Perturbation theory

Yu Lu

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1 Non-degenerate perturbation theory

Often, the Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$ of our interest has a major component $\hat{H}_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle$ whose spectrum can be solved analytically and a perturbative component $\hat{H}^{(1)}$ whose spectrum are unknown. When the perturbation is small ($\left\langle \hat{H}^{(1)} \right\rangle \ll \left\langle \hat{H}^{(1)} \right\rangle$), we could expect an adiabatic change to the original eigenvalues and eigenstates $E_n^{(0)} \to E_n$ and $\left|n^0\right\rangle \to |n\rangle$ such that

$$\begin{aligned} E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \ldots = \sum_{k=1}^{\infty} \lambda^k E_n^{(k)}, \\ |n\rangle &= |n\rangle^{(0)} + \lambda \left|n^{(1)}\right\rangle + \ldots = \sum_{k=1}^{\infty} \lambda^k \left|n^{(k)}\right\rangle \end{aligned},$$

where the λ are just to remind us of the relative magnitude of different terms.

Equating terms of the first order on both sides gives

$$\hat{H}^{(0)} \left|n^{(1)}\right\rangle + \hat{H}^{(1)} \left|n^{(0)}\right\rangle = E_0^{(0)} \left|n^{(1)}\right\rangle + E_n^{(1)} \left|n^{(0)}\right\rangle.$$

Forming an inner product with $\left\langle n^{(0)}\right|$ on both sides and recalling $\left\langle n^{(0)}\right| \hat{H} = \left\langle n^{(0)}\right| E_n^{(0)}$, $\left\langle n^{(0)} \middle| n^{(0)}\right\rangle = 1$ gives the first order correction in energy

$$\boxed{\Delta E_n^{(1)} = \left\langle n^{(0)} \middle| H^{(1)} \middle| n^{(0)} \right\rangle.}$$

Similarly, forming the inner product with $\left\langle m^{(0)}\right|$ on both sides and exploiting the orthogonality gives

$$\left\langle m^{(0)} \middle| n^{(1)} \right\rangle = \frac{\langle m^{(0)} | H^{(1)} | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \implies \boxed{\left|n^{(1)}\right\rangle = \sum_{E_m^{(0)} \neq E_n^{(0)}} \frac{\langle m^{(0)} | H^{(1)} | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \left|m^{(0)}\right\rangle,}$$

where a non-degenerate spectrum is assumed.

Expanding both sides to λ^2 gives the second-order equation

$$\hat{H}^{(0)} \left|n^{(2)}\right\rangle + \hat{H}^{(1)} \left|n^{(1)}\right\rangle = E_0^{(0)} \left|n^{(2)}\right\rangle + E_n^{(1)} \left|n^{(1)}\right\rangle + E_n^{(2)} \left|n^{(0)}\right\rangle.$$

It is convenient to take $\left\langle n^{(0)} \middle| n \right\rangle = 1 \implies \left\langle n^0 \middle| n^i \right\rangle = 0 \quad \forall i > 1$, giving

$$\boxed{E_n^{(2)} = \left\langle n^{(0)} \middle| \hat{H}^{(1)} \middle| n^{(1)} \right\rangle = \sum_{m \neq n}}$$