Problem 5.12

In this problem, we have a Hamiltonian, \( H_0 \), and a perturbation, \( V \), given by

\[
H_0 \rightarrow \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_2 \end{pmatrix}, \quad V \rightarrow \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix}.
\]  (98)

The unperturbed energy eigenkets of \( H_0 \) are given by

\[
|n^{(0)}\rangle = \{ |1\rangle , |2\rangle , |3\rangle \} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}
\]  (99)

The goal of this problem is to calculate the energy eigenvalues of the perturbed Hamiltonian, \( H = H_0 + V \), using three different methods. First, we proceed with non-degenerate perturbation theory for all states. It can be shown with elementary matrix multiplication that the first-order shifts in energy for the three unperturbed eigenkets vanish

\[
\Delta_{1}^{(1)} = \langle 1|V|1\rangle = 0 \quad (100) \\
\Delta_{2}^{(1)} = \langle 2|V|2\rangle = 0 \quad (101) \\
\Delta_{3}^{(1)} = \langle 3|V|3\rangle = 0 \quad (102)
\]

Moving to the second-order shift, we find

\[
\Delta_{1}^{(2)} = \sum_{k \neq 1} \frac{|V_{1k}|^2}{E_{1}^{(0)} - E_{k}^{(0)}} = \text{indeterminate} \quad (103) \\
\Delta_{2}^{(2)} = \sum_{k \neq 2} \frac{|V_{2k}|^2}{E_{2}^{(0)} - E_{k}^{(0)}} = \text{indeterminate} \quad (104) \\
\Delta_{3}^{(2)} = \sum_{k \neq 3} \frac{|V_{3k}|^2}{E_{3}^{(0)} - E_{k}^{(0)}} = \frac{|a|^2 + |b|^2}{E_{2} - E_{1}} \quad (105)
\]

Clearly, this procedure is not correct for the states \( |1\rangle \) and \( |2\rangle \), since we obtain indeterminate results. However, this approach is valid for the state \( |3\rangle \), as it is non-degenerate.

Moving on, we can solve for the eigenvalues of the full Hamiltonian exactly by diagonalizing its matrix representation. This yields

\[
\begin{vmatrix}
E_1 - \eta & 0 & a \\
0 & E_1 - \eta & b \\
a^* & b^* & E_2 - \eta
\end{vmatrix} = 0
\]  (106)

\[
(E_1 - \eta)((E_1 - \eta)(E_2 - \eta) - |b|^2) + a\left(-a^*(E_1 - \eta)\right) = 0
\]  (107)

\[
\therefore \eta_1 = E_1
\]  (108)

\[
(E_1 - \eta)(E_2 - \eta) - |b|^2 - |a|^2 = 0
\]  (109)

\[
\eta^2 - (E_1 + E_2)\eta + E_1E_2 - |a|^2 - |b|^2 = 0
\]  (110)

\[
\eta = \frac{1}{2}(E_1 + E_2) \pm \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4\left(|a|^2 + |b|^2\right)}
\]  (111)

\[
\therefore \eta_2 = \frac{1}{2}(E_1 + E_2) - \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4\left(|a|^2 + |b|^2\right)}(E_2 - E_1)^2
\]  (112)

\[
\therefore \eta_3 = \frac{1}{2}(E_1 + E_2) + \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4\left(|a|^2 + |b|^2\right)}(E_2 - E_1)^2
\]  (113)
Using the fact that \((E_2 - E_1) \gg |a|^2 + |b|^2\), we can Taylor expand the exact energy eigenvalues to second-order to obtain

\[
\eta_2 \approx E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1} \tag{114}
\]

\[
\eta_3 \approx E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1} \tag{115}
\]

Doing this, we see that, to second-order, the eigenvalue \(\eta_3\) matches exactly to the energy of the state \(|3\rangle\) combined with the shift obtained by non-degenerate perturbation theory.

Finally, we move to degenerate perturbation theory. Initial attempts to diagonalize the perturbation in the degenerate subspace yield a null matrix

\[
\begin{pmatrix}
\langle 1|V|1 \rangle & (1|V|2) \\
(2|V|1) & (2|V|2)
\end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \tag{116}
\]

Physically, this means that the degeneracy is not lifted at first order. In order to proceed, we construct a new perturbative matrix

\[
\tilde{V}_{m'm} \equiv V_{m'm} + \sum_{k \in D} \frac{V_{m'k} V_{km}}{E_k - E(0)} , \quad m', m \in D \tag{117}
\]

This matrix has the form

\[
\tilde{V} \rightarrow \frac{1}{E_1 - E_2} \begin{pmatrix} |a|^2 & ab^* \\ ba^* & |b|^2 \end{pmatrix} \tag{118}
\]

Diagonalizing this matrix, we have

\[
\begin{pmatrix} |a|^2 & -\Delta_1^{(2)} \\ E_1 - E_2 & -\Delta_2^{(2)} \end{pmatrix} \begin{pmatrix} |b|^2 \\ E_1 - E_2 \end{pmatrix} - \frac{|a|^2 |b|^2}{(E_1 - E_2)^2} = 0 \tag{119}
\]

\[
(\Delta_1^{(2)})^2 - \frac{|a|^2 + |b|^2}{E_1 - E_2} \Delta_2^{(2)} = 0 \tag{120}
\]

The two solutions to this characteristic equation are

\[
\Delta_1^{(2)} = 0, \quad \Delta_2^{(2)} = -\frac{|a|^2 + |b|^2}{E_2 - E_1} \tag{121}
\]

These shifts combined with the unperturbed energies of \(|1\rangle\) and \(|2\rangle\) correspond perfectly to the exact energy eigenvalues \(\eta_1\) and \(\eta_2\) to second-order.