hw 6 qm2

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(i)

$$P(\lambda) = |[M] - \lambda I| = -\lambda^3 + 4\lambda^2 - 5\lambda + 3\lambda\epsilon^2 - 4\epsilon^2 - \lambda\epsilon + \epsilon + 2 = 0 \tag{1}$$

(ii)

Plugging in (1),

$$P(\lambda)=\left(\lambda_3^{(0)}+\lambda_3^{(2)}\epsilon^2+\lambda_3^{(1)}\epsilon\right)^3+4\left(\lambda_3^{(0)}+\lambda_3^{(2)}\epsilon^2+\lambda_3^{(1)}\epsilon\right)^2+3\epsilon^2\left(\lambda_3^{(0)}+\lambda_3^{(2)}\epsilon^2+\lambda_3^{(1)}\epsilon\right)-\epsilon\left(\lambda_3^{(0)}+\lambda_3^{(2)}\epsilon^2+\lambda_3^{(1)}\epsilon\right)-5\left(\lambda_3^{(0)}+\lambda_3^{(2)}\epsilon^2+\lambda_3^{(1)}\epsilon\right)-4\epsilon^2+\epsilon+2=0 \tag{2}$$

$$=3\epsilon^2\left(\lambda_3^{(0)}+\epsilon\left(\lambda_3^{(1)}+\lambda_3^{(2)}\epsilon\right)\right)-4\epsilon^2-\left(\lambda_3^{(0)}+\epsilon\left(\lambda_3^{(1)}+\lambda_3^{(2)}\epsilon\right)\right)^3+4\left(\lambda_3^{(0)}+\epsilon\left(\lambda_3^{(1)}+\lambda_3^{(2)}\epsilon\right)\right)^2-\epsilon\left(\lambda_3^{(0)}+\epsilon\left(\lambda_3^{(1)}+\lambda_3^{(2)}\epsilon\right)\right)-5\left(\lambda_3^{(0)}+\epsilon\left(\lambda_3^{(1)}+\lambda_3^{(2)}\epsilon\right)\right)+\epsilon+2=0 \tag{3}$$

Keeping only the terms till ϵ^2 and substituting $\lambda_3^{(0)} = 2$ and we have two equations for the coefficients,

$$\text{For } \epsilon : -1 - \lambda_3^{(1)} \tag{4}$$

$$\text{For } \epsilon^2 : -2\lambda_3^{(1)2} - \lambda_3^{(1)} - \lambda_3^{(2)} + 2 \tag{5}$$

Since $P(\lambda) = 0$ and $\lambda \neq 0$ we must have (3)(4)$= 0$. Then it is clear to see that $\lambda_3^{(1)} = -1$ and using this we have $\lambda_3^{(2)} = 1$.

(iii)

Substituting $\lambda_1^{(0)} = 1 = \lambda_2^{(0)}$ in (3) and keeping the terms till ϵ^3, the ϵ terms vanish and the ϵ^2, ϵ^3 terms give us the case choice for both $\lambda_1^{(1)}, \lambda_1^{(2)}$ and $\lambda_2^{(1)}, \lambda_2^{(2)}$,

$$\text{For } \epsilon^2 : \lambda_{1,2}^{(1)2} - \lambda_{1,2}^{(1)} - 1 \tag{6}$$

$$\text{For } \epsilon^3 : -\lambda_{1,2}^{(1)3} + 2\lambda_{1,2}^{(2)}\lambda_1 + 3\lambda_{1,2}^{(1)} - \lambda_{1,2}^{(2)} \tag{7}$$

Using the same argument as in (ii), we set (6),(7)$= 0$. The roots of (6) can be labelled arbitrarily as $\lambda_1^{(1)}$ or $\lambda_2^{(1)}$, then let,

$$\lambda_1^{(1)} = \frac{1}{2}\left(1 - \sqrt{5}\right) \tag{8}$$

$$\lambda_2^{(1)} = \frac{1}{2}\left(1 + \sqrt{5}\right) \tag{9}$$

Substituting (8)(9) in (7)= 0 we have,

$$\lambda_1^{(2)} = \frac{(1-\sqrt{5})\,(3+\sqrt{5})}{4\sqrt{5}} \tag{10}$$

$$\lambda_2^{(2)} = \frac{(\sqrt{5}-3)\,(1+\sqrt{5})}{4\sqrt{5}} \tag{11}$$

(iv)

Using Mathematica Solve function directly on $P(\lambda) = 0$ and adjusting to $\epsilon = 0.01$, we can see which one is smaller and thus, we have,

$$\lambda_1(\epsilon) = -\frac{\sqrt[3]{\sqrt{4(-9\epsilon^2+3\epsilon-1)^3+(9\epsilon-2)^2}+9\epsilon-2}}{3\sqrt[3]{2}} + \frac{\sqrt[3]{2}\left(-9\epsilon^2+3\epsilon-1\right)}{3\sqrt[3]{\sqrt{4(-9\epsilon^2+3\epsilon-1)^3+(9\epsilon-2)^2}+9\epsilon-2}} + \frac{4}{3} \tag{12}$$

$$\lambda_2(\epsilon) = \frac{(1+i\sqrt{3})\sqrt[3]{\sqrt{4(-9\epsilon^2+3\epsilon-1)^3+(9\epsilon-2)^2}+9\epsilon-2}}{6\sqrt[3]{2}} - \frac{(1-i\sqrt{3})\left(-9\epsilon^2+3\epsilon-1\right)}{3\ 2^{2/3}\sqrt[3]{\sqrt{4(-9\epsilon^2+3\epsilon-1)^3+(9\epsilon-2)^2}+9\epsilon-2}} + \frac{4}{3} \tag{13}$$

$$\lambda_3(\epsilon) = \frac{(1-i\sqrt{3})\sqrt[3]{\sqrt{4(-9\epsilon^2+3\epsilon-1)^3+(9\epsilon-2)^2}+9\epsilon-2}}{6\sqrt[3]{2}} - \frac{(1+i\sqrt{3})\left(-9\epsilon^2+3\epsilon-1\right)}{3\ 2^{2/3}\sqrt[3]{\sqrt{4(-9\epsilon^2+3\epsilon-1)^3+(9\epsilon-2)^2}+9\epsilon-2}} + \frac{4}{3} \tag{14}$$

Figure 1 shows a plot of the perturbative eigenvalues and the analytical,

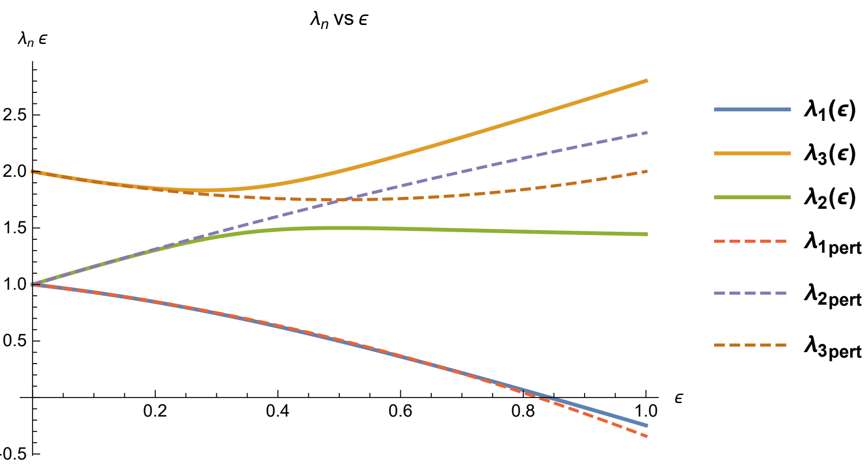

Figure 1: Plots of Eigenvalues

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(i)

We can write H as,

$$H = H^{(0)} + \epsilon H^{(1)} = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & E_0 & 0 \\ 0 & 0 & 2E_0 \end{pmatrix} + \epsilon \begin{pmatrix} E_0 & iE_0 & 0 \\ -iE_0 & 0 & E_0 \\ 0 & E_0 & -E_0 \end{pmatrix} \tag{15}$$

(ii)

In order to find the non-degenerate correction to the energies we must find the eigenvectors, namely by representation, $|\psi_1^{(0)}\rangle, |\psi_2^{(0)}\rangle, |\psi_3^{(0)}\rangle$ of unperturbed hamiltonian corresponding to the energies, which are simply $\begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\end{bmatrix}$. Then,

$$E_3^{(1)} = \epsilon\langle\psi_3^{(0)}|H^{(1)}|\psi_3^{(0)}\rangle = \epsilon\begin{bmatrix}0 & 0 & 1\end{bmatrix}\begin{pmatrix}E_0 & iE_0 & 0\\ -iE_0 & 0 & E_0\\ 0 & E_0 & -E_0\end{pmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix} = -\epsilon E_0 \tag{16}$$

$$E_3^{(2)} = \epsilon^2\left(\frac{|\langle\psi_2^{(0)}|H^{(1)}|\psi_3^{(0)}\rangle|^2}{E^{(0)}} + \frac{|\langle\psi_1^{(0)}|H^{(1)}|\psi_3^{(0)}\rangle|^2}{E^{(0)}}\right) \tag{17}$$

$$= \frac{\epsilon^2}{E_0}\left(\left|\begin{bmatrix}1 & 0 & 0\end{bmatrix}\begin{pmatrix}E_0 & iE_0 & 0\\ -iE_0 & 0 & E_0\\ 0 & E_0 & -E_0\end{pmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}\right|^2 + \left|\begin{bmatrix}0 & 1 & 0\end{bmatrix}\begin{pmatrix}E_0 & iE_0 & 0\\ -iE_0 & 0 & E_0\\ 0 & E_0 & -E_0\end{pmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}\right|^2\right) \tag{18}$$

$$= \epsilon^2 E_0 \tag{19}$$

Then the energy eigenvalue with corrections is $E_3 = 2E_0 - \epsilon E_0 + \epsilon^2 E_0 = E_0(2 - \epsilon + \epsilon^2)$, Which just the eigenvalue that was found in (1) with E_0 factor.

(iii)

Using the non-degenerate formulation for first order correction to eigenvectors and results in (18) we have,

$$|\psi_3^{(1)}\rangle = \epsilon\left[\frac{\langle\psi_2^{(0)}|H^{(1)}|\psi_3^{(0)}\rangle}{E_0}|\psi_2^{(0)}\rangle + \frac{\langle\psi_1^{(0)}|H^{(1)}|\psi_3^{(0)}\rangle}{E_0}|\psi_1^{(0)}\rangle\right] = \epsilon|\psi_2^{(0)}\rangle \tag{20}$$

(iv)

The energy E_0 is two-fold degenerate, so the goal is to find the matrix that acts in this degenerate subspace and its eigenvalues and eigenvectors. Projecting the degenerate eigenvectors onto first order degenerate perturbation equation as,

$$\langle\psi_n^{(0)}|(H^{(0)} - E^{(0)})|\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}|(H^{(1)} - \lambda_n)|\psi^{(Deg)}\rangle = 0 \tag{21}$$

The first term vanishes as all the degenerate eigenvectors have the same eigenvalue $E^{(0)}$, thus, we have,

$$\langle\psi_n^{(0)}|H^{(1)}|\psi^{(Deg)}\rangle = \lambda_n\langle\psi_n^{(0)}|\psi^{(Deg)}\rangle \tag{22}$$

By basis closure and considering that the degenvector belongs to subspace that is orthogonal to all the other basis vectors,

$$\sum_{n=1}^{2}\langle\psi_n^{(0)}|H^{(1)}|\psi_{n'}^{(0)}\rangle\langle\psi_{n'}^{(0)}|\psi^{(Deg)}\rangle = \lambda_n\langle\psi_n^{(0)}|\psi^{(Deg)}\rangle \tag{23}$$

$$H_{nn'}\Psi_{n'}^{Deg} = \lambda_n\Psi_n^{Deg} \tag{24}$$

Then,

$$H_{nn'} = \begin{pmatrix} \langle\psi_1^{(0)}|H^{(1)}|\psi_1^{(0)}\rangle & \langle\psi_1^{(0)}|H^{(1)}|\psi_2^{(0)}\rangle \\ \langle\psi_2^{(0)}|H^{(1)}|\psi_1^{(0)}\rangle & \langle\psi_2^{(0)}|H^{(1)}|\psi_2^{(0)}\rangle \end{pmatrix} = \begin{pmatrix} E_0 & iE_0 \\ -iE_0 & 0 \end{pmatrix} \tag{25}$$

Using mathematica, the eigenvalues of this matrix are,

$$E_1^{(1)} = \lambda_1 = \frac{1}{2}\left(1-\sqrt{5}\right)E_0 \tag{26}$$

$$E_2^{(1)} = \lambda_2 = \frac{1}{2}\left(1+\sqrt{5}\right)E_0 \tag{27}$$

The eigenvalues do match the result in (1) but differ by a factor E_0.

(v)

Since, the other elements of the unrestricted matrix do no correspond to these eigenvalues, then we can diagonalise $H_{nn'}$ and find

$$|\psi_1^{(A)}\rangle = \begin{bmatrix} \frac{1}{2}i(1-\sqrt{5}) \\ 1 \\ 0 \end{bmatrix} \tag{28}$$

$$|\psi_2^{(A)}\rangle = \begin{bmatrix} \frac{1}{2}i(1+\sqrt{5}) \\ 1 \\ 0 \end{bmatrix} \tag{29}$$

Then,

$$|\psi_1^{(B)}\rangle = \frac{\langle\psi_3^{(0)}|H^{(1)}|\psi_1^{(A)}\rangle}{E_0 - 2E_0}|\psi_3^{(0)}\rangle = -|\psi_3^{(0)}\rangle = |\psi_2^{(B)}\rangle \tag{30}$$

Then,

$$|\psi_1\rangle = |\psi_1^{(A)}\rangle - \epsilon|\psi_3^{(0)}\rangle = \begin{bmatrix} \frac{1}{2}i(1-\sqrt{5}) \\ 1 \\ -\epsilon \end{bmatrix} \tag{31}$$

$$|\psi_2\rangle = |\psi_2^{(A)}\rangle - \epsilon|\psi_3^{(0)}\rangle = \begin{bmatrix} \frac{1}{2}i(1+\sqrt{5}) \\ 1 \\ -\epsilon \end{bmatrix} \tag{32}$$

(3)

(i)

Proof. By definition of partial derivative, for the left hand side we must have,

$$\begin{aligned}
\frac{\partial}{\partial\lambda}\langle\psi_1(\lambda)|\psi_2(\lambda)\rangle &= \lim_{\epsilon\to 0}\frac{\langle\psi_1(\lambda+\epsilon)|\psi_2(\lambda+\epsilon)\rangle - \langle\psi_1(\lambda)|\psi_2(\lambda)\rangle}{\epsilon} \\
&+ \lim_{\epsilon\to 0}\frac{\langle\psi_1(\lambda)|\psi_2(\lambda+\epsilon)\rangle}{\epsilon} - \lim_{\epsilon\to 0}\frac{\langle\psi_1(\lambda)|\psi_2(\lambda+\epsilon)\rangle}{\epsilon} \\
&= \lim_{\epsilon\to 0}\frac{\langle\psi_1(\lambda+\epsilon)| - \langle\psi_1(\lambda)|}{\epsilon}|\psi_2(\lambda+\epsilon)\rangle + \lim_{\epsilon\to 0}\langle\psi_1(\lambda)|\frac{|\psi(\lambda+\epsilon)\rangle - |\psi(\lambda)\rangle|}{\epsilon} \\
&= \langle\partial_\lambda\psi_1(\lambda)|\psi_2(\lambda)\rangle + \langle\psi_1(\lambda)|\partial_\lambda\psi_2(\lambda)\rangle \\
&\text{(By the definition given and that } \lim_{\epsilon\to 0}\psi(\lambda+\epsilon) = \psi(\lambda))
\end{aligned}$$

□

(ii)

Proof. Suppose $|\psi(\lambda)\rangle$ is a normalised wave function for any λ. Then we can say,

$$\begin{aligned}
\Re\{(\langle\partial_\lambda\psi(\lambda)|\psi(\lambda)\rangle)\} &= \frac{1}{2}[\langle\partial_\lambda\psi(\lambda)|\psi(\lambda)\rangle + \langle\psi(\lambda)|\partial_\lambda\psi(\lambda)\rangle] \\
&= \frac{1}{2}\lim_{\epsilon\to 0}\frac{\langle\psi(\lambda+\epsilon)|\psi(\lambda)\rangle + \langle\psi(\lambda)|\psi(\lambda+\epsilon)\rangle - 2\langle\psi(\lambda)|\psi(\lambda)\rangle}{\epsilon} \\
&\text{as } \epsilon\to 0,\ \psi(\lambda+\epsilon)|\psi(\lambda)\rangle + \langle\psi(\lambda)|\psi(\lambda+\epsilon)\rangle \text{ converges to } 2\langle\psi(\lambda)|\psi(\lambda)\rangle \\
&\text{then, since } \psi(\lambda) \text{ is normalised,} \\
&\Re\{(\langle\partial_\lambda\psi(\lambda)|\psi(\lambda)\rangle)\} = 0
\end{aligned}$$

□

(iii)

Proof. By using the definition of partial derivative,

$$\begin{aligned}
&\frac{\partial}{\partial\lambda}\langle\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda)\rangle \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\langle\psi_1(\lambda+\epsilon)|\hat{H}(\lambda)(\lambda+\epsilon)|\psi_2(\lambda+\epsilon)\rangle - \langle\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda)\rangle \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\langle\psi_1(\lambda+\epsilon)|\hat{H}(\lambda+\epsilon)|\psi_2(\lambda+\epsilon)\rangle - \langle\psi_1(\lambda)|\hat{H}(\lambda+\epsilon)|\psi_2(\lambda+\epsilon)\rangle + \langle\psi_1(\lambda)|\hat{H}(\lambda+\epsilon)|\psi_2(\lambda+\epsilon)\rangle \\
&+ \langle\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda+\epsilon)\rangle - \langle\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda+\epsilon)\rangle - \langle\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda)\rangle \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\langle\psi_1(\lambda+\epsilon)| - \langle\psi_1(\lambda)|\hat{H}(\lambda+\epsilon)|\psi_2(\lambda+\epsilon)\rangle \\
&+ \lim_{\epsilon\to 0}\frac{1}{\epsilon}\langle\psi_1(\lambda)|\hat{H}(\lambda+\epsilon) - \hat{H}(\lambda)|\psi_2(\lambda+\epsilon)\rangle + \lim_{\epsilon\to 0}\frac{1}{\epsilon}\langle\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda+\epsilon) - \psi_2(\lambda)\rangle \\
&= \langle\partial_\lambda\psi_1(\lambda)|\hat{H}(\lambda)|\psi_2(\lambda)\rangle + \langle\psi_1(\lambda)|\partial_\lambda\hat{H}(\lambda)|\psi_2(\lambda)\rangle + \langle\psi_1(\lambda)|\hat{H}(\lambda)|\partial_\lambda\psi_2(\lambda)\rangle
\end{aligned}$$

□

(iv)

Proof. By (iii) we can say,

$$\begin{aligned}
\frac{\partial E_n(\lambda)}{\partial_\lambda} &= \langle \partial_\lambda \psi_n(\lambda)|\hat{H}(\lambda)|\psi_n(\lambda)\rangle + \langle \psi_n(\lambda)|\partial_\lambda \hat{H}(\lambda)|\psi_n(\lambda)\rangle + \langle \psi_n(\lambda)|\hat{H}(\lambda)|\partial_\lambda \psi_n(\lambda)\rangle \\
&= (\lim_{\epsilon\to 0} \tfrac{1}{\epsilon} \langle \psi_n(\lambda+\epsilon)|\hat{H}(\lambda)|\psi_n(\lambda)\rangle + \langle \psi_n(\lambda)|\hat{H}(\lambda)|\psi_n(\lambda+\epsilon)\rangle - 2\langle \psi_n(\lambda)|\hat{H}(\lambda)|\psi_n(\lambda)\rangle) + \langle \psi_n(\lambda)|\partial_\lambda \hat{H}(\lambda)|\psi_n(\lambda)\rangle \\
&\text{(Expanding first and last term in the limit definition of partial derivative)} \\
&= \langle \psi_n(\lambda)|\partial_\lambda \hat{H}(\lambda)|\psi_n(\lambda)\rangle \text{ (In the limit } \epsilon \to 0\text{, the expansion vanishes)}
\end{aligned}$$

□

(v)

$$\begin{aligned}
&\Rightarrow \frac{\partial E_n}{\partial \alpha} = \langle \psi_{nlm}|\partial_\alpha \hat{H}(\alpha)|\psi_{nlm}\rangle \\
&\Rightarrow -\frac{\alpha}{n^2} m_e c^2 = -\frac{\hbar^2}{2m_e}\langle \psi_{nlm}|\partial_\alpha \nabla^2|\psi_{nlm}\rangle - \hbar c\langle \psi_{nlm}|\frac{1}{r}|\psi_{nlm}\rangle (\nabla^2 \text{ independent of } \alpha) \\
&\Rightarrow \frac{\alpha}{n^2} m_e c^2 = \hbar c\langle \psi_{nlm}|\frac{1}{r}|\psi_{nlm}\rangle \\
&\Rightarrow \langle \psi_{nlm}|\frac{1}{r}|\psi_{nlm}\rangle = \frac{1}{\hbar c}\frac{m_e c^2}{n^2}\frac{e^2}{\hbar c} = \frac{1}{n^2 a_0}
\end{aligned}$$