Perturbation theory

<u>Problem statement</u>: Consider the Hamiltonian $H = H_0 + \lambda H_1$ where $|\lambda| \ll 1$. Suppose we know everything about H_0 (its eigenvectors, eigenvalues), can one obtain properties of H as a <u>power series</u> in λ?

In the <u>time-independent</u> setting, H_1 is independent of time, and one is interested in the eigenvectors and the corresponding eigenvalues of H as a power series in λ in terms of the eigenvectors and eigenvalues of H_0.

In the <u>time-dependent</u> setting, H_1 is either a non-trivial function of time, e.g. $H_1 = \sin(t)\,\hat{O}$ where $\hat{O}$ is some operator, or, H_1 can be 'turned on' at some time t_0 i.e. $H_1 = \hat{O}\,\Theta(t-t_0)$ where Θ is the heaviside step-function.

In either case, one question one may ask is the following: suppose the system is initially prepared in some eigenstate $|\alpha\rangle$ of H_0. What is the probability of finding it in some other eigenstate $|\beta\rangle$ of H_0 at a later time t?

Time-independent Perturbation theory

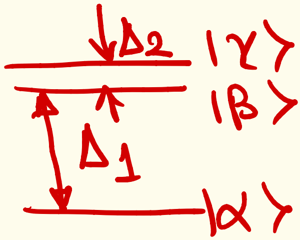
As we will soon see, in this case the structure of the solution depends on whether the 'target state' $|\alpha\rangle$ of H_0 (i.e. the state whose perturbed properties we are interested in) is separated from any nearby state $|\beta\rangle$ by a gap

$$\Delta = |E_\beta - E_\alpha| \gg \lambda \langle\alpha|H_1|\beta\rangle$$

If this condition is satisfied, then one is dealing with 'non-degenerate perturbation' theory. As we will see, in this case, the state $|\alpha\rangle$ will only be modified a little bit for small λ. However, when this condition is not satisfied, then even when

λ is small, the state corresponding to the perturbed system will generically differ dramatically from that of the unperturbed system. This case is called 'degenerate / nearly degenerate state perturbation theory'.

Note that for a given $H = H_0 + \lambda H_1$, one can have some target states that can be dealt with non-degenerate perturbation theory, while others may require degenerate perturbation theory. For example, consider H_0 with the following spectrum:



$$\Delta_1 = E_\beta - E_\alpha$$
$$\Delta_2 = E_\gamma - E_\beta$$

If $\Delta_1 \gg \lambda \langle \alpha | H_1 | \beta \rangle , \lambda \langle \alpha | H_1 | \gamma \rangle$ then one may calculate the effect of the perturbation on $|\alpha\rangle$ using non-degenerate perturbation theory.

At the same time, if $\Delta_2 \ll \lambda \langle \beta | H_1 | \gamma \rangle$, then one resort to the degenerate perturbation theory to calculate the effect of the perturbation on states $|\beta\rangle$ or $|\gamma\rangle$, one need to resort to degenerate state perturbation theory.

Non-degenerate state Perturbation theory

Lets denote the eigenstates of the unperturbed system by $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ etc. and the corresponding perturbed states as $|a\rangle, |b\rangle, |c\rangle$ etc.

i.e. $$H_0 |\alpha\rangle = E_\alpha |\alpha\rangle \quad \text{etc.}$$

$$(H_0 + \lambda H_1)|a\rangle = E_a |a\rangle \quad \text{etc.}$$

and $|a\rangle \to |\alpha\rangle$ as $\lambda \to 0$.

$E_a \longrightarrow \alpha$ as $\lambda \to 0$.

Let's focus on the perturbed state $|a\rangle$. lets expand it in terms of the unperturbed states as

$$|a\rangle = c_\alpha |\alpha\rangle + \sum_{\beta \neq \alpha} d_\beta |\beta\rangle$$

where $c_\alpha = O(1)$ and $d_\beta = O(\lambda)$.

further, since $\langle a | a \rangle = 1 \Rightarrow$

$$|c_\alpha|^2 + \sum_{\beta \neq \alpha} |d_\beta|^2 = 1.$$

The schrodinger's eqn. $H|a\rangle = E_a|a\rangle$

$$\Rightarrow E_a|a\rangle = [H_0 + \lambda H_1][c_\alpha|\alpha\rangle + \sum_{\beta\neq\alpha} d_\beta|\beta\rangle]$$

Taking dot product with $|\gamma\rangle \neq |\alpha\rangle$ on both sides, and using $\langle \gamma | a \rangle = d_\gamma$,

$$\Rightarrow E_a d_\gamma = E_\gamma d_\gamma + \lambda c_\alpha \langle \gamma | H_1 | \alpha \rangle + \lambda \sum_{\beta \neq \alpha} d_\beta \langle \gamma | H_1 | \beta \rangle$$

Since d_β for $\beta \neq \alpha$ is $O(\lambda)$, the last term on the R.H.S. is $O(\lambda^2)$.

Therefore, to $O(\lambda)$, one may neglect it.

$$\Rightarrow \quad d_\beta = \frac{\lambda \, c_\alpha \langle \beta | H_1 | \alpha \rangle}{E_\alpha - E_\beta} + O(\lambda^2)$$

To find c_α we use $|c_\alpha|^2 + \sum_{\beta \neq \alpha} |d_\beta|^2 = 1$. $\Rightarrow |c_\alpha| = 1 - O(\lambda^2)$ One may choose $c_\alpha = 1$ that guarantees that as $\lambda \to 0$, $c_\alpha \to 1$.

$$\Rightarrow \quad d_\beta = \frac{\lambda \langle \beta | H_1 | \alpha \rangle}{E_\alpha - E_\beta} + O(\lambda^2).$$

Substituting this in the expression for $|a\rangle$:

$$|a\rangle = |\alpha\rangle + \lambda \sum_{\beta \neq \alpha} |\beta\rangle \frac{\langle \beta | H_1 | \alpha \rangle}{E_\alpha - E_\beta} + O(\lambda^2)$$

To find $\mathcal{E}_a$, we take the dot product of the aforementioned Schrodinger eqn., namely,

$$\mathcal{E}_a|a\rangle = [H_0 + \lambda H_1][c_\alpha|\alpha\rangle + \sum_{\beta\neq\alpha} d_\beta|\beta\rangle]$$

with $\langle\alpha|$.

$$\Rightarrow \mathcal{E}_a = c_\alpha\langle\alpha|H_0|\alpha\rangle + \lambda\langle\alpha|H_1|\alpha\rangle c_\alpha + \lambda\sum_{\beta\neq\alpha} d_\beta\langle\alpha|H_1|\beta\rangle$$

Substituting $c_\alpha = 1$ and the above obtained expression for d_β,

$$\mathcal{E}_a = E_\alpha + \lambda\langle\alpha|H_1|\alpha\rangle + \lambda^2\sum_{\beta\neq\alpha}\frac{|\langle\beta|H_1|\alpha\rangle|^2}{\mathcal{E}_a - \mathcal{E}_\beta}.$$

Since $\mathcal{E}_a = E_\alpha + O(\lambda)$, one may replace $\mathcal{E}_a$ by E_α in the denominator on the R.H.S. of the above eqn. as well as in the eqn. for $|a\rangle$.

$\Rightarrow$

$$|a\rangle = |\alpha\rangle + \lambda \sum_{\beta \neq \alpha} |\beta\rangle \frac{\langle \beta | H_1 | \alpha \rangle}{E_\alpha - E_\beta} + O(\lambda^2)$$

and

$$\mathcal{E}_a = E_\alpha + \lambda \langle \alpha | H_1 | \alpha \rangle + \lambda^2 \sum_{\beta \neq \alpha} \frac{|\langle \beta | H_1 | \alpha \rangle|^2}{E_\alpha - E_\beta} + O(\lambda^3).$$

More generally, determining $|a\rangle$ to $O(\lambda^n)$, determines $\mathcal{E}_a$ to $O(\lambda^{n+1})$.

These are the main results for non-degenerate perturbation theory.

These equations already illustrate the requirement for the assumption

$$\frac{\lambda|\langle\beta|H_1|\alpha\rangle|}{|E_\alpha - E_\beta|} \ll 1,$$

that we made for the validity of non-degerate perturbation theory. As above equns. show, if this condition is violated, then the terms subleading in λ cannot be ignored even as $\lambda \to 0$, signalling the breakdown of the perturbation theory. Such a violation necessiate a different treatment, namely degenerate perturbation theory, as hinted earlier.