# HW 12: Physics 545

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## 1a

FIGURE ATTACHED

The density of states $D(\epsilon)$ for this 2D dispersion of graphene is:

$$D(\epsilon) = \sum_{\mathbf{k}s} \delta(\epsilon - \epsilon_{\mathbf{k}s}) \tag{1}$$

$$= 2\pi V/(2\pi\hbar)^2 \int dk \quad k(\delta(\epsilon - v_f k) + \delta(\epsilon + v_f k)) \tag{2}$$

$$= D_0|\epsilon| \tag{3}$$

with $D_0 = \frac{V}{2\pi\hbar^2 v_f^2}$, and we note that it is independent of spin $s$

Also, it's kind of "gapped" in that there are no states at zero energy.

## 1b

At zero temperature, with $\mu(0) = 0$, the contribution to number of electrons is only from $s = -1$ because the Fermi distribution function $f_{\mathbf{k}1} = 0$ and $f_{\mathbf{k}-1} = 1$

$$N_0 = D_0 \int_0^\infty d\epsilon \quad \epsilon \tag{4}$$

The above is divergent, but we can still compare with the electron number for finite temperature:

$$
\begin{aligned}
N(T) &= \sum_{\mathbf{k}s} (e^{\beta(\epsilon_{\mathbf{k}s}-\mu)}+1)^{-1} && (5)\\
&= D_0 \int_{-\infty}^{\infty} d\epsilon \quad |\epsilon| (e^{\beta(\epsilon-\mu)}+1)^{-1} && (6)\\
&= D_0 \int_{0}^{\infty} d\epsilon \quad \epsilon \Big[ 1 + (e^{\beta(\epsilon-\mu)}+1)^{-1} - (e^{\beta(\epsilon+\mu)}+1)^{-1} \Big] && (7)\\
&= N_0 + D_0 \int_{0}^{\infty} d\epsilon \quad \epsilon \Big[ (e^{\beta(\epsilon-\mu)}+1)^{-1} - (e^{\beta(\epsilon+\mu)}+1)^{-1} \Big] && (8)\\
&= N_0 + D_0 \Big[ \int_{-\mu}^{\mu} dx \quad \frac{x+\mu}{e^{\beta x}+1} + 2\mu \int_{\mu}^{\infty} dx \quad \frac{1}{e^{\beta x}+1} \Big] && (9)
\end{aligned}
$$

For conservation of particles we require $N(T) = N_0$. Therefore, the term in brackets (8) must be zero, so $\mu = 0$

## 1c

To calculate the specific heat we use the form $C = \frac{dU}{dT}$, U is the internal energy.

$$
\begin{aligned}
U &= D_0 \int_{-\infty}^{\infty} d\epsilon \quad |\epsilon| \epsilon f(\epsilon) && (10)\\
&= D_0 \int_{0}^{\infty} d\epsilon \quad \epsilon^2 (f(\epsilon) - f(-\epsilon)) && (11)\\
&= D_0 \int_{0}^{\infty} d\epsilon \quad \epsilon^2 \; (2f(\epsilon) - 1) && (12)\\
&= 2T^3 D_0 \int_{0}^{\infty} dx \quad \frac{x^2}{e^x+1} - D_0 \int_{0}^{\infty} d\epsilon \quad \epsilon^2 && (13)
\end{aligned}
$$

The second term is the ground state energy $E_0$ and does not contribute to the specific heat because there is no temperature dependence there.

The integral in the first term can be found in tables and the result is

$$\delta U = 3T^3 D_0 \zeta(3) + E_0 \qquad (14)$$

$$C = 9T^2 D_0 \zeta(3) \qquad (15)$$

## 2

The equation for minimum of energy is:

$$\frac{\partial F}{\partial \boldsymbol{\eta}} = 0 = \sum_{i=1,2} \alpha\eta_i + \beta_1(\boldsymbol{\eta}\cdot\boldsymbol{\eta}^*)\eta_i + \beta_2(\boldsymbol{\eta}\cdot\boldsymbol{\eta})\eta_i^* + \beta_3|\eta_i|^2\eta_i \tag{16}$$

for the 4 orientation cases to consider we can write the above as a function of magnitude $\eta_{01}$, $\eta_{10}$, $\eta_{11}$, $\eta_{1i}$, noting that $\eta_{01}$ and $\eta_{10}$ are the same.

$$0 = \alpha\eta_{10} + \beta_1|\eta_{10}|^2\eta_{10} + \beta_2\eta_{10}^2\eta_{10}^* + \beta_3|\eta_{10}|^2\eta_{10} \tag{17}$$

$$\Rightarrow |\eta_{10}|^2 = \frac{-\alpha}{\beta_1+\beta_2+\beta_3} \tag{18}$$

$$0 = \alpha\eta_{11} + 2\beta_1|\eta_{11}|^2\eta_{11} + 2\beta_2\eta_{11}^2\eta_{11}^* + \beta_3|\eta_{10}|^2\eta_{11} \tag{19}$$

$$\Rightarrow |\eta_{11}|^2 = \frac{-\alpha}{2\beta_1+2\beta_2+\beta_3} \tag{20}$$

$$0 = \alpha\eta_{1i} + 2\beta_1|\eta_{1i}|^2\eta_{1i} + \beta_3|\eta_{1i}|^2\eta_{1i} \tag{21}$$

$$\Rightarrow |\eta_{1i}|^2 = \frac{-\alpha}{2\beta_1+\beta_3} \tag{22}$$

The free energy of these states is:

$$F[\eta_{10}] = \frac{-\alpha^2/(2\beta_1)}{1+\beta_2/\beta_1+\beta_3/\beta_1} \tag{23}$$

$$F[\eta_{11}] = \frac{-\alpha^2/(\beta_1)}{2+2\beta_2/\beta_1+\beta_3/\beta_1} \tag{24}$$

$$F[\eta_{1i}] = \frac{-\alpha^2/(\beta_1)}{2+\beta_3/\beta_1} \tag{25}$$

For each possible value of $x = \beta_2/\beta_1$ and $y = \beta_3/\beta 1$ the system will choose the state with lowest free energy. The conditions on this choice are
**choose 10 over 11**: $y < 0$
**choose 10 over 1i**: $y < -2x$
**choose 11 over 1i**: $x < 0$
The regions are mapped out in the figure

## 3a

The diagonalized Hamiltonian is:

$$\mathcal{H} = \sum_{\mathbf{k},s} E_{\mathbf{k}s} b^{\dagger}_{\mathbf{k}s} b_{-\mathbf{k}s} \tag{26}$$

and the $b$ operators are defined through the Bogolioubov transformation:

$$a_{\mathbf{k}s} = u_{\mathbf{k}} b_{\mathbf{k}s} - (i\sigma_y)_{ss'} v_{\mathbf{k}} b_{-\mathbf{k}s'} \tag{27}$$

which results in the Bogolioubov-de Gennes equations

$$E_{\mathbf{k}s} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \xi_{\mathbf{k}} & \Delta^* \\ \Delta & \xi_{\mathbf{k}\bar{s}} \end{pmatrix} \begin{pmatrix} u_{vk} \\ v_{\mathbf{k}} \end{pmatrix} \tag{28}$$

In the above definition for $b$ operators I omitted spin indices on the amplitudes in anticipation of the final result which is

$$u_{\mathbf{k}} = \sqrt{\frac{\Delta}{E}} e^{\theta_E/2} \tag{29}$$

$$v_{\mathbf{k}} = \sqrt{\frac{\Delta}{E}} e^{-\theta_E/2} \tag{30}$$

The eigenvalues are

$$E_{\mathbf{k}s} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta|^2} - \mu_B H s \tag{31}$$

with $\theta_E = cosh^{-1}(E/\Delta)$.

## 3b

After using the form of $a$ operators in terms of the diagonal $b$'s, the spin magnetisation reduces to

$$M = \mu_B \sum_{\mathbf{k}} f_{\mathbf{k}\uparrow} - f_{\mathbf{k}\downarrow} \tag{32}$$

where $f_{\mathbf{k}s} = (e^{\beta E_{\mathbf{k}s}} + 1)^{-1}$ and $\beta = 1/T$. This is good!

We can preform the sum over states by using the density of states for a superconductor $N = N_0|E|/\sqrt{E^2 - \Delta^2}$ and $N_0$ is the normal DOS at the Fermi level.

$$M = \mu_B N_0 \int_{\Delta}^{\infty} dE \frac{E}{\sqrt{E^2 - \Delta^2}} (f_{\mathbf{k}\uparrow} - f_{\mathbf{k}\downarrow}) \tag{33}$$

The linear response to a field will be $M_{lr} = \chi(T)H$ and we can Taylor expand the Fermi functions in H $f_{\mathbf{k}s} \approx f_{\mathbf{k}} + \frac{s\beta}{4cosh^2(\beta E/2)} H$ to get the desired result

$$\begin{aligned}
\chi(T) &= (1/2)\mu_B N_0 \beta \int_{\Delta}^{\infty} dE \frac{E}{\sqrt{E^2 - \Delta^2}} \frac{1}{cosh^2(\beta E/2)} && (34)\\
&= (1/2)\mu_B N_0 \int_{\beta\Delta}^{\infty} dx \frac{x}{\sqrt{x^2 - (\beta\Delta)^2}} \frac{1}{cosh^2(x/2)} && (35)\\
&= (1/2)\mu_B N_0 \int_{\beta\Delta}^{\infty} dx \sqrt{x^2 - (\beta\Delta)^2} \frac{tanh(x/2)}{cosh^2(x/2)} && (36)
\end{aligned}$$

and we integrated by parts in the last step

## 3c

The two limits of interest are $\beta\Delta >> 1$, and $\Delta = \Delta_0 = constant$ for low temperature and $\beta\Delta << 1$ for near $T_c$ when self consistent solution $\Delta(T)$ is first appearing as a second order phase transition. The limit near $T_c$ would not apply if it was a first order transition.

$\beta\Delta_0 >> 1$**, Low Temperature**
The low T limit allows write $tanh(x/2) \approx 1$ and $cosh(x/2) \approx \frac{1}{2}e^{x/2}$

$$\begin{aligned}
\chi(T) &= 2\mu_B N_0 \int_{\beta\Delta}^{\infty} dx \sqrt{x^2 - (\beta\Delta)^2} e^{-x} && (37)\\
&= 2\mu_B N_0 (\beta\Delta)^2 \int_{1}^{\infty} dy \sqrt{y^2 - 1} e^{-\beta\Delta y} && (38)
\end{aligned}$$

The integral is equivalent to the $n = 1$ modified Bessel function of the second kind.

$$K_1(z) = z \int_{1}^{\infty} dy \sqrt{y^2 - 1} e^{-zy} \quad (39)$$

$$\chi(T) = 2\mu_B N_0 \frac{\Delta_0}{T} K_1(\Delta_0/T) \quad (40)$$

$\beta\Delta << 1$**, Near** $T_c$ Here we employ Leibniz rule to Taylor expand the integral

$$\int_{\beta\Delta}^{\infty} dx \sqrt{x^2 - (\beta\Delta)^2} \frac{tanh(x/2)}{cosh^2(x/2)} \approx \int_0^{\infty} dx \quad x \frac{tanh(x/2)}{cosh^2(x/2)} \tag{41}$$

$$- \quad (\beta\Delta)^2/2 \int_0^{\infty} dx \frac{1}{x} \frac{tanh(x/2)}{cosh^2(x/2)} \tag{42}$$

The first integral is easy and evaluates to 2.

The second integral is not easy, but mathematica can do it and the result is $-28\zeta'(-2) \approx .852557$. At this point we can also use the limiting expression for $\Delta(T)$ near $T_c$ which was written in class.

$$\Delta(T) = \sqrt{\frac{2}{7|\zeta'(-2)|}} T_c \sqrt{1 - T/T_c} \tag{43}$$

Now we can finally write the two limits using normal state susceptibility $\chi_N = \mu_B N_0$

$$\frac{\chi^{T_c}(T)}{\chi_N} = 1 - 2\frac{1 - T/T_c}{(T/T_c)^2} \tag{44}$$

$$\frac{\chi^0(T)}{\chi_N} = 2\frac{\Delta_0}{T} K_1(\Delta_0/T) \tag{45}$$

The zero temperature expansion is a very slow growing function of T, and plots show that $\frac{\chi^0(T)}{\chi_0} < 0.04$ for $T < 0.2\Delta_0$. This is expected from the form of the magnetisation in the beginning of part 3b combined with the gapped density of states.

Near $T_c$ the normal state $\chi_N$ is recovered and the temperature dependence of the decrease in $\chi$ is due to the onset of the order parameter $\Delta(T)$. Looking at plots, one can see that the $\chi$ is quickly reduced to near zero for $T/T_c \approx 0.75$

FIGURES ATTACHED