In this problem we are given a 2D surface with electron energies

\[ \epsilon = \epsilon_0 \pm v_F |p| \]

Given fixed \( p \), there are two energies \( \epsilon_\pm \). At each energy there is a four-fold degeneracy, two from spin-1/2 and two from ‘the valley index’. \(^1\)

The figure shows the allowed energies in a graphene lattice. Our energy relation comes from approximating the surface to be a cone near lattice points, in k-space. This is called the Dirac cone in literature. It has slope \( v_F \), dimensions \([p/m]\), and is called the Fermi velocity.

We are asked to find the specific heat as \( T \to 0 \) for (a) electrons with \( p_F > 0 \), (b) electrons at \( p_F = 0 \), and (c) phonons (additional information given below).

(a) To find the specific heat \( c_V = dU/dT \), we need to write down an expression for \( U = \langle \epsilon \rangle \), which is derived from fermi-dirac statistics. Let’s start with the density of states

\[ \rho(\epsilon)d\epsilon = g \frac{d^2k}{(2\pi)^2} = \frac{gkd\epsilon}{2\pi} \]

The degeneracy \( g = 4 \) is given, and

\[ k = \frac{|\epsilon - \epsilon_0|}{\hbar v_F} > 0 \]

Therefore the density of states is

\[ \rho(\epsilon) = \frac{2|\epsilon - \epsilon_0|}{\pi\hbar^2 v_F^2} \]

We can use this to write

\[ U = \int_0^\infty f_{FD}(\epsilon)\rho(\epsilon)d\epsilon = \frac{2}{\pi\hbar^2 v_F^2} \int_0^\infty \frac{\epsilon|\epsilon - \epsilon_0|d\epsilon}{e^{\beta(\epsilon - \mu)} + 1} \]

At low temperature \( \beta \to \infty \) and \( \mu = \epsilon_F \), which necessarily takes the positive energy band

\[ \epsilon_F = \epsilon_0 + v_F p_F \]

\(^1\)This arises from the lattice structure. 2D graphene atoms arrange themselves in a hexagonal honeycomb. The ‘smallest site’ has two atoms (a line segment), whether the electron occupies atom A or atom B produces the same energy. This gives a factor of 2 to degeneracy. You can read more about graphene here.
We approach this integral using the Sommerfield expansion

\[ U = \int_{-\infty}^{\mu} \rho(\epsilon) e \, d\epsilon + \frac{\pi^2}{6}(kT)^2 \frac{d}{d\epsilon} [\rho(\epsilon)|_{\mu} + O(T^4)] \]

The first term is an integral that blows up at \( \epsilon \to -\infty \). We can ignore this for two reasons: (1) this term is constant with respect to \( T \), and therefore disappears from the specific heat (2) the singularity for large \( |\epsilon| \) is unphysical. It appears only as a relic from the Dirac cone approximation, but energy and \( \rho(\epsilon) \) are clearly bounded everywhere in the lattice (see figure).

So we can compute the derivative

\[ \frac{d}{d\epsilon} [\rho(\epsilon)|_{\mu}] = \frac{2(\epsilon_0 + 2v_F p_F)}{\pi \hbar^2 v_F^2} \]

where we have taken \( \mu = \epsilon_0 + v_F p_F \). Now

\[ U = U_0 + \frac{\pi(\epsilon_0 + 2v_F p_F)}{3h^2 v_F^2} (kT)^2 \]

therefore the low temperature heat capacity is

\[ c_V = \frac{\partial U}{\partial T} = \frac{2\pi k^2 (\epsilon_0 + 2v_F p_F)}{3h^2 v_F^2} T \]

Since the zero-point energy is arbitrary, we could set \( \epsilon_0 = 0 \) and have

\[ c_V = \frac{4\pi k^2 p_F}{3h^2 v_F} T \]

here \( v_F \) is the Fermi velocity and \( p_F > 0 \) is the Fermi momentum.

(b) When \( p_F = 0 \) we cannot use the Sommerfield expansion, because \( \frac{d}{d\epsilon}(\rho e) \) is undefined at the cusp of the cone. Instead we have the special case \( \mu = \epsilon_F = \epsilon_0 \). This means \( \mu \) is independent of \( T \), and we can take \( d/dT \) inside the integral. \(^3\) As before

\[ U = \frac{2}{\pi \hbar^2 v_F^2} \int_{0}^{\infty} \frac{\epsilon|\epsilon - \epsilon_0| \, d\epsilon}{e^{\beta(\epsilon - \mu)} + 1} \]

setting \( \mu = \epsilon_0 \) and collecting constants \( A = 2/\pi \hbar^2 v_F^2 \)

\[ U = A \int_{-\epsilon_0}^{\infty} \frac{(x + \epsilon_0)}{e^{\beta x} + 1} \, dx \]

Now

\[ \frac{dU}{dT} = Ak^2 \int_{-\epsilon_0}^{\infty} \frac{e^{\beta x}}{(e^{\beta x} + 1)^2} x(x + \epsilon_0) \, dx \]

\(^2\)derived below

\(^3\)Here we only need to take derivatives of \( \beta \). In part (a), there was have been an additional \( \mu(T) \) dependence. That’s why we had to use the Sommerfield expansion to do the integral first, before taking \( d/dT \).
Recognize that \( e^y/(e^y+1)^2 \) is even. \(^4\) In the low temperature limit \( \beta \to \infty \) we can stretch the integration bound to \( \int_{-\infty}^{\infty} d\epsilon \). Now the second term

\[
I_2 = Ak\beta^2 \int_{-\infty}^{\infty} \frac{e^{\beta x}}{(e^{\beta x} + 1)^2} x |x| dx = 0
\]

because \( x |x| \) is odd. So we are left with just the first term

\[
I_1 = Ak\beta^2 \int_{-\infty}^{\infty} \frac{e^{\beta x}}{(e^{\beta x} + 1)^2} x^2 |x| dx
\]

\[
= 2Ak\beta^2 \int_{0}^{\infty} \frac{e^{\beta x}}{(e^{\beta x} + 1)^2} x^3 dx
\]

\[
= 2A \frac{\partial}{\partial T} \int_{0}^{\infty} \frac{x^2}{e^{\beta x} + 1} dx
\]

\[
= 2A \frac{\partial}{\partial T} \left( \frac{1}{\beta^3} \int_{0}^{\infty} \frac{y^2 dy}{e^y + 1} \right)
\]

Define a family of integrals

\[
C_m^\pm = \int_{0}^{\infty} \frac{y^m}{e^y \pm 1} dy
\]

Although \( y = \beta(\epsilon - \epsilon_0) \), the \( \beta \) dependence vanishes in this dimensionless integral. Therefore

\[
I_1 = 2AC_2^+ \frac{\partial}{\partial T} (kT)^3 = 6AC_2^+ k^3 T^2
\]

recalling \( c_V = dU/dT = I_1 + I_2 \) one finds

\[
c_V = \left( \frac{12k^3 C_2^+}{\pi h^2 v_F^2} \right) T^2
\]

In summary \( c_V \propto T \) for \( p_F > 0 \), but \( c_V \propto T^2 \) when \( p_F = 0 \). These are the electronic contributions to specific heat of graphene at low temperatures.

\(^4\) \[
\frac{e^y}{(e^y+1)^2} = \frac{1}{(e^y+1)(e^{-y}+1)}
\]
Phonons have 2D longitudinal and transverse waves
\[ \omega = v_L q \]
\[ \omega = v_T q \]
where \( q = |\vec{q}| \) is the wavenumber magnitude. There is also a low frequency mode with displacements normal to the sheet
\[ \omega = K q^2 \]
Let us compute the density of states independently. For the linear modes \( E = \hbar \omega = \hbar v q \). Therefore
\[ \frac{qdq}{2\pi} = \frac{\hbar^2 v^2}{2\pi} EdE \]
and
\[ \rho_1(\epsilon) = \frac{\hbar^2 v^2}{2\pi} \epsilon \]
For the quadratic modes \( E = \hbar \omega = \hbar K q^2 \). Therefore
\[ \frac{qdq}{2\pi} = \frac{dE}{4\pi\hbar K} \]
and
\[ \rho_2(\epsilon) = \frac{1}{4\pi\hbar K} \]
the density of states is constant! \(^5\) Phonons are bosons. We can compute the Bose-Einstein statistics
\[ U = \int_0^\infty \frac{1}{e^{\beta(\epsilon - \mu)} - 1} \rho(\epsilon) \epsilon d\epsilon \]
We need \( \mu < 0 \) for convergence. But at low temperatures we can put \( \mu \) arbitrarily close to 0. \(^6\) Then
\[ U_2 = \int_0^\infty \frac{\epsilon}{e^{\beta \epsilon} - 1} \frac{d\epsilon}{4\pi\hbar K} = \frac{C_1^-}{4\pi\hbar K} \frac{1}{\beta^2} \]
and
\[ U_1 = \frac{\hbar^2 v^2}{2\pi} \int_0^\infty \frac{e^{\beta \epsilon} - 1}{e^{\beta \epsilon} - 1} = \frac{\hbar^2 v^2 C_2^+}{2\pi} \frac{1}{\beta^3} \]
At low temperatures \( \beta \to \infty \) and the quadratic modes dominate. Therefore the heat capacity \( dU/dT \) is to leading order
\[ c_V = \left( \frac{k^2 C_1^-}{2\pi\hbar K} \right) T \]

\(^5\)this must be a low frequency approximation
\(^6\)I have no proof for this
1 note

Given a Fermi-Dirac distribution, the Sommerfeld expansion solves integrals

$$I = \int_0^\infty f_{FD}(\epsilon) \phi(\epsilon) d\epsilon$$

where $\phi$ is any smooth function of $\epsilon$ (in our problem $\phi = \rho_\epsilon$). Let us recall the Fermi-Dirac distribution

$$f_{FD} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

looks like a step function, and its derivative $F = df_{FD}/d\epsilon$ behaves like a $\delta$-function centered at $\epsilon = \mu$ with width $1/\beta = kT$. To leverage this we take an integration by parts

$$I = [f(\epsilon)\psi(\epsilon)]_0^\infty - \int_0^\infty F(\epsilon)\psi(\epsilon) d\epsilon = - \int_{-\infty}^\infty F(\epsilon)\psi(\epsilon) d\epsilon$$

where

$$\psi(\epsilon) = \int_0^\epsilon \phi(\epsilon') d\epsilon'$$

is defined such that $d\psi/d\epsilon = \phi(\epsilon)$. Evidently $\psi(0) = 0$ and $F(\pm \infty) = 0$. This allows us to drop the constant and stretch the integration bound, which will be useful later on.

Now letting $x = \epsilon - \mu$ we compute

$$F = \frac{-\beta e^{\beta x}}{(e^{\beta x} + 1)^2} = \frac{-\beta}{(e^{\beta x} + 1)(e^{-\beta x} + 1)}$$

and Taylor expand about $\mu$

$$\psi = \sum_{m=0}^{\infty} \frac{1}{m!} \left. \frac{d^m \psi}{de^m} \right|_{\mu} (\epsilon - \mu)^m$$

Since $F$ is even, all odd terms in $\psi$ drop from $\int_{-\infty}^\infty d\epsilon$. Now

$$I = - \int_{-\infty}^\infty F(\epsilon)\psi(\epsilon) d\epsilon = \int_0^\infty \sum_{m=0}^{\infty} \frac{\psi^{(m)}(0)}{m!} \frac{\beta x^m}{(e^{\beta x} + 1)(e^{-\beta x} + 1)} dx$$

$$= \sum_{m=0}^{\infty} \frac{\psi^{(m)}(0)}{m!\beta^m} \int_{-\infty}^\infty \frac{y^m dy}{(e^y + 1)(e^{-y} + 1)}$$

$$= \sum_{m=0}^{\infty} \frac{\psi^{(m)}(0)}{m!\beta^m} I_m$$

Here we access known dimensionless integrals

$$I_m = \int_{-\infty}^\infty \frac{y^m dy}{(e^y + 1)(e^{-y} + 1)}$$

where $I_0 = 1$, $I_2 = \pi^2/3$, and $I_m = 0$ if $m$ is odd. Therefore

$$I = \psi(\mu)I_0 + \frac{1}{2!\beta^2} \psi''(\mu)I_2 + \frac{1}{4!\beta^4} \psi^{(4)}(\mu)I_4 + \ldots$$

$$= \int_0^\mu \phi(\epsilon) d\epsilon + \frac{\pi^2}{6} \phi'(\mu)(kT)^2 + O(T^4)$$

This is the Sommerfeld expansion. \footnote{Big thanks to Yichen Fu and Fang Xie for their insights on this problem.}