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 $|n(\lambda)\rangle$:

$$\begin{aligned} E_n(\lambda) &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots , \\ |N(\lambda)\rangle &= |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots , \end{aligned} \tag{5}$$

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 $H = H_0 + \lambda V$:

$$\begin{aligned} &(H_0 + \lambda V) \cdot (|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n(2)\rangle + \cdots) \\ &\qquad = (E_n^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots) \cdot (|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots), \end{aligned} \tag{6}$$

do not contain λ, Equation (1.6) $\Rightarrow H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(o)}\rangle$, for λ^1 term we can get:

$$H_0 |n^{(1)}\rangle + V |n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle , \tag{7}$$

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

$$\boxed{\langle n^{(0)}|V|n^{(0)}\rangle = E_n^{(1)},} \tag{8}$$

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

$$E_n = E_n^{(0)} + \langle n^{(0)}|\lambda V|n^{(0)}\rangle \rightarrow \boxed{E_n = E^{(0)} + \langle n^{(0)}|H'|n^{(0)}\rangle\,.} \tag{9}$$

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

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

λV in the same basis can express as:

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

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

Now we try to find first order pertubrbation for state. From Equation (1.7) and (1.8):

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

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

$$\begin{aligned} \langle k^{(0)}|H_0|n^{(1)}\rangle + \langle k^{(0)}|V|n^{(0)}\rangle &= E_n^{(0)}\,\langle k^{(0)}|n^{(1)}\rangle + E_n^{(1)}\,\langle k^{(0)}|n^{(0)}\rangle\,, \\ E_k^{(0)}\,\langle k^{(0)}|n^{(1)}\rangle + \langle k^{(0)}|V|n^{(0)}\rangle &= E_n^{(0)}\,\langle k^{(0)}|n^{(1)}\rangle\,. \end{aligned} \tag{10}$$

The term $\langle k^{(0)}|n^{(1)}\rangle$ is a 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 (5.10) we can solve $\langle k^{(0)}|n^{(1)}\rangle$, which qual to C_k :

$$\boxed{C_k = \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}},} \tag{11}$$

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

$$\boxed{|n^{(1)}\rangle = \sum_{k\neq m} \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle\,,} \tag{12}$$

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

$$\boxed{|n\rangle = |n^{(0)}\rangle + \sum_{k\neq m} \frac{\langle k^{(0)}|H'|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle\,,} \tag{13}$$

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 $\{\ |\ n^{(0)}\rangle\ \}$:

$$H_0 + H' \xrightarrow{matirx\ \ in\ \ \{\,|n^{(0)}\rangle\,\}} \left(\begin{matrix} E_{ka}^{(0)} & H_{kn}^{(0)} \\ & E_{bn}^{(0)} \end{matrix}\right).$$

Example: Spin - $\dfrac{1}{2}$ system

We have

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

The Hamiltonian is

$$H = H_0 + H' \to \begin{pmatrix} \Omega & \lambda \\ \lambda & \Omega \end{pmatrix}, and \quad \Omega \gg \lambda$$

we can solve eigenenergy

$$E_1 = \Omega + \frac{\lambda^2}{2\Omega}, \quad E_2 = -\Omega - \frac{\lambda^2}{2\Omega},$$

and the eigenstates

$$|\psi\rangle_1 = \begin{pmatrix} 1 - \frac{\lambda^2}{2\Omega^2} \\ \frac{\lambda}{2\Omega} \end{pmatrix},$$

$$|\psi\rangle_2 = \begin{pmatrix} -\frac{\lambda}{2\Omega} \\ 1 - \frac{\lambda^2}{2\Omega^2} \end{pmatrix}.$$