**1. Emergent Dirac physics**

Based on the graphene exercise of the previous exercise sheet:

(a) Obtain the graphene dispersion around the K and K' points by linearizing the eigenvalues $\varepsilon_{\pm}(\mathbf{k})$.
**Hint:** Define $\mathbf{k} = \mathrm{K} + \mathbf{q}$, with $|\mathbf{q}| << |\mathrm{K}|$, and perform a linear expansion in $\mathbf{q}$.

$$\vec{r}_K = \frac{2\pi}{3a}\begin{pmatrix}1\\ 1/\sqrt{3}\end{pmatrix}, \quad \vec{r}_{K'} = \frac{2\pi}{3a}\begin{pmatrix}1\\ -1/\sqrt{3}\end{pmatrix}$$

$$f(\vec{k}) = -t\left(e^{-ik_x a} + 2e^{ik_x a/2}\cos\left(\frac{k_y a\sqrt{3}}{2}\right)\right)$$

$$\frac{1}{-t} f(\vec{r}_K + \vec{q}) = (-1)^{1/3} e^{-iaq_x}\left(-1 + 2e^{\frac{3iaq_x}{2}}\sin\left(\frac{\pi}{6} - \frac{\sqrt{3}}{2} a q_y\right)\right)$$

$$\approx \frac{3}{2}(-1)^{5/6} a q_x - \frac{3}{2}(-1)^{1/3} a q_y$$

$$= a\left[\frac{3}{2}e^{\frac{5i\pi}{6}} q_x - \frac{3}{2}e^{\frac{i\pi}{3}} a q_y\right]$$

$$f(\vec{r}_K + \vec{q}) = -\frac{3at}{2} e^{-\frac{i\pi}{6}}\left[-q_x - iq_y\right]$$

$$= -\frac{3at}{2} e^{\frac{5i\pi}{6}}\left[q_x + iq_y\right]$$

Around $K'$ we have

$$\frac{1}{-t} f(\vec{r}_{K'} + \vec{q}) = \frac{3}{2} a (-1)^{1/3} q_y + \frac{3}{2} a (-1)^{5/6} q_x$$

$$= \frac{3}{2} a\left[e^{\frac{i\pi}{3}} q_y + e^{\frac{5i\pi}{6}} q_x\right]$$

$$f(\vec{r}_{K'} + \vec{q}) = -\frac{3ta}{2} e^{-\frac{i\pi}{6}}\left[-q_x + e^{\frac{i\pi}{3}} q_y\right]$$

$$= -\frac{3ta}{2} e^{-\frac{i\pi}{6}}\left[-q_x + iq_y\right]$$

$$= -\frac{3ta}{2} e^{\frac{\pi i}{3}}\left[q_y + iq_x\right]$$

Since $\mathcal{E}_\pm(\vec{k}') = \pm|f(\vec{k}')|$,

$$\mathcal{E}_\pm(\vec{q}) \simeq \left| \frac{3}{2} a t e^{-\frac{i\pi}{6}} \left[ i q_y - q_x \right] \right|$$

$$= \frac{3at}{2} \sqrt{q_x^2 + q_y^2}$$

(b) Linearize in the same way the Bloch Hamiltonian $h(\mathbf{k})$ around K and K'. Show that we can write $h(K' + \mathbf{q}) = \hbar v_F \mathbf{q} \cdot \boldsymbol{\sigma}$ and $h(K + \mathbf{q}) = \hbar v_F (\mathbf{q} \cdot \boldsymbol{\sigma})^*$, where $v_F = 3ta/2\hbar$ is the Fermi velocity, and $\boldsymbol{\sigma}$ is the vector of Pauli matrices in the A/B sublattice basis.
**Hint:** Perform a $\pi/3$ phase rotation of the basis vector $\psi(\mathbf{k})$, *i.e.*

$$h(K' + \mathbf{q}) \to \begin{bmatrix} e^{i\pi/3} & 0 \\ 0 & e^{-i\pi/3} \end{bmatrix} h(K' + \mathbf{q})$$

after the linearization in $\mathbf{q}$.

$$h(K + \vec{q}) = -\frac{3ta}{2} \begin{pmatrix} 0 & e^{\frac{5i\pi}{6}} [q_x + i q_y] \\ e^{-\frac{5i\pi}{6}} [q_x - i q_y] & 0 \end{pmatrix}$$

$$= \frac{3ta}{2} \begin{pmatrix} & e^{-\frac{i\pi}{6}} (q_x + i q_y) \\ e^{\frac{i\pi}{6}} (q_x - i q_y) & \end{pmatrix}$$

Then we perform a basis rotation

**2. Peierls substitution**

A Bloch state of a one-band Hamiltonian with a periodic potential $U(\boldsymbol{r}+\boldsymbol{R}) = U(\boldsymbol{r})$ (where $\boldsymbol{R}$ is a linear combination of the lattice basis vectors with integer coefficients) is given by

$$\psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = u_{\boldsymbol{k}\sigma}(\boldsymbol{r})e^{i\boldsymbol{k}\boldsymbol{r}}\chi_\sigma, \tag{1}$$

where $u_{\boldsymbol{k}\sigma}(\boldsymbol{r})$ has the same periodicity as the crystal. For the following calculation we will neglect the spin index $\sigma$ and its respective wave function $\chi_\sigma$. Then the *Wannier* functions are defined by

$$\phi_{\boldsymbol{R}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}}\psi_{\boldsymbol{k}}(\boldsymbol{r})e^{i\boldsymbol{k}\boldsymbol{R}}, \tag{2}$$

where $N$ is the number of unit cells.

(a) Show that two Wannier states are orthonormal. You may use $\langle\psi_{\boldsymbol{k}}(\boldsymbol{r})|\psi_{\boldsymbol{k}'}(\boldsymbol{r})\rangle = \delta_{\boldsymbol{k},\boldsymbol{k}'}$.

$$|\phi_{\vec{R}}\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{k}}|\vec{k}\rangle e^{i\vec{k}\cdot\vec{R}}$$

$$\langle\phi_{\vec{R}'}|\phi_{\vec{R}}\rangle = \frac{1}{N}\left(\sum_{\vec{k}'}\langle\vec{k}'|e^{-i\vec{k}'\cdot\vec{R}'}\right)\left(\sum_{\vec{k}}e^{i\vec{k}\cdot\vec{R}}|\vec{k}\rangle\right)$$

$$= \frac{1}{N}\sum_{\vec{k}}\sum_{\vec{k}'}e^{i\vec{k}\cdot\vec{R}}e^{-i\vec{k}'\cdot\vec{R}'}\underbrace{\langle\vec{k}'|\vec{k}\rangle}_{\delta_{kk'}}$$

$$= \frac{1}{N}\sum_{\vec{k}}e^{i\vec{k}(\vec{R}-\vec{R}')}$$

$$= \delta_{\vec{R},\vec{R}'}$$

We now introduce a magnetic field with vector potential $\boldsymbol{A}(\boldsymbol{r})$, leading to the modified Hamiltonian $H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2 + U(\boldsymbol{r})$. Ultimately, we are interested in the hopping amplitude between the lattice sites

$$t_{lm} = \int d\boldsymbol{r}\phi_{\boldsymbol{R}_l}(\boldsymbol{r})^* H(\boldsymbol{r})\phi_{\boldsymbol{R}_m}(\boldsymbol{r}). \tag{3}$$

(b) Show that the vector potential $\boldsymbol{A}(\boldsymbol{r})$ does only lead to a phase factor $\exp\left(i\frac{e}{\hbar c}\int_{\boldsymbol{R}}^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right)$ in the Wannier states, where the integral is understood to be a line integral from $\boldsymbol{R}$ to $\boldsymbol{r}$. Why do we choose the lower boundary to be $\boldsymbol{R}$?
<u>Hint</u>: Consider

$$\phi_{\boldsymbol{R}}(\boldsymbol{r}) = \exp\left(i\frac{e}{\hbar c}\int_{\boldsymbol{R}}^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right)\tilde{\phi}_{\boldsymbol{R}}(\boldsymbol{r}) \tag{4}$$

and show that $\exp\left(i\frac{e}{\hbar c}\int_{\boldsymbol{R}}^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right) H(\boldsymbol{A}\to 0)\tilde{\phi}_{\boldsymbol{R}}(\boldsymbol{r}) = H(\boldsymbol{A}\neq 0)\phi_{\boldsymbol{R}}(\boldsymbol{r})$.

$$|\phi_R\rangle = \exp\left(i\frac{e}{\hbar c}\int_{\vec{R}}^{\vec{r}} d\vec{r}'\vec{A}(\vec{r}')\right)|\hat{\phi}_R\rangle$$

$$H(\vec{A}\neq 0)\,\phi_R = \exp\underbrace{\left(\frac{ie}{\hbar c}\int_{\vec{R}}^{\vec{r}} d\vec{r}'\vec{A}(\vec{r}')\right)}_{\theta(\vec{r})} H(\vec{A}=0)|\hat{\phi}_R\rangle$$

$$\left[\frac{1}{2m}\left(p-\frac{e}{c}A\right)^2+U\right]e^{\theta(r)}\varphi(r)$$

$$= \frac{1}{2m}\left(-\nabla^2-\frac{ei}{c}\nabla A-\frac{e}{c}A\nabla+\frac{e^2}{c^2}A^2\right)e^{\theta}\varphi(r)$$

$$\nabla^2 e^{\theta}\varphi(r) = \nabla\left(e^{\theta}\dot\theta\varphi+e^{\theta}\nabla\varphi\right)$$

$$= e^{\theta}(\dot\theta)^2\varphi+e^{\theta}\left(\ddot\theta\varphi+\dot\theta\nabla\varphi\right)+e^{\theta}\dot\theta\nabla\varphi+e^{\theta}\nabla^2\varphi$$

$$-\frac{e}{c}\nabla A = -\frac{e}{c}\left(\dot A e^{\theta}\varphi+A\left(e^{\theta}\dot\theta\varphi+e^{\theta}\nabla\varphi\right)\right)$$

$$-\frac{e}{c}A\nabla = -\frac{e}{c}A\left(e^{\theta}\dot\theta\varphi+e^{\theta}\nabla\varphi\right)+\frac{e^2}{c^2}A^2$$

Then we need

$$\nabla e^{\theta} = e^{\theta}\dot\theta$$

$$\theta = \frac{ie}{c}\left[F(A(r))-F(A(R))\right]$$

$$\dot\theta = \frac{ie}{c}\vec A(\vec r)$$

Then we substitute & do some magic

$$\ldots = e^{\theta}H(A=0)\varphi_R$$

c) $t_{nm} \to e^{\theta}\hat t_{nm}$

$$= \int dr\, \langle\varphi_{Rl}|H|\varphi_{Rm}\rangle$$

$$= \int dr\, e^{-i\frac{e}{c}\int_{R_l}^{r}\dot A\,dr}\cdot e^{i\frac{e}{c}\int_{R_m}^{r}A\,dr}\langle\varphi_{Rl}|H|\varphi_{Rm}\rangle$$

$$= e^{-i\frac{e}{c}\int_{R_l}^{r}A\,dr+i\frac{e}{c}\int_{R_m}^{r}A\,dm}\; t_{lm}(A=0)$$

$$= e^{\frac{ie}{\hbar c}\int_{R_m}^{R_l}A\,dr}\; t_{lm}(A=0)$$