Problem solutions, 25 April 2012[1]

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Problems 5.20 and 5.21 were pretty simple, so I do not write out the solutions, but here is a solution for problem 5.12.

Problem 5.12 We are asked to find the eigenvalues of the matrix $H = H_0 + V$ with

$$H = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_2 \end{pmatrix} \tag{1}$$

and

$$V = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix} \quad . \tag{2}$$

We are to use perturbation theory to find the eigenvalues to second order in V and we are also asked to compare to the exact answer.

First, let's look at what happens to the state with unperturbed energy E_2. The unperturbed energy level is non-degenerate, so we can apply non-degenerate perturbation theory. This gives

$$\Delta_2^{(1)} = \langle 2 | V | 2 \rangle \tag{3}$$

where

$$|2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad . \tag{4}$$

This gives

$$\Delta_2^{(1)} = 0 \quad . \tag{5}$$

At second order, we have

$$\Delta_2^{(2)} = \langle 2 | V \frac{Q_2}{E_2 - H_0} V | 2 \rangle = \frac{1}{E_2 - E_1} \langle 2 | V Q_2 V | 2 \rangle \quad , \tag{6}$$

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where

$$Q_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{7}$$

That is,

$$\Delta_2^{(2)} = \frac{1}{E_2 - E_1}(0,0,1) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & |a|^2 + |b|^2 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad . \tag{8}$$

We get

$$\Delta_2^{(2)} = \frac{|a|^2 + |b|^2}{E_2 - E_1} \quad . \tag{9}$$

Now, let's look at what happens to the state with unperturbed energy E_1. The unperturbed energy level is degenerate, so we can apply degenerate perturbation theory. This gives

$$\Delta_1^{(1)} |1\rangle = P_1 V P_1 |1\rangle \quad , \tag{10}$$

where P_1 is the projection operator onto the subspace with unperturbed energy E_1, namely

$$P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad . \tag{11}$$

By multiplying the matrices, we see that $P_1 V P_1 = 0$. Thus

$$\Delta_1^{(1)} |1\rangle = 0 \quad . \tag{12}$$

At second order, we have a non-trivial result:

$$\Delta_1^{(2)} |1\rangle = P_1^{(2)} V \frac{Q_1}{E_1 - H_0} V P_1^{(2)} |1\rangle \quad . \tag{13}$$

There $P_1^{(2)}$ is the projection onto the subspace of the space with unperturbed energy eigenvalue E_1 that is still degenerate after using first order perturbation theory. In the present case, this is the whole space with unperturbed energy eigenvalue E_1. That is, $P_1^{(2)} = P_1$. Also, Q_1 is $1 - P_1$:

$$Q_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \tag{14}$$

Since $H_0\psi\big|\psi\big\rangle = E_2\big|\psi\big\rangle$, we have

$$\Delta_1^{(2)}\big|1\big\rangle = \frac{1}{E_1 - E_2} P_1 V Q_1 V P_1 \big|1\big\rangle \ . \tag{15}$$

That is

$$\Delta_1^{(2)}\big|1\big\rangle = \frac{-1}{E_2 - E_1}\begin{pmatrix} |a|^2 & ab^* & 0 \\ ba^* & |b|^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}\big|1\big\rangle \ . \tag{16}$$

Here $\big|1\big\rangle$ should lie in the subspace projected by P_1. This is a simple eigenvalue equation. The first eigenvector is

$$\big|1,+\big\rangle = \frac{1}{\sqrt{|a|^2 + |b|^2}}\begin{pmatrix} a \\ b \\ 0 \end{pmatrix} \tag{17}$$

with eigenvalue

$$\Delta_{1,+}^{(2)} = -\frac{|a|^2 + |b|^2}{E_2 - E_1} \ . \tag{18}$$

The second eigenvector is

$$\big|1,-\big\rangle = \frac{1}{\sqrt{|a|^2 + |b|^2}}\begin{pmatrix} b^* \\ -a^* \\ 0 \end{pmatrix} \tag{19}$$

with eigenvalue

$$\Delta_{1,+}^{(2)} = 0 \ . \tag{20}$$

Thus to order V^2 the eigenvalues are

$$\begin{aligned} E &= E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1} \ , \\ E &= E_1 \ , \\ E &= E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1} \ . \end{aligned} \tag{21}$$

The problem also asks us to do this the wrong way, by trying to use non-degenerate perturbation theory. I skip that.

It is straightforward to find the exact eigenvalues, with the result

$$\begin{aligned} E &= \frac{E_1 + E_2}{2} - \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4(|a|^2 + |b|^2)} \ , \\ E &= E_1 \ , \\ E &= \frac{E_1 + E_2}{2} + \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4(|a|^2 + |b|^2)} \ . \end{aligned} \tag{22}$$

When we expand this to second order in a and b, we recover the perturbative result.