TFY4245/FY8917 Solid State Physics, Advanced Course

Problemset 9

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SUGGESTED SOLUTION

Problem 1

(a) The key observation here is to realize that since the dispersion is given by

$$E_{n,k_x,k_y,k_z} = \hbar\omega_c(n+1/2) + \frac{\hbar^2 k_z^2}{2m}, \tag{1}$$

the density of states will be the sum of the density of states for a 1D electron gas (due to the k_z^2 term) shifted to the minimum energies $\hbar\omega_c(n+1/2)$. Recall that we have a massive degeneracy in the k_x and k_y indices. So let us first briefly derive the 1D density of states for free electrons, using the same approach is done in the textbook 3D case.

The k-space volume taken up by a single state (generalized ”cube” in k-space) is in 1D equal to π/L for a system with length L and using periodic boundary conditions. The latter gives that the allowed k-values are separated by π/L. The k-space volume of a generalized ”sphere” in 1D is simply $V_{\text{line}} = k$. Therefore, the number of filled states in the sphere is

$$N = V_{\text{line}}/V = kL/\pi. \tag{2}$$

Since $\varepsilon = \hbar^2k^2/2m$, we get

$$N = \sqrt{2m\varepsilon}^{1/2}\frac{L}{\hbar\pi}. \tag{3}$$

The density per unit energy is then

$$\frac{dN}{d\varepsilon} = \frac{dN}{dk}\frac{dk}{d\varepsilon} = \frac{mL}{\hbar\pi\sqrt{2mE}}. \tag{4}$$

The density of states (DOS) $D(\varepsilon)$ per unit volume is then found by dividing on the ”volume” L of the crystal:

$$D(\varepsilon) = \frac{1}{\hbar\pi}\sqrt{\frac{m}{2\varepsilon}}. \tag{5}$$

This is per spin.

In our case, we have a 3D system. To get the DOS per unit volume, we thus should divide on L^3 rather than L. We should also take into account the degeneracy in k_x, k_y: namely, we have $N_L = eBL^2/h$ number of modes for each n and k_z value.

Thus, we arrive that the final value for the density of states (per unit volume) and per spin:

$$D(\varepsilon) = \frac{N_L}{L^2}\sum_{n=0}^{\infty}\frac{1}{\pi\hbar}\sqrt{\frac{m}{2(\varepsilon-[n+1/2]\hbar\omega_c)}}\Theta\Big(\varepsilon-[n+1/2]\hbar\omega_c\Big). \tag{6}$$

The step-function is there because the minimum value of the energy for each value of n is $\hbar\omega_c(n+1/2)$.

(b) The total zero-temperature energy of the system should be the integral over the energy of each state times the density of states (times a factor 2 for spin):

$$E = 2V\int_0^{\mu} d\varepsilon\, \varepsilon\, D(\varepsilon). \tag{7}$$

An integration by parts gives

$$E = 2V\Big[\mu P_1(\mu) - \int_0^{\mu} d\varepsilon\, P_1(\varepsilon)\Big] = \mu N - 2V P_2(\mu). \tag{8}$$

The explicit expression for $P_2(\mu)$ is

$$P_2(\mu) = \frac{1}{\pi\hbar}\sqrt{\frac{m}{2}}\frac{N_L}{L^2}\sum_{n=0}^{\infty}\frac{4}{3}\Big(\mu-(n+1/2)\hbar\omega_c\Big)^{3/2}\Theta(\mu-(n+1/2)\hbar\omega_c\Big). \tag{9}$$

Since we could assume $\hbar\omega_c \ll \mu$, we can replace this sum over n by an integral. The Poisson summation formula given in the problem text provides us with:

$$P_2(\mu) = \frac{1}{\pi\hbar}\sqrt{\frac{m}{2}}\frac{N_L}{L^2}\frac{4}{3}\Big\{\int_0^{\mu/\hbar\omega_c} dx\,(\mu-x\hbar\omega_c)^{3/2} + 2\sum_{s=1}^{\infty}(-1)^s\int_0^{\mu/\hbar\omega_c} dx\,(\mu-x\hbar\omega_c)^{3/2}\cos(2\pi sx)\Big\}. \tag{10}$$

Let $p \equiv \mu/\hbar\omega_c$. We then have

$$P_2(\mu) = C_0\Big[(\hbar\omega_c)^{3/2}\int_0^p (p-x)^{3/2}dx + 2\sum_{s=1}^{\infty}(-1)^s(\hbar\omega_c)^{3/2}\int_0^p (p-x)^{3/2}\cos(2\pi sx)dx\Big], \tag{11}$$

where we defined $C_0 \equiv \frac{1}{\pi\hbar}\sqrt{\frac{m}{2}}\frac{N_L}{L^2}\frac{4}{3}$ for brevity. Use that

$$\int_0^p (p-x)^{3/2}dx = \frac{2p^{5/2}}{5}. \tag{12}$$

Then, we use a partial integration to show that

$$\int_0^p (p-x)^{3/2}\cos(2\pi sx)dx = \frac{\sin(2\pi sx)}{2\pi s}(p-x)^{3/2}\Big|_0^p - \int_0^p \frac{\sin(2\pi sx)}{2\pi s}\Big(-\frac{3}{2}\Big)(p-x)^{1/2}dx. \tag{13}$$

The surface term vanishes. Performing a variable shift $u \equiv p-x$, we obtain for the remaining term:

$$\begin{aligned}\int_0^p (p-x)^{3/2}\cos(2\pi sx)dx &= \frac{3}{2}\frac{1}{2\pi s}\int_0^p du\sqrt{u}\sin[2\pi s(p-u)]\\ &= \frac{3\sqrt{p}}{8\pi^2 s^2} - \frac{3}{16\pi^2 s^{5/2}}\Big[\cos(2\pi ps)C(2\sqrt{sp}) + \sin(2\pi ps)S(2\sqrt{sp})\Big]\end{aligned} \tag{14}$$

where in the second line we defined the Fresnel integrals $C(z)$ and $S(z)$ which are two transcendental functions. Plugging the above results back into our expression for $P_2(\mu)$ gives:

$$P_2(\mu) = C_0\Big\{(\hbar\omega_c)^{3/2}\int_0^p (p-x)^{3/2}dx + 2\sum_{s=1}^{\infty}(-1)^s(\hbar\omega_c)^{3/2}\frac{3\sqrt{p}}{8\pi^2 s^2} - 2(\hbar\omega_c)^{3/2}\frac{3}{16\pi^2}\sum_{s=1}^{\infty}\frac{(-1)^s}{s^{5/2}}\Big[\cos(2\pi ps)C(2\sqrt{sp}) + \sin(2\pi ps)S(2\sqrt{sp})\Big]\Big\}. \quad (15)$$

Now use

$$\sum_{s=1}^{\infty}\frac{(-1)^s}{s^2} = -\frac{\pi^2}{12}: \quad (16)$$

to obtain

$$P_2(\mu) = C_0\Big\{(\hbar\omega_c)^{3/2}\frac{2p^{5/2}}{5} - 2(\hbar\omega_c)^{3/2}\Big(\frac{\sqrt{p}}{32} + \frac{3}{16\pi^2}\sum_{s=1}^{\infty}\frac{(-1)^s}{s^{5/2}}\Big[\cos(2\pi ps)C(2\sqrt{sp}) + \sin(2\pi ps)S(2\sqrt{sp})\Big]\Big)\Big\}. \quad (17)$$

Compare now $\frac{\sqrt{p}}{32}$ with the term containing the sum. As p increases, the first term increase linearly. On the other hand, the Fresnel integrals $C(x)$ and $S(x)$ both have asymptotes 0.5 as $x \to \infty$. Numerically, one verifies that the term with the sum is indeed much smaller than $\frac{\sqrt{p}}{32}$ in the limit $p \gg 1$, corresponding to $\mu \gg \hbar\omega_c$, that we are considering (in effect, $B \to 0$). Therefore, this term can safely be neglected and we are left with

$$P_2(\mu) = \frac{1}{\pi\hbar}\sqrt{\frac{m}{2}}\frac{N_L}{L^2}\frac{4}{3}\Big(\frac{2}{3}\frac{\mu^{5/2}}{\hbar\omega_c} - \frac{1}{16}(\hbar\omega_c)\sqrt{\mu}\Big). \quad (18)$$

(c) Since $N_L \propto B$ and $\hbar\omega_c \propto B$, the first term is of order B^0 and thus determines the energy in the absence of a magnetic field. We therefore get

$$E = E(B=0) + 2V\frac{1}{\pi\hbar}\sqrt{\frac{m}{2}}\frac{N_L}{L^2}\frac{4}{3}\frac{1}{16}\hbar\omega_c\sqrt{\mu}, \quad (19)$$

allowing us to identify

$$\kappa = \frac{1}{12\pi^2}V\frac{e^2\sqrt{\mu}}{\sqrt{2m}\hbar}. \quad (20)$$

Problem 2

If $j = j'$, the exponential is 1, so the sum is $N \cdot 1 = N$. If $j \neq j'$, consider the summand which is

$$e^{ik(j-j')a} = e^{i\frac{2\pi}{Na}m(j-j')a} \equiv x^m \quad (21)$$

where $x \equiv e^{i2\pi(j-j')/N}$ and we used that $r_j = ja$ in 1D.

Since both j and j' can only take values between 1 and N, and we have assumed $j \neq j'$, we get $0 < |j-j'| < N$, and therefore $x \neq 1$. We now rewrite the sum as

$$\sum_k e^{ik(j-j')a} = \sum_{m=-N/2}^{N/2-1} x^m = x^{-N/2}\sum_{m=0}^{N-1} x^m = x^{-N/2}\frac{1-x^N}{1-x}. \quad (22)$$

We used above the formula for the sum of a geometric seriers. Since $x \neq 1$ the denominator $1-x$ is nonzero. Furthermore, $x^N = 1$, so $1-x^N$ vanishes. This completes the proof.