Physics 212b, Ken Intriligator lecture 11, Feb 21, 2018

• Last time: time independent, a.k.a. stationary state perturbation theory, continued $H = H_0 + H_1$, with $H_0 \sim \epsilon^0$ and $H_1 \sim \epsilon^1$, and that we can do an expansion order-by-order in the small parameter, making corrections to the H_0 case. To first order, $E_{n,1} = \langle E_{n,0}|H_1|E_{n,0}\rangle$ and

$$\langle E_{m\neq n,0}|E_{n,1}\rangle = \frac{1}{E_{n,0}-E_{m,0}}\langle E_{m\neq n,0}|H_1|E_{n,0}\rangle, \qquad \langle E_{n,0}|E_{n,1}\rangle = 0,$$

where the last condition is by a choice of overall phase. So

$$|E_{n,1}\rangle = {\sum_m}' \frac{|E_{m,0}\rangle\langle E_{m,0}|H_1|E_{n,0}\rangle}{E_{n,0}-E_{m,0}} = \frac{P_{n\perp}}{E_{n,0}-H_0}H_1|E_{n,0}\rangle$$

where ${\sum_m}'$ means all states with $E_{m,0} \neq E_{n,0}$ and $P_{n\perp} \equiv 1 - |E_{n,0}\rangle\langle E_{n,0}|$. Note that $|E_{n,1}\rangle \equiv |n_1\rangle$ is not an eigenstate of either H_0 or H_1; it is the order ϵ correction to the eigenstate of H. To second order

$$E_{n,2} = \langle E_{n,0}|H_1|E_{n,1}\rangle = {\sum_m}' \frac{|\langle E_{m,0}|H_1|E_{n,0}\rangle|^2}{E_{n,0}-E_{m,0}}.$$

Note that this is always negative for the ground state.

• Show that to the above order we have the expected result

$$E_n = \langle n|H|n\rangle = (\langle n_0| + \langle n_1| + \ldots)(H_0 + H_1)(|n_0\rangle + |n_1\rangle + \ldots).$$

$\langle n|n\rangle = \langle n_0|n_0\rangle = 1$ gives $\langle n_0|n_2\rangle + \langle n_2|n_0\rangle + \langle n_1|n_1\rangle = 0$, so $\langle n_2|H_0|n_0\rangle + \langle n_0|H_0|n_2\rangle + \langle n_1|H_0|n_1\rangle = \langle n_1|H_0 - E_{n,0}|n_1\rangle = -E_{n,2}$, so to $\mathcal{O}(\epsilon^2)$ get $2E_{n,2} - E_{n,2} = E_{n,2}$.

• Example: two-state system with $H = \begin{pmatrix} E_{1,0} & V_{12} \\ V_{12}^* & E_{2,0}\end{pmatrix}$. We can diagonalize this matrix to find the exact eigenvalues

$$E_{1,2} = \tfrac{1}{2}(E_{1,0}+E_{2,0}) \pm \sqrt{(\tfrac{1}{2}(E_{1,0}-E_{2,0}))^2 + |V_{12}|^2}.$$

The perturbative expansion follows by taking $V_{12} = \mathcal{O}(\epsilon)$ and Taylor expanding this expression. Find

$$E_1 = E_{1,0} + \frac{|V_{12}|^2}{E_{1,0}-E_{2,0}} + \ldots, \qquad E_2 = E_{2,0} + \frac{|V_{12}|^2}{E_{2,0}-E_{1,0}}$$

In agreement with our above expressions. The first order correction to E vanishes, and the second order correction is BTW negative for the groundstate. The first order correction to the eigenstates to zeroth and first order are

$$|E_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{V_{12}^*}{E_{1,0}-E_{2,0}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} + \ldots, \qquad |E_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \frac{V_{12}}{E_{2,0}-E_{1,0}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \ldots$$

Can check that it agrees with above.

• Example: SHO with $H_1 = \frac{1}{2}\epsilon m\omega^2 x^2$, i.e. replace $\omega \to \sqrt{1+\epsilon}\omega$. The ground state of the perturbed theory, to order ϵ is computed from

$$V_{00} = \langle 0^{(0)}|H_1|0^{(0)}\rangle = \epsilon\hbar\omega/4, \qquad V_{2,0} = \langle 2^{(0)}|H_1|0^{(0)}\rangle = \epsilon\hbar\omega/2\sqrt{2}.$$

Compute $E_0^{(1)} = \frac{1}{4}\epsilon\hbar\omega$, and $|0^{(1)}\rangle = -\epsilon|2^{(0)}\rangle/4\sqrt{2}$ and $E_0^{(2)} = -\hbar\omega\epsilon^2/16$, which indeed agrees with expanding $\frac{1}{2}\hbar\omega\sqrt{1+\epsilon}$.

• Stark effect: put an atom in an external electric field, treating eE_0 as a perturbation. Take $H_1 = eE_0 z$ for an electric field along the $\hat{z}$ axis (the electron charge here is $-e$). Then $E_{n,1} = eE_0\langle E_{n,0}|z|E_{n,0}\rangle$, which is zero by parity symmetry if the state is non-degenerate (e.g. in the ground state of the hydrogen atom). To second order,

$$E_{n,2} = e^2 E_0^2 \sum_m{}' \frac{|\langle E_{m,0}|z|E_{n,0}\rangle|^2}{E_{n,0}-E_{m,0}}.$$

It follows from the Wigner-Eckart theorem that $\langle n', \ell', m'|z|n, \ell, m\rangle \propto \delta_{m',m}\delta_{(\ell'-\ell)^2,1}$.. The second order shift can be understood as polarizing the system, and the change in energy is $-\frac{1}{2}\alpha E_0^2$ (you'll check this in HW examples).

For degenerate states, there is generally an effect already at first order; we need to use degenerate perturbation theory.

• Degenerate perturbation theory: especially interesting case, where H_1 splits the degenerate spectrum of H_0. Suppose the H_0 eigenstates are $|n_{0,k}\rangle$, where k runs over the degenerate space of H_0 eigenvectors with eigenvalue $E_{n,0}$, say $k = 1\ldots K$. Now H_1's matrix elements on this space of states is a $K\times K$ matrix. If we naively apply the above expressions, we run into problems with the denominator of e.g. $\langle E_{m\neq n,0}|E_{n,1}\rangle = \frac{1}{E_{n,0}-E_{m,0}}\langle E_{m\neq n,0}|H_1|E_{n,0}\rangle$ in the degenerate subspace. The solution is to diagonalize the H_1 matrix elements on this space, so we get $0/0$ instead of $1/0$. Also, diagonalizing H_1 in the degenerate space is needed for a smooth $\epsilon\to 0$ limit, since for any $\epsilon \to 0^+$ the states are not eigenstates unless they diagonalize H_1. The eigenvalues of the H_1 matrix are the first order correction $E_{n,1,k}$ values. The expression for $|n,1\rangle$ is similar to that in the non-degenerate case, where the $\sum_m'$ is understood to be over states with $E_{m,0} \neq E_{n,0}$, i.e. excluding all of the states with energy $E_{n,0}$.

If some degeneracy remains at first order, one needs to diagonalize the matrix $V_{n',n} + \sum_m{}' V_{nm}V_{mn'}/(E_{n,0} - E_{m,0})$ where we take $H_1 \to V$ to reduce index clutter.