Graphene

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PROBLEM

Graphene is a two-dimensional sheet of carbon atoms. Both electronic and phonon degrees of freedom contribute to the low-temperature specific heat per unit area. The electron states resembe the states of the massless Dirac equation, with energies

$$\epsilon_{\pm} = \epsilon_0 \pm v_f p \,, \quad p \equiv |\vec{p}|$$

where $\vec{p} = (p_x, p_y)$ is the analog of the momentum carried by a Dirac electron. (There are two energy bands, $\epsilon_+(\vec{p}) \geq \epsilon_0$ and $\epsilon_-(\vec{p}) \leq \epsilon_0$ which become degenerate at $\vec{p} = 0$). These states have a fourfold degeneracy (the usual two-fold spin degeneracy is doubled by an additional "valley" index).

a) If the Fermi energy E_F is $\epsilon_0 + v_F p_F$, with $p_F > 0$, what is the leading behavior of the electronic specific heat as $T \to 0$?

b) What is the low-temperature electronic specific heat when $p_F = 0$?

(The next calculation is independent of parts a), b) above). Recently, freely suspended graphene sheets have been studied. These have an unusual phonon spectrum: in addition to longitudinal and transverse sound waves with frequencies $\omega = v_L q, v_T q$ (where q is the magnitude of the wavenumber $\vec{q}$), there is an extra low-frequency mode $\omega = Kq^2$ where atomic displacements are normal to the sheet.

c) Obtain the leading behavior of the phonon contribution to be specific heat as $T \to 0$.

You may express your answers in terms of the numerical constants

$$C_n^{\pm} = \int_0^{\infty} dx \frac{x^n}{e^x \pm 1} \,, \quad n > 0 \,.$$

SOLUTION TO PART A

First of all we use the defination $\int d^2k/(2\pi)^2 = \int \rho(\epsilon) d\epsilon$ to derive the density of state of graphene. The result is

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

Then the total energy (per area) of the graphene is given by

$$U = \int_{-\infty}^{\infty} \frac{1}{e^{\beta(\epsilon-\mu)+1}} \rho(\epsilon) \epsilon d\epsilon$$

Now we can use the Sommerfeld's expansion for Fermi statistics:

$$U = \int_{-\infty}^{\mu} \rho(\epsilon)\epsilon d\epsilon + \frac{\pi^2}{6}(k_B^2 T^2)\frac{d}{d\epsilon}\left(\rho(\epsilon)\epsilon\right)\Big|_{\epsilon=\mu} + \mathcal{O}\left(T^4\right)$$

Notice that the first term is infinity but it doesn't depend on temperature, so it has no contribution to the heat capacity. For low temperature we have $\mu = \epsilon_0 + v_F p_F$, then we get

$$U = U_0 + \frac{2\pi p_F}{3\hbar^2}(k_B T)^2$$

then we get the heat capacity at low temperature is

$$c_V = \frac{\partial U}{\partial T} = \frac{4\pi^2 p_F^2 k_B^2}{3\hbar^2} T\,.$$

SOLUTION TO PART B

When $p_F = 0$, we cannot use the Sommerfeld's expansion. But an important fact for us is that the chemical potential μ is not changing when the temperature is changing. The particle number is given by the following integral

$$N = \int_{-\infty}^{\infty} \frac{1}{e^{\beta\epsilon}+1}\frac{2|\epsilon|}{\pi v_F^2 \hbar^2} d\epsilon$$

We then take the derivative of T, and it turns out that the integrand of $\partial N/\partial T$ is an odd function, thus the integral value is zero. That means the chemical potential is not changing and we can directly take the derivative of the internal energy and get the heat capacity. So we first write down the internal energy as an integral

$$U = \int_{-\infty}^{\infty} \frac{1}{e^{\beta\epsilon}+1}\frac{2|\epsilon|}{\pi v_F^2 \hbar^2}\epsilon d\epsilon$$

Then take the derivative of temperature T:

$$\begin{aligned}
c_V = \frac{\partial U}{\partial T} &= \int_{-\infty}^{\infty} \frac{e^{\beta\epsilon}}{(e^{\beta\epsilon}+1)^2}\frac{\epsilon^2}{k_B T^2}\frac{2|\epsilon|}{\pi v_F^2 \hbar^2} d\epsilon \\
&= 2\int_{0}^{\infty} \frac{e^{\beta\epsilon}}{(e^{\beta\epsilon}+1)^2}\frac{\epsilon^2}{k_B T^2}\frac{2|\epsilon|}{\pi v_F^2 \hbar^2} d\epsilon \\
&= \frac{4}{\pi v_F^2 \hbar^2}\frac{\partial}{\partial T}\left(\int_0^{\infty} \frac{\epsilon^2}{e^{\beta\epsilon}+1} d\epsilon\right) \\
&= \frac{4}{\pi v_F^2 \hbar^2}\frac{\partial}{\partial T}(k_B T)^3 \int_0^{\infty} \frac{x^2}{e^x+1} dx \\
&= \frac{12 k_B^3 T^2}{\pi v_F^2 \hbar^2} C_2^+
\end{aligned}$$

SOLUTION TO PART C

The leading order contribution to the phonon heat capacity comes from the quadratic mode. So the corresponding internal energy is

$$U = \int_0^{\infty} \frac{\epsilon}{e^{\beta\epsilon}-1}\frac{d\epsilon}{4\pi\hbar K} = \frac{(k_B T)^2}{4\pi\hbar K} C_1^-$$

Then obviously the heat capacity is

$$c_V = \frac{\partial U}{\partial T} = \frac{k_B^2 T}{2\pi\hbar K} C_1^- \, .$$