Physics 140A: TakeHome Exam: Solutions

3/1/05. Due 3/8/05.

1. Vibrating Chain of Atoms. 15 points.
Consider a chain of identical atoms of mass M, spacing a.
(a) Write the *form* of solution for the atomic displacements that we use to obtain wavelike solutions to Newton's 2nd law.
Answer.

$$u_j(t) = Ue^{i(jka-\omega t)}$$

(b) Draw a diagram and label atoms. Then consider a chain whose 2nd neighbor force constant is K_2, and 3rd neighbor force constant is K_3 (no nearest neighbor spring). Determine the phonon dispersion relation $\omega(k)$ and calculate the sound velocity ($k \to 0$).
Answer. Each pair of j-th neighbor atoms contributes to the force side of the equation a term $2K_j[cos(jka) - 1]U$, and the U will cancel out. Solution is

$$\omega(k) = a\sqrt{\frac{2K_2(1 - cos(2ka) + 2K_3(1 - cos(3ka)}{M}}$$

The velocity can be calculated most directly by using $1 - cosx = 2sin^2\frac{x}{2}$ and then expanding sine to lowest order in $x = ka$ (all that is needed). Alternatively, one can directly take the derivative $d\omega_k/dk$ and taking the $k \to 0$ limit using L'Hopital's rule. The result is $c = \sqrt{(4K_2 + 9K_3)/M}$.
(c) Is the chain stable for every positive value of K_2 and K_3?
Answer. Stability means stable vibrations: $\omega(k) > 0$ everywhere except for the acoustic modes at $K = 0$ where zero is normal (uniform translational modes). Since $cosx \leq 1$, $1 - cos(jka)$ is positive except where the cosine is unity. To get zero (at some $k > 0$) each cosine term that appears must be equal to unity. If K_2 and K_3 are nonzero (and positive) as implied in the statement of the problem, then the chain is stable. Check this for yourself. That was a sufficient answer. *Extra comment:* if K_3=0, there is an instability ($\omega = 0$) at the zone boundary $ka = \pi$. This was discussed a bit in class: with only a K_2, the chain breaks up into two unconnected chains made up of every other atom; atom j is not connected to $j \pm 1$. For K_2=0, there is an instability ($\omega = 0$) 2/3 of the way to the zone boundary; the system breaks up now into three separate chains comprising third neighbors.

2. Debye Model of Phonons. 20 points.
Use the Debye phonon dispersion $\omega(k) = c|\vec{k}|$ for a 3D simple cubic lattice.
(a) Determine the Debye wavevector k_D such that the "Debye sphere" contains the same number of states as the Brillouin zone does. Express it in terms of the lattice constant a.
Answer. The distribution of states in k-space ("density of states in k-space") is constant, hence the condition of equal number of states reduces to finding the Debye sphere with the same volume as the Brillouin zone:

$$\frac{4\pi}{3}k_D^3 = (\frac{2\pi}{a})^3 \rightarrow (k_D a)^3 = 6\pi^2.$$

Simple cubic was given, hence the Brillouin zone volume that was used.
(b) Evaluate the density of states *per primitive cell* $\rho(\omega)$. Assume that all three branches are "degenerate," that is, they all have the same energy, *i.e.* they are identical.
Answer. For the N unit cell system ("sample"),

$$\begin{aligned}\rho(\omega) &= 3\sum_k \delta(\omega - ck) = 3\frac{V}{(2\pi)^3}\int_0^{k_D} d^3k\delta(\omega - ck) = 3\frac{V}{(2\pi)^3}\int_0^{k_D} d^3k\frac{\delta(k-\omega/c)}{|c|} \quad (1)\\ &= 3\frac{V}{(2\pi)^3}4\pi k(\omega)^2\frac{1}{c} = 3\frac{Na^3}{(2\pi)^3}3\frac{4\pi}{3}k_D^3\frac{\omega^2}{\omega_D^3} = 9N\frac{\omega^2}{\omega_D^3}.\end{aligned}$$

(c) Sketch the result, showing the correct behavior both as $\omega \rightarrow 0$ and $\omega \rightarrow \omega_D \equiv ck_D$.
Answer. It is a continuous curve starting from ω=0, and going as ω^3 out to ω_D, where it ends (discontinuously). It does not diverge to infinity.

3. Einstein Oscillators and Internal Energy. 20 points.
(a) Write the Bose-Einstein thermal occupation function, defining what it is and what enters it.
Answer. $n(\omega) = 1/(e^{\hbar\omega/k_b T} - 1)$. This is the relative probability in thermal equilibrium at temperature T that a state with frequency ω (energy $\hbar\omega$) will be occupied (excited).
(b) Consider an Einstein optical branch $\omega(k) = \Omega$, a constant. First write the density of states for a system of N oscillators in a volume V.
Answer. Simple way: all oscillators are at frequency $\omega = \Omega$, hence the density of states is proportional to $\delta(\omega - \Omega)$. The integral over all states (all frequencies) must be the total number of oscillators, which is given in the question as N. Thus

$$\rho(\omega) = N\delta(\omega - \Omega),$$

because the integral over the δ-function will be one. This is the density of states for the volume V corresponding to N oscillators.
(c) Then evaluate the energy $U(T)$ of the vibrational system. Point out its high temperature and low temperature limits, and argue why these results make physical sense.

Answer. The energy $U(T)$ is the sum over all states, times the energy of the state, times the probability that it is thermally occupied:

$$U(T) = \int d\omega \rho(\omega)\ \hbar\omega\ n(\omega) = N\hbar\Omega \frac{1}{e^{\hbar\Omega/k_b T} - 1}.$$

Low T implies $\hbar\Omega >> k_B T$ so $n(\omega) \rightarrow exp(-\hbar\Omega/k_B T)$.
High T implies $\hbar\Omega << k_B T$ so $n(\omega) \rightarrow 1/(1 + [\hbar\Omega/k_B t] + ... - 1) = k_B T/\hbar\Omega$.
Then for low T: $U(T) = N\hbar\Omega exp(-\hbar\Omega/k_B T)$ and get exponentially small at $T \rightarrow 0$: none of the states (at the finite frequency Ω) are occupied.
For high T: $U(T) \rightarrow Nk_B T$, the result from classical physics; the heat capacity is Nk_B.

4. Debye Specific Heat. 5 points.
Given: in 2D the phonon density of states of an elemental simple square lattice is $\rho(\omega) = P\omega$ per unit cell, in the Debye approximation.
(a) Determine the constant P such that the "Debye circle" contains the correct number of states.
Answer. Simple way: use the fact that the integral over all states, which can be done as an integral over all frequencies including the density of states per unit frequency, must integrate to the total number of oscillators. The total number of oscillators for an elemental (one atom per cell) simple square (2D) lattice is 2/cell. Thus

$$2 = \int^{\omega_D} P\omega d\omega = \frac{P}{2}\omega_D^2 \rightarrow P = \frac{4}{\omega_D^2}.$$

One can of course go back to the Debye spectrum $\omega(k) = ck$ and calculate $\rho(\omega)$ directly and get the same result.
(b) Write the expression in general form for the heat capacity per unit cell, in terms of the dispersion relation, cell parameters, etc.
Answer. General expression: $U(T)$ is the sum over all states of the energy, times the probability that the state is thermally excited (occupied); then the heat capacity is the temperature derivative.

$$C_V = \frac{d}{dT}\sum_k \hbar\omega(k) n(\omega(k)) = \frac{d}{dT}\int d\omega \rho(\omega)\hbar\omega n(\omega).$$

Either answer is a correct general expression. The derivative of course acts only on $n(\omega)$ and can be taken inside the sum/integral if desired.
(c) What is the T-dependence of the phonon heat capacity for a 3D solid in the lot-T limit (which is given correctly by the Debye model).
Answer. This is something that you should remember, and all that is wanted is the answer; you probably won't have time to work it out and are not expected to (on the in-class exam). The low T heat capacity of solids is normally fit to the form $C = \gamma T + \beta T^3$,

with the first term giving the *electronic contribution* and the second giving the phonon part (1D form).
Of course on a takehome exam you have the time. This is worked out in detail in the text (pp. 135-136): $C_V \propto T^3$.

5. Free Electron Gas (FEG). 10 points.
Consider a 1D free electron gas.
(a) Consider the energy derivative $df/d\varepsilon$ of the Fermi-Dirac thermal distribution function in the T=0 case. Show that it is proportional to the δ-function $\delta(\varepsilon - \varepsilon_F)$, and find the proportionality constant. Refer to the defining properties of the δ-function.
Answer. For T=0, $f(E) = 1$ for $E < E_F$ and $f(E) = 0$ for $E > E_F$, and it is discontinuous at $E = E_F$. Thus its derivative is zero everywhere except at $E = E_F$, where it is undefined. Hmmmmm...almost like the δ-function. Integrate:

$$\int_{-\varepsilon}^{\varepsilon} \frac{df(E)}{dE} dE = f(\varepsilon) - f(-\varepsilon) = 0 - 1 = -1,$$

where ε can be any positive number. Thus df/dE has the properties of the δ-function except for the minus sign: $-\frac{df(E)}{dE} = \delta(E - E_F)$. It is instructive to plot $-\frac{df(E)}{dE}$ versus E for several temperatures (set E_F=0 for plotting, and see how its behavior (continuous for any finite T) approaches that of the δ-function.
(b) Write the FEG dispersion relation, then calculate the density of states.
Answer. $E_k = \hbar^2 k^2/2m$ is the starting point.

$$\begin{aligned} \rho(E) &= 2\sum_k \delta(E - E_k) = 2\frac{L}{2\pi}\int_{-\infty}^{\infty} dk\delta(E - E_k) = 2 \times 2\frac{L}{2\pi}\int_0^{\infty} dk \frac{\delta(k - k(E))}{|\nabla_k E_k|} \quad (2) \\ &= 4\frac{L}{2\pi}\int_0^{\infty} dk \frac{\delta(k - k(E))}{\hbar^2 |k(E)|/m} = L\frac{2m}{\pi\hbar^2}\sqrt{\frac{\hbar^2}{2mE}}. \end{aligned}$$

The constants can be gathered; the essential result is $\rho(E)/V \propto 1/\sqrt{(E)}$ in one dimension.
(c) Suppose the electron density of states for some system has the form $\rho(E) = AE^g$, where g is a positive constant. For a Fermi energy $E_F >> k_B T$, what is the T-dependence of the heat capacity to lowest order (smallest exponent of T)? Hint: this is a rather simple question, don't do a lot of calculating because you don't need to.
Answer. OK, perhaps not simple in the way one might think, but the result was discussed in the text in some detail in the free electron section. Answer: The given function of $\rho(E)$ is a smooth function of E around the Fermi enegy $E_F >> k_B T$. The temperature dependence enters the heat capacity only through $df(E)/dT$ which is strongly peaked at

E_F. The internal energy $U(T)$ is a constant plus a T^2 term, the latter depending only on $\rho(E_F)$ and does not even depend on dimension! Thus $C_V \propto T$.

6. Liquid Helium. 10 points.
Liquid ^{3}He (helium) is a fermion (spin 1/2) and, perhaps surprisingly, is a very good "free fermion gas", i.e. free electron gas except no electric charge. But we have nelgected interactions anyway. Its **mass** density is 0.08 g/cm^3. Calculate the Fermi wavevector k_F and Fermi energy E_F; what is the corresponding Fermi temperature? Helpful numbers: $\hbar \approx 10^{-27} erg\ s$, electron mass $m \approx 0.9 \times 10^{-27} g$. Also, $\hbar/m \approx 1.2\ cm^2/s$, and 1 eV = $1.6{\times}10^{-12} erg$. Make numerical approximations, no calculator, answer within a factor of ten is fine. *Remember*, this is ^{3}He!
Answer. One must use the He mass here; the electron mass was given explicitly expecting you to know that the protom mass $M_p \approx 2000 m_e$, and of course ^3He mass $M = 3M_p$. The mass density was given, to convert it to the *number density*, which is what is crucial in the free fermion gas one only needs the value of M. It converts to n=$1.5{\times}10^{22}/\mathrm{cm}^3$. Then $k_F = (3\pi^2 n)^{1/3} \approx 7{\times}10^7/cm = 0.7\mathring{A}^{-1}$. From this follows $E_F = \hbar^2 k_F^2/2M \approx (1/3)$ meV. Using 1 meV $\approx$ 12 K gives for ^3He: $T_F \approx 4$ K. The superfluid transition in ^3He in fact occurs only when T<<T_F, around T = 1 mK!