PHZ6426: Fall 2013
MIDTERM: Solutions

Please help your instructor by doing your work neatly. Every (algebraic) final result must be supplemented by a check of units. Without such a check, no more than 75% of the credit will be given even for an otherwise correct solution.

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The energy spectrum of charge carriers in graphene is described by the Dirac-like dispersion relation (see Fig. 1):
\[ \varepsilon_k = \pm \hbar v_0 |k|. \]

Find the \( T \) dependence of the electronic part of the specific heat for several positions of the Fermi energy with respect to the “Dirac point” (\( \varepsilon_k = 0 \)):

a) \( \varepsilon_F = 0; \)
b) \( \varepsilon_F > 0; \)
c) \( \varepsilon_F < 0. \)

For cases b) and c), consider only the low-temperature limit: \( k_B T \ll |\varepsilon_F| \). You may need to use the fact that
\[ \int_0^{\infty} dx \frac{x^2}{e^x + 1} = \frac{3}{2} \zeta(3) \approx 1.803, \]
where \( \zeta(z) \) is the Riemann zeta-function.

**Solution** The grand-canonical free energy of an electron gas with \( \varepsilon_F = 0 \) is given by
\[ F = -2k_B T \sum_{j = \pm} \int \frac{d^2 k}{(2\pi)^2} \ln \left( 1 + e^{-\varepsilon_{j,k}/k_B T} \right), \]
where \( j = (+/-) \) corresponds to the conduction (valence) band. The density of states in graphene is found from the Pauli principle:
\[ g(\varepsilon) = \frac{1}{\pi} \frac{k(\varepsilon)}{|d\varepsilon/dk|} = \frac{1}{\pi \hbar^2 v_0^2} |\varepsilon|. \]

Apparently, \( g \) is an even function of energy. Switching from an integration over \( k \) to that over \( \varepsilon \), and taking into account both the conduction and valence bands, we obtain
\[ F = -k_B T \left[ \int_0^{\infty} d\varepsilon g(\varepsilon) \ln \left( 1 + e^{-\varepsilon/k_B T} \right) + \int_{-\infty}^0 d\varepsilon g(\varepsilon) \ln \left( 1 + e^{\varepsilon/k_B T} \right) \right] \]
\[ = -k_B T \int_0^{\infty} d\varepsilon g(\varepsilon) \ln \left( 1 + e^{-\varepsilon/k_B T} \right) - \frac{2}{\pi \hbar^2 v_0^2} k_B T \int_0^{\infty} d\varepsilon \ln \left( 1 + e^{\varepsilon/k_B T} \right) \]

Integration by parts gives
\[ F = -\frac{1}{\pi \hbar^2 v_0^2} k_B T \int_0^{\infty} d\varepsilon \frac{\varepsilon^2}{e^{\varepsilon/k_B T} + 1} = -\frac{1}{\pi \hbar^2 v_0^2} \frac{(k_B T)^3}{v_0^2} \int_0^{\infty} dx \frac{x^2}{e^x + 1}, \]
where \( \zeta(z) \) is the Riemann function.

\[ C_V = -T \frac{\partial^2 F}{\partial T^2} = \frac{9}{\pi \hbar^2 v_0^2} \zeta(3) \frac{k_B^2 T^2}{v_0^2}. \]

For cases b) and c), there is no need to re-do the calculation from the scratch. It suffices to recall that \( C_V \) for a Fermi gas with arbitrary dispersion and at \( k_B T \ll |\varepsilon_F| \) is given by
\[ C_V = \frac{\pi^2}{3} g(\varepsilon_F) k_B^2 T = \frac{\pi}{3 \hbar^2 v_0^2} |\varepsilon_F| k_B^2 T. \]
P2  a) Identify the primitive unit cell of a two-dimensional triangular lattice. Find the basis vectors.
    b) Construct the basis vectors of the reciprocal unit cell.

**Solution**

See Fig. 2. Denoting the side of an equilateral triangle as \( a \), the basis vectors can be chosen as

\[
\mathbf{a}_1 = a \hat{x}; \quad \mathbf{a}_2 = \frac{a}{2} \hat{x} + \frac{\sqrt{3}}{2} a \hat{y}.
\]

The reciprocal lattice vectors are defined by the condition

\[
\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}
\]

or, in components,

\[
\begin{align*}
a_{1x}b_{1x} + a_{1y}b_{1y} &= 2\pi \\
a_{2x}b_{2x} + a_{2y}b_{2y} &= 2\pi \\
a_{1x}b_{2x} + a_{1y}b_{2y} &= 0 \\
a_{2x}b_{1x} + a_{2y}b_{1y} &= 0.
\end{align*}
\]

We then obtain \( b_{2x} = 0, b_{2y} = 2\pi/a_{2y} = 4\pi/a\sqrt{3}, b_{1x} = 2\pi/a_{1x} = 2\pi/a, b_{1y} = -\frac{a_{2x}}{a_{2y}}b_{1x} = -2\pi/a\sqrt{3} \)

or

\[
\begin{align*}
\mathbf{b}_1 &= \frac{2\pi}{a} \hat{x} - \frac{2\pi}{a\sqrt{3}} \hat{y} \\
\mathbf{b}_2 &= \frac{4\pi}{a\sqrt{3}} \hat{y}.
\end{align*}
\]

The reciprocal primitive unit cell is a parallelogram obtained by rotating the unit cell in the coordinate space by \( \pi/2 \) and by rescaling the sides by a factor of \( 2\pi/a \).
FIG. 2: Primitive unit cell (shaded) and basis vectors.