Massachusetts Institute of Technology
Physics Department

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Perturbation Theory Summary

A quick summary of perturbation theory in the presence of degeneracies.

1 Steps

We assume that the eigenstates of H_0 are known and are discrete.

$$H_0 |n_0\rangle = E_n^0 |n_0\rangle$$

Suppose H_0 has a *degenerate subspace*, $\mathcal{D}$,

$$H_0 |n_0\rangle = \bar{E}_0 |n_0\rangle \;\text{ for all }\; |n_0\rangle \in \mathcal{D}$$

We want to construct the perturbation expansion for the eigenstates and eigenvalues of

$$H = H_0 + V.$$

To solve the problem, take the following steps:

- Diagonalize the perturbation in the degenerate subspace:
  Find a new basis for $\mathcal{D}$ such that V is diagonal in $\mathcal{D}$: $V_{mn} = \delta_{mn} V_{nn}$ for $m, n \in \mathcal{D}$.
- Lump the diagonal elements of V in $\mathcal{D}$ into the zeroth order eigenvalues:
  $$E_n^0 \to E_n^{\prime 0} \equiv E_n^0 + V_{nn}, \text{ if } n \in \mathcal{D}$$
  (and then for simplicity drop the $'$ notation, remembering that E_n^0 contains V_{nn} if n is in $\mathcal{D}$).
- Proceed as before in the derivation of the perturbation expansion.

2 Results

Here are the resulting formulas for the energy through third order and the wavefunction through second order:

Energy

For $n \notin \mathcal{D}$ the standard formula is unchanged. For $n \in \mathcal{D}$:

$$E_n = E_n^0 + \sum_{k \notin \mathcal{D}} \frac{V_{nk}V_{kn}}{(E_n^0 - E_k^0)} + \sum_{k,l \notin \mathcal{D}} \frac{V_{nk}V_{kl}V_{ln}}{(E_n^0 - E_k^0)(E_n^0 - E_l^0)} - V_{nn} \sum_{k \notin \mathcal{D}} \frac{V_{nk}V_{kn}}{(E_n^0 - E_k^0)^2}$$

Wavefunction

Once again, if the state under investigation is not in $\mathcal{D}$ nothing changes. For $n \in \mathcal{D}$, and for $m \notin \mathcal{D}$:

$$\langle m^0 | n \rangle = \frac{V_{mn}}{(E_n^0 - E_m^0)} + \sum_{k \notin \mathcal{D}} \frac{V_{mk}V_{kn}}{(E_n^0 - E_m^0)(E_n^0 - E_k^0)} - V_{nn} \frac{V_{mn}}{(E_n^0 - E_m^0)^2}$$

And for $m \in \mathcal{D}$ (only through the first non-trivial order):

$$\langle m^0 | n \rangle = \sum_{k \notin \mathcal{D}} \frac{V_{mk}V_{kn}}{(E_n^0 - E_m^0)(E_n^0 - E_k^0)}$$

Note that the (explicitly) first order term, V_{mn} vanishes. Note also, that the term written above while naively second order is actually first order because $E_n^0 - E_m^0 = V_{nn} - V_{mm}$.

3 If the degeneracy is not completely removed

Suppose that diagonalizing V in $\mathcal{D}$ does not completely remove the degneracy, so the new zeroth order Hamiltonian remains degenerate in a subspace, $\mathcal{D}_1 \subset \mathcal{D}$. So all the basis states in $\mathcal{D}_1$ have the same energy $\bar{E}$. Troubles will appear in the form of vanishing energy denominators if you go to high enough order in perturbation theory. For the perturbative expansion of the energy the difficulty first appears at fourth order. Here is one of the fourth order terms (the most obvious one), for $n \in \mathcal{D}_1$,

$$E_n^4 = \sum_{k,l \notin \mathcal{D}_1, p} \frac{V_{nk}V_{kp}V_{pl}V_{ln}}{(E_n^0 - E_k^0)(E_n^0 - E_p^0)(E_n^0 - E_l^0)}$$

The problem is that the state $|p_0\rangle$ can be in $\mathcal{D}_1$ because the matrix elements V_{kp} and V_{pl} are not zero (remember $|k\rangle$ and $|l\rangle$ are not in $\mathcal{D}_1$). So the energy difference $E_n^0 - E_p^0$ vanishes.

The solution is (offered without proof), to choose a new basis for $\mathcal{D}_1$ where the (Hermitian) operator V_{np}^2, defined by

$$V_{np}^2 = \sum_k \frac{V_{nk}V_{kp}}{(\bar{E} - E_k^0)}, \text{ for } n, p \in \mathcal{D}_1$$

is diagonal in $\mathcal{D}_1$. You can see that if this matrix is diagonal, then the expression for E_n^4 no longer can have a zero in the denominator.

This process can be continued indefinitely to remove all problems with degenerate perturbation theory. In fact, the formal reassurance that this is possible is more important than the actual construction, which is rarely, if ever, used.