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## Simplest perturbation two by two Hamiltonian

Q: two state Hamiltonian. Given a two-state system

$$H = H_0 + \lambda V$$

$$= \begin{bmatrix} E_1 & \lambda \Delta \\ \lambda \Delta & E_2 \end{bmatrix}$$
(1.1)

- a Solve the system exactly.
- b Find the first order perturbed states and second order energy shifts, and compare to the exact solution.
- c Solve the degenerate case for  $E_1 = E_2$ , and compare to the exact solution.

A: part (a) The energy eigenvalues  $\epsilon$  are given by

$$0 = (E_1 - \epsilon)(E_2 - \epsilon) - (\lambda \Delta)^2, \tag{1.2}$$

or

$$\epsilon^2 - \epsilon (E_1 + E_2) + E_1 E_2 = (\lambda \Delta)^2. \tag{1.3}$$

After rearranging this is

$$\epsilon = \frac{E_1 + E_2}{2} \pm \sqrt{\left(\frac{E_1 - E_2}{2}\right)^2 + (\lambda \Delta)^2}.$$
 (1.4)

Notice that for  $E_2 = E_1$  we have

$$\epsilon = E_1 \pm \lambda \Delta.$$
 (1.5)

Since a change of basis can always put the problem in a form so that  $E_1 > E_2$ , let's assume that to make an approximation of the energy eigenvalues for  $|\lambda\Delta| \ll (E_1 - E_2)/2$ 

$$\epsilon = \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \sqrt{1 + \frac{(2\lambda\Delta)^2}{(E_1 - E_2)^2}}$$

$$\approx \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \left(1 + 2\frac{(\lambda\Delta)^2}{(E_1 - E_2)^2}\right)$$

$$= \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \pm \frac{(\lambda\Delta)^2}{E_1 - E_2}$$

$$= E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2}, E_2 + \frac{(\lambda\Delta)^2}{E_2 - E_1}.$$
(1.6)

For the perturbed states, starting with the plus case, if

$$|+\rangle \propto \begin{bmatrix} a \\ b \end{bmatrix}$$
, (1.7)

we must have

$$0 = \left(E_1 - \left(E_1 + \frac{(\lambda \Delta)^2}{E_1 - E_2}\right)\right) a + \lambda \Delta b$$

$$= \left(-\frac{(\lambda \Delta)^2}{E_1 - E_2}\right) a + \lambda \Delta b,$$
(1.8)

so

$$|+\rangle \to \begin{bmatrix} 1\\ \frac{\lambda\Delta}{E_1 - E_2} \end{bmatrix}$$

$$= |+\rangle + \frac{\lambda\Delta}{E_1 - E_2} |-\rangle.$$
(1.9)

Similarily for the minus case we must have

$$0 = \lambda \Delta a + \left( E_2 - \left( E_2 + \frac{(\lambda \Delta)^2}{E_2 - E_1} \right) \right) b$$
  
=  $\lambda \Delta b + \left( -\frac{(\lambda \Delta)^2}{E_2 - E_1} \right) b$ , (1.10)

for

$$|-\rangle \to |-\rangle + \frac{\lambda \Delta}{E_2 - E_1} |+\rangle.$$
 (1.11)

*A*: part (b) For the pertubation the first energy shift for pertubation of the  $|+\rangle$  state is

$$E_{+}^{(1)} = |+\rangle V |+\rangle$$

$$= \lambda \Delta \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= \lambda \Delta \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= 0.$$
(1.12)

The first order energy shift for the pertubation of the  $|-\rangle$  state is also zero. The perturbed  $|+\rangle$  state is

$$|+\rangle^{(1)} = \frac{\overline{P}_{+}}{E_{1} - H_{0}} V |+\rangle$$

$$= \frac{|-\rangle \langle -|}{E_{1} - E_{2}} V |+\rangle$$
(1.13)

The numerator matrix element is

$$\langle -|V|+\rangle = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \Delta \end{bmatrix}$$

$$= \Delta,$$
(1.14)

so

$$|+\rangle \rightarrow |+\rangle + |-\rangle \frac{\Delta}{E_1 - E_2}.$$
 (1.15)

Observe that this matches the first order series expansion of the exact value above. For the perturbation of  $|-\rangle$  we need the matrix element

$$\langle + | V | - \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \Delta \\ 0 \end{bmatrix}$$

$$= \Delta,$$
(1.16)

so it's clear that the perturbed ket is

$$|-\rangle \rightarrow |-\rangle + |+\rangle \frac{\Delta}{E_2 - E_1},$$
 (1.17)

also matching the approximation found from the exact computation. The second order energy shifts can now be calculated

$$\langle + | V | + \rangle' = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\Delta} \\ \overline{E_1 - E_2} \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\Delta^2}{E_1 - E_2} \\ \Delta \end{bmatrix}$$

$$= \frac{\Delta^2}{E_1 - E_2},$$
(1.18)

and

$$\langle -|V|-\rangle' = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} \frac{\Delta}{E_2 - E_1} \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta \\ \frac{\Delta^2}{E_2 - E_1} \end{bmatrix}$$

$$= \frac{\Delta^2}{E_2 - E_1}'$$
(1.19)

The energy perturbations are therefore

$$E_1 \to E_1 + \frac{(\lambda \Delta)^2}{E_1 - E_2}$$
  
 $E_2 \to E_2 + \frac{(\lambda \Delta)^2}{E_2 - E_1}$ . (1.20)

This is what we had by approximating the exact case.

A: part (c) For the  $E_2 = E_1$  case, we'll have to diagonalize the perturbation potential. That is

$$V = U \wedge U^{\dagger}$$

$$\wedge = \begin{bmatrix} \Delta & 0 \\ 0 & -\Delta \end{bmatrix}$$

$$U = U^{\dagger} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$
(1.21)

A change of basis for the Hamiltonian is

$$H' = U^{\dagger} H U$$

$$= U^{\dagger} H_0 U + \lambda U^{\dagger} V U$$

$$= E_1 U^{\dagger} + \lambda U^{\dagger} V U$$

$$= H_0 + \lambda \bigwedge.$$
(1.22)

We can now calculate the perturbation energy with respect to the new basis, say  $\{|1\rangle, |2\rangle\}$ . Those energy shifts are

$$\Delta^{(1)} = \langle 1 | V | 1 \rangle = \Delta$$

$$\Delta^{(2)} = \langle 2 | V | 2 \rangle = -\Delta.$$
(1.23)

The perturbed energies are therefore

$$E_1 \to E_1 + \lambda \Delta$$
  
 $E_2 \to E_2 - \lambda \Delta$ , (1.24)

which matches eq. (1.5), the exact result.

## Bibliography