Department of physics, NTNU
TFY4340 Mesoscopic Physics
Spring 2010

Solution to Exercise 3

Question 1

We have the band structure

$$E(k_x, k_y) = -8\gamma + 4\gamma \cos\frac{k_x a}{2}\left(\cos\frac{k_x a}{2} + \cos\frac{\sqrt{3}k_y a}{2}\right)$$

for the 2D triangular lattice in the single–band nn TB model. We expand E around the Γ–point to second order in $\boldsymbol{k}$, using $\cos\alpha \simeq 1 - \alpha^2/2$ for $\alpha \ll 1$:

$$\begin{aligned}
E &\simeq -8\gamma + 4\gamma\left(1 - \frac{k_x^2 a^2}{8}\right)\left(1 - \frac{k_x^2 a^2}{8} + 1 - \frac{3k_y^2 a^2}{8}\right) \\
&\simeq -8\gamma + 4\gamma\left(2 - \frac{3k_x^2 a^2}{8} - \frac{3k_y^2 a^2}{8}\right) \\
&= -\frac{3}{2}\gamma a^2\left(k_x^2 + k_y^2\right) \\
&= -\frac{3}{2}\gamma a^2 k^2
\end{aligned}$$

Hence, the inverse effective mass tensor is diagonal and isotropic, i.e., with both diagonal elements equal to

$$1/m^* = \frac{3|\gamma|a^2}{\hbar^2}$$

since we had assumed $\gamma < 0$. Anisotropy would require different coefficients in front of k_x^2 and k_y^2. A non–diagonal inverse effective mass tensor would require a term in E proportional with $k_x k_y$.

Question 2

a) We take the hints given in the text and expand E to lowest order in deviations from $\boldsymbol{k}_K$:

$$\begin{aligned}
\cos\frac{3k_x a}{2} &= \cos\left(\pi + \frac{3}{2}\varepsilon_x\right) = -\cos\frac{3}{2}\varepsilon_x \\
&\simeq -1 + \frac{9}{8}\varepsilon_x^2 \\
\cos\frac{\sqrt{3}k_y a}{2} &= \cos\left(\frac{\pi}{3} + \frac{\sqrt{3}}{2}\varepsilon_y\right)
\end{aligned}$$

$$
\begin{aligned}
&= \cos\frac{\pi}{3}\cos\frac{\sqrt{3}}{2}\varepsilon_y - \sin\frac{\pi}{3}\sin\frac{\sqrt{3}}{2}\varepsilon_y \\
&\simeq \frac{1}{2}\cdot\left(1-\frac{3}{8}\varepsilon_y^2\right) - \frac{\sqrt{3}}{2}\cdot\frac{\sqrt{3}}{2}\varepsilon_y \\
&= \frac{1}{2} - \frac{3}{4}\varepsilon_y - \frac{3}{16}\varepsilon_y^2
\end{aligned}
$$

The expression under the square root becomes, to second order in ε_x and ε_y,

$$
\begin{aligned}
& 1+4\cos\frac{3k_x a}{2}\cos\frac{\sqrt{3}k_y a}{2} + 4\cos^2\frac{\sqrt{3}k_y a}{2} \\
\simeq\ & 1+4\left(-1+\frac{9}{8}\varepsilon_x^2\right)\left(\frac{1}{2}-\frac{3}{4}\varepsilon_y-\frac{3}{16}\varepsilon_y^2\right)+4\left(\frac{1}{2}-\frac{3}{4}\varepsilon_y-\frac{3}{16}\varepsilon_y^2\right)^2 \\
\simeq\ & \frac{9}{4}\left(\varepsilon_x^2+\varepsilon_y^2\right) \\
=\ & \frac{9}{4}a^2(\Delta\boldsymbol{k})^2
\end{aligned}
$$

Here, $\Delta\boldsymbol{k} = \boldsymbol{k} - \boldsymbol{k}_K = (\varepsilon_x\hat{x} + \varepsilon_y\hat{y})/a$. Hence,

$$
E^{\pm} \simeq \pm\frac{3}{2}|\gamma|a\Delta k,
$$

and the constant is $C = 3|\gamma|a/2$.

b) As in Exercise 1, Question 3, we have a constant density of states in 2D,

$$
D_2(\boldsymbol{k}) = \frac{A}{2\pi^2},
$$

which means that the number of states with $|\boldsymbol{k} - \boldsymbol{k}_K|$ less than a given Δk is

$$
N_2(\Delta k) = \pi(\Delta k)^2 \cdot D_2 = \frac{A(\Delta k)^2}{2\pi}.
$$

With the linear dispersion found in *a*), we have

$$
N_2(E) = \frac{A}{2\pi}\left(\frac{E}{C}\right)^2,
$$

and therefore

$$
D_2(E) = \frac{dN_2}{dE} = \frac{A}{\pi}\frac{E}{C^2} = \frac{4AE}{9\pi\gamma^2 a^2}.
$$

c) Photons are massless particles, so the energy–momentum relation for photons is simply $E = pc$. For electrons in a crystal, we know that the wavenumber, measured relative to the energy band minimum, and multiplied by $\hbar$, is the crystal momentum. More precisely,

$$p = \hbar \Delta k,$$

so we may write for the graphene electrons at the Fermi level, near the conduction band minimum,

$$E = \frac{3}{2}|\gamma| a \Delta k = v_F p,$$

with Fermi velocity

$$v_F = \frac{3|\gamma|a}{2\hbar}.$$

The nearest neighbour distance in graphene is $a \simeq 1.4$ Å, so if $\gamma \sim 3$ eV, the velocity of the electrons is

$$v_F \sim \frac{3 \cdot 3 \cdot 1.6 \cdot 10^{-19} \cdot 1.4 \cdot 10^{-10}}{2 \cdot 1.05 \cdot 10^{-34}} \simeq 10^6 \text{ m/s}.$$