$P_K = \sum_G (K+G) e^{i(K+G)}$, $\phi_{K+G}(r) = \phi_K(r)$

$\frac{\hbar^2}{2m} |C(K)|^2 + \sum_G U_G (K-G) = \varepsilon_K C(K)$.

$\to U_G = \frac{1}{V} \int U(r) e^{-iG \cdot r} dr$.

$\left[-\frac{\hbar^2}{2m} \nabla^2 + U(r) \right] \phi_K(r) = \varepsilon_K \phi_K(r)$

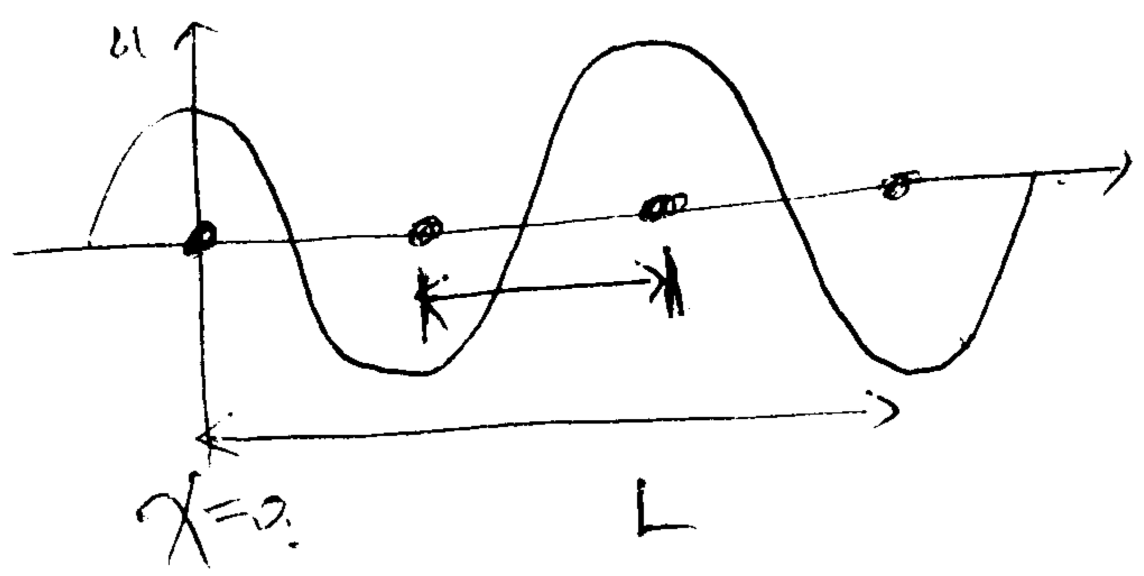
$U(r) = U(r+R)$.

$U(r) = 0$.

$\to \phi_K(r) = C(K) e^{iK \cdot r} \Rightarrow \frac{1}{\sqrt{V}} e^{iK \cdot r}$

$\phi_K(r) = C(K) e^{iK \cdot r}$
$+ C(K-G_1) e^{iG_1 \cdot r} + C(K+G_1) e^{-iG_1 \cdot r} + C(K+G_2) e^{-iG_2 \cdot r} + C(K+G_2) e^{-iG_2 \cdot r}$.

$G_i = \left(\frac{2\pi}{a_x} n_{xi}, \frac{2\pi}{a_y} n_{yi}, \frac{2\pi}{a_z} n_z \right)$.



In metal ;

$U(r) \Rightarrow U(x) = \cos\left(\frac{2\pi}{a} x\right)$
$= \cos(G_1 x)$

$\frac{\hbar^2}{2}(K \mp G)^2 \leq E_{cutt}$.

$U(x) = C(K) e^{iK \cdot x} + C(K-G) e^{i(K-G)x}$

$U_G = \frac{1}{a} \int_0^a \cos\left(\frac{2\pi}{a} x\right) \cdot e^{-i\frac{2\pi}{a} x} dx$

$= \frac{1}{a} \int_0^a \cos G_1 x \, e^{-iG \cdot x} dx$.

$\frac{\hbar^2 K^2}{2m} C(K) + \sum_G U_G C(K-G) = \varepsilon_K C(K)$

$\frac{\hbar^2 K^2}{2m} C(K) + U_{G_1} C(K-G) = \varepsilon_K C(K)$

$\frac{\hbar^2 (K-G_1)^2}{2m} C(K-G) + U_{G_1} C(K) = \varepsilon_K C(K-G_1)$

$\varepsilon_K^0 = \frac{\hbar^2 K^2}{2m}$

$\varepsilon_{K-G}^0 = \frac{\hbar^2 (K-G_1)^2}{2m}$

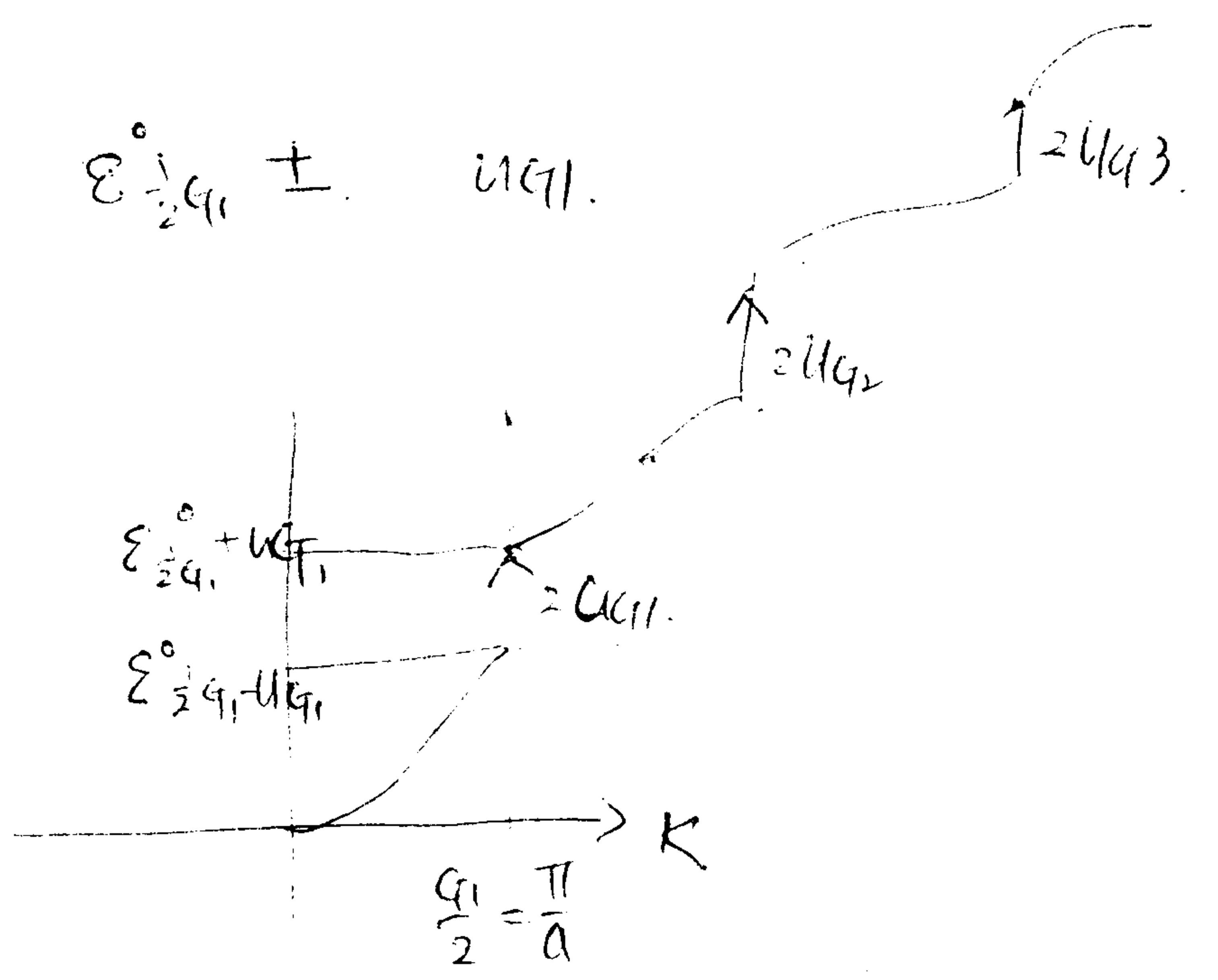
$\begin{pmatrix} \varepsilon_K^0 - \varepsilon & U_{G_1} \\ U_{-G_1} & \varepsilon_{K-G}^0 - \varepsilon \end{pmatrix} \begin{pmatrix} C(K) \\ C(K-G_1) \end{pmatrix} = 0$.

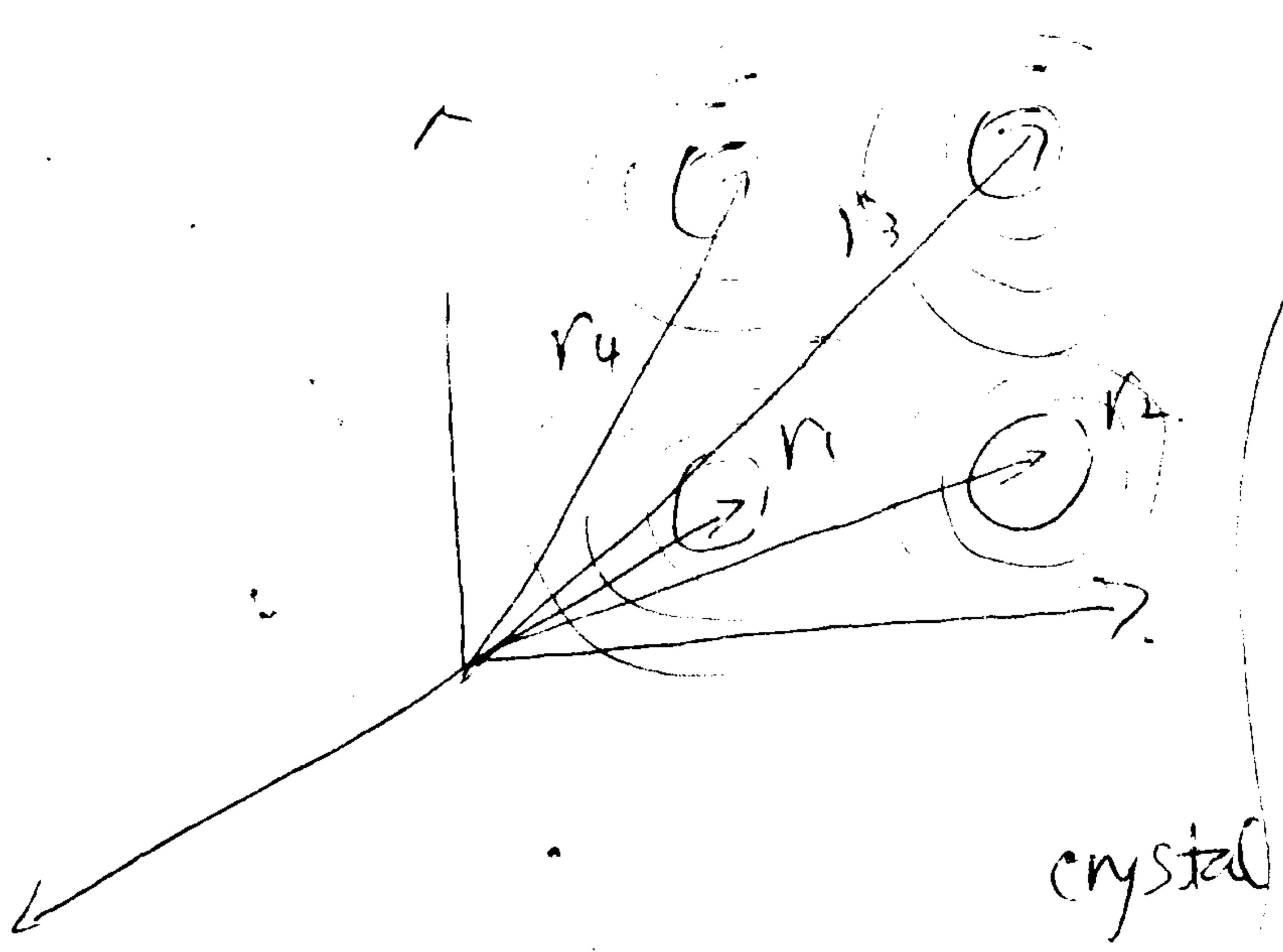
$\varepsilon^2 - (\varepsilon_K^0 + \varepsilon_{K-G_1}^0) \varepsilon + (\varepsilon_K^0 \varepsilon_{K-G_1}^0 - U_G U_{-G_1}) = 0$

($U_G U_{-G_1} = U_{G_1}^2$)

$\varepsilon = \varepsilon_K^0 + \varepsilon_{K-G}^0 \pm \sqrt{(\varepsilon_K^0 - \varepsilon_{K-G})^2 + 4 U_G^2}$

$= \varepsilon^{\circ}_{\frac{1}{2}G_1} \pm U_{G_1}$





$\phi(r) = \sum C(K, r_j)\, \varphi(r - r_j)$

atomic

$\phi_k(r+R) = V(r+R) \cdot e^{ik\cdot(r+R)} \rightarrow \frac{2\pi}{L}(n_x, n_y, n_z)$

$= V(r)\, e^{ik\cdot r} \cdot e^{ik\cdot R}$

$= \phi_k(r) \cdot e^{ik\cdot R}$

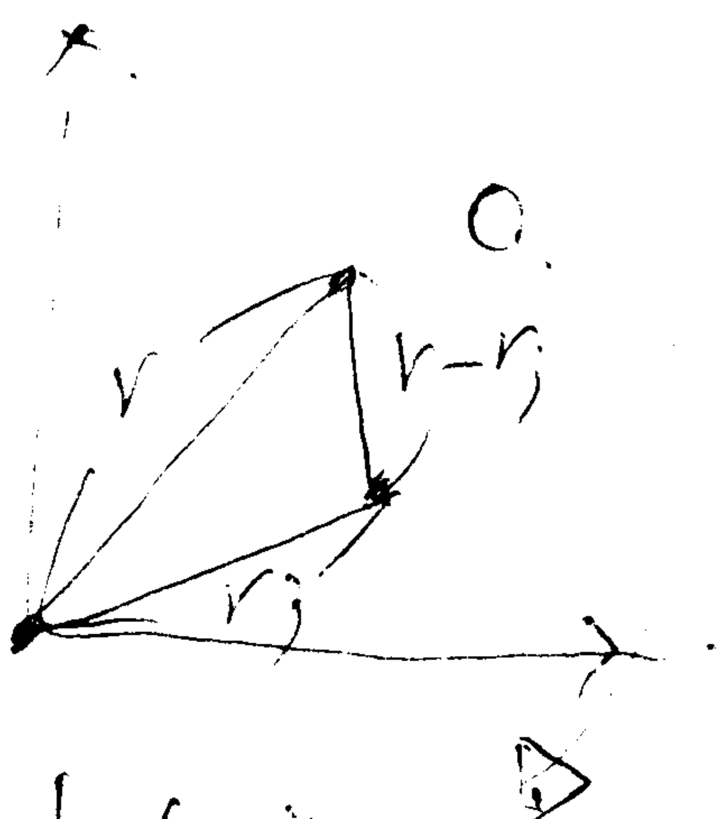
crystal

$\phi(r+R) = e^{ik\cdot R} \phi(r)$

$R - r_j = r_j'$
$r_j' = r_j - R$
$\Rightarrow r_j = r_j' + R$

$\phi(r+R) = \sum_j C(K, r_j)\, \varphi(r + R - r_j)$

$= e^{ik\cdot R} \sum_l C(K, r_l)\, \varphi(r - r_l)$



$\phi_k(r) = \sum C(k, r_j + R)\, \rho(r - r_j)$

$\phi_k(r) = \sum C(k, r_j)\, \rho(r, r_j)$

$= \sum_{j=1}^{N} \frac{1}{\sqrt{N}} e^{ik\cdot r_j} \rho(r - r_j)$

$\frac{1}{\sqrt{N}}\left(e^{ik\cdot r_1} \rho(r - r_1) + e^{ik\cdot r_2} \rho(r - r_2)\right)$

$\langle p \rangle = \langle k | \hat{p} | k \rangle$

$\varepsilon = \langle k | \hat{H} | k \rangle$

$\varepsilon_k = \langle k | h(r) | k \rangle = -\alpha - r \sum C$

$\frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{ik\cdot r_j} \rho(r - r_j)$