Department of Physics University of Maryland College Park, MD 20742-4111

Physics 603

37.73

HOMEWORK ASSIGNMENT #7

Spring 2014

Due date for problems on Tuesday, April 15 [deadline on April 17]. This may be delayed by one lecture depending on progress in class.

- 0. (Do not turn in) Convince yourself that, in 3D, $N_{ex}/V = \lambda_T^{-3} \operatorname{Li}_{3/2}(z)$ and $U/V = (3/2) \ N_i \ k_B T \ \operatorname{Li}_{5/2}(z) / \operatorname{Li}_{3/2}(z)$, where N_i is N above T_c ; below T_c , N_i is N_{ex} and z=1.
- 1. (10) PB 7.4 For the first equation, start with Eq. 7.1.7 and use Eq. D.10. For the second, note that at constant N, S = S(z) (cf. Eq. 7.1.44), so that, with the appropriate subscripts, $C = T(\partial S/\partial z)(\partial z/\partial T)$. For the last part, note Eq. (D.8); in PB notation, α is $-\beta\mu$.
- 2. (15) PB 7.14. Once you have C_V, use your results from the previous problem to find C_P.
- 3. (5) PB 7.24 ·
- 4. (10) PB 7.25 Hint: After setting up the integral explicitly, expand $\frac{\hbar\omega}{\exp(\hbar\omega/k_BT)-1}$ (in the high-temperature limit) to first order in ω . For $C_V(\infty)$ make use of the classical result for U. You do not need, and should not use, the Debye approximation.

5. (15) from a recent Qualifier Exam. In part b), cast the integral for U(T) into dimensionless form.

Consider a two-dimensional (2D) periodic crystal lattice consisting of a large number N of equivalent atoms and occupying an area A. The ratio $A/N \equiv a^2$ defines the characteristic length a of the order of interatomic distance. In this problem, we study contributions of lattice vibrations (phonons) to the thermal energy U and heat capacity C_V of the 2D crystal.

First consider the in-plane vibrations, where the atoms move in the 2D plane of the crystal. In the long-wavelength limit (for small k), the frequencies ω of these vibrational modes depend linearly on the 2D wavevector $\mathbf{k} = (k_x, k_y)$:

$$\omega_{\rm in}(k) = v\sqrt{k_x^2 + k_y^2} = vk, \tag{1}$$

where v is the speed of sound. There are two such modes (transverse and longitudinal), but we assume for simplicity that they are degenerate and have the same v.

- (a) [5 points] In the Debye model, Eq. (1) is assumed to hold up to the Debye wavenumber k_D , i.e., to be valid for $k < k_D$. The value of k_D is determined by the requirement that the total number of vibrational modes in the circular domain $k < k_D$ is equal to the number 2N of the 2D spatial degrees of freedom of the atoms. Show that $k_D = 2\sqrt{\pi}/a$.
- (b) [8 points] In the Debye theory, write an integral expression for the phonon energy U(T), valid for all temperatures T. Also, write a general thermodynamic formula for the heat capacity at constant volume, $C_V(T)$, in terms of U(T).

- (c) [8 points] i) From your expressions in Part (b), find U(T) and $C_V(T)$ in the low-temperature limit. ii) How does the T-dependence of $C_V(T)$ differ from the usual expression in three dimensions? iii) What is the relationship between the exponent of T-in U(T) and the spatial dimension? iv) What is the physical origin of this relationship?
- (d) [7 points] From your expressions in Part (b), find U(T) and $C_V(T)$ in the high-temperature limit and verify that they agree with the classical equipartition theorem.
- (e) [5 points] Draw a sketch of $C_V(T)$ in the full range of temperatures, from low to high T, including T=0. What is the characteristic temperature scale T_D (the Debye temperature) separating the low- and high-temperature limits?

The Nobel Prize in Physics in 2010 was awarded for the discovery of graphene, a 2D honeycomb lattice of carbon atoms. The figure on the next page shows the experimentally measured dispersion relations $\omega_n(k)$, $n=1,\ldots,6$, for the 6 vibrational eigenmodes in graphene. The modes represented by Eq. (1), with different values of v, correspond to the second and third lowest curves near the origin. (The upper three branches are due to the two-atom unit cell in a honeycomb lattice. Ignore these three upper branches, because they are not excited at low temperatures.) The lowest branch originates from the out-of-plane motion of the atoms perpendicular to the 2D plane. Similarly to perpendicular vibrations of an elastic plate, this mode has the following dispersion relation for small k:

$$\omega_{\text{out}}(\mathbf{k}) = b \, k^2, \tag{2}$$

where b is a coefficient.

(f) [7 points]. Determine temperature dependences of the contributions from the mode in Eq. (2) to U(T) and $C_V(T)$ at low T. Sketch the contribution to $C_V(T)$ by a dashed line on your plot in Part (e) for low T only. Which mode gives the predominant contribution to $C_V(T)$ at low T, the in-plane mode (1) or the out-of-plane mode (2)?

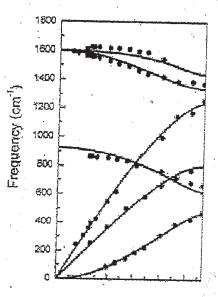


Figure 1: Phonon dispersion relations $\omega_n(k)$, $n=1,\ldots,6$, in graphene.