Chapter 5: Approximation methods

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1 Time-independent perturbation theory

We start with the problem really close to a solved problem, then we can use the solution at hand to do approximation.

Box 1.1: Recap for Taylor expansion

$$f(x) \simeq f(x_0) + f'(x_0)(x - x_0) + \cdots + \frac{f^n(x_0)}{n!}(x - x_0)^n + \cdots . \tag{1}$$

If keep all the way to $(x - x_0)^2$, then we can do a fit with a polynomial function.

For quantum mechanics:

$$H = H_0 + H' \tag{2}$$

H_0 has a known solution for eigen energy $E_n^{(0)}$, and eigenstates $\{|n^{(0)}\rangle\}$:

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle \tag{3}$$

H' is perturbational part of Hamiltonian, it can express as:

$$H' = \lambda V \tag{4}$$

where λ is a number, and $\lambda \ll 1$. V is another part of Hamiltonian. Then we try to find $H |n\rangle = E_n |n\rangle$. E_n must be a function of H, which is a function of λ, so as $|n\rangle$. Therefore we can make a Taylor expansion of $E_n(\lambda)$ and $|n(\lambda)\rangle$:

$$E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \tag{5}$$

$$|n(\lambda)\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots \tag{6}$$

where $\lambda E_n^{(1)}$ is first order energy shift. $\lambda E_n^{(2)}$ is second order energy shift. Plug the expansion back to $H |n\rangle = E |n\rangle$ with $H = H_0 + \lambda V$:

$$\begin{aligned}(H_0 + \lambda V) \cdot \left(|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots\right) \\ = (E_n^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots) \cdot (|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots)\end{aligned} \tag{7}$$

do not contain λ, equation (7) $\Rightarrow H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$, for λ^1 term we can get:

$$H_0 |n^{(1)}\rangle + V |n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle \tag{8}$$

apply $\langle n^{(0)}|$ to the left:

$$\boxed{\langle n^{(0)}|V|n^{(0)}\rangle = E_n^{(1)}} \tag{9}$$

which is **first order perturbation for** E_n, plug in to $E_n = E_n^{(0)} + \lambda E_n^{(1)}$, we can get:

$$E_n = E_n^{(0)} + \langle n^{(0)}|\lambda V|n^{(0)}\rangle \rightarrow \boxed{E_n = E^{(0)} + \langle n^{(0)}|H'|n^{(0)}\rangle} \tag{10}$$

For $H = H_0 + \lambda V$, we can express it in the energy representation in $\{|n^{(0)}\rangle\}$,

$$H_0 = \begin{pmatrix} E_0^{(0)} & 0 & 0 & \dots & 0 \\ 0 & E_1^{(0)} & 0 & \dots & 0 \\ 0 & 0 & E_2^{(0)} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & E_n^{(0)} \end{pmatrix} \tag{11}$$

λV in the same basis can express as:

$$\lambda V = \begin{pmatrix} \lambda V_{11} & \lambda V_{12} & \dots & \lambda V_{1n} \\ \lambda V_{21} & \lambda V_{22} & \dots & \lambda V_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda V_{n1} & \lambda V_{n2} & \dots & \lambda V_{nn} \end{pmatrix} \tag{12}$$

For $n = 0$, $E_0 \simeq E_0^{(0)} + \lambda V_{11}$. First order perturbation is just n row, n columm for matrix $H_0 + \lambda V$ in $\{|n^{(0)}\rangle\}$ basis.

Now we try to find first order pertubrbation for state. Recall equation (8) and (9):

$$\begin{cases} H_0 |n^{(1)}\rangle + V |n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle \\ \langle n^{(0)}|V|n^{(0)}\rangle = E_n^{(1)} \end{cases}$$

we try to solve $|n^{(1)}\rangle$, we can apply $\langle k^{(0)}|$ to left, with $k \neq n$, then $\langle k^{(0)}|n^{(0)}\rangle = 0$. We also require $E^{(0)} \neq E^{(0)}$, we can get

$$\langle k^{(0)}|H_0|n^{(1)}\rangle + \langle k^{(0)}|V|n^{(0)}\rangle = E_n^{(0)} \langle k^{(0)}|n^{(1)}\rangle + E_n^{(1)} \langle k^{(0)}|n^{(0)}\rangle \tag{13}$$

$$\Rightarrow E_k^{(0)} \langle k^{(0)}|n^{(1)}\rangle + \langle k^{(0)}|V|n^{(0)}\rangle = E_n^{(0)} \langle k^{(0)}|n^{(1)}\rangle \tag{14}$$

The term $\langle k^{(0)}|n^{(1)}\rangle$ is an inner product between an unknown state $|n^{(1)}\rangle$ and a state in the known basis, it called "amplitude".

We want to solve the state $|n^{(1)}\rangle$, from the **Superposition Principle**, we know that $|n^{(1)}\rangle = \sum_k C_k |k^{(0)}\rangle$, since $\{|k^{(0)}\rangle\}$ form a basis. If we can solve every C_k, the state $|n^{(1)}\rangle$ is known. We can easily observe that $\langle k^{(0)}|n^{(1)}\rangle \rightarrow \sum_k C_k \langle k^{(0)}|n^{(0)}\rangle \rightarrow \sum_k C_k \delta_{k,n} \rightarrow C_k$, so all we need is to solve $\langle k^{(0)}|n^{(1)}\rangle$.

From equation (14) we can solve $\langle k^{(0)}|n^{(1)}\rangle$, which qual to C_k:

$$\boxed{C_k = \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}} \tag{15}$$

notice that $k \neq n$. Therefore, we can get the **first order perturbation for state** $|n\rangle$

$$\boxed{|n^{(1)}\rangle = \sum_{k\neq m} \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle} \tag{16}$$

plug it and $H' = \lambda V$ back to $|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle$ we get

$$\boxed{|n\rangle = |n^{(0)}\rangle + \sum_{k\neq m} \frac{\langle k^{(0)}|H'|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle} \tag{17}$$

where $\langle k^{(0)}|H'|n^{(0)}\rangle$ can be the matrix element in the k row and n colum of matrix H' in the basis of $\{|n^{(0)}\rangle\}$:

$$H_0 + H' \xrightarrow{\text{matrix in } \{|n^{(0)}\rangle\}} \begin{pmatrix} E_{ka}^{(0)} & H_{kn}^{(0)} \\ & E_{bn}^{(0)} \\ & \end{pmatrix} \tag{18}$$

Box 1.2: Example for spin - $\frac{1}{2}$ system

We have

$$H_0 = \Omega\sigma_z = \begin{pmatrix} \Omega & 0 \\ 0 & \Omega \end{pmatrix}, \; H' = \lambda\sigma_x = \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix} \tag{19}$$

The Hamiltonian is

$$H = H_0 + H' = \begin{pmatrix} \Omega & \lambda \\ \lambda & \Omega \end{pmatrix}, \text{ and } \Omega \gg \lambda \tag{20}$$

we can solve eigenenergy

$$E_1 = \Omega + \frac{\lambda^2}{2\Omega}, \; E_2 = -\Omega - \frac{\lambda^2}{2\Omega} \tag{21}$$

and the eigenstates

$$|\psi_1\rangle = \begin{pmatrix} 1 - \frac{\lambda^2}{2\Omega^2} \\ \frac{\lambda}{2\Omega} \end{pmatrix}, \; |\psi_2\rangle = \begin{pmatrix} -\frac{\lambda}{2\Omega} \\ 1 - \frac{\lambda^2}{2\Omega^2} \end{pmatrix} \tag{22}$$