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Simplest perturbation two by two Hamiltonian

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

$$\begin{aligned} H &= H_0 + \lambda V \\ &= \begin{bmatrix} E_1 & \lambda\Delta \\ \lambda\Delta & E_2 \end{bmatrix} \end{aligned} \tag{1.1}$$

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 ϵ 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

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

Notice that for $E_2 = E_1$ we have

$$\epsilon = E_1 \pm \lambda\Delta. \tag{1.5}$$

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 $|\lambda\Delta| \ll (E_1 - E_2)/2$

$$
\begin{aligned}
\epsilon &= \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \sqrt{1 + \frac{(2\lambda\Delta)^2}{(E_1 - E_2)^2}} \\
&\approx \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \left(1 + 2 \frac{(\lambda\Delta)^2}{(E_1 - E_2)^2} \right) \\
&= \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \pm \frac{(\lambda\Delta)^2}{E_1 - E_2} \\
&= E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2}, E_2 + \frac{(\lambda\Delta)^2}{E_2 - E_1}.
\end{aligned}
\tag{1.6}
$$

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

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

we must have

$$
\begin{aligned}
0 &= \left(E_1 - \left(E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2} \right) \right) a + \lambda\Delta b \\
&= \left(-\frac{(\lambda\Delta)^2}{E_1 - E_2} \right) a + \lambda\Delta b,
\end{aligned}
\tag{1.8}
$$

so

$$
\begin{aligned}
|+\rangle &\rightarrow \begin{bmatrix} 1 \\ \frac{\lambda\Delta}{E_1 - E_2} \end{bmatrix} \\
&= |+\rangle + \frac{\lambda\Delta}{E_1 - E_2} |-\rangle.
\end{aligned}
\tag{1.9}
$$

Similarily for the minus case we must have

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

for

$$
|-\rangle \rightarrow |-\rangle + \frac{\lambda\Delta}{E_2 - E_1} |+\rangle.
\tag{1.11}
$$

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

$$\begin{aligned} E_+^{(1)} &= |+\rangle V |+\rangle \\ &= \lambda\Delta \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \lambda\Delta \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &= 0. \end{aligned} \tag{1.12}$$

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

$$\begin{aligned} |+\rangle^{(1)} &= \frac{\overline{P}_+}{E_1 - H_0} V |+\rangle \\ &= \frac{|-\rangle \langle -|}{E_1 - E_2} V |+\rangle \end{aligned} \tag{1.13}$$

The numerator matrix element is

$$\begin{aligned} \langle -| V |+\rangle &= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \Delta \end{bmatrix} \\ &= \Delta, \end{aligned} \tag{1.14}$$

so

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

Observe that this matches the first order series expansion of the exact value above.

For the perturbation of $|-\rangle$ we need the matrix element

$$\begin{aligned} \langle +| V |-\rangle &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \Delta \\ 0 \end{bmatrix} \\ &= \Delta, \end{aligned} \tag{1.16}$$

so it's clear that the perturbed ket is

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

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

$$
\begin{aligned}
\langle + | \, V \, | + \rangle' &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{\Delta}{E_1 - E_2} \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\Delta^2}{E_1 - E_2} \\ \Delta \end{bmatrix} \\
&= \frac{\Delta^2}{E_1 - E_2},
\end{aligned}
\tag{1.18}
$$

and

$$
\begin{aligned}
\langle - | \, V \, | - \rangle' &= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} \frac{\Delta}{E_2 - E_1} \\ 1 \end{bmatrix} \\
&= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta \\ \frac{\Delta^2}{E_2 - E_1} \end{bmatrix} \\
&= \frac{\Delta^2}{E_2 - E_1},
\end{aligned}
\tag{1.19}
$$

The energy perturbations are therefore

$$
\begin{aligned}
E_1 &\rightarrow E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2} \\
E_2 &\rightarrow E_2 + \frac{(\lambda\Delta)^2}{E_2 - E_1}.
\end{aligned}
\tag{1.20}
$$

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

$$
\begin{aligned}
V &= U \bigwedge U^\dagger \\
\bigwedge &= \begin{bmatrix} \Delta & 0 \\ 0 & -\Delta \end{bmatrix} \\
U = U^\dagger &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.
\end{aligned}
\tag{1.21}
$$

A change of basis for the Hamiltonian is

$$
\begin{aligned}
H' &= U^\dagger H U \\
&= U^\dagger H_0 U + \lambda U^\dagger V U \\
&= E_1 U^\dagger + \lambda U^\dagger V U \\
&= H_0 + \lambda \bigwedge.
\end{aligned}
\tag{1.22}
$$

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

$$
\begin{aligned}
\Delta^{(1)} &= \langle 1| V |1\rangle = \Delta \\
\Delta^{(2)} &= \langle 2| V |2\rangle = -\Delta.
\end{aligned} \tag{1.23}
$$

The perturbed energies are therefore

$$
\begin{aligned}
E_1 &\to E_1 + \lambda\Delta \\
E_2 &\to E_2 - \lambda\Delta,
\end{aligned} \tag{1.24}
$$

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

Bibliography