_3 = A\hbar^2 - B\hbar^2$$

a

We can write

$$\hat{H} = \hat{H}_o + \hat{V} = E_o \begin{pmatrix} -5 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & -8 \end{pmatrix} + \lambda E_o \begin{pmatrix} 0 & 3 & 0 & 0 \\ 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

Since $\hat{H}_o$ is diagonal, it is clear that the eigenvalues and associated eigenvectors are

$$E_1 = -5E_o$$
$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$
$$E_2 = 5E_o$$
$$|2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$
$$E_3 = 8E_o$$
$$|1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$
$$E_4 = -8E_o$$
$$|4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

b

From Mathematica, the exact eigenvalues of $\hat{H}$ are

$$E = \pm E_o\sqrt{64+\lambda^2}, \pm E_o\sqrt{25+9\lambda^2}$$

Taylor expanding gives

$$E \approx \pm E_o(8+\frac{1}{2}\frac{\lambda^2}{8}), \pm E_o(5+\frac{1}{2}\frac{9\lambda^2}{5})$$

c

The first order energy is given by

$$\langle n|\,\hat{V}\,|n\rangle = 0$$

since the diagonal entries in $\hat{V}$ are all zero. To second order, the only nonzero terms are

$$\langle 1|\,\hat{V}\,|2\rangle = \langle 2|\,\hat{V}\,|1\rangle = 3\lambda E_o$$
$$\langle 3|\,\hat{V}\,|4\rangle = \langle 4|\,\hat{V}\,|3\rangle = -\lambda E_o$$

The second order correction is given by

$$\sum_{m\neq n}\frac{\left|\langle n|\,\hat{V}\,|m\rangle\right|^2}{\epsilon_n-\epsilon_m}$$

So for $n=1$ and $m=2$ this gives

$$\frac{(3\lambda E_o)^2}{-10E_o}$$

For $n=2$ and $m=1$ this gives

$$\frac{(3\lambda E_o)^2}{10E_o}$$

For $n = 3$ and $m = 4$ this gives

$$\frac{(-\lambda E_o)^2}{16E_o}$$

For $n = 4$ and $m = 3$ this gives

$$\frac{(-\lambda E_o)^2}{-16E_o}$$

Thus the energies to second order, obtained by adding the second order term to the eigenvalue of $\hat{H}_o$, are

$$E_1 = -E_o(5 + \frac{1}{2}\frac{9\lambda^2}{5})$$
$$E_2 = E_o(5 + \frac{1}{2}\frac{9\lambda^2}{5})$$
$$E_3 = E_o(8 + \frac{1}{2}\frac{\lambda^2}{8})$$
$$E_4 = -E_o(8 + \frac{1}{2}\frac{\lambda^2}{8})$$

These match the Taylor expansions to second order of the exact solution above.

Variational Method

Consider a particle that has the Hamiltonian $\hat{H} = \hat{H}_0 + \lambda\hbar\omega(\hat{a}^2 + \hat{a}^{\dagger 2})$, where $\hat{H}_0$ is the Hamiltonian of the simple one-dimensional harmonic oscillator, and where $\hat{a}$ and $\hat{a}^\dagger$ are the usual annihilation and creation operators which obey $[\hat{a}, \hat{a}^\dagger] = 1$; λ is a very small real number.

(a) Calculate the ground state energy to second order in λ

(b) Find the energy of the nth excited state, E_n, to second order in λ and the corresponding eigenstate $|\psi_n\rangle$ to first order in λ.

Solution

(a) For a simple harmonic oscillator, we have

$$H_0 = E_n|n\rangle, \qquad E_n = \hbar\omega(n + \frac{1}{2}) \tag{1}$$

The first order corrections to the unperturbed energy levels are given by

$$E_n^{(1)} = \langle n|\hat{V}|n\rangle = \lambda\hbar\omega\langle n|(\hat{a}^2 + \hat{a}^{\dagger 2})|n\rangle. \tag{2}$$

Because the unperturbed states are orthogonal, all first order corrections are zero. The second order corrections are given by

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\langle n|\hat{V}|m\rangle|^2}{E_n - E_m} \tag{3}$$

$$= \frac{\lambda^2\hbar^2\omega^2}{E_n - E_{n-2}}|\langle n-2|\sqrt{n(n-1)}|n-2\rangle|^2 + \frac{\lambda^2\hbar^2\omega^2}{E_n - E_{n+2}}|\langle n+2|\sqrt{(n+1)(n+2)}|n+2\rangle|^2 \tag{4}$$

For ground state, we have n=0, and the first term disappears, and we are left with

$$E_0^{(2)} = \lambda^2\hbar^2\omega^2\frac{|\langle 2|\sqrt{2}|2\rangle|^2}{-2\hbar\omega} = \lambda^2\hbar\omega \tag{5}$$

The corrected ground state is therefore

$$E_0 = \frac{\hbar\omega}{2} - \lambda^2\hbar\omega = \hbar\omega(\frac{1}{2} - \lambda^2) \tag{6}$$

(b) The second order correction of the nth unperturbed energy is again given by equation 4. The corrected energy is of the nth energy level is therefore

$$E_n^{(2)} = \hbar\omega \left((n + \frac{1}{2}) + \frac{\lambda^2}{2}(n(n-1) - (n+1)(n+2)) \right). \tag{7}$$

For $n > 2$. For $n < 2$, the $n(n-1)$ term disappears, and we are left with

$$E_n^{(2)} = \hbar\omega \left((n + \frac{1}{2}) - \frac{\lambda^2}{2}(n+1)(n+2) \right). \tag{8}$$

The first order corrections to the corresponding eigenstates are given by

$$|N^{(1)}\rangle = \sum_{m \neq n} |m\rangle \frac{\langle n|\hat{V}|m\rangle}{E_n - E_m} \tag{9}$$

The corrected eigenstates are therefore

$$|n^{(2)}\rangle = |n\rangle + \frac{\lambda}{2}\langle\sqrt{n(n-1)}|n-2\rangle - \frac{\lambda}{2}\sqrt{(n+1)(n+2)}|n+2\rangle \tag{10}$$

for $n \geq 2$ and

$$|n^{(2)}\rangle = |n\rangle + -\frac{\lambda}{2}\sqrt{(n+1)(n+2)}|n+2\rangle \tag{11}$$

for $n < 2$.