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Physics 603 | **HOMEWORK ASSIGNMENT #7** | Spring 2012

Due date for problems on Tuesday, April 17 [deadline on April 19].

1. PB 7.14

Consider an n-dimensional Bose gas whose single-particle energy spectrum is given by $\varepsilon \propto p^s$, where s is some positive number. Discuss the onset of Bose–Einstein condensation in this system, especially its dependence on the numbers n and s. Study the thermodynamic behavior of this system and show that,

$$P = \frac{s}{n}\frac{U}{V}, \quad C_V(T \to \infty) = \frac{n}{s}Nk, \quad \text{and} \quad C_P(T \to \infty) = \left(\frac{n}{s} + 1\right)Nk.$$

2. PB 7.25 Hint: After setting up the integral explicitly, expand $\dfrac{\hbar\omega}{\exp(\hbar\omega / k_B T) - 1}$ (in the high-temperature limit) to first order in ω.

Figure 7.20 is a plot of $C_V(T)$ against T for a solid, the limiting value $C_V(\infty)$ being the classical result $3Nk$. Show that the shaded area in the figure, namely

$$\int_0^\infty \{C_V(\infty) - C_V(T)\} dT,$$

is exactly equal to the zero-point energy of the solid. Interpret the result physically.

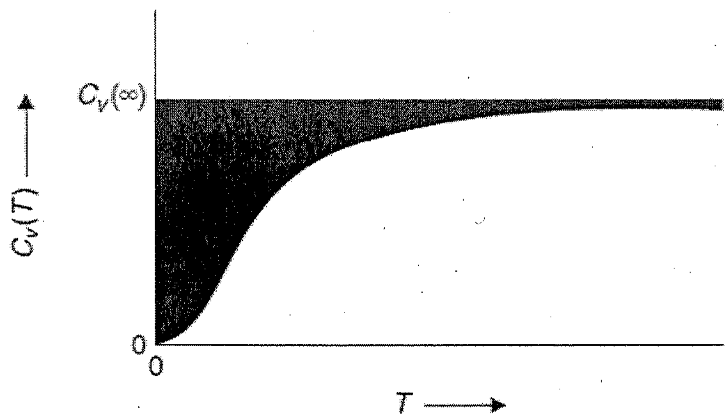

FIGURE 7.20

3. from the most 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 $\boldsymbol{k} = (k_x, k_y)$:

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

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 $\omega_n(\boldsymbol{k})$, $n = 1, \ldots, 6$, 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:

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

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)?

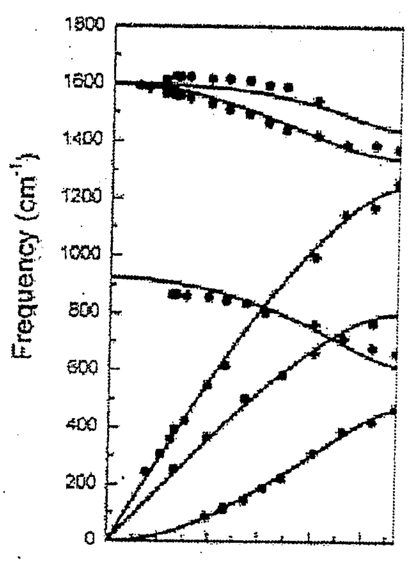

Figure 1: Phonon dispersion relations $\omega_n(\boldsymbol{k})$, $n = 1, \ldots, 6$, in graphene.

4. An unidentified molecular, or possibly monatomic, material (call it **J**, with a molecular mass m_J) has been studied via various thermodynamic measurements. In the gaseous phase and at laboratory temperatures, the constant volume specific heat (or the heat capacity) is specified by

$$C_V = c_J R = c_J N_0 k_B \, ,$$

with the numerical parameter c_J close to 2.50.

(a) Name the symbols R, N_0, and k_B appearing in the equation above. **[1.5 points]**

(b) Explain why the value of c_J suffices to prove that **J** is not monatomic. **[2 points]**

(c) It follows that **J** might be diatomic, triatomic, or polyatomic. Which possibility is the most plausible and why? **[3 points]**

At low temperatures the vapor **J** condenses into a uniaxial solid crystalline phase. The density of the vapor in equilibrium with the solid is then found to vanish with decreasing T as

$$n_0(T) \sim T^{3/2} \exp\left(-T_J/T\right) .$$

(d) What information about **J** is contained in T_J? **[2 points]**

(e) Measurements of the molecular entropy, $S(T)$, of the solid reveal that it extrapolates to a (non-negligible) value S_0 at $T = 0$. Explain (*i*) why this violates the Third Law of Thermodynamics and (*ii*) what this observation suggests about the homo- or heteroatomic character of **J**. **[4 points]**

(f) In light of the conclusions drawn in parts (c) and (e) above, determine the magnitude of S_0 that should be anticipated. **[2 points]**

(g) As expected, the low-T specific heat of solid **J** obeys a Debye T^3 law. However, when molecules of **J**, at an overall density well below that of the crystal, are trapped in a deep three-dimensional optical lattice, the specific heat in the millikelvin range is observed to vanish exponentially fast as $\exp\left(-\varepsilon/k_B T\right)$. If, in a leading approximation, each well of the optical lattice imposes a potential

$$V(x, y, z) = \frac{1}{2} K(x^2 + 4y^2 + 4z^2)$$

on an individual **J** molecule located near the origin, $(x, y, z) = (0, 0, 0)$, find an expression for the energy ε in terms of parameters given.

[4 points]

(h) If the vapor phase of **J** is subjected to an electric field E, and the induced polarization, P, is measured, what, if any, other molecular properties of **J** might be determined? **[1.5 points]**

NOT assigned, but of interest

In a three-dimensional solid, there exists a class of propagating excitation modes (unspecified) which have a dispersion relation, at small values of wave vector k, of the form $\omega = Ak^m$. Assume that these excitations obey Bose-Einstein statistics.

a) What is the number of modes between ω and $\omega + d\omega$ for a solid of unit volume?

b) Show that the mean energy density at temperature $T \ll E_{max}/k_B$ is of the form $E(T) = BT^n$ and determine n. (E_{max} is the maximum of E(k), k_B is the Boltzman constant, and B is a constant that you need not determine).

c) Does your result agree with the Debye result for phonons (m = 1)?

d) What is the temperature dependence of the specific heat when m = 2?

e) What is the relation of your result for m = 1 to the Stefan-Boltzman law for black body radiation?

III. Consider a square thin film of solid material – only one atom thick – of area $A = L^2$ deposited on an inert substrate. The N atoms may vibrate parallel to the surface, but not perpendicular to it. The speed of sound in the solid is c_s.

(a) Find the vibration frequency ν as a function of L and c_s. [2 points]

(b) Show that the density of vibration modes as a function of vibration frequency ν is $D(\nu) = 4\pi A\nu/c_s^2$ [4 points]

(c) Verify that the maximum vibration frequency $\nu_{\max}$ is

$$\nu_{\max} = \left(\frac{c_s^2 N}{\pi A}\right)^{1/2} \text{ Hz.}$$ [3points]

(d) What is the temperature of the system at which all modes are excitable (Debye temperature)? What does the Debye temperature tell us about the heat capacity of the material? [2 points]

(e) Calculate the average energy $\langle E\rangle$ and the heat capacity at constant area C_A in the limit of
i. high temperature $kT \gg h\nu_{\max}$ [3 points]
Note that for small x, $e^x = 1 + x$
ii. low temperature $kT \ll h\nu_{\max}$ [4 points]

$$\text{Note that} \int_0^\infty \frac{x^2}{e^x - 1}\, dx = 2.404$$

(f) How is the heat capacity of a system measured experimentally (briefly describe the general approach in no more than three sentences)? [2 points]