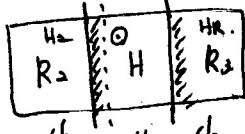


① 

$\psi_{II} \quad H \quad \psi_{III}$

→ 장계작용 interaction .

$H\psi_{II} + \tau\psi_{III} + \tau_{II}\psi_{II} = E\psi_{II}$.

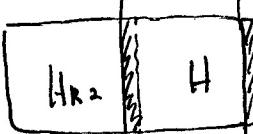
$H_2\psi_{II} + 0\psi_{III} + \tau_{II}'\psi_{II} = E\psi_{II}$.

$$\left[\begin{array}{ccc} H & \tau_{II} & \tau_{II} \\ \tau_{II}' & H_{R_2} & 0 \\ \tau_{II} & 0 & H_{R_3} \end{array} \right] \begin{pmatrix} \psi_I \\ \psi_{II} \\ \psi_{III} \end{pmatrix} = E \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \psi_I \\ \psi_{II} \\ \psi_{III} \end{pmatrix} \quad (* \text{ 일부분은 } ② \text{ 뒤집음}).$$

$$H = -\frac{\hbar^2}{2m} \nabla^2 + \sum_{\alpha \in II} \frac{g_{\alpha}(-e)}{4\pi\epsilon_0} + \sum_{j \in II} \int \frac{e^2 \phi_j^*(r_j) \phi_j(r_j) dr_j}{4\pi\epsilon_0 |r_j - r|} + E_x^2(r) + E_c^2(r).$$

$(E - H)\psi = 0 \rightarrow \text{solution} \quad H\psi_{\alpha} = E_{\alpha}\psi_{\alpha}$

$(E - H)\psi = g \Rightarrow \quad " \quad \psi(r) = \int \frac{\frac{\phi_{\alpha}(r)\phi_{\alpha}(r')}{E - E_{\alpha}}}{g(r')} dr'$

② 

→ matrix × 일부분에서 2행짜기.

$H\psi_I + \tau_{II}\psi_{II} = E\psi_I$.

$\tau_{II}\psi_I + H_{R_2}\psi_{II} = E\psi_{II}$.

$\psi_{II}(r) = \int \left(\sum_{\alpha} \frac{\frac{\phi_{\alpha}(r)\phi_{\alpha}(r')}{E - E_{\alpha}}}{G(r, r')} \right) \tau_{II}' \psi_I(r') dr' \quad G(r, r')$

$H\psi_I + \int \tau_{II} G(r, r') \tau_{II}' dr' = E\psi_I$.

$H\psi_I + \int_{I_1} \underbrace{\psi_{II}(r)r' \tau_{II}' dr'}_{\psi_{II}(r')} + \int_{I_2} \underbrace{\psi_{II}(r)r' \tau_{II}' dr'}_{\psi_{II}(r')} =$

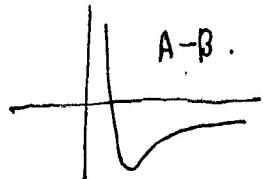
$\sum_{\alpha} \frac{\phi_{\alpha}^2(r) \phi_{\alpha}^*(r')}{E - E_{\alpha}^2}$.

$\sum_{\beta} \frac{\phi_{\beta}^2(r) \phi_{\beta}^*(r')}{E - E_{\beta}^2}$.

$\tau_{II}' = \sum_{k \in II} \frac{g_k(-e)}{4\pi\epsilon_0 |r_k - r|} + \sum_{j, r_j \in II, i \neq j} \frac{e^2 \phi_j^*(r_j) \phi_j(r_i)}{4\pi\epsilon_0 |r_j - r_i|} + f_x^2(r) + f_c^2$.

$$E = \sum_{jk} \sum_{ij} \frac{f(s_{ij})}{r} \frac{g(s_{ij}, s_{jk})}{\theta} \frac{h(s_{ij}, s_{jk}, s_{kj})}{\phi}$$

+ J^{Monopole} + V^{Dipole}



\downarrow
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Final. $22^\circ \text{ CR} \rightarrow 11^\circ \Sigma$. $12:00$, $1^{\text{m}} 21$
type.

$$\left[H\psi(r) + \int \nabla^2 \phi(r, r') \nabla' \phi(r') \right] = E[\phi(r)]$$

basis set $\psi(r) = \sum_i C_i b_i(r)$

solution $\psi_1, \psi_2, \dots, \psi_{\infty}$

$$\begin{pmatrix} \psi_1(r) \\ \psi_2(r) \\ \vdots \\ \psi_K(r) \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & \dots & C_{1K} \\ C_{21} & C_{22} & \dots & C_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ C_{K1} & C_{K2} & \dots & C_{KK} \end{pmatrix} \begin{pmatrix} b_1(r) \\ b_2(r) \\ \vdots \\ b_K(r) \end{pmatrix}$$

$$P(r) = \sum_i \frac{\psi_i^*(r) \psi_i(r)}{1 + e^{(\varepsilon_i - \mu)/T}} f(\varepsilon_i - \mu)$$

$$P(r) = \text{trace} \left[(b_1^* \dots b_K^*) \begin{pmatrix} C_{11}^* & C_{12}^* & \dots & C_{1K}^* \\ C_{21}^* & C_{22}^* & \dots & C_{2K}^* \\ \vdots & \vdots & \ddots & \vdots \\ C_K^* & C_{K2}^* & \dots & C_{KK}^* \end{pmatrix} \begin{pmatrix} f(\varepsilon_1 - \mu) & 0 & \dots & 0 \\ 0 & f(\varepsilon_2 - \mu) & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & f(\varepsilon_K - \mu) \end{pmatrix} \begin{pmatrix} C_{11} & C_{12} & \dots & C_{1K} \\ C_{21} & C_{22} & \dots & C_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ C_{K1} & C_{K2} & \dots & C_{KK} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_K \end{pmatrix} \right]$$

doping $\frac{[N_A(r) - P(r)]}{\epsilon}$

\Rightarrow effect of μ & T & ϵ .

$$\boxed{II} \quad J_i = V^+ \left(\begin{smallmatrix} J_{ii} & 0 \\ 0 & 0 \end{smallmatrix} \right) V$$

