Solid State Physics HW 7

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Problem 1

Consider transverse vibrations of a square lattice with a distance between nn atoms to be "a". All atoms and force constants are equal (mass M and force constant C respectively). Find the equation of motion for nearest neighbor coupling and determine the dispersion relations. Determine the first Brillouin zone. What is the maximum magnitude of the k vector? Draw 6 equipotential lines (k-points with equal energy), approximately evenly spaced between a minimum and maximum values of k.

See attached sketch for details on the equations of motion on the square lattice. We have that the maximum allowed values for k are $k = \pm\frac{\pi}{a}$ and so the first Brillouin zone is the region in $\mathbb{R}^2$ given by $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right] \times \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$. The equation of motion for nearest neighbor coupling is given by

$$M\frac{d^2u_{m,n}}{dt^2} = C[u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{n,m}]$$

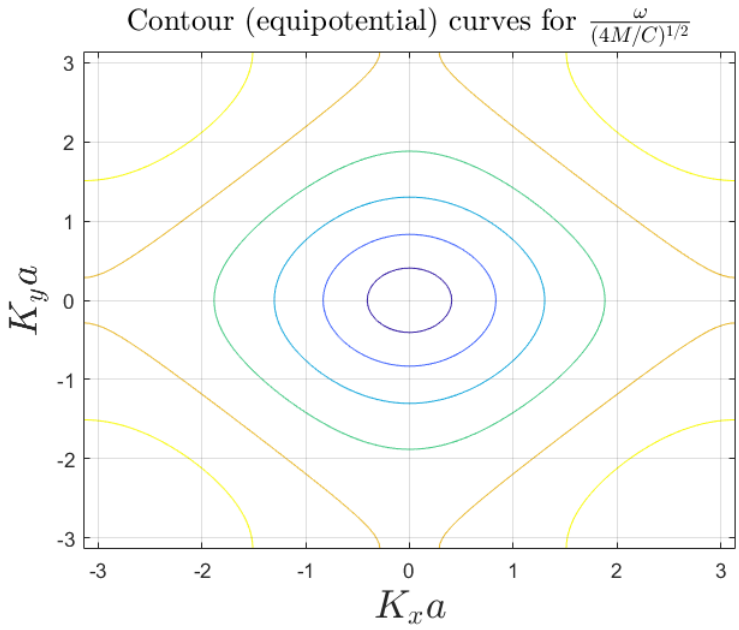
We seek traveling wave solutions of the form

$$u_{m,n} = u_0 e^{i(mk_xa + nk_ya - \omega t)}$$

Then substituting this into our equation of motion, we find

$$\begin{aligned}
-\omega^2 M &= C\left[e^{ik_xa} + e^{-1k_xa} + e^{ik_ya} + e^{-ik_ya} - 4\right] \\
&= [2\cos(k_xa) + 2\cos(k_ya) - 4] \\
\omega^2 &= \frac{2C}{M}[(1 - \cos(k_xa)) + (1 - \cos(k_ya))] \\
&= \frac{4C}{M}\left[\sin^2\left(\frac{1}{2}k_xa\right) + \sin^2\left(\frac{1}{2}k_ya\right)\right] \\
\omega &= \pm\sqrt{\frac{4C}{M}}\left[\sin^2\left(\frac{1}{2}k_xa\right) + \sin^2\left(\frac{1}{2}k_ya\right)\right]^{1/2}
\end{aligned}$$

And finally, below is a plot for 6 equipotential curves:



Problem 5.1

Singularity in density of states. (a) From the dispersion relation derived in Chapter 4 for a monatomic linear lattice of N atoms with nearest-neighbor interactions, show that the density of modes is

$$\mathcal{D}(\omega) = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}}$$

where ω_m is the maximum frequency.

Recall from Chapter 4 that the dispersion relation for a monatomic linear lattice of N atoms is given by

$$\omega = \sqrt{\frac{4C}{M}} \sin^2 (1/2Ka)$$

Clearly, from the above equation, we have $\omega_m = 4C/M$. Solving this equation for K, we find

$$K = \frac{2}{a} \arcsin \left(\frac{\omega}{\omega_m} \right)$$

Then

$$\begin{aligned} \frac{dK}{d\omega} &= \frac{2}{a} \left(\frac{1}{(1 - \omega^2/\omega_m^2)^{1/2}} \right) \left(\frac{1}{\omega_m} \right) \\ &= \frac{2}{a} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}} \end{aligned}$$

Then our density of states takes the form

$$\mathcal{D}(\omega) = \frac{2L}{\pi a} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}}$$

And since $L = Na$ for a linear lattice, we have

$$\mathcal{D}(\omega) = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}}$$

Which is what we wanted to show.

(b) Suppose that an optical phonon branch form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $\mathcal{D}(\omega) = (L/(2\pi))^3(2\pi/A^{3/2})(\omega_0 - \omega)^{1/2}$ for $\omega < \omega_0$ and $\mathcal{D}(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

To begin, suppose that $\omega < \omega_0$ and recall that for a three dimensional cubic lattice that

$$\mathcal{D}(\omega) = \frac{\partial N}{\partial \omega}$$

and

$$N = \frac{4\pi}{3} K^3 \left(\frac{L}{2\pi}\right)^3$$

Thus,

$$\begin{aligned}
\frac{\partial N}{\partial \omega} &= 4\pi K^2 \frac{\partial K}{\partial \omega} \left(\frac{L}{2\pi}\right)^3 \\
\frac{\partial K}{\partial \omega} &= \frac{\partial}{\partial \omega} \left(\frac{\omega_0 - \omega}{A}\right)^{1/2} \\
&= -\frac{1}{2A^{1/2}(\omega_0 - \omega)^{1/2}}
\end{aligned}$$

so

$$\begin{aligned}
\frac{\partial N}{\partial \omega} &= 4\pi \left(\frac{L}{2\pi}\right)^3 \frac{\omega_0 - \omega}{A} \frac{-1}{2A^{1/2}(\omega_0 - \omega)^{1/2}} \\
&= \left(\frac{L}{2\pi}\right)^3 \left(\frac{2\pi}{A^{3/2}}\right) \frac{\omega_0 - \omega}{(\omega_0 - \omega)^{1/2}} \\
&= \left(\frac{L}{2\pi}\right)^3 \left(\frac{2\pi}{A^{3/2}}\right) (\omega_0 - \omega)^{1/2}
\end{aligned}$$

Thus $\mathcal{D}(\omega) = (L/2\pi)^3(2\pi/A^{3/2})(\omega_0 - \omega)^{1/2}$ which is what we wished to show.

Problem 5.2

Rms thermal dilation of crystal cell. (a) Estimate for 300 K the root mean square thermal dilation $\Delta V/V$ for a primitive cell of sodium. Take the bulk modulus as 7×10^{10} erg cm^{-3}. Note that the Debye temperature 158 K is less than 300 K, so that the thermal energy is of the order of $k_B T$.

Recall that $U_{thermal} = \frac{1}{2} B \delta^2 a^3$ where $\delta \equiv \Delta V/V$. We also have that $U_{thermal} = \frac{1}{2} k_b T$, so we have

$$\frac{1}{2} B \left(\frac{\Delta V}{V}\right)^2 a^3 = \frac{1}{2} k_b T$$

Solving, we have

$$\frac{\Delta V}{V} = \sqrt{\frac{k_b T}{B a^3}}$$

Using $k_b = 1.38062 \times 10^{-16}$ erg K^{-1}, we find

$$\frac{\Delta V}{V} \approx 0.0886$$

(b) Use this result to estimate the root mean square thermal fluctuation $\Delta a/a$ of the lattice parameter.

In the limit where ΔV is "small", we have $\Delta V/V = 3\Delta a/a$, so from part (a), we find

$$\frac{\Delta a}{a} \approx 0.02953$$

Problem 4

Grüneisen Parameter. Calculate the Grüneisen parameter, $\gamma = -d\ln(\omega)/d\ln(L)$, for a linear chain of length L, lattice spacing a, and only nearest-neighbor interaction. Assume that the interaction potential has a form of $U(x) = U_0 + 0.5\kappa x^2 + \lambda x^3$, where $x = d - a$, and d is the distance between nearest neighbors.

To begin, recall that the maximum frequency for the equation of motion for a linear lattice is given by $\omega_m = \sqrt{4C/M}$. For us, our force constant is given by $C = F = -dU/dx = -\kappa x - 3\lambda x^2$. Rewriting, we see

$$F = -x(\kappa + 3\lambda x^2)$$

which is of the form of Hooke's law with spring (force) constant $\kappa + 3\lambda x^2$. Thus ω_m takes the form

$$\omega_m = \sqrt{\frac{4(\kappa + 3\lambda x)}{M}}$$

Now, the Grüneisen parameter is given by (using the chain rule):

$$\gamma = -\frac{L}{\omega}\frac{d\omega}{dL}$$

Further using the chain rule, we have

$$\frac{d\omega}{dL} = \frac{1}{2\sqrt{4(\kappa + 3\lambda x)/M}}\left(3\lambda \frac{dx}{dL}\right)$$

Since $x = d - a$, and we have a one dimensional lattice of length L with lattice spacing a, we have $N = aL$ where N is the number of atoms in the lattice. Solving for a, we have $a = L/N$ and so $x = d - L/N$ and $dx/dL = -1/N$. Thus,

$$-\frac{L}{\omega}\frac{d\omega}{dL} = -\frac{L}{\omega}\frac{1}{2\sqrt{4(\kappa + 3\lambda x)/M}}\left(-\frac{3\lambda}{N}\right)$$

$$\gamma = \frac{3L\lambda}{2N}$$