PH423 Assignment 4

Parth Sastry 180260026 | Sahas Kamat 180260030 | Sankalp Gambhir 180260032

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Question 2.

(a) The given Hamiltonian $H(\epsilon)$ is

$$H(\epsilon) = V_0 \cdot \begin{pmatrix} (1-\epsilon) & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} \tag{1}$$

and the unperturbed Hamiltonian H_0

$$H_0 = H(0) = V_0 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{2}$$

is diagonal, so the eigenvectors of the unperturbed system are simply $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ with eigenvalues V_0, V_0, and $2V_0$ respectively.

The perturbation H' is thus

$$H' = H(\epsilon) - H_0 = V_0 \cdot \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \tag{3}$$

Eigenvalues of the whole system are given by the equation in ϵ and $lambda$, the eigenvalues themselves,

$$\left|(H(\epsilon) - \lambda\ \hat{\mathbf{1}})\right| = 0 \text{ , or,} \tag{4}$$

$$\begin{vmatrix} (V_0(1-\epsilon) - \lambda) & 0 & 0 \\ 0 & V_0 - \lambda & V_0\epsilon \\ 0 & V_0\epsilon & 2V_0 - \lambda \end{vmatrix} = 0 \tag{5}$$

$$((1-\epsilon)V_0 - \lambda)((V_0 - \lambda)(2V_0 - \lambda) - V_0^2\epsilon^2) = 0 \tag{6}$$

This gives $\lambda = (1-\epsilon)V_0$, $\frac{V_0}{2}(3 - \sqrt{4\epsilon^2 + 1})$, $\frac{V_0}{2}(3 + \sqrt{4\epsilon^2 + 1})$ as the eigenvalues of H. Call these $\lambda_{1,2,3}$ respectively.

Evaluating to second order in ϵ, we get

$$(\lambda_1, \lambda_2, \lambda_3) = V_0(1-\epsilon, 1-\epsilon^2, 2+\epsilon^2) \tag{7}$$

(b) The last eigenvalue, $2V_0$, is non degenerate, so we attempt to approximate its perturbed analogue using non-degenerate perturbation theory as required, using both first and second order theories.

The first order correction is given simply by

$$\begin{aligned}\langle v_3|H'|v_3\rangle &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \epsilon\\ 0 & \epsilon & 0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\\ &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\\epsilon\\0\end{pmatrix}\\ &= 0\,.\end{aligned} \tag{8}$$

That is, there is no first-order correction to the eigenvalue, which is expected, given the calculation from part a.

Moving on, representing the n^th order correction to the i^th eigenket as $\left|v_{i,n}\right\rangle$, the second-order correction is

$$\left\langle v_{3,0}\right| H' \left|v_{3,1}\right\rangle = \left\langle v_{3,0}\right| H' \sum_{m\neq 3} \frac{\left\langle v_{m,0}\right| H' \left|v_{3,1}\right\rangle}{E_3^{(0)} - E_m^{(0)}} \left|v_{m,0}\right\rangle \tag{9}$$

Since our eigenvectors are basis vectors, this basically filters components. Since we know $H'\left|v_{3,1}\right\rangle$, the calculation trivially reduces to

$$\begin{aligned}\left\langle v_{3,0}\right| H' \left|v_{3,1}\right\rangle &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \epsilon\\ 0 & \epsilon & 0\end{pmatrix}\begin{pmatrix}0\\\epsilon\\0\end{pmatrix}\\ &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\0\\\epsilon^2\end{pmatrix}\\ &= \epsilon^2\end{aligned} \tag{10}$$

Thus the second order correction is ϵ^2, exactly matching the result from part a.

(c) As for the degenerate levels, corresponding to $\left|v_{1,0}\right\rangle$ and $\left|v_{2,0}\right\rangle$, we apply the degenerate thoery. That is, compute the matrix W, with elements $\left\langle v_{i,0}\right| H' \left|v_{j,1}\right\rangle$ for $i, j \in \{1, 2\}$.

We get

$$W = \begin{pmatrix} -\epsilon & 0 \\ 0 & 0 \end{pmatrix} . \tag{11}$$

Since this matrix is diagonal, we simply read off the eigenvalues, ϵ and 0. These are the first order corrections to the energy values. Both of them match the exact results we got in part a. The first one matching exactly, and the second one missing a second order correction.

Question 3.

The 3D isotropic oscillator has a potential profile that looks like the follows -

$$V(x, y, z) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2)$$

We know that for the 1D harmonic oscillator ($V(x) = 1/2 m\omega^2 x^2$), the eigenfunctions for the same take the following form

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} . e^{-\frac{m\omega x^2}{2\hbar}} . H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right)$$

where $H_n(x)$ are the Hermite polynomials.

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2})$$
$$\text{with } H_0(x) = 1 \, , \; H_1(x) = 2x$$

The potential profile in the 3D Harmonic oscillator is a separable function in x, y and z. Which means that the eigenfunctions to the Hamiltonian for the 3D harmonic oscillator can be derived as a direct product of the eigenfunctions of the 1D harmonic oscillators in x, y and z directions.

$$\psi_{n_x n_y n_z} = \frac{1}{\sqrt{2^{n_x+n_y+n_z} n_x! n_y! n_z!}} \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} . e^{-\frac{m\omega(x^2+y^2+z^2)}{2\hbar}} . H_{n_x}\left(\sqrt{\frac{m\omega}{\hbar}} x\right) . H_{n_y}\left(\sqrt{\frac{m\omega}{\hbar}} y\right) . H_{n_z}\left(\sqrt{\frac{m\omega}{\hbar}} z\right)$$

with the energy of the eigenstate being

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right) \hbar\omega$$

Thus, the ground state for the 3D Harmonic oscillator is -

$$\psi_{000} = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{\frac{-m\omega(x^2+y^2+z^2)}{2\hbar}}$$

with energy $3/2\hbar\omega$

The first excited state is triply degenerate, since any of n_x, n_y and n_z can be changed to 1 and thus we have three degenerate eigenstates

$$\psi_{100} = \frac{2}{\pi^{3/4}}\left(\frac{m\omega}{\hbar}\right)^{5/4} xe^{\frac{-m\omega(x^2+y^2+z^2)}{2\hbar}}$$
$$\psi_{010} = \frac{2}{\pi^{3/4}}\left(\frac{m\omega}{\hbar}\right)^{5/4} ye^{\frac{-m\omega(x^2+y^2+z^2)}{2\hbar}}$$
$$\psi_{001} = \frac{2}{\pi^{3/4}}\left(\frac{m\omega}{\hbar}\right)^{5/4} ze^{\frac{-m\omega(x^2+y^2+z^2)}{2\hbar}}$$

with energies $5/2\hbar\omega$

We now introduce a perturbation to this system, given as

$$H' = \lambda x^2 yz$$

for a constant λ. Since the ground state is non-degenerate, we can use the non-degenerate perturbation theory to calculate the correction to the energy eigenvalue. So

$$\begin{aligned} E_{000,1} &= \langle\psi_{000}|H'|\psi_{000}\rangle \\ &= \lambda \int\int\int |\psi_{000}(x,y,z)|^2 x^2 yz\, dx\, dy\, dz \end{aligned}$$

The integrals over y and z are zero, because ψ_{000} is an even function over x, y and z, and the perturbation H' is odd in y and z. Which makes the integrals over y and z odd, and thus they equate to 0. Thus

$$E_{000,1} = 0$$

and thus, there is no correction to the ground state energy. $E'_{000} = E_{000} = \frac{3}{2}\hbar\omega$

For the first excited state, we use the degenerate perturbation theory. We thus need to calculate the matrix elements $W_{ab} = \left\langle n_x n_y n_z \middle| H' \middle| m_x m_y m_z \right\rangle$. This means

$$W_{ab} = \lambda \left\langle n_x \middle| x^2 \middle| m_x \right\rangle \left\langle n_y \middle| y \middle| m_y \right\rangle \left\langle n_z \middle| z \middle| m_z \right\rangle$$

We just consider the matrix elements where one of n_x, n_y, n_z is 1 and the others are 0, and likewise for the m_x, m_y, m_z

Now we know that

$$\begin{aligned}\langle n_x|\, x\, |n_x\rangle &= \int \psi_{n_x}(x) x \psi_{n_x}(x)\, dx \\ &= \int |\psi_{n_x}|^2 x\, dx = 0\end{aligned}$$

since the integrand is an odd function.

For $n_x =\neq m_x$, we know that

$$\begin{aligned}\langle n_x|\, x\, |m_x\rangle &= \int \psi_{n_x}(x) x \psi_{m_x}(x)\, dx \\ &= \sum_{m_x \neq n_x} \frac{|\langle n_x|\, x\, |m_x\rangle|^2}{(m_x - n_x)\hbar\omega} \\ &= \sqrt{\frac{\hbar}{2m\omega}} \sum_{m_x \neq n_x} \frac{\left[\sqrt{m_x+1}\delta_{n_x,m_x+1} + \sqrt{m_x}\delta_{n_x,m_x-1}\right]^2}{(m_x - n_x)} \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{m_x+1}\delta_{n_x,m_x+1} + \sqrt{m_x}\delta_{n_x,m_x-1}\right)\end{aligned}$$

$\langle n_x|\, x^2\, |m_x\rangle = 0$, if $n_x \neq m_x$, since the integrand becomes an odd function, with an x^3 inside. Thus, for the overall W_{ab}, the only non-zero elements will have $n_x = m_x$, $n_y \neq m_y$ and $n_z \neq m_z$. The elements that satisfy this are

$$\begin{aligned}W_{010,001} &= \lambda\, \langle 0|\, x^2\, |0\rangle \langle 1|\, y\, |0\rangle \langle 0|\, z\, |1\rangle \\ W_{001,010} &= \lambda\, \langle 0|\, x^2\, |0\rangle \langle 0|\, y\, |1\rangle \langle 1|\, z\, |0\rangle\end{aligned}$$

For $\langle 0|\, x^2\, |0\rangle$, we have

$$\begin{aligned}\langle 0|\, x^2\, |0\rangle &= \int \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} .e^{-\frac{m\omega x^2}{\hbar}} x^2\, dx \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega x^2}{\hbar}}\, dx\end{aligned}$$

let $\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = y$

$$\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\int_{-\infty}^{\infty}x^2e^{-\frac{m\omega x^2}{\hbar}}\,dx = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} * \left(\frac{\hbar}{m\omega}\right) * \left(\sqrt{\frac{\hbar}{m\omega}}\right)\int_{-\infty}^{\infty}y^2e^{-y^2}\,dy$$
$$= \frac{1}{\sqrt{\pi}} * \left(\frac{\hbar}{m\omega}\right) * \frac{\sqrt{\pi}}{2}$$
$$= \frac{\hbar}{2m\omega}$$

Thus, the W_{ab} matrix becomes -

$$W_{ab} = \lambda\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & \left(\frac{\hbar}{2m\omega}\right)^2\\ 0 & \left(\frac{\hbar}{2m\omega}\right)^2 & 0\end{bmatrix}$$

Thus, the energy corrections, are the eigenvalues of W_{ab}, which are computed as

$$-E\left(E^2 - \left(\frac{\hbar}{2m\omega}\right)^4\right) = 0$$

$$\implies E_1 = 0, \pm\lambda\left(\frac{\hbar}{2m\omega}\right)^2$$

Thus, the perturbation splits the degeneracy. It leaves $E'_{100} = E_{100} = \frac{5}{2}\hbar\omega$ while the degeneracy in ψ_{010} and ψ_{001} is lifted with their energy eigenvalues changing to $E = \frac{5}{2}\hbar\omega \pm \lambda\left(\frac{\hbar}{2m\omega}\right)^2$.

This is the effect of the perturbation on the ground state and the first excited state of the isotropic oscillator.

Question 4.

We use the following expression for the Kinetic energy T:

$$\begin{aligned}T &= E - mc^2\\ &= \sqrt{p^2c^2 + m^2c^4} - mc^2\\ &= \left(mc^2\right)\sqrt{1 + \frac{p^2}{m^2c^2}} - mc^2\\ &= \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \mathcal{O}(p^6)\end{aligned} \tag{12}$$

Using the first two terms to find the lowest order relativistic correction, we get the following Hamiltonian for the 1-D harmonic oscillator:

$$H = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \frac{1}{2}m\omega^2x^2 \tag{13}$$

We treat $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$ as our unperturbed Hamiltonian and $H_1 = -\frac{p^4}{8m^3c^2}$ as the perturbation.

The resulting energy levels will be of the from $E_n = E_n^0 + E_n^1$ where E_n^1 is the relativistic correction.

This requires calculation of terms of the form:

$$\begin{aligned} E_n^1 &= \left\langle n^0 \right| H_1 \left| n^0 \right\rangle \\ &= \left\langle n^0 \right| \left(\frac{-\hbar^2\omega^2}{32mc^2} \right) \left(a^\dagger - a \right)^4 \left| n^0 \right\rangle \end{aligned} \tag{14}$$

Here we have used the ladder operators $a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right)$ and $a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right)$

Since states of different n are orthogonal to each other, we only select terms that have equal creation and annihilation operators from $(a^\dagger - a)^4$. There are ${}^4C_2 = 6$ terms of this kind:

$$\begin{gathered} a^\dagger a^\dagger a a \\ a^\dagger a a^\dagger a \\ a a^\dagger a^\dagger a \\ a^\dagger a a a^\dagger \\ a a^\dagger a a^\dagger \\ a a a^\dagger a^\dagger \end{gathered} \tag{15}$$

Inserting these terms into the equation for E_n^1 and using $a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $a\,|n\rangle = \sqrt{n}\,|n-1\rangle$ we get:

$$\begin{aligned} E_n^1 &= \left(\frac{-\hbar^2\omega^2}{32mc^2} \right) \left(n\sqrt{n^2-1} + n^2 + n(n+1) + (n+1)n + (n+1)^2 + (n+2)(n+1) \right) \\ &= \left(\frac{-\hbar^2\omega^2}{32mc^2} \right) \left(n\sqrt{n^2-1} + 5n^2 + 7n + 3 \right) \end{aligned} \tag{16}$$

Thus energies with first order relativistic corrections for the Harmonic oscillator are:

$$E_n = \hbar\omega \left(\frac{1}{2} + n \right) + \left(\frac{-\hbar^2\omega^2}{32mc^2} \right) \left(n\sqrt{n^2-1} + 5n^2 + 7n + 3 \right) \tag{17}$$

Question 6.

$$V(r) = \begin{cases} -\frac{Ze^2}{r}, & r \geq a \\ -\frac{Ze^2}{a}\left(\frac{3}{2} - \frac{r^2}{2a^2}\right), & r \leq a \end{cases}$$

where Z is the nuclear charge and a is the nuclear radius. Assuming that $a \ll \frac{\hbar^2}{me^2} = a_0$ (typically , $a \sim 10^{-13}$cm, while $a_0 \sim 10^{-8}$cm calculate the first order change in the ground state energy from its value for a point nucleus.

Ans. The Hamiltonian for such a system will be given by:

$$\begin{aligned} H &= \frac{p^2}{2m} + V(r) \\ &= \frac{p^2}{2m} - \frac{Ze^2}{r} + \left(V(r) + \frac{Ze^2}{r}\right) \end{aligned} \tag{18}$$

We regard $H_0 = \frac{p^2}{2m} - \frac{Ze^2}{r}$ as the unperturbed Hamiltonian and $H_1 = V(r) + \frac{Ze^2}{r}$ as the perturbation. The perturbation term may be explicitly written as follows to verify that it is small (it is only non zero and finite over a small region, hence any integrals involving it will be small).

$$\begin{aligned} H_1(r) &= 0 \text{ for } r > a \\ &= \frac{-Ze^2}{a}\left(\frac{3}{2} - \frac{a}{r} - \frac{r^2}{2a^2}\right) \text{ for } r \leq a \end{aligned} \tag{19}$$

We can now write the perturbation to the ground state as:

$$E_0^{(1)} = \langle \psi_0 | H_1 | \psi_0 \rangle \tag{20}$$

Where ψ_0 is the ground state wavefunction for the hydrogen atom. Substituting the position basis expressions for relevant quantities, we get the following integral:

$$E_0^{(1)} = \frac{-Ze^2 \times 4\pi}{\pi {a_0}^3 a} \int_0^a \left(\frac{3}{2} - \frac{a}{r} - \frac{r^2}{2a^2}\right) e^{-2r/a_0} r^2 dr \tag{21}$$

Since $a << a_0$ we get

$$E_0^{(1)} = \frac{-4Ze^2}{{a_0}^3 a} \int_0^a \left(\frac{3r^2}{2} - ar - \frac{r^4}{2a^2}\right)(1 + \mathcal{O}(a/a_0))dr \tag{22}$$

Ignoring the $\mathcal{O}(a/a_0)$ term,

$$\begin{aligned} E_0^{(1)} &= \frac{-4Ze^2}{{a_0}^3 a}\int_0^a \left(\frac{3r^2}{2} - ar - \frac{r^4}{2a^2}\right)dr \\ &= \frac{2Ze^2a^2}{5a_0^3} \end{aligned} \tag{23}$$

Question 8.

The original Hamiltonian is of the form $H_0 = AL^2 + BL_z$. There's a small perturbation added to this Hamiltonian of the form $H_1 = CL_y$, where C is a constant. Thus, we have

$$\begin{aligned} H_0 &= AL^2 + BL_z \\ L_y &= \left(\frac{L_+ - L_-}{2i}\right) \end{aligned}$$

The eigenkets of H_0 are the simultaneous eigenkets of L^2 and L_z, $|l, m\rangle$. The energy eigenvalues here are $E_{l,m} = A\hbar^2 l(l+1) + B\hbar m$.

$L_y = \left(\frac{L_+ - L_-}{2i}\right)$, on the other hand, is off-diagonal in the $|l, m\rangle$ basis (owing to the ladder operators seen). Due to this, the first order energy shift $\langle l, m| CL_y |l, m\rangle$ vanishes, and we are left with the second order energy shifts

$$\begin{aligned} E'_{l,m} &= E^{(0)}_{l,m} + C^2 \sum_{m' \neq m} \frac{|\left\langle l, m'\right| \left(\frac{L_+ - L_-}{2i}\right) |l, m\rangle|^2}{E^{(0)}_{l,m} - E^{(0)}_{l,m'}} + O(C^3) \\ &= E^{(0)}_{l,m} + (C\hbar)^2 \frac{(l-m)(l+m+1)}{-4B\hbar} + (C\hbar)^2 \frac{(l+m)(l-m+1)}{4B\hbar} + O(C^3) \\ &= E^{(0)}_{l,m} + \hbar m \frac{C^2}{2B} + O(C^3) \end{aligned}$$

Similarly, the shifts in the eigenfunctions are

$$\begin{aligned} |l, m\rangle &= |l, m\rangle_0 + C \sum_{m' \neq m} \frac{\langle l, m'| \left(\frac{L_+ - L_-}{2i}\right) |l, m\rangle}{E^{(0)}_{l,m} - E^{(0)}_{l,m'}} \left|l, m'\right\rangle \\ &= |l, m\rangle_0 + \frac{C}{2i} \sum_{m' \neq m} \frac{\langle l, m'| (L_+ - L_-) |l, m\rangle}{E^{(0)}_{l,m} - E^{(0)}_{l,m'}} \left|l, m'\right\rangle \\ &= |l, m\rangle_0 + \frac{C\hbar}{2i} \sum_{m' \neq m} \frac{\sqrt{l(l+1) - m(m+1)}\,\langle l, m'|l, m+1\rangle - \sqrt{l(l+1) - m(m-1)}\,\langle l, m'|l, m-1\rangle}{E^{(0)}_{l,m} - E^{(0)}_{l,m'}} \left|l, m'\right\rangle \end{aligned}$$

We make these calculations for the case $l = 1$. Thus, the corrections in each state corresponding to $m = -1, 0, +1$ are -

$$E'_{1,-1} = E_{1,-1} - \frac{C^2\hbar}{2B} = 2A\hbar^2 - \frac{(C^2 + 2B^2)\hbar}{2B}$$
$$E'_{1,0} = E_{1,0} = 2A\hbar^2$$
$$E'_{1,1} = E_{1,1} + \frac{C^2\hbar}{2B} = 2A\hbar^2 + \frac{(C^2 + 2B^2)\hbar}{2B}$$

$$|1,-1\rangle' = |1,-1\rangle - \frac{C}{\sqrt{2}Bi}|1,0\rangle$$
$$|1,0\rangle' = |1,0\rangle - \frac{C}{\sqrt{2}Bi}(|1,1\rangle + |1,-1\rangle)$$
$$|1,1\rangle' = |1,1\rangle - \frac{C}{\sqrt{2}Bi}|1,0\rangle$$

Solving the system exactly, we recognize that the new states must be withing the linear span of the $|l, m\rangle$ states. We then write the effect of the Hamiltonian on an arbitrary such state to obtain the eigenvalue condition.

$$H\sum_{l,m} a_{l,m}|l,m\rangle = (A\,\hat{\mathbf{L}}^2 + B\,\hat{\mathbf{L}}_z + C\,\hat{\mathbf{L}}_y)\sum_{l,m} a_{l,m}|l,m\rangle \tag{24}$$

Define $c_{+,l,m}$ and $c_{-,l,m}$ as $\hat{\mathbf{L}}_+|l,m\rangle = \hbar c_{+,l,m}|l,m\rangle$ and similarly for the negative. We write $\hat{\mathbf{L}}_y = \frac{\hat{\mathbf{L}}_+ - \hat{\mathbf{L}}_-}{2i}$ and absorb the $2i$ into C as $D = \frac{C}{2i}$ to get

$$\begin{aligned} H\sum_{l,m}|l,m\rangle &= (A\,\hat{\mathbf{L}}^2 + B\,\hat{\mathbf{L}}_z + D\,\hat{\mathbf{L}}_+ - D\,\hat{\mathbf{L}}_-)\sum_{l,m} a_{l,m}|l,m\rangle \\ &= \hbar\sum_{l,m} a_{l,m}((\hbar Al(l+1) + Bm)|l,m\rangle + Dc_{+,l,m}|l,m+1\rangle - Dc_{-,l,m}|l,m-1\rangle) \\ &= \hbar\sum_{l,m}(a_{l,m}(\hbar Al(l+1) + Bm) + Da_{l,m-1}c_{+,l,m-1} - Da_{l,m+1}c_{-,l,m+1})|l,m\rangle \end{aligned} \tag{25}$$

$$\tag{26}$$

This gives us a form for the matrix representation of H, which has diagonal terms, and terms one above and one below the diagonal. The eigenvalues of this matrix can be obtained (painfully) via brute force calculation.

We use $l = 1$ for this case to construct the matrix representation of H

$$H = \hbar \begin{pmatrix} 2\hbar A - B & -Dc_{-,1,0} & 0 \\ Dc_{+,1,-1} & 2\hbar A & -Dc_{-,1,1} \\ 0 & Dc_{+,1,0} & 2\hbar A + B \end{pmatrix} . \tag{27}$$

All the $c_{\pm,l,m}$ equal $\sqrt{2}$ when appearing in the matrix (zero elements are outside 3×3). And replacing back $D = \frac{C}{2i}$ we get

$$H = \hbar \begin{pmatrix} 2\hbar A - B & -\frac{C}{\sqrt{2}i} & 0 \\ \frac{C}{\sqrt{2}i} & 2\hbar A & -\frac{C}{\sqrt{2}i} \\ 0 & \frac{C}{\sqrt{2}i} & 2\hbar A + B \end{pmatrix} . \tag{28}$$

Eigenvalues of this matrix, using a symbolic solver, were found to be

$$\lambda_1 = 2A\hbar^2 , \tag{29}$$

$$\lambda_2 = 2A\hbar^2 - \hbar\sqrt{B^2 + C^2} , \tag{30}$$

$$\lambda_3 = 2A\hbar^2 + \hbar\sqrt{B^2 + C^2} . \tag{31}$$

At first sight, these seem very different from the previously calculated values, but a trivial factorisation of the square root and binomial approximation to first order gives us exactly the values calculated via perturbation theory!