PHY555 Fall 2007 Midterm Exam Friday October 26 10:30-11:25

1. Consider N atoms of type A located at positions $x=a_n=2nc$ $(n=1,2,...N)$, and an equal number of type B located at $x=b_n=(2n+1)c$. Each atom has one electron and one orbital, $\psi_A(x-a_m)=|mA>$, and $\psi_B(x-b_p)=|pB>$. Orbitals are all orthonormal, $<mA|nA>= \delta_{mn}$, $<mB|nB>=\delta_{mn}$, and $<mA|nB>=0$. There are periodic boundary conditions on the wavefunctions $\psi(x+2Nc)=\psi(x)$. The Hamiltonian for each electron is $H=p^2/2m+V(x)$ where $V(x+2a)=V(x)$. The Hamiltonian matrix elements are $<mA|H|nA>=\delta_{mn}\varepsilon_A$, $<mB|H|nB>=\delta_{mn}\varepsilon_B$, and $<mA|H|nB>=0$ unless a_m and b_n are nearest neighbors, in which case $<mA|H|nB>=-t$. Find the Bloch state eigenvalues $\varepsilon_n(k)$, and sketch $\varepsilon_n(k)/t$ for the case t=1 eV and ε_A-ε_B=t.
2. The graph below is from a neutron scattering experiment on solid crystalline (rare gas) krypton (M_{Kr}=83.8 amu). The paper is J. Skalyo, Y. Endoh, and G. Shirane, Phys. Rev. B **9**, 1797 (1974). Kr has fcc crystal structure, and lattice constant a=5.7Å

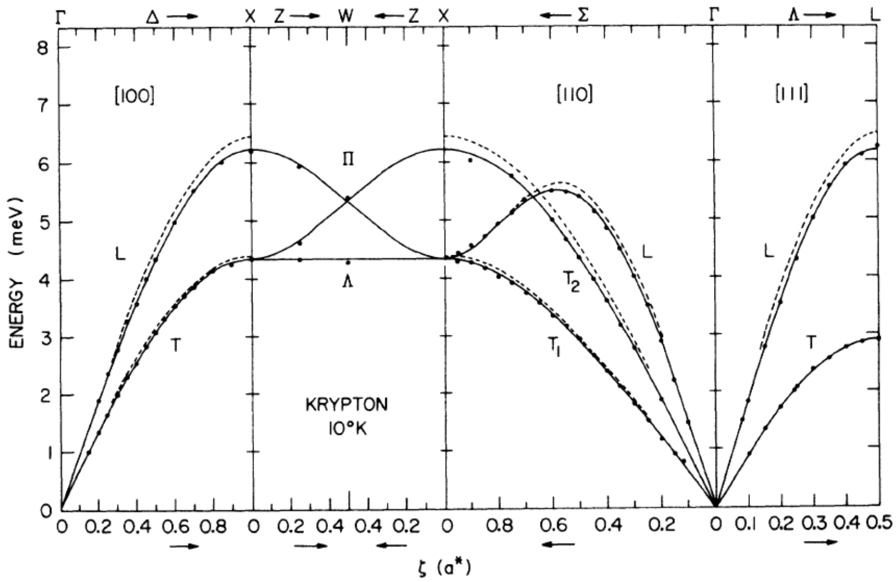

FIG. 3. Phonon dispersion of krypton at 10°K. ζ is the reduced wave vector. The solid line is a three-nearest-neighbor general force-constant fit to the data and the dashed line is a theoretical calculation by Barker *et al.* (Ref. 8).

a. At what temperature T are you approximately in the classical limit for heat capacity?
b. What is the value of the classical heat capacity (in J/moleK and in J/kgK)?
c. The left-most panel (Γ to X along Δ) is the (100) direction, and the point "X" is the Brillouin zone boundary along (100) with $k=(2\pi/a)(1,0,0)$. What is the velocity of longitudinally-polarized sound (in m/s) in this direction?
d. Why are only two branches shown in the left and right, while three are shown in the two middle panels?
e. Are there "optical" phonons not shown here?
f. Estimate the magnitude $\sqrt{<u^2>}$ of zero point vibration of Kr atoms in this crystal.
g. Make an intelligent guess about the energy gap E_g for electronic excitations in Kr.