5.73

Quiz 16 ANSWERS

1.

<u>Non-degenerate Perturbation Theory</u>

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = \mathbf{H}_{nn}^{(0)} + \mathbf{H}_{nn}^{(1)} + \sum_m{}' \frac{\mathbf{H}_{nm}^{(1)}\mathbf{H}_{mn}^{(1)}}{E_n^{(0)} - E_m^{(0)}}$$

$$\psi_n = \psi_n^{(0)} + \psi_n^{(1)} = \sum_m{}' \frac{\mathbf{H}_{nm}^{(1)}}{E_n^{(0)} - E_m^{(0)}} \psi_n^{(0)}$$

<u>Quasi-degenerate Perturbation Theory</u> (Van Vleck transformation)

$$\mathbf{H}_P^{(2)} = \sum_{s,P'} \frac{\mathbf{H}_{ns}^{(1)}\mathbf{H}_{sm}^{(1)}}{\frac{E_n^{(0)} + E_m^{(0)}}{2} - E_s^{(0)}}$$ where n, m belong to P and s belongs to P′.

A. Use non-degenerate perturbation theory to find the eigenvalues and eigenvectors of $\begin{pmatrix} 0 & 5 \\ 5 & 20 \end{pmatrix}$.

$$E_+ = 20 + \frac{5^2}{20} = 21.25 \qquad \psi_+ = \psi_2^{(0)} + 0.25\psi_1^{(0)}$$

$$E_- = 0 - \frac{5^2}{20} = -1.25 \qquad \psi_- = \psi_1^{(0)} - 0.25\psi_2^{(0)}$$

B. Find the eigenvalues of the 2×2 matrix in part **A** by diagonalization.

$$0 = \begin{vmatrix} 0-E & 5 \\ 5 & 20-E \end{vmatrix}$$

$$0 = E^2 - 21E - 25$$

$$E_\pm = \frac{21 \pm [441+100]^{1/2}}{2} = 10.5 \pm 11.63$$

$E_+ = 21.13 \qquad E_- = -1.13$

C. Perform the Van Vleck transformation on

$$\mathbf{H} = \left(\begin{array}{cc|c} 0 & 0 & 10.02 \\ 0 & 1 & 14.18 \\ \hline 10.02 & 14.18 & 100.5 \end{array}\right)$$

$$\begin{pmatrix} 0+\dfrac{(10.02)^2}{0.5-100.5} & \dfrac{(10.02)(14.18)}{0.5-100.5} \\ \text{sym} & 1+\dfrac{(14.18)^2}{0.5-100.5} \end{pmatrix} = \begin{pmatrix} -1.004 & -1.42 \\ \text{sym} & -1.011 \end{pmatrix}$$

D. If you were successful on part **C**, you would have obtained a matrix of the form

$$\mathbf{H}^{\text{eff}} = \begin{pmatrix} A & B & 0 \\ B & A & 0 \\ 0 & 0 & C \end{pmatrix} \text{ where } |C| \gg |A| + |B|.$$

What are the two lowest energy eigenvalues and eigenvectors of $\mathbf{H}^{\text{eff}}$?
[**HINT**: You should be able to solve this problem by inspection!]

$E_- = A - B \qquad \psi_- = 2^{-1/2}\left(\psi_1^{(0)} - \psi_2^{(0)}\right)$

$E_+ = A + B \qquad \psi_+ = 2^{-1/2}\left(\psi_1^{(0)} + \psi_2^{(0)}\right)$

verify $E_\mp \leftrightarrow \psi_\mp$

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} A-B \\ B-A \end{pmatrix} = (A-B)\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

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