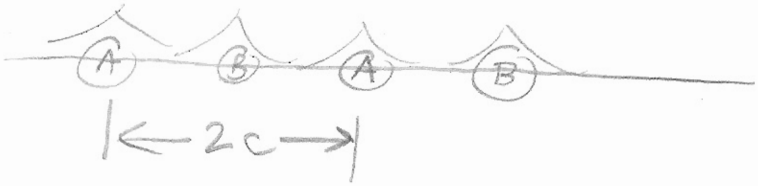
Physics 555 Midterm 10/26/07 answers



The lattice constant $a = 2c$

k-vectors obey $e^{ik\cdot 2Nc} = e^{ik\cdot Na} = 1$

$k = \frac{2\pi}{Na} \times$ integer. Brillouin Zone is $-\frac{\pi}{a}$ to $\frac{\pi}{a}$

or $-\frac{\pi}{2c}$ to $\frac{\pi}{2c}$

Bloch basis functions are

$$|kA\rangle = \frac{1}{\sqrt{N}} \sum_n e^{ik\cdot 2nc} |nA\rangle$$

$$|kB\rangle = \frac{1}{\sqrt{N}} \sum_p e^{ik\cdot(2p+1)c} |pB\rangle$$

These are orthonormal. also H is k-diagonal.

$\langle kA|\mathcal{H}|k', A \text{ or } B\rangle = 0$ unless $k = k'$

$$\psi_{kn} = C_A(k)|kA\rangle + C_B(k)|kB\rangle$$

where $\mathcal{H}\begin{pmatrix} C_A \\ C_B \end{pmatrix} = \epsilon \begin{pmatrix} C_A \\ C_B \end{pmatrix}$ and $\mathcal{H} = \begin{pmatrix} \langle kA|H|kA\rangle & \langle kB|H|kA\rangle \\ \langle kA|H|kB\rangle & \langle kB|H|kB\rangle \end{pmatrix}$

$$\langle kA|H|kA\rangle = \frac{1}{N}\sum_{nm} (\ )^*(\ )\langle nA|H|mA\rangle = \epsilon_A$$

$$\langle kA|H|kB\rangle = \epsilon_B$$

$$\langle kA|H|kB\rangle = \frac{1}{N}\sum_{nm} \left(e^{ik2nc}\right)^*\left(e^{ik(2m+1)c}\right)\langle nA|H|mB\rangle$$

2m+1 must equal 2n ± 1

$$= \left(e^{ikc} + e^{-ikc}\right)(-t)$$

$$= -2t\cos kc$$

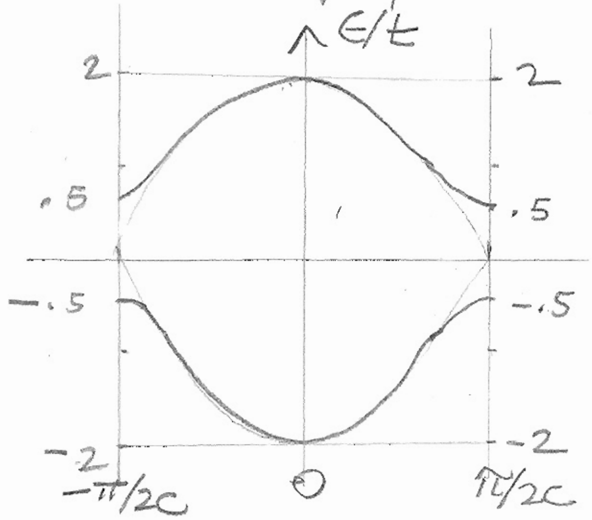
$$H = \begin{pmatrix} \epsilon_A & -2t\cos kc \\ -2t\cos kc & \epsilon_B \end{pmatrix}$$

$$\epsilon_{nk} = \frac{\epsilon_A + \epsilon_B}{2} \pm \sqrt{\left(\frac{\epsilon_A - \epsilon_B}{2}\right)^2 + (2t\cos kc)^2}$$

choose $\frac{\epsilon_A + \epsilon_B}{2} = 0$, $\epsilon_A - \epsilon_B = t$

$$\epsilon_{nk}/t = \pm\sqrt{\frac{1}{4} + 4\cos^2 kc} \approx 2|\cos kc| \text{ unless}$$

kc is close to $\pi/2$



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

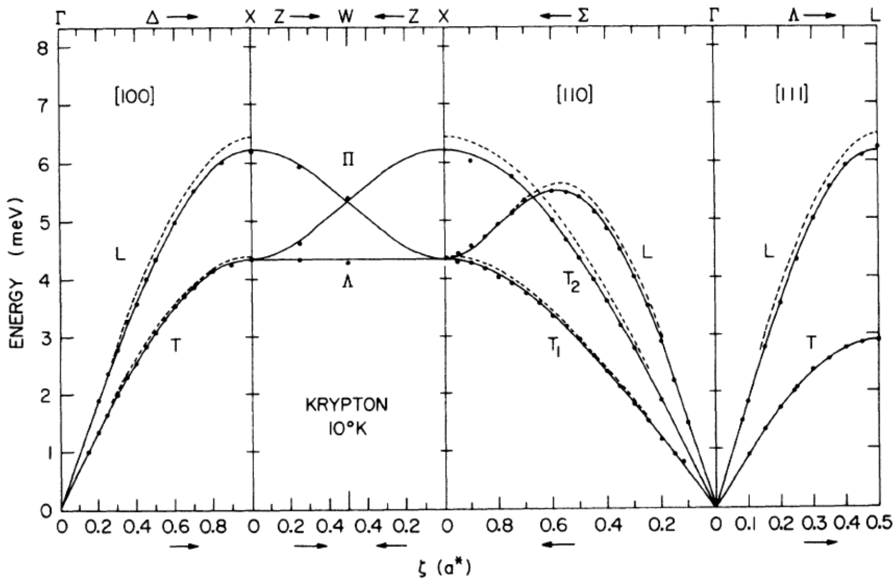


FIG. 3. Phonon dispersion of krypton at 10°K. ζ is the reduced wave vector. The solid line is a three-nearest-neighbor general force-constant fit to the data and the dashed line is a theoretical calculation by Barker *et al.* (Ref. 8).

a. At what temperature T are you approximately in the classical limit for heat capacity?
   6 meV corresponds to 45 K, so for T > 45 K, it's fairly classical.
b. What is the value of the classical heat capacity (in J/moleK and in J/kgK)?
   $3N_Ak_B$ = 24.9 J/molK. There are 1000/83.8 moles per kg, so 297 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?
   I get the slope of the LA branch in the left panel to be 126 m/s (slow for a solid.)_
d. Why are only two branches shown in the left and right, while three are shown in the two middle panels?
   The TA branch is doubly degenerate along (100) and (111).
e. Are there "optical" phonons not shown here?
   No. fcc crystal structure has 1 atom per primitive cell.
f. Estimate the magnitude $\sqrt{\langle u^2\rangle}$ of zero point vibration of Kr atoms in this crystal.
   $\sqrt{\hbar/2M\omega}$=0.10Å if you take ω=4 meV
g. Make an intelligent guess about the energy gap E_g for electronic excitations in Kr.
   Bigger than 10 eV, less than 20 eV. The 1s to 2s excitation of He is 22 eV(?) and Kr should have a smaller value.