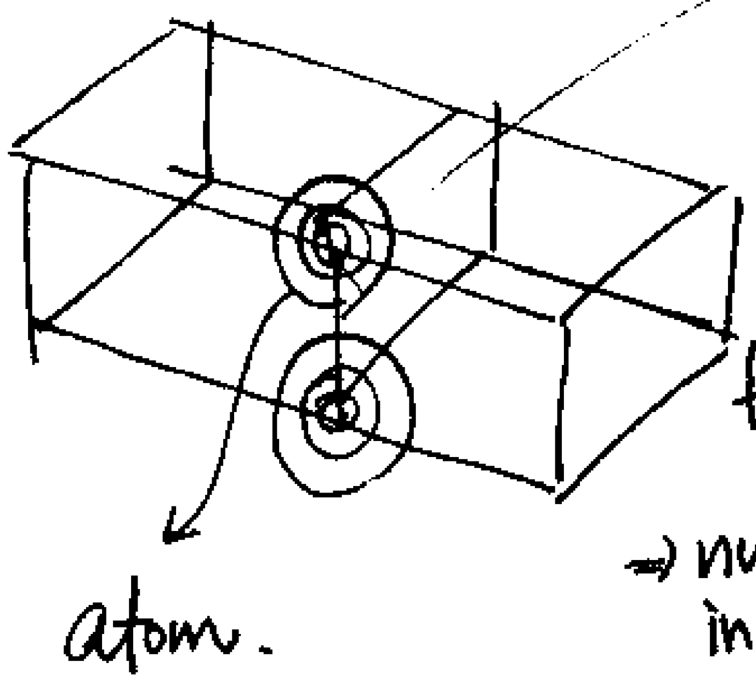
Quiz : Next Wed.

Home : Next Mon.

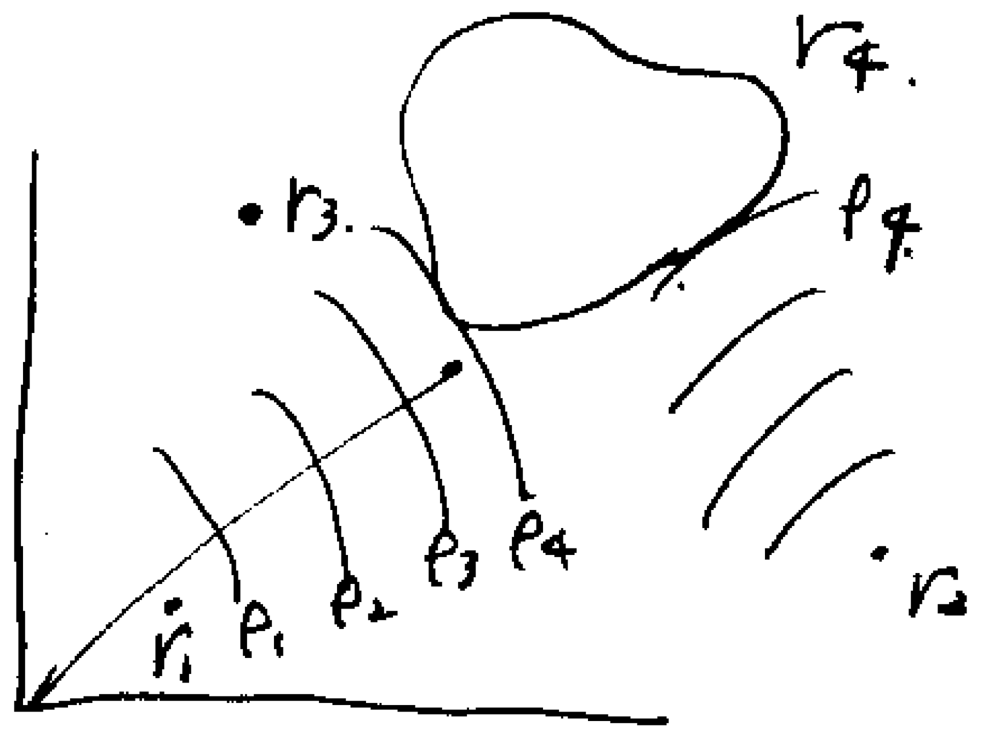


$$\underbrace{\varphi_k(r)}_{\uparrow} \sum_j \frac{e^{i\underset{\sim}{k}\cdot r_j}}{\sqrt{N}} \varphi(r-r_j).$$

for single body

→ nucleus 사이 interaction (x).

$$\left(\frac{2\pi}{l}n_x, \frac{2\pi}{l}n_y, \frac{2\pi}{l}n_z\right).$$



$E = \langle \varphi | H | \varphi \rangle$.

crystal

$\hookrightarrow E_k + E_{Ne} + E_J + E_x + E_c \Rightarrow -\frac{\hbar^2}{2m}\nabla^2 + \underline{\underline{u(r)}}$

$u(r) = u(r+k)$

$$E = \frac{1}{N}\langle \sum_m e^{ik\cdot r_m}\varphi(r-r_m) \,|\, -\frac{\hbar^2}{2m}\nabla^2 + u(r) \,|\, \sum_j e^{ik\cdot r_j}\varphi(r-r_j)$$

$$= \frac{1}{M}\sum_m\sum_j \int e^{ik\cdot \underbrace{(r_j - r_m)}_{s_m}} \langle \varphi(r-r_m) | \underbrace{-\frac{\hbar^2}{2m}\nabla^2 + u(r)}_{r} | \underbrace{\varphi(r-r_j)}_{s_m + r_m} \rangle$$

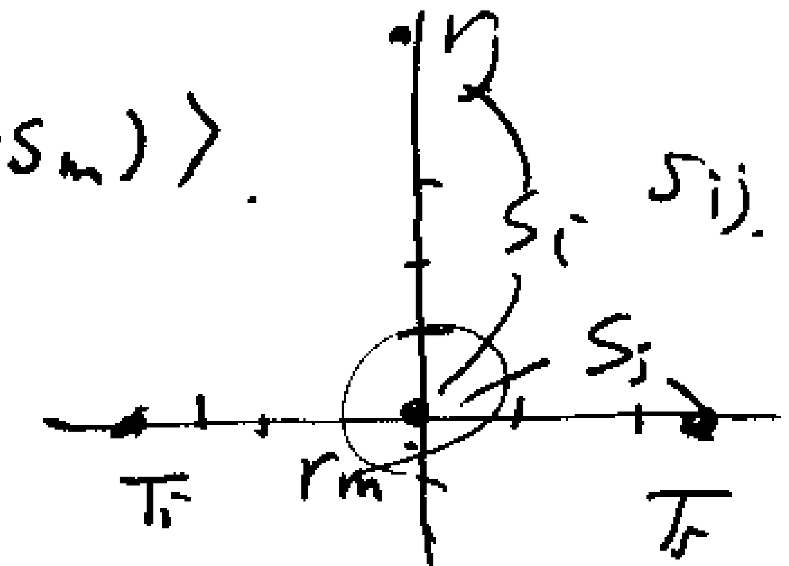
$r_j - r_m = s_m$

$$= \sum_j e^{ik\cdot s_m} \langle \varphi(r-r_m) | -\frac{\hbar^2}{2m}\nabla^2 + u(r) | \varphi(r - r_m - s_m) \rangle$$

"

$$\int \varphi^*(r-r_m) H(r) \varphi(r - r_m - s_m)\, dr.$$

$$= \sum_j e^{ik\cdot s_m} \langle \varphi(r) | -\frac{\hbar^2}{2m}\nabla^2 + u(r) | \varphi(r-s_m) \rangle.$$



$$E_k = \sum_j e^{ik\cdot s_m} \langle \varphi(r) | H(r) | \varphi(r - s_m) \rangle.$$

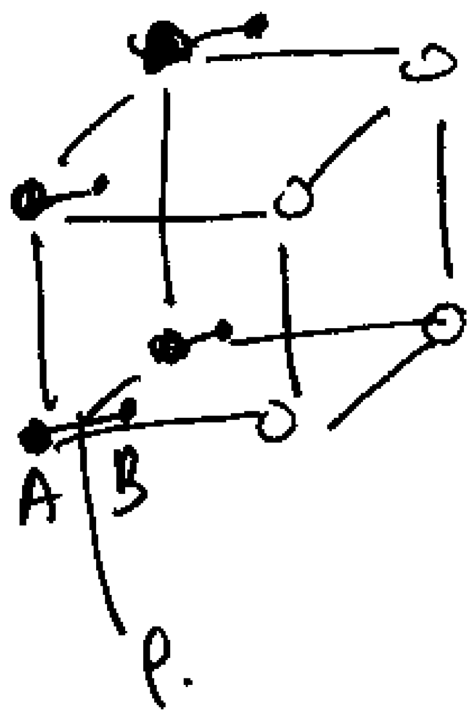
$$= e^{ik\cdot \underset{\uparrow}{0}} \langle \varphi(r) | H(r) | \varphi(r-0) \rangle + \sum_{j \neq m} e^{ik\cdot s_m} \langle \varphi(r) | H(r) \varphi(r - s_2) \rangle + \cdots$$

only 2nd-neighbors

$$= \underbrace{\langle \varphi(r) | H(r) | \varphi(r) \rangle}_{-\alpha} + \sum_{j\neq m} e^{ik\cdot s_1} \underbrace{\langle \varphi(r) | H(r) | \varphi(r - s_1) \rangle}_{-\beta} + \sum_{j\neq m} e^{ik\cdot 2} \underbrace{\langle \varphi | H | \varphi - s_2 \rangle}_{-r}.$$

but only 1st neighbor

$$\cong -r - r\sum e^{ik\cdot s_1} \langle \varphi | H | \varphi(r - s_i) \rangle$$



$$\rho_k(r) = \frac{1}{\sqrt{2N}}\left[\sum_j e^{ik\cdot r_j}\rho_a(r-r_j) + \sum_j e^{ik\cdot(r_j+\rho)}\rho_b(r-(r_j+\rho))\right]$$

$$S(n) = [\pm a.0.0]\ [0.\pm a.0]\ [0\ 0\ \pm a]$$

$$E_k = -\alpha - \gamma\sum e^{ik\cdot S(n)} = \left(\underbrace{e^{ik[\pm a\,0.0]}}_{2\cos k_x\cdot a} + \underbrace{e^{ik\cdot[0.\pm a.0]}}_{2\cos k_y\cdot a} + \underbrace{e^{ik\cdot[0\,0.\pm a]}}_{2\cos k_z\cdot a}\right)$$

$$e^{ik\cdot\pm a} = 2\cos k_x\cdot a.$$

$$E_k = -\alpha - 2\gamma\left[\cos k_x\cdot a + \cos k_y\cdot a + \cos k_z\cdot a\right].$$

$\vec{k} = [111]$.

$k_x = \frac{k}{\sqrt{3}}$

$k_y = \frac{k}{\sqrt{3}}$ $k_z = \frac{k}{\sqrt{3}}$

$$E_{k[111]} = -\alpha - 6\alpha\cdot\cos\frac{k}{\sqrt{3}}\cdot a$$