Midterm 2 Solutions

1) a) A Bravais lattice is the set of all points

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 ,$$

where $\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 \neq 0$ and $n_i \in \mathbb{Z}$.

b) $e^{i \vec{G} \cdot \vec{R}} = 1 \quad \forall \vec{R} \in BL$.

c) $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$

$\vec{b}_2 = b \hat{y}$ $\qquad \vec{a}_2 \cdot \vec{b}_2 = \frac{\sqrt{3}\, ab}{2} = 2\pi$

$b = \frac{4\pi}{\sqrt{3}\, a}$ $\qquad \boxed{\vec{b}_2 = \frac{4\pi}{\sqrt{3}\, a} \hat{y}}$

Let $\vec{b}_1 = \alpha \hat{x} + \beta \hat{y}$

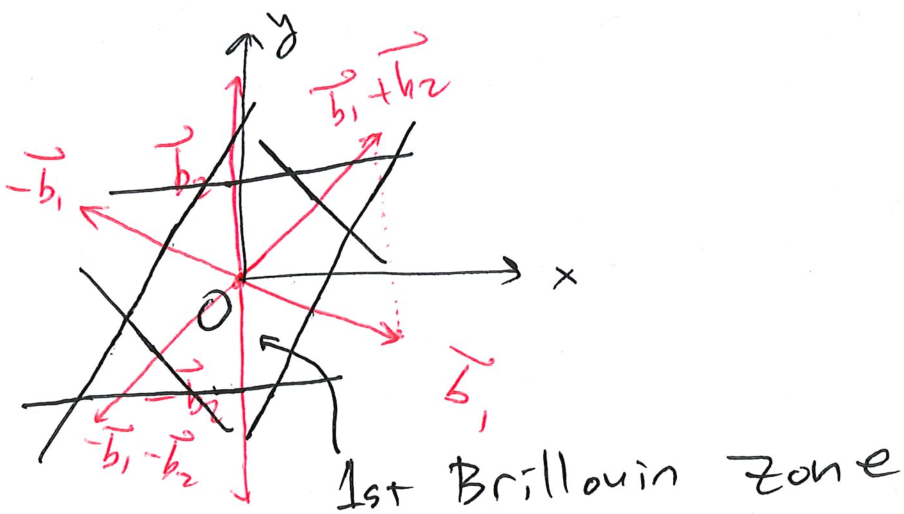
$0 = \vec{a}_2 \cdot \vec{b}_1 = \alpha \frac{a}{2} + \beta \frac{\sqrt{3}\, a}{2}$ $\qquad 0 = \alpha + \beta \sqrt{3}$

$\beta = - \frac{\alpha}{\sqrt{3}}$

$$\vec{b}_1 = \alpha\left(\hat{x} - \frac{\hat{y}}{\sqrt{3}}\right)$$

$$2\pi = \vec{a}_1 \cdot \vec{b}_1 = a\alpha \qquad \alpha = \frac{2\pi}{a}$$

$$\boxed{\vec{b}_1 = \frac{2\pi}{a}\left(\hat{x} - \frac{\hat{y}}{\sqrt{3}}\right)}$$



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2) a) $\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{x})\right]\psi(\vec{x}) = \varepsilon\,\psi(\vec{x})$

$$U(\vec{x}) = \sum_{\vec{G}} U_{\vec{G}}\, e^{i\vec{G}\cdot\vec{x}}, \qquad \psi(\vec{x}) = \sum_{\vec{k}} C(\vec{k})\, e^{i\vec{k}\cdot\vec{x}}$$

$$\boxed{\left(\frac{\hbar^2 \vec{k}^2}{2m} - \varepsilon\right) C(\vec{k}) + \sum_{\vec{G}} U_{\vec{G}}\, C(\vec{k} - \vec{G}) = 0}$$

$$\Longrightarrow \quad \psi_{\vec{k}}(\vec{x}) = \sum_{\vec{G}} C(\vec{k} + \vec{G})\, e^{i(\vec{k}+\vec{G})\cdot\vec{x}}$$

The central equation implies that energy eigenstates must be of the above form.

$$\psi_{\vec{k}}(\vec{x}+\vec{R}) = \sum_{\vec{G}} C(\vec{k}+\vec{G})\, e^{i(\vec{k}+\vec{G})\cdot\vec{x}} \times e^{i(\vec{k}+\vec{G})\cdot\vec{R}}$$

But $e^{i\vec{G}\cdot\vec{R}} = 1$, so

$$\psi_{\vec{k}}(\vec{x}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\,\psi_{\vec{k}}(\vec{x}) \qquad \text{Q.E.D.}$$

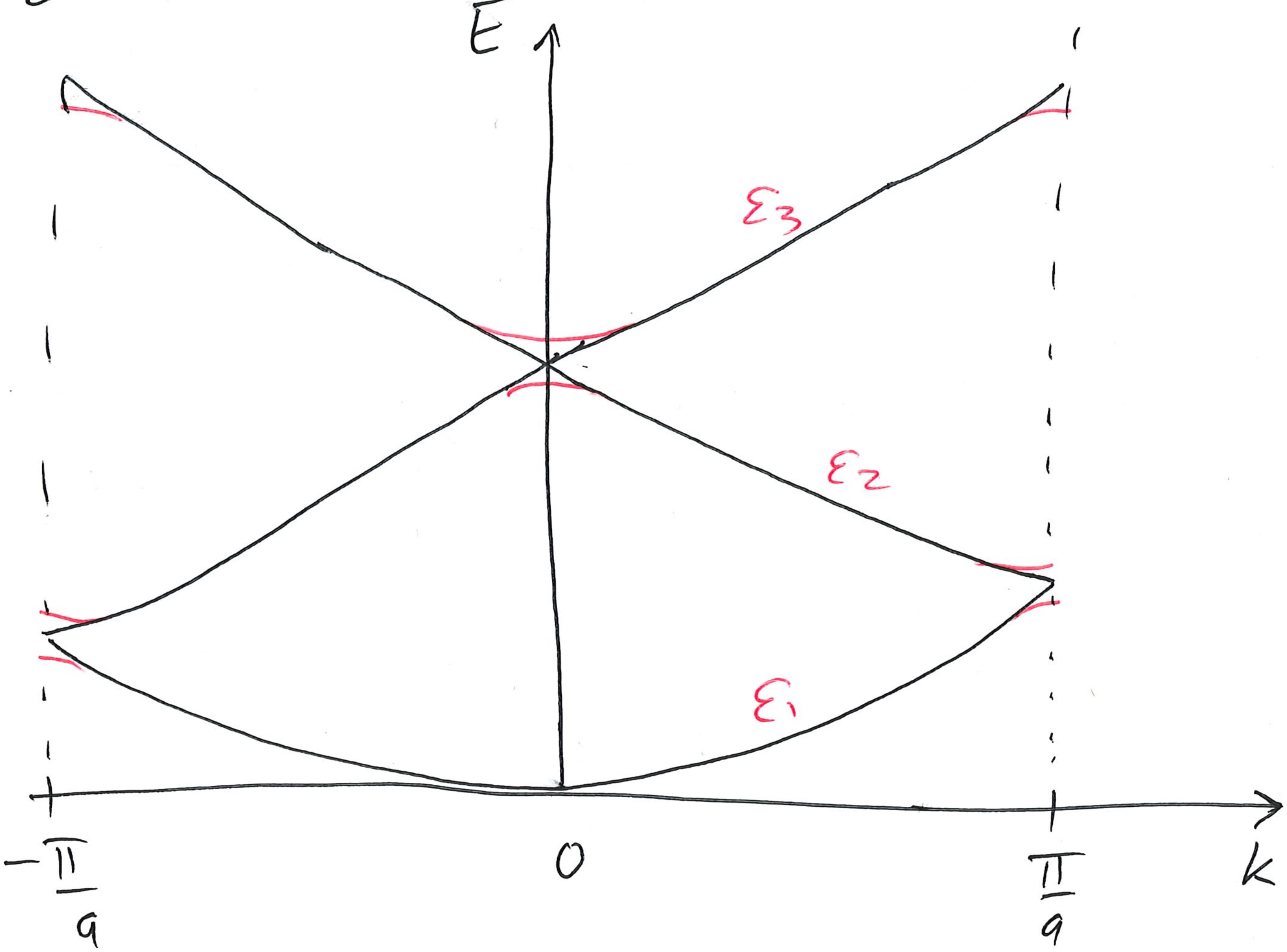
or

$$\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} \underbrace{\sum_{\vec{G}} C(\vec{k}+\vec{G})\, e^{i\vec{G}\cdot\vec{x}}}_{\phi_{\vec{k}}(\vec{x})}$$

$$\phi_{\vec{k}}(\vec{x}+\vec{R}) = \sum_{\vec{G}} C(\vec{k}+\vec{G})\, e^{i\vec{G}\cdot\vec{x}}\, \underbrace{e^{i\vec{G}\cdot\vec{R}}}_{1}$$

$$= \phi_{\vec{k}}(\vec{x}) \qquad \text{Q.E.D.}$$

2 b)



c) If the # of electrons per primitive cell is odd, the material must be a metal. If the # of electrons per primitive cell is even, then it is an insulator if the bands do not overlap, but is a metal if the bands overlap at the Fermi energy.

3) $\varepsilon(k) = \varepsilon_{at}^{*} - 2t\cos ka$

a) $$V = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k} = \frac{2ta}{\hbar}\sin ka$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k^2} = \frac{2ta^2}{\hbar^2}\cos ka$$

b) $$\hbar\frac{dk}{dt} = F$$

$$k(t) = k(0) + \frac{Ft}{\hbar} = \frac{Ft}{\hbar} \qquad (k(0)=0)$$

$$V(t) = \frac{2ta}{\hbar}\sin\left(\frac{Fat}{\hbar}\right)$$

$$X(t) = X(0) + \int_0^t dt'\, V(t')$$

$$= X(0) - \frac{\hbar}{Fa}\frac{2ta}{\hbar}\cos\left(\frac{Fat}{\hbar}\right)\Big|_0^t$$

$$X(t) - X(0) = \frac{2t}{F}\left(1 - \cos\Omega t\right)$$

$\Omega = \frac{Fa}{\hbar}$ = characteristic frequnacy

$\frac{2t}{F}$ = characteristic amplitude