Discussion 6 solutions

by Eli Chertkov

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(a) $$H = V_0 \begin{pmatrix} 1-\varepsilon & & \\ & 1 & \varepsilon \\ & \varepsilon & 2 \end{pmatrix} = H_0 + H'$$

$$H_0 = V_0 \begin{pmatrix} 1 & & \\ & 1 & \\ & & 2 \end{pmatrix} \Rightarrow |e_1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |e_2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$ are degenerate eigenvectors with energy $E_1^{(0)} = E_2^{(0)} = V_0$.

The third eigenvector of H_0 is $|e_3^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ with energy eigenvalue $E_3^{(0)} = 2V_0$.

$$H' = V_0 \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix}$$

(b) The eigenvalues of H are given by

$$\det(H - IE) = 0$$

$$\det\left[V_0 \begin{pmatrix} 1-\varepsilon-E & & \\ & 1-E & \varepsilon \\ & \varepsilon & 2-E \end{pmatrix} \right] = 0$$

$$V_0^3 (1-\varepsilon-E) \underbrace{[(1-E)(2-E) - \varepsilon^2]}_{[E^2 - 3E + 2 - \varepsilon^2]} = 0$$

There are three solutions for E:

$$E_1 = (1-\varepsilon) V_0$$

$$E_{2,3} = \frac{3 \mp \sqrt{9 - 4(2-\varepsilon^2)}}{2} V_0 = \frac{1}{2}\left(3 \mp \sqrt{1+4\varepsilon^2}\right) V_0.$$

1con For small $\varepsilon \ll 1$, we can expand the
(b_con) square root as follows:

$$\sqrt{1+4\varepsilon^2} = 1 + 4\left(\tfrac{1}{2}\varepsilon^2\right) + \mathcal{O}(\varepsilon^4)$$
$$= 1 + 2\varepsilon^2 + \mathcal{O}(\varepsilon^4).$$

To second-order in ε, the energy eigenvalues are therefore

$$E_1 = (1-\varepsilon)V_0$$
$$E_2 = \tfrac{1}{2}\left(3 - \sqrt{1+4\varepsilon^2}\right)V_0 = \tfrac{V_0}{2}\left(3 - (1+2\varepsilon^2+\mathcal{O}(\varepsilon^4))\right)$$
$$= \tfrac{1}{2}\left(2 - 2\varepsilon^2 + \mathcal{O}(\varepsilon^4)\right)V_0$$
$$= (1-\varepsilon^2)V_0 + \mathcal{O}(\varepsilon^4)$$
$$E_3 = \tfrac{1}{2}\left(3 + (1+2\varepsilon^2+\mathcal{O}(\varepsilon^4))\right)V_0$$
$$= (2+\varepsilon^2)V_0 + \mathcal{O}(\varepsilon^4).$$

(c) First-order non-degenerate perturbation theory tells us that, to order ε, the nondegenerate state $|e_3^{(0)}\rangle$'s energy gets shifted by

$$E_3^{(1)} = \langle e_3^{(0)} | H' | e_3^{(0)} \rangle$$
$$= (0,0,1)\, V_0 \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$
$$= 0.$$

l_{con} which means that the 3rd eigenstate's total
(c_{con}) corrected energy is

$$E_3 = E_3^{(0)} + E_3^{(1)} + \mathcal{O}(\varepsilon^2)$$
$$= 2V_0 + \mathcal{O}(\varepsilon^2).$$

The second-order correction to the energy eigenvalue of state $|e_3^{(0)}\rangle$ is

$$E_3^{(2)} = \langle e_3^{(0)}|H'|e_3^{(1)}\rangle = \sum_{m \neq n_3} \frac{|\langle e_m^{(0)}|H'|e_3^{(0)}\rangle|^2}{E_m^{(0)} - E_3^{(0)}}$$

$$= \frac{|\langle e_1^{(0)}|H'|e_3^{(0)}\rangle|^2}{E_3^{(0)} - E_1^{(0)}} + \frac{|\langle e_2^{(0)}|H'|e_3^{(0)}\rangle|^2}{E_3^{(0)} - E_2^{(0)}}$$

$$= \frac{\left|(1,0,0)\, V_0 \begin{pmatrix} -\varepsilon & & \varepsilon \\ & \varepsilon & \\ & & \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right|^2}{2V_0 - V_0} + \frac{\left|(0,1,0)\, V_0 \begin{pmatrix} -\varepsilon & & \varepsilon \\ & \varepsilon & \\ & & \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right|^2}{2V_0 - V_0}$$

$$= 0 + V_0\varepsilon^2 = V_0\varepsilon^2.$$

To second-order, the 3rd eigenstate's energy is

$$E_3 = E_3^{(0)} + E_3^{(1)} + E_3^{(2)} + \mathcal{O}(\varepsilon^3)$$

$$= 2V_0 + V_0\varepsilon^2 = (2+\varepsilon^2)V_0 + \mathcal{O}(\varepsilon^3)$$

which agrees with the result from part (b).

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(d) Suppose we try applying the non-degenerate perturbation theory formulae to the two degenerate states $|e_1^{(0)}\rangle, |e_2^{(0)}\rangle$. What happens?

Their energy corrections are

$$E_1^{(1)} = \langle e_1^{(0)} | H' | e_1^{(0)} \rangle$$

$$= (1,0,0)\, V_0 \begin{pmatrix} -\varepsilon & & \varepsilon \\ & & \\ \varepsilon & & \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -\varepsilon V_0$$

$$E_2^{(1)} = \langle e_2^{(0)} | H' | e_2^{(0)} \rangle$$

$$= (0,1,0)\, V_0 \begin{pmatrix} -\varepsilon & & \varepsilon \\ & & \\ \varepsilon & & \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0.$$

Their total corrected energies are then

$$E_1 = E_1^{(0)} + E_1^{(1)} + \mathcal{O}(\varepsilon^2)$$

$$= V_0 - \varepsilon V_0 + \mathcal{O}(\varepsilon^2) = (1-\varepsilon)V_0 + \mathcal{O}(\varepsilon^2)$$

and

$$E_2 = E_2^{(0)} + E_2^{(1)} + \mathcal{O}(\varepsilon^2)$$

$$= V_0 + 0 + \mathcal{O}(\varepsilon^2) = V_0 + \mathcal{O}(\varepsilon^2).$$

These both <u>happen to</u> agree with the exact result from part (b).

(Icon) The main thing to realize is that,

(e) in the degenerate subspace of $|e_1^{(0)}\rangle, |e_2^{(0)}\rangle$, the perturbation matrix is

$$\langle e_i^{(0)}|H'|e_j^{(0)}\rangle = \begin{pmatrix} \langle e_1^{(0)}|H'|e_1^{(0)}\rangle & \langle e_1^{(0)}|H'|e_2^{(0)}\rangle \\ \langle e_2^{(0)}|H'|e_1^{(0)}\rangle & \langle e_2^{(0)}|H'|e_2^{(0)}\rangle \end{pmatrix} = \begin{pmatrix} -\varepsilon & 0 \\ 0 & 0 \end{pmatrix},$$

which is diagonal.

The 1st-order non-degenerate PT formula worked in this case because we worked with a "good basis", one that already diagonalized the above matrix. In a sense, it was as if we already did the first step of degenerate PT without realizing it. If the $\langle e_\alpha^{(0)}|H'|e_\beta^{(0)}\rangle$ matrix was not diagonal for a set of degenerate states $\{|e_\alpha^{(0)}\rangle\}$, then we would have needed to diagonalize the matrix and find its eigenvectors to find the "good basis."

②

(a) $H = V_0 \begin{pmatrix} 1-\varepsilon & & \\ & 2 & \varepsilon \\ & \varepsilon & 2 \end{pmatrix} = H_0 + H'$

$H_0 = V_0 \begin{pmatrix} 1 & & \\ & 2 & \\ & & 2 \end{pmatrix} \rightarrow$ eigenvectors and eigenvalues of H_0

$|e_1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \; E_1 = V_0$

$|e_2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \; E_2 = 2V_0$

$|e_3^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \; E_3 = 2V_0$

$H' = V_0 \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix}$

(b) The exact eigenvalues are given by

$$\det(H - IE) = 0 = V_0^3 (1-\varepsilon-E) \left(\underbrace{(2-E)^2 - \varepsilon^2}_{E^2 - 2E + 4 - \varepsilon^2}\right)$$

The three solutions for E are:

$$E_1 = (1-\varepsilon)V_0, \; E_2 = (2-\varepsilon)V_0, \; E_3 = (2+\varepsilon)V_0.$$

These are already linear in ε, so there is no need to apply an approximation. These are exact energies.

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(c) Naively applying non-degenerate PT gives us

$$\tilde{E}_1^{(1)} = \langle e_1^{(0)} | H' | e_1^{(0)} \rangle$$

$$= (1,0,0)\, V_0 \begin{pmatrix} -\varepsilon & & \\ & & \varepsilon \\ & \varepsilon & \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$= -\varepsilon V_0$$

$$\tilde{E}_2^{(1)} = \langle e_2^{(0)} | H' | e_2^{(0)} \rangle$$

$$= (0,1,0)\, V_0 \begin{pmatrix} -\varepsilon & & \\ & & \varepsilon \\ & \varepsilon & \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$= 0$$

$$\tilde{E}_3^{(1)} = \langle e_3^{(0)} | H' | e_3^{(0)} \rangle = (0,0,1)\, V_0 \begin{pmatrix} -\varepsilon & & \\ & & \varepsilon \\ & \varepsilon & \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= 0.$$

Note that $\tilde{E}_2^{(1)}$ and $\tilde{E}_3^{(1)}$ are <u>wrong</u>, they do not match the results of (b).

(d) $|e_2^{(0)}\rangle, |e_3^{(0)}\rangle$ do not diagonalize $H'_{ij} = \langle e_i^{(0)} | H' | e_j^{(0)} \rangle$.

The first step of degenerate PT requires us to find a basis that diagonalizes H'_{ij}.

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(e) The relevant matrix that we need to compute and diagonalize for deg. PT is

$$\begin{pmatrix} H'_{22} & H'_{23} \\ H'_{32} & H'_{33} \end{pmatrix} = \begin{pmatrix} \langle e_2^{(0)} | H' | e_2^{(0)} \rangle & \langle e_2^{(0)} | H' | e_3^{(0)} \rangle \\ \langle e_3^{(0)} | H' | e_2^{(0)} \rangle & \langle e_3^{(0)} | H' | e_3^{(0)} \rangle \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}.$$

Its eigenvectors are

$$|e_2'\rangle = \frac{1}{\sqrt{2}}\left(|e_2^{(0)}\rangle - |e_3^{(0)}\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \qquad (\text{eigenvalue } \underline{\underline{-\varepsilon}})$$

$$|e_3'\rangle = \frac{1}{\sqrt{2}}\left(|e_2^{(0)}\rangle + |e_3^{(0)}\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}. \qquad (\text{eigenvalue } \underline{\underline{+\varepsilon}})$$

The first-order corrections to the degenerate energy levels $E_2^{(0)} = E_3^{(0)} = 2V_0$ are then

$$E_2^{(1)} = -\varepsilon V_0, \quad E_3^{(1)} = +\varepsilon V_0.$$

This agrees with the exact result of part (b).