北京大學
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No 5. 1. $\hat{H}\Psi = E\Psi$

$\therefore \hat{H}(c_1\psi_a + c_2\psi_b) = E(c_1\psi_a + c_2\psi_b)$

$\therefore (\hat{H}-E)c_1|\psi_a\rangle + (\hat{H}-E)c_2|\psi_b\rangle = 0.$

$\therefore \begin{cases} (\mathcal{E}_a - \mathcal{E})c_1 + H_{ab}c_2 = 0 \\ H_{ab}^* c_1 + (\mathcal{E}_b - \mathcal{E})c_2 = 0 \end{cases}$

$\therefore \mathcal{E}_a\mathcal{E}_b - (\mathcal{E}_a + \mathcal{E}_b)\mathcal{E} + \mathcal{E}^2 - H_{ab}^2 = 0$

代入,有: $\mathcal{E}^2 + \mathcal{E} - 2 = 0 \Rightarrow \mathcal{E}_+ = -2eV \quad \mathcal{E}_- = 1eV$

当 $\mathcal{E}_+ = -2eV$, $2c_1 + \sqrt{2}c_2 = 0 \Rightarrow c_2 = -\sqrt{2}c_1$

$\therefore \Psi_+ = \sqrt{\frac{1}{3}}\psi_A - \sqrt{\frac{2}{3}}\psi_B$

当 $\mathcal{E}_- = 1eV$ $-c_1 + \sqrt{2}c_2 = 0$

$\therefore \Psi_- = \sqrt{\frac{2}{3}}\psi_A + \sqrt{\frac{1}{3}}\psi_B.$

2. Pf: $\begin{vmatrix} (\mathcal{E}_A - \mathcal{E}) & H_{AB} \\ H_{AB}^* & (\mathcal{E}_B - \mathcal{E}) \end{vmatrix} = \mathcal{E}^2 - (\mathcal{E}_A + \mathcal{E}_B)\mathcal{E} + \mathcal{E}_A\mathcal{E}_B - |H_{AB}|^2 = 0$

$\therefore$ 令 $\Delta = \sqrt{\mathcal{E}_A^2 + \mathcal{E}_B^2 - 2\mathcal{E}_A\mathcal{E}_B + 4|H_{AB}|^2} = \sqrt{(\mathcal{E}_A - \mathcal{E}_B)^2 + 4|H_{AB}|^2}$

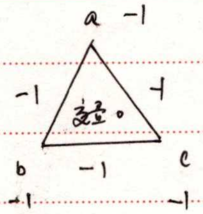
有: $\mathcal{E}_- = \dfrac{\mathcal{E}_A + \mathcal{E}_B + \Delta}{2}$

$\therefore -\dfrac{\mathcal{E}_B - \mathcal{E}_A + \Delta}{2}c_1 + H_{AB}c_2 = 0$

$c_2 = +\dfrac{\mathcal{E}_B - \mathcal{E}_A + \sqrt{(\mathcal{E}_B - \mathcal{E}_A)^2 + 4|H_{AB}|^2}}{2H_{AB}}c_1$

$|c_2|^2 = \dfrac{4|H_{AB}|^2 + (\Delta\mathcal{E})^2 + \cancel{4|H_{AB}|^2 \Delta\mathcal{E}}\,(\Delta\mathcal{E})^2 + 2\Delta\mathcal{E}\cdot\sqrt{(\Delta\mathcal{E})^2 + 4|H_{AB}|^2}}{4|H_{AB}|^2}|c_1|^2$

$> |c_1|^2$. 证毕.

3. 

$$\begin{vmatrix} -1-\varepsilon & -1 & -1 \\ -1 & -1-\varepsilon & -1 \\ -1 & -1 & -1-\varepsilon \end{vmatrix} = 0$$

$=\!=$ 0 (2)

—— −3 (1)

$\therefore (-1-\varepsilon)^3 - 1 - 1 + 3(\varepsilon+1)$

$= -\varepsilon^3 - 3\varepsilon^2 - 3\varepsilon - 3 + 3\varepsilon + 3$

$= -\varepsilon^3 - 3\varepsilon^2 = 0 \Rightarrow \varepsilon_1 = -3,\ \varepsilon_2 = 0,\ \varepsilon_3 = 0.$

i) $\varepsilon_1 = -3$.

$$\begin{cases} 2c_1 + c_2 + c_3 = 0 \\ c_1 + 2c_2 + c_3 = 0 \end{cases} \quad \therefore \begin{cases} 2c_1 + c_2 = -c_3 \\ c_1 + 2c_2 = -c_3 \end{cases}$$

$$\therefore \begin{cases} c_1 + c_2 = -\frac{2}{3}c_3 \\ c_1 - c_2 = 0 \end{cases} \Rightarrow c_1 = c_2 = -\frac{1}{3}c_3$$

$\Psi_1 = -\frac{1}{3}\psi_a - \frac{1}{3}\psi_b + \psi_c$ (未归一化)

ii) $\varepsilon_2 = 0$ $\quad c_1 + c_2 + c_3 = 0 \quad c_1 = -c_2 - c_3$

$\therefore \Psi_2 = \sqrt{\frac{1}{2}}\psi_a - \sqrt{\frac{1}{2}}\psi_b$

$\Psi_3 = \sqrt{\frac{1}{2}}\psi_a - \sqrt{\frac{1}{2}}\psi_c.$