Physics 155- Winter 2016

Introduction to Condensed Matter Physics

Solution of Test-1
100 points, Time 1.20 hours 20 Jan, 2016

1. *For the standard nearest neighbor one dimensional lattice (spectrum given below in* **Notes***), following Debye, we can rewrite the summation over wave vectors as*

$$\sum_k \to \int_0^{\omega_D} g_D(\omega)\, d\omega.$$

Show that the Debye density of states $g_D(\omega)$ is given by

$$g_D(\omega) = N/\omega_D, \ \ \ldots\ldots\ldots [5]$$

and the Debye frequency by

$$\omega_D = 2\pi\, v/a, \ \ \ldots\ldots\ldots [10]$$

where v is the velocity and a is the lattice constant. Assuming (without proof) that the exact density of states $g(\omega)$ is given by

$$g(\omega) = 2N/\pi \frac{1}{\sqrt{\omega_{max}^2 - \omega^2}},$$

show that at low ω the Debye result underestimates the density of states by half , i.e.

$$\lim_{\omega\to 0} g_D(\omega) \to \frac{1}{2}\, g(\omega). \ \ \ldots\ldots\ldots [10]$$

Explain in brief *how the above result* and *the divergence of $g(\omega)$ relative to g_D can be reconciled with the fact that both densities of states integrate to the same number of degrees of freedom N.* ....[15]

{ *Hint: For the last part, a rough sketch of the two functions can be helpful.*}

Solution:

Since we are in 1-dimension $\omega_k = vk$ is assumed for all k. The simplest version of Debye's treatment is to write $dk = d\omega/v$ so that

$$N = L\int dk/(2\pi) = L/(2\pi v)\int_0^{\omega_D} d\omega = L/(2\pi v)\omega_D, \quad (1)$$

giving us

$$g_D = N/\omega_D \quad \text{and} \quad \omega_D = 2\pi v/a, \quad (2)$$

where we used $L = aN$.

For the next part we note that $g(0) = 2N/(\pi\omega_{max})$. We learn from the given dispersion that $\omega_{max} = 2\sqrt{K/m}$, as well as $v = a\sqrt{K/m}$ so that $\omega_{max} = 2v/a$. Combining we see that

$$g(0) = Na/(\pi v).$$

Comparing with the expression above, we see that

$$g_D = 1/2g(0).$$

We note that g_D is smaller than the exact value $g(\omega \to 0)$, and all the way up to ω_{max}. At the ω_{max} the true $g(\omega)$ truncates, but the Debye function does not- and continues to be non zero up to ω_D. However the Debye theory gives the same total area since the magnitude of ω_D exceeds ω_{max} (by a factor of π), so it has a greater region of frequencies to play with.

Special Comment If we use the fact that k and $-k$ have the same energy, then the third and fourth terms of Eq(1) will pick up an extra factor of 2 and thereby change to

$$N = L\int dk/(2\pi) = L/(\pi v)\int_0^{\omega_D} d\omega = L/(\pi v)\omega_D, \quad (1')$$

giving us

$$g'_D = N/\omega'_D \quad \text{and} \quad \omega'_D = \pi v/a, \quad (2')$$

this is smaller than the unprimed value by a factor of 2. Here again the ω'_D exceeds the ω_{max}. However now the excess is by a factor of $\pi/2$ rather than π. One can then verify that it has the same area, made possible by a larger range of ω.

2. *Using the Debye results of Problem 1, show that the heat capacity of a 1-D lattice is*

$$C = Nk_B, \quad \textit{when } T \gg T_D, \quad \ldots\ldots\ldots [20]$$

where $T_D = \hbar\omega_D/k_B$ *and at low temperature* $T \ll T_D$

$$C = Nk_B \times \mathcal{J} \times (T/T_D) \quad \ldots\ldots\ldots [20]$$

where $\mathcal{J} = \int_0^\infty dx\, x^2 \exp(x)/(\exp(x) - 1)^2$. { *Hint: In this problem you will need the formula for heat capacity per mode.*}

Solution: This is very simple when we recall that with $x = \hbar\omega/k_B T$, the heat capacity per mode is

$$C(x) = k_B x^2 \exp x/(\exp x - 1)^2,$$

while the total heat capacity in the Debye model is

$$C = N/\omega_D \int_0^\infty C(\omega)\, d\omega.$$

Changing variables in the integral $\omega = x\ (k_B T)/\hbar$ we get

$$C/(Nk_B) = T/T_D \int_0^{T_D/T} x^2 \exp x/(\exp x - 1)^2\, dx,$$

where $T_D = \hbar\omega_D/k_B$.

At high T/T_D the integral is over a small interval and hence $x \ll 1$, we can then Taylor expand the integrand as $x^2 \exp x/(\exp x - 1)^2 = 1 - (x^2)/12$. Plugging in we find

$$C \sim Nk_B \times (1 - 1/(36) \times (T_D/T)^3).$$

The correction to the leading term (1) is not required in the problem, but it was pretty easy to get- right?

At low T/T_D, we can extend the upper limit to infinity and hence get the required result

$$C = Nk_B \times \mathcal{J} \times (T/T_D).$$

3. *In the 1-d Harmonic lattice problem, assuming that ω reaches its maximum allowed value, show that the amplitudes u_n satisfy a simple equation*

$$u_n = -\frac{1}{2}(u_{n+1} + u_{n-1}). \quad \ldots\ldots\ldots [10]$$

What is the spatial solution of this equation? .... [10]

Solution: This is very straightforward- we start with the equation of motion for the displacements of the atoms

$$M\ddot{u}_n = K(u_{n+1} + u_{n-1} - 2u_n).$$

We can now use the harmonic time dependence and deduce $\ddot{u}_n = -\omega^2 u_n$. At the peak frequency $\omega \to \omega_{max} = 2\sqrt{K/M}$. Plugging in and cancelling K we get the required equation

$$u_n = -\frac{1}{2}(u_{n+1} + u_{n-1}).$$

The spatial solution of this is easy to guess- we write $u_n = u_0 \times (-1)^n$ with an arbitrary amplitude u_0. We see that $u_{n\pm1} = -u_n$ and hence this guess satisfies the equation. Of course the solution found in the class reduces to this simple form when we set k at the boundary of the Brillouin zone.

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