

## DEGENERATE PERTURBATION THEORY

[φ 15.4, H 7.2, G 7.2]

If the unperturbed states are degenerate, our derived perturbation theory fails:

We risk having  $E_n^0 - E_{n'}^0 = 0$ , in which case the corrections to  $|n\rangle$  and  $\tilde{E}_n$  blow up [unless  $\langle n|V|n\rangle = 0$ , a convenient loophole]. We therefore need to handle the problem in a different way.

We consider an unperturbed system for which level  $n$  with energy  $E_n^0$  is degenerate,

$$H_0 |n, r\rangle = E_n^0 |n, r\rangle, \quad r=1, \dots, g_n,$$

where  $g_n$  is the degree of degeneracy, and we assume orthonormalized states

$$\langle n, r | n, s \rangle = \delta_{rs} \quad r, s = 1, \dots, g_n$$

[Remember that we can always construct orthogonal states from linear combinations of degenerate states.] We use  $g=g_n$ .

Again we assume that the exact wavefunctions can be written as a power series in  $\lambda$ :

$$|\psi_{n\alpha}\rangle = |\psi_{n\alpha}^{(0)}\rangle + \lambda |\psi_{n\alpha}^{(1)}\rangle + \lambda^2 |\psi_{n\alpha}^{(2)}\rangle + \dots \quad (1)$$

where  $\alpha = 1, \dots, g$ . Since we have many degenerate states  $|n, r\rangle$  when  $\lambda = 0$ , we do not know which state  $|\psi_{n\alpha}\rangle$  evolves to when  $\lambda \rightarrow 0$ .

We also expand

$$E_{n\alpha} = E_n^0 + \lambda E_{n\alpha}^{(1)} + \lambda^2 E_{n\alpha}^{(2)} + \dots, \quad (2)$$

where we can have different corrections for the different states with index  $\alpha$  which are degenerate in the unperturbed case ( $\lambda = 0$ ).

We now insert eq's (1) and (2) into the eigenvalue equation

$$\hat{H}|\psi_{n\alpha}\rangle = (H_0 + \lambda V)|\psi_{n\alpha}\rangle = E_{n\alpha}|\psi_{n\alpha}\rangle,$$

The resulting equation must be satisfied to each order in  $\lambda$  separately, as before. Collecting terms with the same power of  $\lambda$ , we get

$$H_0 |2f_{n\alpha}^{(0)}\rangle = E_n^0 |2f_{n\alpha}^{(0)}\rangle,$$

to lowest order. Since  $|2f_{n\alpha}^{(0)}\rangle$  satisfy the same equation as the unperturbed states  $|n,r\rangle$ , we can write

$$\begin{aligned} |2f_{n\alpha}^{(0)}\rangle &= \sum_{r=1}^g c_r |n,r\rangle = \\ &= \sum_{r=1}^g \langle n,r |2f_{n\alpha}^{(0)}\rangle |n,r\rangle \\ &= \sum_{r=1}^g U_{r\alpha} |n,r\rangle, \quad (\alpha=1, \dots, g) \end{aligned}$$

Thus, the state  $|2f_{n\alpha}\rangle$  in general tends to a linear combination of the unperturbed states in the limit  $\lambda \rightarrow 0$ .

The first order part of the eigenvalue equation is

$$(H_0 - E_n^{(0)}) |2f_{n\alpha}^{(1)}\rangle + (V - E_{n\alpha}^{(1)}) |2f_{n\alpha}^{(0)}\rangle = 0.$$

We now multiply the  $\lambda'$  equation by  $\langle n, s |$  from the left:

$$\underbrace{\langle n, s | H_0 - E_n^{(0)} | 2f_{n\alpha}^{(1)} \rangle}_{= 0}$$

$$+ \langle n, s | V - E_{n\alpha}^{(0)} | 2f_{n\alpha}^{(0)} \rangle = 0$$

$$\Rightarrow \langle n, s | [V - E_{n\alpha}^{(1)}] \sum_r U_{r\alpha} |n, r\rangle \\ = \sum_r [V_{sr} - E_{n\alpha}^{(0)} S_{sr}] U_{r\alpha} = 0, \quad (3)$$

where we have defined the matrix elements

$$V_{sr} = \langle n, s | V | n, r \rangle,$$

which we can calculate since we know the unperturbed states  $|n, r\rangle$ .

Considering that also  $s = 1, \dots, g$ , we get from (3):

$$(V_{11} - E_{n\alpha}^{(0)}) U_{1\alpha} + V_{12} U_{2\alpha} + \dots = 0$$

$$V_{21} U_{1\alpha} + (V_{22} - E_{n\alpha}^{(0)}) U_{2\alpha} + \dots = 0$$

which can be written on matrix form:

$$\begin{pmatrix} V_{11} - E_n^{(1)} & V_{12} & \cdots & V_{1g} \\ V_{21} & V_{22} - E_n^{(1)} & \cdots & \\ \vdots & \ddots & \ddots & \vdots \\ V_{g1} & \cdots & V_{gg} - E_n^{(1)} & \end{pmatrix} \begin{pmatrix} U_{1\alpha} \\ U_{2\alpha} \\ \vdots \\ U_{g\alpha} \end{pmatrix} = 0. \quad (4)$$

A non-trivial solution is obtained when the system determinant is zero, i.e.

$$\det \begin{pmatrix} V_{\alpha} - E_n^{(1)} & \cdots \\ \vdots & \ddots \end{pmatrix} = 0.$$

This results in an equation of degree  $g$ , with solutions  $E_n^{(1)}$ ,  $\alpha = 1, \dots, g$   
— the first order energy corrections!

If all  $E_n^{(1)}$  are different, the degeneracy is completely removed to first order in the perturbation. If some (or all) are identical, the degeneracy is partially (or not at all) removed.

When we have found the  $\bar{E}_{n\alpha}^{(1)}$ , we can determine the coefficients  $U_{r\alpha}$  by inserting the values for  $\bar{E}_{n\alpha}^{(1)}$  into (4) consecutively and solving for the coefficients and requiring normalization. The coeff.  $U_{r\alpha}$  are unique only if the degeneracy is completely removed.

In some cases, all the off-diagonal matrix elements  $V_{sr} = \langle n,s | V | n,r \rangle, (r \neq s)$  vanish. In that case the matrix in (4) already is diagonal, and we get the first order corrections

$$E_{nr}^{(1)} = \langle n,r | V | n,r \rangle, \quad (r=1, \dots, g).$$

directly. The perturbation  $V$  does not connect the unperturbed states  $|n,r\rangle$  to first order, and we have simply  $|z_{nr}^{(0)}\rangle = |n,r\rangle$ . This happens whenever the unperturbed states can be uniquely specified in terms of a set of operators that all commute with  $V$ .

To be more specific: If there exists a set of Hermitian operators  $F_i$ ,  $i = 1, 2 \dots$ , which commute with  $H_0$  and  $V$ , and we choose a set of states  $|n,r\rangle$  which are eigenstates of  $H_0$  and  $F_i \forall i$ ,

$$F_i |n,r\rangle = f_{ir} |n,r\rangle$$

and  $f_{ir} \neq f_{is}$  if  $s \neq r$ , then the states  $|n,r\rangle$  are "good" states — they already diagonalize the matrix in (4).

See Griffiths p. 292 for a proof, and detailed note posted on the homepage.

## EXAMPLE — 2D Perturbed Harmonic Oscillator

A particle with mass  $m$  is placed in a 2D harmonic potential,

$$H_0 = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2 + y^2),$$

which is perturbed by the potential

$$V = em\omega^2 xy.$$

The eigenvalues and eigenstates of  $H_0$  are

$$E_{n_x n_y}^0 = \hbar\omega [n_x + n_y + 1]$$

$$|n_x n_y\rangle = |n_x\rangle |n_y\rangle.$$

The first excited state is doubly degenerate,  $E_{10}^0 - E_{01}^0 = 2\hbar\omega$ , with possible unperturbed basis vectors

$$|1,1\rangle \equiv |1^0\rangle \equiv |10\rangle, \quad |1,2\rangle \equiv |2^0\rangle \equiv |01\rangle,$$

which are orthonormal.

We express the perturbation in terms of the raising and lowering operators, using

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a_x + a_x^+)$$

$$y = \sqrt{\frac{\hbar}{2m\omega}} (a_y + a_y^+),$$

resulting in

$$V = \frac{I\hbar\omega\epsilon}{2} [a_x + a_x^+] [a_y + a_y^+].$$

Using (4) for a doubly degenerate state, we get

$$\begin{pmatrix} V_{11} - E_{1\alpha}^{(1)} & V_{12} \\ V_{21} & V_{22} - E_{1\alpha}^{(1)} \end{pmatrix} \begin{pmatrix} U_{1\alpha} \\ U_{2\alpha} \end{pmatrix} = 0, \quad (\alpha=1,2) \quad (5)$$

where

$$V_{sr} = \langle s^o | V | r^o \rangle, \quad r, s = 1, 2.$$

Requiring a determinant equal to zero, we get

$$(V_{11} - E_{1\alpha}^{(1)}) (V_{22} - E_{1\alpha}^{(1)}) - V_{12} V_{21} = 0$$

$$\Rightarrow E_{1\alpha}^{(1)} = \frac{V_{11} + V_{22}}{2} \pm \frac{1}{2} \sqrt{(V_{11} - V_{22})^2 + 4|V_{12}|^2}$$

For the matrix elements, we get:

$$\begin{aligned} V_{11} &= \frac{\hbar \omega \epsilon}{2} \langle 1^0 | [a_x + a_x^\dagger] [a_y + a_y^\dagger] | 1^0 \rangle \\ &= \frac{\hbar \omega \epsilon}{2} \langle 1^0 | [a_x + a_x^\dagger] [a_y + a_y^\dagger] | 1^0 \rangle \\ &= \frac{\hbar \omega \epsilon}{2} \langle 1^0 | [a_x + a_x^\dagger] | 1^1 \rangle \\ &= \frac{\hbar \omega \epsilon}{2} \langle 1^0 | [1^0 1\rangle + \sqrt{2} |2^1\rangle] = 0 \end{aligned}$$

and

$$V_{22} = 0,$$

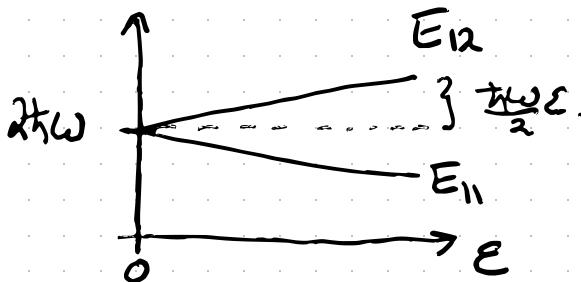
for the same reason.

$$\begin{aligned}
 V_{12} &= \frac{\hbar\omega\varepsilon}{2} \langle 1^0 | [a_x + a_x^+] [a_y + a_y^+] | 2^0 \rangle \\
 &= \frac{\hbar\omega\varepsilon}{2} \langle 1^0 | [a_x + a_x^+] [a_y + a_y^+] | 0^1 \rangle \\
 &= \frac{\hbar\omega\varepsilon}{2} \langle 1^0 | [a_x + a_x^+] [|00\rangle + \sqrt{2} |02\rangle] \\
 &= \frac{\hbar\omega\varepsilon}{2} \langle 1^0 | [0 + |10\rangle + \sqrt{2} \cdot 0 + \sqrt{2} |12\rangle] \\
 &= \frac{\hbar\omega\varepsilon}{2} \langle 1^0 | 1^0 \rangle = \frac{\hbar\omega\varepsilon}{2} = V_{21}^*.
 \end{aligned}$$

Hence, we get the corrections

$$E_{11}^{(1)} = -\frac{\hbar\omega\varepsilon}{2},$$

$$E_{12}^{(1)} = +\frac{\hbar\omega\varepsilon}{2}.$$



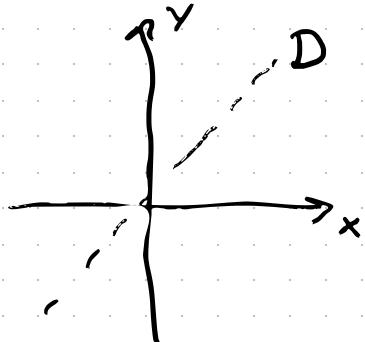
A small comment:  
 We could have gone on  
 to solve for the "limit"  
 states by inserting the  
 eigenvalues back into (5)  
 and solving for  $U_{12}$ .  
 The result would agree  
 with the "good" states we  
 find on the following pages.

The perturbation lifts the degeneracy of  
 the first excited state.

What would be the "good" states in this case that would give the first-order corrections directly? We need an operator that commutes with both  $H_0$  and  $V$ . One such operation is the interchanging of  $x$  and  $y$ , that is, a reflection about a  $45^\circ$  diagonal of the well:

$$D H_0 = H_0$$

$$D V = V$$



where we have called the operator  $D$ .

For the states we have

$$D |1^{\circ}\rangle = D |10\rangle = |01\rangle = |2^{\circ}\rangle$$

$$D |2^{\circ}\rangle = D |01\rangle = |10\rangle = |1^{\circ}\rangle,$$

which are not eigenstates of  $D$ .

However, we can construct linear combinations that are:

$$|\pm^{\circ}\rangle = \frac{|\text{1}^{\circ}\rangle + |\text{2}^{\circ}\rangle}{\sqrt{2}}$$

such that

$$\begin{aligned} D|\pm^{\circ}\rangle &= \frac{|\text{2}^{\circ}\rangle + |\text{1}^{\circ}\rangle}{\sqrt{2}} \\ &= \pm \left( \frac{|\text{1}^{\circ}\rangle + |\text{2}^{\circ}\rangle}{\sqrt{2}} \right) = \pm |\pm^{\circ}\rangle \end{aligned}$$

Hence,  $|\pm^{\circ}\rangle$  are "good" states, since they are eigenstates of  $D$  with distinct eigenvalues ( $\pm 1$ ), and  $D$  commutes with both  $H_0$  and  $V$ .

If we use these states in our perturbation theory, we need the matrix elements  $\langle \pm^{\circ} | V | \pm^{\circ} \rangle$ .

We begin by calculating

$$\begin{aligned}
 & [a_x + a_x^+] [a_y + a_y^+] |\pm^{\circ}\rangle \\
 &= \frac{1}{\sqrt{2}} [a_x + a_x^+] [a_y + a_y^+] [\pm|10\rangle + |01\rangle] \\
 &= \frac{1}{\sqrt{2}} [a_x + a_x^+] [\pm|11\rangle + |00\rangle + \sqrt{2}|02\rangle] \\
 &= \frac{1}{\sqrt{2}} [\pm|01\rangle \pm \sqrt{2}|21\rangle + |10\rangle + \sqrt{2}|12\rangle] \\
 &= [\pm|\pm^{\circ}\rangle \pm |21\rangle + |12\rangle]
 \end{aligned}$$

Hence, we get:

$$\langle +^{\circ} | V | +^{\circ} \rangle = +\frac{\hbar\omega\varepsilon}{2}$$

$$\langle -^{\circ} | V | -^{\circ} \rangle = -\frac{\hbar\omega\varepsilon}{2}$$

$$\langle +^{\circ} | V | -^{\circ} \rangle = \langle -^{\circ} | V | +^{\circ} \rangle = 0,$$

meaning that we directly get the first order corrections

$$E_{1\pm}^{(1)} = \langle \pm^{\circ} | V | \pm^{\circ} \rangle = \pm \frac{\hbar\omega\varepsilon}{2}.$$

The states  $| \pm \rangle$  are therefore the "good" or "limit" states, which the exact solution approaches when the perturbation is turned off,  $\epsilon \rightarrow 0$ .

It's possible to solve this problem exactly by rotating coordinates

$$x' = \frac{x+y}{\sqrt{2}}, \quad y' = \frac{x-y}{\sqrt{2}}.$$

Try it yourself as an exercise, or see Griffiths Example 7.2.

In this example, we have degeneracy for  $H_0$  due to rotational symmetry. However,  $V$  breaks this symmetry and therefore lifts the degeneracy.

The moral is: We make our life a bit easier by finding the "good" states from the outset.

