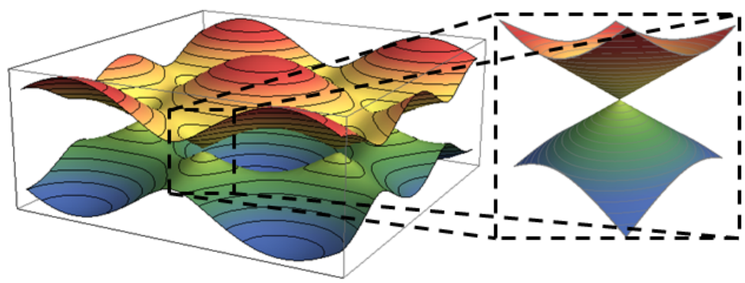
In this problem we are given a 2D surface with electron energies

$$\epsilon = \epsilon_0 \pm v_F |p|$$

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

$$\rho(\epsilon) d\epsilon = g \frac{d^2 k}{(2\pi)^2} = \frac{g k dk}{2\pi}$$

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

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

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 [2]

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

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 every where in the lattice (see figure).

So we can compute the derivative

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

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

$$U = U_0 + \frac{\pi(\epsilon_0 + 2v_F p_F)}{3\hbar^2 v_F^2}(kT)^2$$

therefore the low temperature heat capacity is

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

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

$$c_V = \frac{4\pi k^2 p_F}{3\hbar^2 v_F} T$$

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 $\frac{d}{d\epsilon}(\rho\epsilon)$ is undefined at the cusp of the cone. Instead we have the special case $\mu = \epsilon_F = \epsilon_0$. This means μ 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 $A = 2/\pi\hbar^2 v_F^2$

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

Now

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

[2] derived below

[3] Here we only need to take derivatives of β. 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

$$\begin{aligned} I_1 &= Ak\beta^2 \int_{-\infty}^{\infty} \frac{e^{\beta x}}{(e^{\beta x}+1)^2} x^2|x|dx \\ &= 2Ak\beta^2 \int_0^{\infty} \frac{e^{\beta x}}{(e^{\beta x}+1)^2} x^3 dx \\ &= 2A\frac{\partial}{\partial T} \int_0^{\infty} \frac{x^2}{e^{\beta x}+1} dx \\ &= 2A\frac{\partial}{\partial T} \left(\frac{1}{\beta^3} \int_0^{\infty} \frac{y^2 dy}{e^y+1} \right) \end{aligned}$$

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 β 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

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

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]
$$\frac{e^y}{(e^y+1)^2} = \frac{1}{(e^y+1)(e^{-y}+1)}$$

(c) 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 an also a low frequency mode with displacements normal to the sheet

$$\omega = Kq^2$$

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 μ 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

$$U_1 = \frac{\hbar^2 v^2}{2\pi}\int_0^\infty \frac{\epsilon^2 d\epsilon}{e^{\beta\epsilon} - 1} = \frac{\hbar^2 v^2}{2\pi}\frac{C_2^+}{\beta^3}$$

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 Sommerfield expansion solves integrals

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

where ϕ is any smooth function of ϵ (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 δ-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 μ

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

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

$$\begin{aligned} I = -\int_{-\infty}^\infty F(\epsilon)\psi(\epsilon)d\epsilon &= \int_{-\infty}^\infty \sum_{m=0}^\infty \frac{\psi^{(m)}(0)}{m!} \frac{\beta x^m}{(e^{\beta x}+1)(e^{-\beta x}+1)}dx \\ &= \sum_{m=0}^\infty \frac{\psi^{(m)}(0)}{m!\beta^m} \int_{-\infty}^\infty \frac{y^m dy}{(e^y+1)(e^{-y}+1)} \\ &= \sum_{m=0}^\infty \frac{\psi^{(m)}(0)}{m!\beta^m} I_m \end{aligned}$$

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

$$\begin{aligned} I &= \psi(\mu)I_0 + \frac{1}{2\beta^2}\psi''(\mu)I_2 + \frac{1}{4!\beta^4}\psi^{(4)}(\mu)I_4 + \dots \\ &= \int_0^\mu \phi(\epsilon)d\epsilon + \frac{\pi^2}{6}\phi'(\mu)(kT)^2 + O(T^4) \end{aligned}$$

This is the Sommerfield expansion. [7]

[7] Big thanks to Yichen Fu and Fang Xie for their insights on this problem.