UNOFFICIAL SOLUTIONS BY TheLongCat

C3: CONDENSED MATTER PHYSICS

TRINITY TERM 2015

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Disclaimer: due to its unofficial nature, the author does not warrant the accuracy of the presented solutions in any form. However, the author is happy to discuss the typos and errors should one arises.

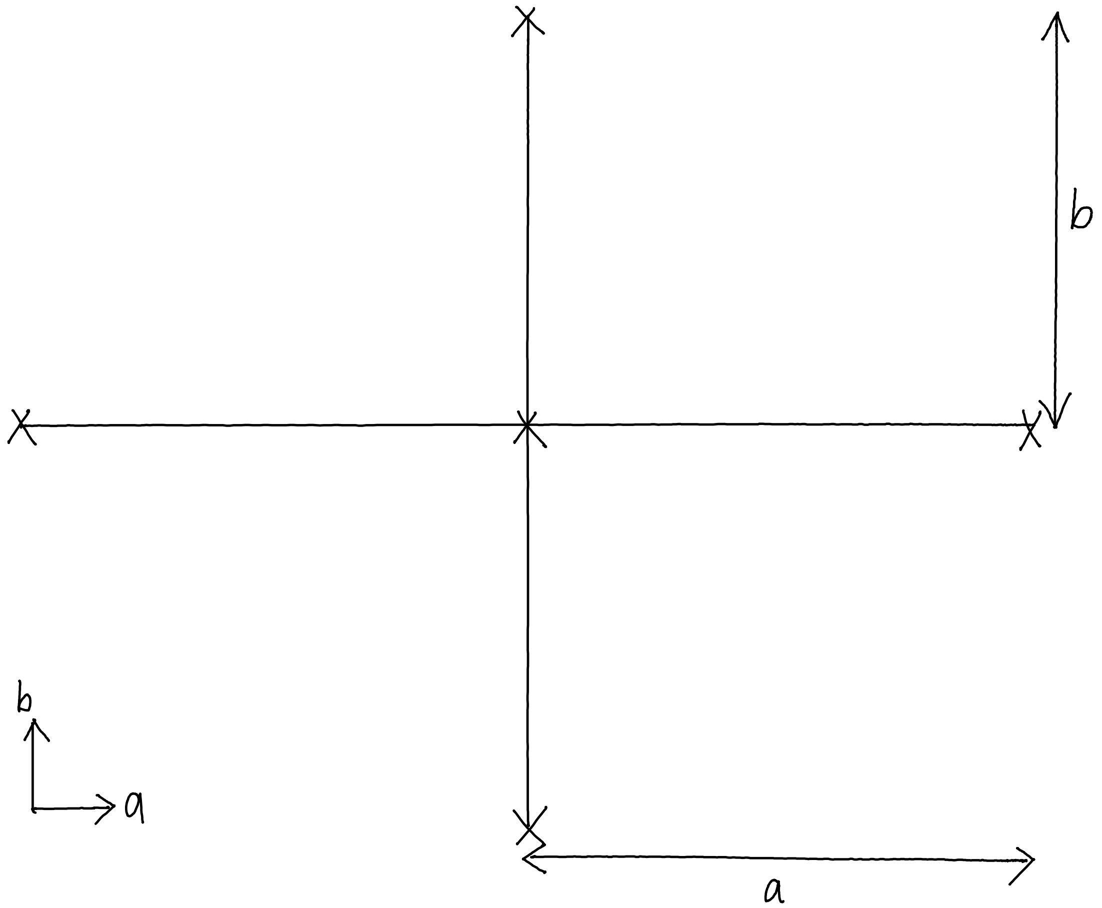
Turn over as you please – we are NOT under exam conditions here.

6. **(DRAFT)** Tight-binding model and Fermi surface.

(a) E_0: unperturbed energy of an atom.

$t(\mathbf{T})$: transfer integral, that is the overlap between orbitals of different atoms weighted by their potentials.

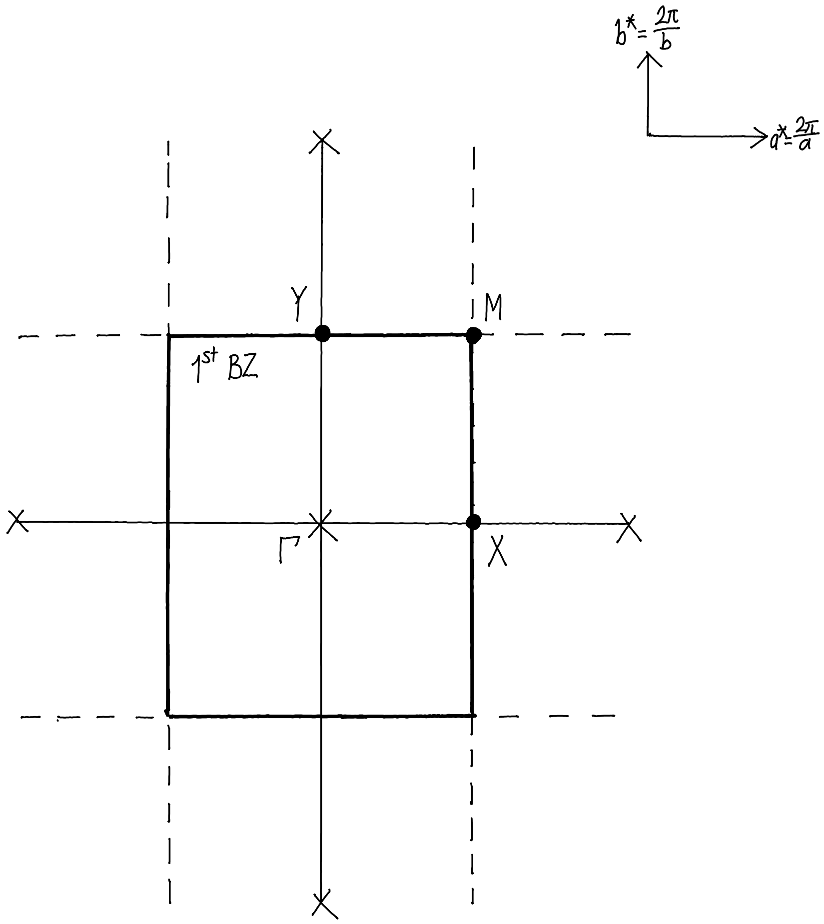
Sketch of the direct lattice:



$$\begin{aligned}E(\mathbf{k}) &= E_0 - t(\mathbf{a})e^{i\mathbf{k}\cdot\mathbf{a}} - t(-\mathbf{a})e^{-i\mathbf{k}\cdot\mathbf{a}} - t(\mathbf{b})e^{i\mathbf{k}\cdot\mathbf{b}} - t(-\mathbf{b})e^{-i\mathbf{k}\cdot\mathbf{b}} \\ &= E_0 - 2t_x \cos k_x a - 2t_y \cos k_y a\end{aligned}$$

where $t_x = t(\mathbf{a}) = t(-\mathbf{a})$, $t_y = t(\mathbf{b}) = t(-\mathbf{b})$ by translational symmetry.

Sketch of the reciprocal lattice:



Along $\Gamma - M$:

$$\frac{k_y}{k_x} = \frac{b^*}{a^*} = \frac{a}{b}$$
$$\Rightarrow E = E_0 - 2t_x \cos(k_x a) - t_x \underbrace{\cos\left(\frac{a}{b}k_x b\right)}_{\cos(k_x a)} = E_0 - 3t_x \cos(k_x a)$$
$$= \begin{cases} E_0 - 3t_x & \text{at } \Gamma \\ E_0 + 3t_x & \text{at } M \end{cases}$$

Along $M - X$:

$$k_x = \frac{\pi}{a} \Rightarrow E = E_0 - 2t_x \cos\pi - t_x \cos(k_y b)$$
$$= E_0 + 2t_x - t_x \cos(k_y b)$$
$$= \begin{cases} E_0 + 3t_x & @M \\ E_0 + t_x & @X \end{cases}$$

Along $X - \Gamma$:

$$k_y = 0 \Rightarrow E = E_0 - 2t_x \cos(k_x a) - t_x$$
$$= \begin{cases} E_0 + t_x & @X \\ E_0 - 3t_x & @\Gamma \end{cases}$$

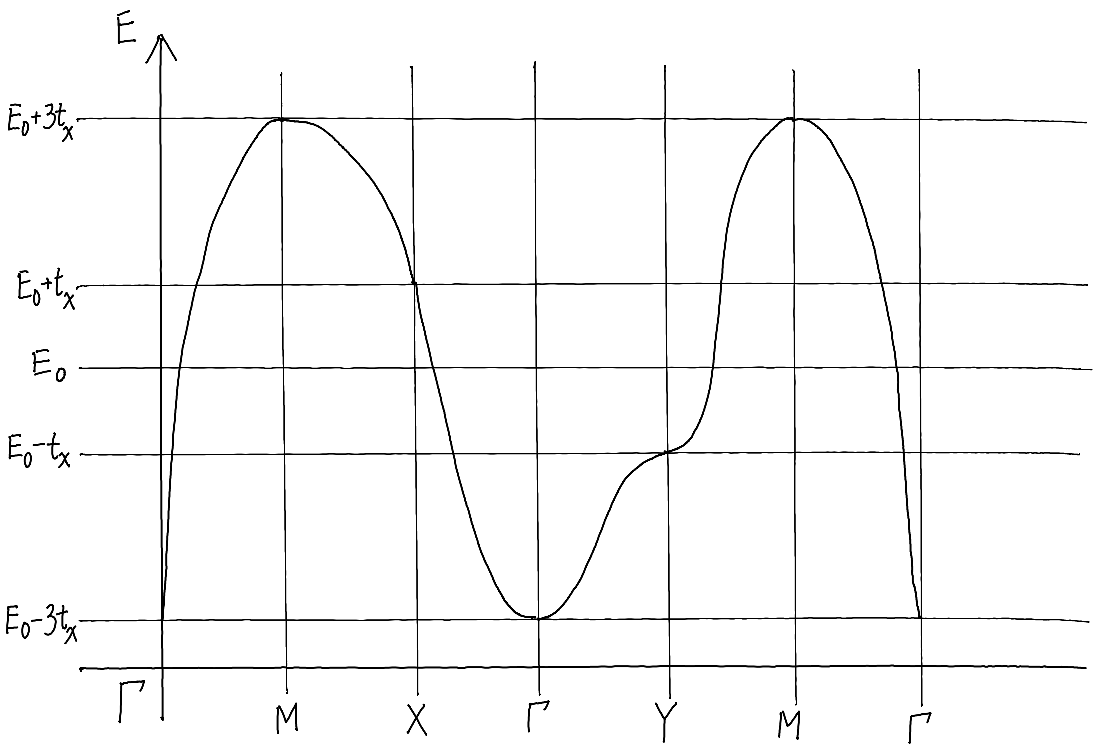
Along $\Gamma - Y$:

$$k_x = 0 \Rightarrow E = E_0 - 2t_x - t_x \cos(k_y b)$$
$$= \begin{cases} E_0 - 3t_x & @\Gamma \\ E_0 - t_x & @Y \end{cases}$$

Along $Y - M$:

$$k_y = \frac{\pi}{b} \Rightarrow E = E_0 - 2t_x \cos(k_x a) + t_x$$
$$= \begin{cases} E_0 - t_x & @Y \\ E_0 + 3t_x & @M \end{cases}$$

Sketch of dispersion:



TO BE CONTINUED...