PH423 Assignment 4

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Question 2.

[Sankalp: Got it]

(a) The given Hamiltonian $H(\epsilon)$ is

$$H(\epsilon) = V_0 \cdot \begin{pmatrix} (1-\epsilon) & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} \tag{1}$$

and the unperturbed Hamiltonian H_0

$$H_0 = H(0) = V_0 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{2}$$

is diagonal, so the eigenvectors of the unperturbed system are simply $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ with eigenvalues V_0, V_0, and $2V_0$ respectively.

The perturbation H' is thus

$$H' = H(\epsilon) - H_0 = V_0 \cdot \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \tag{3}$$

Eigenvalues of the whole system are given by the equation in ϵ and $lambda$, the eigenvalues themselves,

$$\left|(H(\epsilon) - \lambda\ \hat{\mathbf{1}})\right| = 0 \text{ , or,} \tag{4}$$

$$\begin{vmatrix} (V_0(1-\epsilon) - \lambda) & 0 & 0 \\ 0 & V_0 - \lambda & V_0\epsilon \\ 0 & V_0\epsilon & 2V_0 - \lambda \end{vmatrix} = 0 \tag{5}$$

$$((1-\epsilon)V_0 - \lambda)((V_0 - \lambda)(2V_0 - \lambda) - V_0^2\epsilon^2) = 0 \tag{6}$$

This gives $\lambda = (1-\epsilon)V_0$, $\frac{V_0}{2}(3 - \sqrt{4\epsilon^2 + 1})$, $\frac{V_0}{2}(3 + \sqrt{4\epsilon^2 + 1})$ as the eigenvalues of H. Call these $\lambda_{1,2,3}$ respectively.

Evaluating to second order in ϵ, we get

$$(\lambda_1, \lambda_2, \lambda_3) = V_0(1-\epsilon, 1-\epsilon^2, 2+\epsilon^2) \tag{7}$$

(b) The last eigenvalue, $2V_0$, is non degenerate, so we attempt to approximate its perturbed analogue using non-degenerate perturbation theory as required, using both first and second order theories. The first order correction is given simply by

$$\begin{aligned}\langle v_3|H'|v_3\rangle &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \epsilon\\ 0 & \epsilon & 0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\\ &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\ \epsilon\\ 0\end{pmatrix}\\ &= 0\ .\end{aligned} \tag{8}$$

That is, there is no first-order correction to the eigenvalue, which is expected, given the calculation from part a.

Moving on, representing the n^th order correction to the i^th eigenket as $\left|v_{i,n}\right\rangle$, the second-order correction is

$$\left\langle v_{3,0}\right| H' \left|v_{3,1}\right\rangle = \left\langle v_{3,0}\right| H' \sum_{m\neq 3} \frac{\left\langle v_{m,0}\right| H' \left|v_{3,1}\right\rangle}{E_3^{(0)} - E_m^{(0)}} \left|v_{m,0}\right\rangle \tag{9}$$

Since our eigenvectors are basis vectors, this basically filters components. Since we know $H'\left|v_{3,1}\right\rangle$, the calculation trivially reduces to

$$\begin{aligned}\left\langle v_{3,0}\right| H' \left|v_{3,1}\right\rangle &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \epsilon\\ 0 & \epsilon & 0\end{pmatrix}\begin{pmatrix}0\\ \epsilon\\ 0\end{pmatrix}\\ &= \begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\ 0\\ \epsilon^2\end{pmatrix}\\ &= \epsilon^2\end{aligned} \tag{10}$$

Thus the second order correction is ϵ^2, exactly matching the result from part a.

(c) As for the degenerate levels, corresponding to $\left|v_{1,0}\right\rangle$ and $\left|v_{2,0}\right\rangle$, we apply the degenerate thoery. That is, the secular equation, as follows

$$\sum_{i=1}^{2} a_i(\left\langle v_{j,0}\right| H' \left|v_{i,0}\right\rangle - E_i^{(0)}\delta_{ij}) = 0 \text{ for } j \in \{1, 2\} \tag{11}$$

Question 3.

Question 4.

Question 6.

Question 8.