Karlsruhe Institute of Technology
Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

Prof. Dr. A. Shnirman
Dr. D. Shapiro, Dr. H. Perrin

Sheet 4
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Category A

1. Van Hove singularity on a square lattice $(3 + 5 + 2 + 10 = 20$ points$)$

(a) Determine the tight-binding hamiltonian of the square lattice where we consider only nearest neighbour hopping, one orbital per atom and isotropic coupling.

Solution: A general tight-binding hamiltonian is written as:

$$\mathcal{H} = \sum_{m_1,m_2,\mathbf{R}_1,\mathbf{R}_2} t_{m_1,m_2}(\mathbf{R}_1 - \mathbf{R_2}) \left|m_1\mathbf{R}_1\right\rangle \left\langle m_2\mathbf{R_2}\right| \ , \qquad (*)$$

where $\mathbf{R_i}$ are Bravais lattice vectors and m_i denote possible internal indices. In the case of the exercise we have one atom per cell with one orbital, there is no need of internal indice m_i. The Bravais vectors of the square lattice are

$$\mathbf{a_1} = \begin{pmatrix} a \\ 0 \end{pmatrix} \ , \quad \mathbf{a_2} = \begin{pmatrix} 0 \\ a \end{pmatrix} \ .$$

We set in the following the lattice constant $a = 1$. We also consider isotropic and nearest neighbour hopping denoted by $-t$. The Hamiltonian reads :

$$\mathcal{H} = -t \sum_{x,y} \left|x, y+1\right\rangle \left\langle x, y\right| + \left|x+1, y\right\rangle \left\langle x, y\right| + \text{h.c.}$$

where (x, y) are the cartesian coordinate of the Bravais vectors .

(b) Find the band structure (dispersion relation) $\epsilon(\vec{k})$ of this Hamiltonian.

Solution: In this notation, the Bloch states are given by $\psi_{k_x,k_y} = \sum_{x,y} e^{i(k_x x + k_y y)} \left|x, y\right\rangle$ and satisfies $\mathcal{H}\psi_{k_x,k_y} = \epsilon(k_x, k_y)\psi_{k_x,k_y}$. Projecting this equation onto a bra $\left\langle x, y\right|$ gives:

$$\epsilon(k_x, k_y) = -2t \left(\cos(k_x) + \cos(k_y)\right)$$

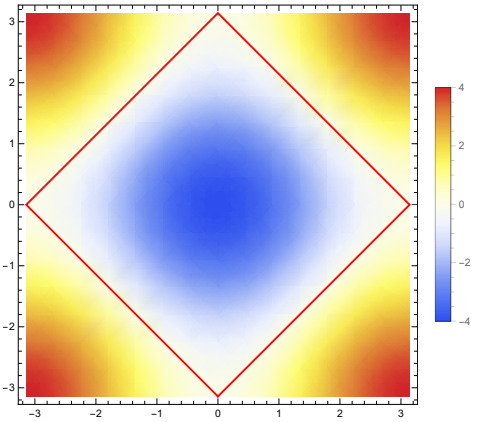
(c) Determine the iso-energy line at $\epsilon = 0$ in the Brillouin zone and plot a sketch of it.

Solution: When $\epsilon = 0$, the above equation equation becomes

$$\cos(k_y) = -\cos(k_x) = \cos(\pm\pi + k_x) \Rightarrow k_y = \begin{cases} \pm\pi + k_x \\ \mp\pi - k_x \end{cases}$$

k_x and k_y runs into the Brillouin zone $[-\pi, \pi]$. When $k_x \in [-\pi, 0]$ then $k_y = \pm(\pi + k_x)$, when $k_x \in [0, \pi]$, $k_y = \pm(-\pi + k_x)$. The iso-energy $E = 0$ is the red square on the

figure below.



(d) Show that the density of states $\rho(E) = \dfrac{1}{(2\pi)^2}\displaystyle\int_{1\ B.Z} \mathrm{d}\vec{k}\ \delta(E - \epsilon(\vec{k}))$ at the energy $E = 0$ diverges. What are the points in the Brillouin zone which cause this divergence? Expand the dispersion relation around one of these points and show that the divergence is logarithmic. Compute the group velocity at these peculiar points.

Solution:

$$\begin{aligned}
\rho(E) &= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\mathrm{d}k_x\int_{-\pi}^{\pi}\mathrm{d}k_y\ \delta(E + 2t(\cos k_x + \cos k_y)) \\
&= \frac{1}{\pi^2}\int_{0}^{\pi}\mathrm{d}k_x\int_{0}^{\pi}\mathrm{d}k_y\ \delta(E + 2t(\cos k_x + \cos k_y)) \\
&= \frac{1}{2\pi^2 t}\int_{0}^{\pi}\mathrm{d}k_x\int_{0}^{\pi}\mathrm{d}k_y\ \delta(\tilde{E} + \cos k_x + \cos k_y)
\end{aligned}$$

where $\tilde{E} = \dfrac{E}{2t}$. Let us change the variable and define $p_x = -\cos k_x$ and $p_y = -\cos k_y$

$$\rho(E) = \frac{1}{2\pi^2 t}\int_{-1}^{1}\frac{\mathrm{d}p_x}{\sqrt{1-p_x^2}}\int_{-1}^{1}\frac{\mathrm{d}p_y}{\sqrt{1-p_y^2}}\ \delta(\tilde{E} - p_x - p_y)$$

The delta function imposes $p_y = \tilde{E} - p_x$ and $-1 \leq p_y \leq 1$ so $\tilde{E} - 1 \leq p_x \leq 1 + \tilde{E}$. We also have $-1 \leq p_x \leq 1$, if we consider $\tilde{E} \geq 0$ we obtain

$$\rho(E) = \frac{1}{2\pi^2 t}\int_{\tilde{E}-1}^{1}\frac{\mathrm{d}p_x}{\sqrt{1-p_x^2}}\frac{1}{\sqrt{1-(\tilde{E}-p_x)^2}}$$

When $E \neq 0$, (here $E > 0$), the integral can be evaluated and gives a finite value (because the divergence of the function under the integral diverges as $\underset{\epsilon\to 0}{\propto}\dfrac{1}{\sqrt{\epsilon}}$ When we try to evaluate this function at $E = 0$ we have that:

$$\rho(0) = \frac{1}{2\pi^2 t}\int_{-1}^{1}\frac{\mathrm{d}p_x}{1-p_x^2}$$

The divergence of the integral is due to the point $p_x^2 = 1 \to k_x = 0, \pm\pi$. We deduce from question (c) that the points located at such k_x and on the iso-energy $E = 0$ are

$(k_x, k_y) = (-\pi, 0)$ (or equivalently $(\pi, 0)$ due to the periodicity of the Brillouin zone and $(k_x, k_y) = (0, \pi)$ or $(k_x, k_y) = (0, -\pi)$. They are the corner of the square iso-energy $E = 0$. One way to compute the behavior of the divergence around $E = 0$ is to expand the dispersion relation around these problematic points in the Brillouin zone. We expand the dispersion relation around the points $(k_x^0, k_y^0) = (0, \pm\pi)$:

$$\epsilon(k_x, k_y) \sim t(k_x^2 - \tilde{k}_y^2)$$

where $\tilde{k_y} = k_y - \pi$

$$\begin{aligned}\rho(E \to 0) &\approx C + \frac{1}{(2\pi)^2}\int_{-\epsilon}^{\epsilon} dk_x \int_{-\epsilon}^{\epsilon} d\tilde{k}_y \delta\left(E - tk_x^2 + t\tilde{k}_y^2\right) = C + \frac{1}{2\pi^2 t}\int_0^{\epsilon'} \frac{d\tilde{k}_y}{\sqrt{2\tilde{E} + \tilde{k}_y^2}} \\ &\approx C + \frac{1}{2\pi^2 t}\int_0^{\frac{\epsilon'}{\sqrt{2\tilde{E}}}} \frac{dk'_y}{\sqrt{1 + k'^2_y}} = C + \frac{\operatorname{asinh}(\epsilon'/\sqrt{2\tilde{E}})}{2\pi^2 t}\end{aligned}$$

where C denotes the regular part of the integral, $\epsilon' = \sqrt{\epsilon^2 - 2\tilde{E}}$. We integrate the diverging part in the vicinity of these points but out of the iso-energy $E = 0$ (because we know that here the integral does not diverge). Furthermore, $\sinh(x) \underset{x\to\infty}{\sim} e^x \to \operatorname{asinh}(y) \underset{y\to\infty}{\sim} \ln(y)$. We obtain:

$$\rho(E) \underset{E\to 0}{\sim} \frac{1}{4\pi^2 t} \ln \frac{t}{E}$$

The group velocity is : $\begin{cases} v_x = \dfrac{\partial \epsilon}{\partial k_x} = 2t \sin k_x \\ v_y = \dfrac{\partial \epsilon}{\partial k_y} = 2t \sin k_y \end{cases}$. At these points of the Brillouin zone it evaluates to 0.

2. Bloch oscillations (10 points)

Consider the semiclassical dynamics of electrons in one one-dimensional lattice in the tight-binding approach (with the nearest neighbors hopping amplitude γ and one state per unit cell). Find the energy spectrum ϵ_k. Then consider the effect of a homogeneous and constant electric field E solving the Bloch's equation of motion, $\dfrac{d}{dt}k = -eE$. Show that the location of an electron oscillates. Find the period and amplitude of the oscillations. *Hint:* use that the velocity, $v \equiv \dfrac{dr}{dt}$, satisfies the relation $v = \dfrac{\partial \epsilon_k}{\partial k}$.

Solution:

The dispersion relation of 1D band is:

$$\epsilon_k = -2\gamma \cos(ka)$$

The bloch equation of motion gives $\dfrac{d}{dt}k = -eE$ .Therefore, $k = -eEt + k_0$.
Moreover we have:

$$\frac{d}{dt}r \approx \frac{\partial \epsilon_k}{\partial k},$$

Therefore the velocity is:

$$v = 2\gamma a \sin(-eEta + k_0 a)$$

and the position is

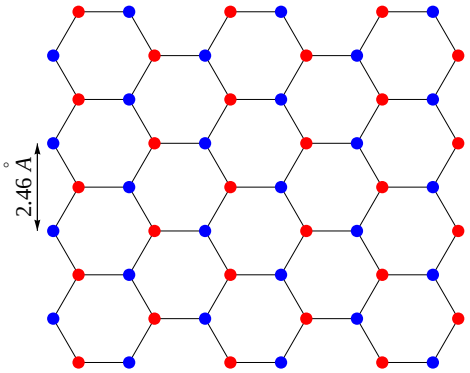
$$r = \frac{2\gamma}{eE}\cos(eEta + k_0 a) + r_0.$$

The electron oscillates with an amplitude $\frac{2\gamma}{eE}$ and a period $\frac{2\pi}{eEa}$.

Category B

3. Band structure of graphene (7 + 8 + 5 = 20 points)

Graphene is a two-dimensional material consisting of a honeycomb lattice of carbon atoms. We will study some of its fundamental electronic properties within the tight-binding approximation, where we restrict the model to nearest-neighbor hopping and a single orbital per atom with isotropic couplings. The honeycomb lattice is not a Bravais lattice. Note that each unit cell contains two atoms – let us denote them as site A and site B. These are shown in different colors in the sketch (although all atoms are carbon atoms). It turns out that all nearest neighbors of atoms at A-sites are located at B-sites, and vice versa. A lattice with this property is also called a *bipartite* lattice.

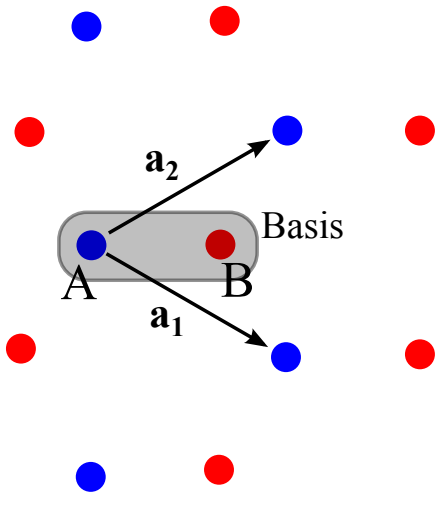


(a) Determine the tight-binding Hamiltonian of graphene. Find the Bloch states and express the Hamiltonian in reciprocal space in the basis of the Bloch states.
Hint: You will be able to write the Hamiltonian as a 2×2 *matrix.*

Solution: The tight-binding Hamiltonian is, in general,

$$\mathcal{H} = \sum_{m_1, m_2, \mathbf{R}_1, \mathbf{R}_2} t_{m_1,m_2}(\mathbf{R}_1 - \mathbf{R_2}) \, |m_1 \mathbf{R}_1\rangle \, \langle m_2 \mathbf{R_2}| \ , \qquad (*)$$

where $\mathbf{R_i}$ are Bravais lattice vectors and $m_i \in \{\mathrm{A}, \mathrm{B}\}$ internal indices specifying the atoms within the unit cell. Now we apply this on the honeycomb lattice. Let us denote the nearest-neighbor spacing a (Not the lattice constant in this case!).



With the restriction to nearest-neighbor hopping, we keep only $t_{AB}(\mathbf{0}), t_{AB}(\mathbf{R}_1), t_{AB}(\mathbf{R_2})$. The Bravais vectors of the lattice are

$$\mathbf{a_1} = \frac{\sqrt{3}}{2}\begin{pmatrix}\sqrt{3}\\-1\end{pmatrix} a \ , \quad \mathbf{a_2} = \frac{\sqrt{3}}{2}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix} a \ .$$

All distances between A and B atoms are equal, thus

$$t_{AB}(\mathbf{0}) = t_{BA}(\mathbf{0}) = t_{AB}(\mathbf{a}_1) = t_{AB}(\mathbf{a}_2) = t_{BA}(-\mathbf{a}_1) = t_{BA}(-\mathbf{a}_2) \equiv -t \ .$$

The Bloch states are given by $\psi_{\mathbf{k}} = \sum_{\mathbf{R}} e^{i\mathbf{kR}} \sum_m b_m \, |m\mathbf{R}\rangle$. Inserting them into the Schrödinger equation, $\mathcal{H}\psi_{\mathbf{k}} = E_{\mathbf{k}}\psi_{\mathbf{k}}$ we find

$$\sum_{m_1,\mathbf{R}} e^{i\mathbf{kR}} t_{m_1,m_2}(\mathbf{R}) b_{m_1} = E_{\mathbf{k}} b_{m_2} \, .$$

In our case, this can be written in matrix form,

$$h_{\mathbf{k}} \begin{pmatrix} b_A \\ b_B \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} b_A \\ b_B \end{pmatrix} \ ,$$

where

$$\Delta_{\mathbf{k}} = 1 + e^{-i\mathbf{ka_1}} + e^{-i\mathbf{ka_2}} \text{ and } h_{\mathbf{k}} = \begin{pmatrix} 0 & -t\Delta_{\mathbf{k}} \\ -t\Delta^*_{\mathbf{k}} & 0 \end{pmatrix}.$$

The coefficients b_m of the Bloch states are given by the eigenfunctions of the (first-quantized) Hamiltonian $h_{\mathbf{k}}$:

$$\begin{pmatrix} b_A \\ b_B \end{pmatrix} = \frac{1}{\sqrt{2}|\Delta_{\mathbf{k}}|} \begin{pmatrix} \sqrt{\Delta_{\mathbf{k}}} \\ \mp\sqrt{\Delta^*_{\mathbf{k}}} \end{pmatrix}.$$

(b) Now use the Hamiltonian which you found in (a) to calculate the band structure. Show that there are special points in the Brillouin zone where the band gap vanishes. Show that the spectrum is approximately linear in proximity to these points.

Solution: The eigenvalues of the Hamiltonian are

$$E_{\mathbf{k}} = \pm t\sqrt{\Delta_{\mathbf{k}}\Delta^*_{\mathbf{k}}},$$

$$\begin{aligned} |\Delta_{\mathbf{k}}|^2 &= 1 + 4\cos(3k_x a/2)\cos\Big(\sqrt{3}k_y a/2\Big) + 4\cos^2(\sqrt{3}k_y a/2) \\ &= 3 + 4\cos(3k_x a/2)\cos\Big(\sqrt{3}k_y a/2\Big) + 2\cos\Big(\sqrt{3}k_y a\Big). \end{aligned} \tag{1}$$

Gap closing occurs when

$$E_{\mathbf{k}} = 0 \quad \Rightarrow \quad \Delta_{\mathbf{k}} = 0$$

From Eq. (1), you can solve the second degree equation

$$0 = 1 + 4XY + 4Y^2$$

where $-1 \leq X = \cos(3k_x a/2) \leq 1$ and $-1 \leq Y = \cos\left(\sqrt{3}k_y a/2\right) \leq 1$. You find

$$Y_{\text{sol}} = \frac{-X \pm i\sqrt{1-X^2}}{2}$$

which is real only when $X = \pm 1$. Eventully at the end you find gap closing at the corners K and K' of the Brillouin zone:

$$\mathbf{K} = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right), \quad \mathbf{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right).$$

The other corners are equivalent to either K or K' due to symmetry (i.e., identical up to a reciprocal lattice vector).
The expansion at the $\mathbf{K}$ point yields

$$\mathbf{k} = \mathbf{K} + \mathbf{q},$$

$$\Delta_{\mathbf{k}} \approx -ia\frac{3}{2}e^{-iK_x a}(q_x + iq_y).$$

The constant phase factor $-ie^{-iK_x a}$ does not matter. Therefore, the low-energy Hamiltonian close to K reads

$$\mathcal{H} = v\begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix}, \quad v = \frac{3}{2}ta.$$

The Hamiltonian at $\mathbf{K}'$ is derived analogously. Owed to its linearity in momentum, the low-energy Hamiltonian of graphene is often referred to as a two-dimensional massless Dirac Hamiltonian: it is mathematically equivalent to the Hamiltonian of a relativistic fermion without a mass (recall that, in 2D, the Dirac algebra reduces to Pauli matrices). However, in graphene and other *Dirac materials* the speed of light is replaced by the Fermi velocity $v_F \ll c$. It is remarkable that quasi-relativistic physics emerges in an entirely non-relativistic range of speed!

(c) Now include next-nearest neighbors in the model and recalculate the band structure. Expand the eigenenergies to second order for momenta close to one of the gap-closing points found in (b).

Solution: We start again from Eq. (∗), but include next-nearest neighbors (A-A and B-B hopping terms). The distances to all next-nearest neighbors are equal, but differ from the nearest-neighbor distance, thus:

$$\begin{aligned} &t_{AB}(\mathbf{0}) = t_{AB}(\mathbf{0}) = t_{AB}(\mathbf{a}_1) = t_{AB}(\mathbf{a}_2) = t_{BA}(-\mathbf{a}_1) = t_{BA}(-\mathbf{a}_2) \equiv -t\ , \\ &t_{AA}(\pm\mathbf{a}_1) = t_{AA}(\pm\mathbf{a}_2) = t_{AA}(\pm[\mathbf{a}_1 - \mathbf{a}_2]) \\ =&t_{BB}(\pm[\mathbf{a}_1 - \mathbf{a}_2]) = t_{BB}(\pm\mathbf{a}_1) = t_{BB}(\pm\mathbf{a}_2) \equiv -t'\ . \end{aligned}$$

We arrive at the Hamiltonian 2×2 matrix

$$h_{\mathbf{k}} = -t\begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & 0 \end{pmatrix} - 2t'\Delta'_{\mathbf{k}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\Delta'_{\mathbf{k}} = \cos(\mathbf{k}\cdot\mathbf{a}_1) + \cos(\mathbf{k}\cdot\mathbf{a}_2) + \cos[\mathbf{k}\cdot(\mathbf{a}_1 - \mathbf{a_2})]$$

with eigenenergies

$$
\begin{aligned}
E_{\mathbf{k}} &= \pm t\sqrt{3+f_{\mathbf{k}}} - t' f_{\mathbf{k}}\,, \\
f_{\mathbf{k}} &= 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_x a\right),
\end{aligned}
$$

The expansion at the corners ($\mathbf{q} = \mathbf{k} - \mathbf{K}$) leads to:

$$
E_{\mathbf{q}}^{\pm} \simeq 3t' \pm v_F\,|\mathbf{q}| - \left[\frac{9t'a^2}{4} \pm \frac{3ta^2}{8}\sin(3\theta_{\mathbf{q}})\right]|\mathbf{q}|^2\,,
$$

where

$$
\theta_{\mathbf{q}} = \arctan\left(\frac{q_x}{q_y}\right).
$$