Quiz 5: Solutions

1. Perturbation theory: three level system

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

(a) For $\epsilon = 0$,

$$H = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \equiv H_0$$

The eigenvalues and eigenvectors are:

- V_0 for eigenvector $(1\ 0\ 0)^T$
- V_0 for eigenvector $(0\ 1\ 0)^T$
- $2V_0$ for eigenvector $(0\ 0\ 1)^T$

(b) To solve for the exact eigenvalues of H, we need to diagonalize the subspace of H

$$V_0 \begin{pmatrix} 1 & \epsilon \\ \epsilon & 2 \end{pmatrix}.$$

$$\begin{aligned}
\det\left| V_0 \begin{pmatrix} 1 & \epsilon \\ \epsilon & 2 \end{pmatrix} - \lambda \mathbf{1} \right| &= 0 \\
\lambda &= V_0\Big(\frac{3}{2} \pm \frac{1}{2}\sqrt{1+4\epsilon^2}\Big) \\
&\approx V_0\left(\frac{3}{2} \pm \frac{1}{2}\Big(1 + \frac{1}{2}(4\epsilon^2) + \mathcal{O}(\epsilon^4)\Big)\right) \\
\lambda_+ &= V_0(2+\epsilon^2) + \mathcal{O}(\epsilon^4) \\
\lambda_- &= V_0(1-\epsilon^2) + \mathcal{O}(\epsilon^4)
\end{aligned}$$

Last eigenvalue is $\lambda_3 = V_0(1-\epsilon)$.

(c) Rewrite H as

$$H = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + \underbrace{V_0 \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix}}_{V} \tag{2}$$

The non-degenerate eigenvector of H_0 is $(0\ 0\ 1)^T$. Let $|1\rangle = (1\ 0\ 0)^T$, $|2\rangle = (0\ 1\ 0)^T$ and $|3\rangle = (0\ 0\ 1)^T$. Note that $\langle m|V|n\rangle = V_{mn}$, the matrix element in matrix V.

$$\begin{aligned}
E_3^{(1)} &= \langle 3|V|3\rangle = 0 \\
E_3^{(2)} &= \sum_{m\neq 3} \frac{|\langle m|V|3\rangle|^2}{E_3^0 - E_m^0} \\
&= \frac{1}{2V_0 - V_0}(|\langle 1|V|3\rangle|^2 + |\langle 2|V|3\rangle|^2) \\
&= \frac{1}{V_0}(0 + \epsilon^2 V_0^2) \\
&= V_0\epsilon^2
\end{aligned}$$

The approximate eigenvalue obtained using first- and second-order non-degenerate perturbation theory is thus $2V_0$ and $V_0(2+\epsilon^2)$ respectively. The latter is the same as λ_+ in (b), to $\mathcal{O}(\epsilon^2)$.

(d) For the two degenerate eigenvalues of H_0, we need to diagonalize the submatrix

$$\tilde{V} = V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & 0 \end{pmatrix}$$

But $\tilde{V}$ is already diagonal. So the first-order corrections to the eigenvalues are the eigenvalues of $\tilde{V}$: $E_1^{(1)} = -V_0\epsilon, E_2^{(1)} = 0$.
From (b), we have $\lambda_3 = V_0(1-\epsilon)$ and $\lambda_- = V_0(1-\epsilon^2)$. The first order term in λ_3 is $-V_0\epsilon$, corresponding to $E_1^{(1)}$ and the first order term in λ_- is 0, corresponding to $E_2^{(1)}$.

(e) The second order correction to the degenerate eigenvalues can be calculated with:

$$\begin{aligned}
E_1^{(2)} &= \sum_p \frac{|\langle p|V|1\rangle|^2}{E_1^0 - E_p^0} \\
E_2^{(2)} &= \sum_p \frac{|\langle p|V|1\rangle|^2}{E_2^0 - E_p^0}
\end{aligned}$$

where $|p\rangle = |3\rangle$ is the non-degenerate eigenvector within the non-degenerate subspace of H_0.

So

$$\begin{aligned} E_1^{(2)} &= \frac{|\langle 3|V|1\rangle|^2}{E_1^0 - E_3^0} = 0 \\ E_2^{(2)} &= \frac{|\langle 3|V|2\rangle|^2}{E_2^0 - E_3^0} = \frac{V_0^2\epsilon^2}{-V_0} = -V_0\epsilon^2 \end{aligned}$$

Thus, to $\mathcal{O}(\epsilon^2)$, the eigenvalues are:

$$\begin{aligned} (V_0 - V_0\epsilon + 0) = V_0(1-\epsilon) \\ \text{and } (V_0 + 0 - V_0\epsilon^2) = V_0(1-\epsilon^2) \end{aligned}$$

corresponding to λ_3 and λ_- respectively, and the respective second order terms match.