Quiz 5

Due in class, at the beginning of class on Tue 29 Oct, 2024

1. Perturbation theory: three level system

This question is adapted from Griffith's *Introduction to Quantum Mechanics.*

Consider a quantum system with just three linearly independent states. Suppose the Hamiltonian, in the matrix form, is

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

where V_0 is a real, positive constant, and ϵ is some small positive number ($\epsilon \ll 1$). We suppose that the part of the matrix arising from ϵ is a perturbation.

(a) Write down the eigenvectors and eigenvalues of the unperturbed Hamiltonian ($\epsilon = 0$).

(b) Solve for the exact eigenvalues of H. Expand each of them as a power series in ϵ up to second order.

(c) Use first- and second-order non-degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the non-degenerate eigenvector of H_0. Compare your results with those in part (b).

(d) Use degenerate perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare your results with those in part (b).

(e) Find, using perturbation theory (refer to the Appendix below), the second-order corrections to the two initially degenerate eigenvalues. You are required to show your working clearly. Compare your results with those in part (b).

Appendix: Second-order correction to the energy eigenvalue in degenerate perturbation theory

Consider a Hamiltonian H_0 with known eigenvalues. The eigenvalue E_n^0 is M-fold degenerate.
Let us call the degenerate subspace $\mathcal{V}_M$.

$$H_0|\psi\rangle = E_n^0|\psi\rangle \text{ for all } |\psi\rangle \in \mathcal{V}_M$$

Let the Hilbert space of all eigenvectors of H_0 be $\mathcal{H}$.
We can write $\mathcal{H} = \mathcal{V}_M \oplus \mathcal{V}_M^\perp$.

Consider a perturbation $V' = \lambda V$.
We know that to proceed to obtain eigenvectors that vary smoothly in λ from the degenerate subspace, we should choose the eigenvectors of H_0 that diagonalize V' in $\mathcal{V}_M$.
Let these eigenvectors be $\mathcal{B}_M = \left\{|n^{(0)}, 1\rangle, |n^{(0)}, 2\rangle, \cdots, |n^{(0)}, M\rangle\right\}$
i.e. $\langle n^{(0)}, k|V'|n^{(0)}, m\rangle = 0$ for $k \neq m$.
$\mathcal{B}_M$ is an orthonormal basis for $\mathcal{V}_M$.
The set of (non-degenerate) eigenvectors $\mathcal{B}_{M^\perp} = \left\{|p^{(0)}\rangle\right\}$ spans $\mathcal{V}_M^\perp$.
$\mathcal{B}_M \bigcup \mathcal{B}_{M^\perp}$ forms an orthonormal basis for $\mathcal{H}$.

Write

$$|n, k\rangle_\lambda = |n^{(0)}, k\rangle + \lambda|n^{(1)}, k\rangle + \lambda^2|n^{(2)}, k\rangle + \cdots, k = 1, \cdots, M$$

where as usual, all corrections to $|n^{(0)}, k\rangle$ are orthogonal to $|n^{(0)}, k\rangle$.

Coefficients of λ:

$$H_0|n^{(1)}, k\rangle + V|n^{(0)}, k\rangle = E_n^0|n^{(1)}, k\rangle + E_n^{(1)}|n^{(0)}, k\rangle \tag{2}$$

Coefficients of λ^2:

$$H_0|n^{(2)}, k\rangle + V|n^{(1)}, k\rangle = E_n^0|n^{(2)}, k\rangle + E_n^{(1)}|n^{(1)}, k\rangle + E_n^{(2)}|n^{(0)}, k\rangle \tag{3}$$

Goal: Find $E_n^{(2)}$
Apply $\langle n^{(0)}, k|$ to (3):

$$\langle n^{(0)}, k|H_0|n^{(2)}, k\rangle + \langle n^{(0)}, k|V|n^{(1)}, k\rangle = 0 + 0 + E_n^{(2)}$$

$$\langle n^{(0)}, k|H_0|n^{(2)}, k\rangle = E_n^0\langle n^{(0)}, k|n^{(2)}, k\rangle = 0.$$

So $E_n^{(2)} = \langle n^{(0)}, k|V|n^{(1)}, k\rangle$

We know that $|n^{(1)}, k\rangle$ has a component $|n^{(1)}, k\rangle|_{\mathcal{V}_M}$ in $\mathcal{V}_M$ and a component $|n^{(1)}, k\rangle|_{\mathcal{V}_M^\perp}$ in $\mathcal{V}_M^\perp$.
But

$$\langle n^{(0)}, k|n^{(1)}, k\rangle = 0 \tag{4}$$

and $\left\{|n^{(0)}, 1\rangle, \cdots, |n^{(0)}, M\rangle\right\}$ diagonalizes V in $\mathcal{V}_M$.
Therefore

$$\langle n^{(0)}, k|V\left(|n^{(1)}, k\rangle|_{\mathcal{V}_M}\right) = 0$$

((4) implies that $|n^{(1)}, k\rangle = \sum_{m\neq k} c_m |n^{(0)}, m\rangle + |n^{(1)}, k\rangle|_{\mathcal{V}_M^\perp}$)
Thus,

$$E_n^{(2)} = \langle n^{(0)}, k|V\left(|n^{(1)}, k\rangle|_{\mathcal{V}_M^\perp}\right)$$

To find $|n^{(1)}, k\rangle|_{\mathcal{V}_M^\perp}$, we use Eq. (2).
Apply $\langle p^{(0)}| \in \mathcal{V}_M^\perp$ to (2):

$$\begin{aligned}
&\langle p^{(0)}|H_0|n^{(1)}, k\rangle + \langle p^{(0)}|V|n^{(0)}, k\rangle = E_n^0 \langle p^{(0)}|n^{(1)}, k\rangle + 0 \\
&(E_n^0 - E_p^0)\langle p^{(0)}|n^{(1)}, k\rangle = \langle p^{(0)}|V|n^{(0)}, k\rangle
\end{aligned}$$

So

$$\langle p^{(0)}|n^{(1)}, k\rangle = \frac{\langle p^{(0)}|V|n^{(0)}, k\rangle}{(E_n^0 - E_p^0)}$$

Thus

$$|n^{(1)}, k\rangle = \underbrace{\sum_p \frac{\langle p^{(0)}|V|n^{(0)}, k\rangle}{(E_n^0 - E_p^0)} |p^{(0)}\rangle}_{|n^{(1)}, k\rangle|_{\mathcal{V}_M^\perp}} + |n^{(1)}, k\rangle|_{\mathcal{V}_M}$$

Thus,

$$\boxed{\begin{aligned} E_n^{(2)} &= \langle n^{(0)}, k|V\left(|n^{(1)}, k\rangle|_{\mathcal{V}_M^\perp}\right) \\ &= \sum_p \frac{|\langle p^{(0)}|V|n^{(0)}, k\rangle|^2}{E_n^0 - E_p^0} \end{aligned}} \tag{5}$$

where $\langle p^{(0)}| \in \mathcal{V}_M^\perp$.