SS2019: Solid State Theory
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Problem Set 4

1. **Tight-binding model on the square lattice** (3+3+2 points)

Consider a tight-binding model on the square lattice

$$H = -t \sum_{\vec{r} \in \vec{R}_n} \sum_{\vec{\delta} = \vec{a}_1, \vec{a}_2} \sum_{\sigma = \uparrow, \downarrow} (c^\dagger_{\vec{r},\sigma} c_{\vec{r}+\vec{\delta},\sigma} + c^\dagger_{\vec{r}+\vec{\delta},\sigma} c_{\vec{r},\sigma}),$$

where $t > 0$. The primitive vectors are $\vec{a}_1 = a\hat{x}$ and $\vec{a}_2 = a\hat{y}$.

(a) Show that the energy band is given by

$$E_{\vec{k}} = -2t[\cos(k_x a) + \cos(k_y a)].$$

(b) When the number of electrons per site is $n_e = 1$ (so-called "half-filling"), sketch the shape of the Fermi surface.

Hint: In this case, the Fermi energy is zero (why?).

(c) Sketch the shape of the Fermi surface when the Fermi energy is $\varepsilon_F = -0.2t$. Note that the number of electrons per site satisfies $n_e < 1$.

2. **Tight-binding model on the kagome lattice** (3+4+3 points)

There are a number of materials whose crystal structure forms a kagome lattice (see Fig. 1). It has a unit cell with three atoms, denoted by A, B, C. The primitive vectors can be chosen as $\vec{a}_1 = a\hat{x}$ and $\vec{a}_2 = \frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$.

(a) Calculate the primitive vectors $\vec{b}_1$, $\vec{b}_2$ for the reciprocal space. Sketch the reciprocal lattice and the first Brillouin zone (FBZ).

(b) Consider a tight-binding model (spin index suppressed)

$$H = -t \sum_{\langle \vec{r}, \vec{r}' \rangle} (c^\dagger_{\vec{r}} c_{\vec{r}'} + c^\dagger_{\vec{r}'} c_{\vec{r}})$$

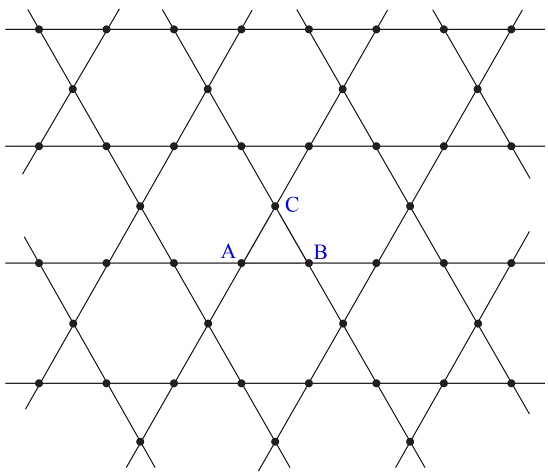

Figure 1: The kagome lattice.

restricted to nearest-neighbors with $t > 0$. Diagonalize the Hamiltonian and find the energy bands $E_\alpha(\vec{k})$ ($\alpha = 1, 2, 3$).

Check your result: $E_1(\vec{k}) = 2t$ and $E_{2,3}(\vec{k}) = -t \pm t\sqrt{4[\cos^2(\vec{k} \cdot \vec{\delta}_1) + \cos^2(\vec{k} \cdot \vec{\delta}_2) + \cos^2(\vec{k} \cdot \vec{\delta}_3)] - 3}$, where $\delta_1 = \frac{1}{2}\vec{a}_1$, $\delta_2 = \frac{1}{2}\vec{a}_2$, and $\vec{\delta}_3 = \vec{\delta}_2 - \vec{\delta}_1$. Note that $E_1(\vec{k})$ is a flat band.

(c) Sketch the band structure in the FBZ. Where do band-touching points appear?