Solid State Physics

112-1 Second-Term Exam

Fermi-Dirac distribution function at low temperatures. The electrons in a metal obey the Fermi-Dirac distribution

$$n_F(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1}.$$

(1) Find the Fermi-Dirac distribution function $n_F^0(\varepsilon)$ at $T = 0$ by taking explicitly the $T \to 0$ limit of $n_F(\varepsilon)$. Note that $\mu(T = 0) \equiv \varepsilon_F$.

(2) Plot $n_F^0(\varepsilon)$ and $n_F(\varepsilon)$ as functions of $\varepsilon/\varepsilon_F$. For $n_F(\varepsilon)$, neglect the temperature dependence of μ and plot it at $T = 0.01\varepsilon_F/k_B$ and $T = 0.1\varepsilon_F/k_B$.

(3) Differentiate $n_F(\varepsilon)$ with respect to ε. Plot $-\partial n_F(\varepsilon)/\partial\varepsilon$ as a function of $\varepsilon/\varepsilon_F$ at $T = 0.01\varepsilon_F/k_B$, neglecting the temperature dependence of μ.
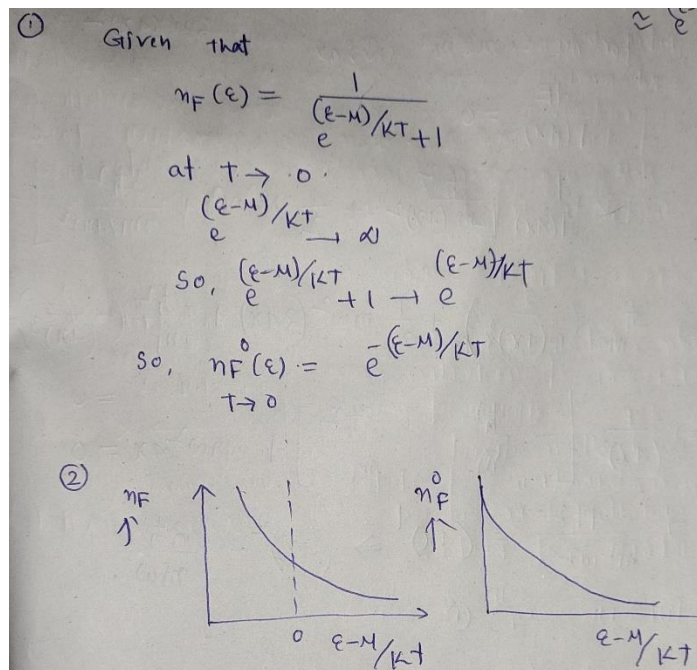
Phonon density of states for an optical branch. Assume that the dispersion relation of an optical phonon branch in a solid takes on the form $\omega(k) = \omega_0 - Ak^2$ near $k = 0$, where ω_0 and A are positive constants. Find the phonon density of states for $\omega < \omega_0$ and $\omega > \omega_0$, respectively.

$$g(\omega) = \frac{1}{\mathcal{V}} \sum_k \delta\big(\omega - \omega(k)\big)$$

Explanation:

Step 1: Define the Problem For an optical phonon branch, we are given the quadratic dispersion relation $\omega(k) = \omega 0 - A \times k^2$, where $\omega 0$ and A are constants.

Finding the phonon density of states for both $\omega > \omega 0$ and $\omega < \omega 0$ is our objective.

Step 2: Relation of Dispersion

A parabolic curve with a downward opening in k-space represents the dispersion relation that is given. There will be two equivalent k values, a positive and a negative one, for each frequency ω below $\omega 0$.

Step 3: Formula for Density of States (DOS)

The formula $g(\omega) = \left(\frac{1}{V}\right) \times$ sum over k of $\delta(\omega - \omega(k))$ defines the phonon density of states, $g(\omega)$. Here, V represents the solid's volume and δ is the Dirac delta function.

Explanation:

Step 4: Calculating k We solve the equation $\omega = \omega 0 - A \times k^2$ for k when ω is smaller than $\omega 0$. Two solutions for k are obtained as a result: $k = \sqrt{\frac{\omega 0 - \omega}{A}}$ and $k = -\sqrt{\frac{\omega 0 - \omega}{A}}$.

Using the Delta Function in Step Five

Selecting values of k for which the dispersion relation matches the frequency ω is done using the delta function, $\delta(\omega - \omega(k))$. There are two such k values for each ω, hence both should be included in the density of states.

Explanation:

Step 6: Totaling States

Formally, the density of states is expressed as the sum of the delta functions at the k solutions. Given the continuous nature of the k states, in reality this would be converted into an integral over the Brillouin zone to account for the actual density of states.

Procedure 7: DOSf or $\omega > \omega 0$

The equation $\omega = \omega 0 - A \times k^2$ does not have any real k solutions when ω is larger than $\omega 0$, suggesting that the density of states $g(\omega)$ is zero at these frequencies.

In practice, the density of states would be computed by integrating the delta function over k while accounting for the shape of the Brillouin zone; however, this overview does not include such intricate computations. Two k states are found to be contributing to the DOS for frequencies below $\omega 0$, whereas the contribution is zero for frequencies above $\omega 0$.

To sum up,
the answer describes how to determine the phonon density of states with a quadratic dispersion relation. It outlines the essential procedures, including summing over k values, utilizing the Dirac delta function, and solving for k. It also says that at frequencies above $\omega 0$, the density of states is zero. In-depth computations would need to integrate over the Brillouin zone and take into account the unique properties of the system.

2-3 Approximate expression for the Fermi-Dirac distribution function. The internal energy density of the electron gas in a metal at temperature T is given by $u = \int_0^\infty d\varepsilon\, \varepsilon g(\varepsilon) n_F(\varepsilon)$ with $g(\varepsilon)$ the density of states per unit volume. The Fermi-Dirac distribution function $n_F(\varepsilon)$ is here approximated as

$$n_F(\varepsilon) = \begin{cases} 1, & \varepsilon < \varepsilon_F - 2k_B T, \\ 1/2 - (\varepsilon - \varepsilon_F)/4k_B T, & \varepsilon_F - 2k_B T \le \varepsilon \le \varepsilon_F + 2k_B T, \\ 0, & \varepsilon > \varepsilon_F + 2k_B T. \end{cases}$$

Compute the specific heat per unit volume of the electron gas, $c_v = \partial u/\partial T$, to the lowest order in $k_B T/\varepsilon_F$.

Solution

$$U = \int_0^\infty \varepsilon\, g(\varepsilon)\, n_F(\varepsilon)\, d\varepsilon \qquad g(\varepsilon) = \frac{g(\varepsilon)}{V}$$

where $g(\varepsilon)$ - density of states per unit volume

$$g(\varepsilon) = \frac{Vm^{3/2}}{\pi^2\hbar^3}\sqrt{2\varepsilon} \qquad \text{or } g(\varepsilon) = \frac{g(\varepsilon)}{V} \propto \sqrt{\varepsilon} \quad \Rightarrow \quad g(\varepsilon) \propto \sqrt{\varepsilon}$$

Fermi-Dirac distribution function given as -

$$n_F(\varepsilon) = \begin{cases} 1 & \varepsilon < \varepsilon_F - 2k_B T \\ \frac{1}{2} - \left(\frac{\varepsilon - \varepsilon_F}{4k_B T}\right) & \varepsilon_F - 2k_B T \le \varepsilon \le \varepsilon_F + 2k_B T \\ 0 & \varepsilon > \varepsilon_F + 2k_B T \end{cases}$$

$$\Rightarrow U = \int_0^{\varepsilon_F - 2k_B T} \varepsilon\, g(\varepsilon)(1)\, d\varepsilon + \int_{\varepsilon_F - 2k_B T}^{\varepsilon_F + 2k_B T} \varepsilon\, \frac{m^{3/2}}{\pi^2 \hbar^2}\sqrt{2\varepsilon}\left[\frac{1}{2} - \frac{(\varepsilon - \varepsilon_F)}{4k_B T}\right] d\varepsilon \quad + \; 0$$

$$\Rightarrow \quad \text{Let} \quad A = \frac{\sqrt{2}\, m^{3/2}}{\pi^2 \hbar^3}$$

Now,

$$U = A \int_0^{\varepsilon_F - 2k_B T} \varepsilon^{3/2}\, d\varepsilon + A \int_{\varepsilon_F - 2k_B T}^{\varepsilon_F + 2k_B T} \varepsilon\sqrt{\varepsilon}\left(\frac{1}{2} - \frac{\varepsilon}{4k_B T} + \frac{\varepsilon_F}{4k_B T}\right) d\varepsilon$$

$$= A\,\frac{2}{5}\varepsilon^{5/2}\Big|_0^{\varepsilon_F - 2k_B T} + A\left[\int_{\varepsilon_F - 2k_B T}^{\varepsilon_F + 2k_B T}\frac{1}{2}\varepsilon^{3/2}\,d\varepsilon - \int\frac{\varepsilon}{4k_B T}d\varepsilon + \frac{\varepsilon_F}{4k_B T}\int\varepsilon^{3/2}d\varepsilon\right]$$

$$= \frac{2A}{5}[\varepsilon_F - 2k_B T]^{5/2} + \frac{A}{2}\times\frac{2}{5}\varepsilon^{5/2}\Big|_{\varepsilon_F - 2k_B T}^{\varepsilon_F + 2k_B T} - \frac{2A}{7(4k_B T)}\varepsilon^{7/2}\Big|_{\varepsilon_F - 2k_B T}^{\varepsilon_F + 2k_B T}$$

$$+ \frac{A\varepsilon_F}{4k_B T}\cdot\frac{2}{5}\varepsilon^{5/2}\Big|_{\varepsilon_F - 2k_B T}^{\varepsilon_F + 2k_B T}$$

$$= \frac{2A}{5}(\varepsilon_F - 2k_B T)^{5/2} + \frac{A}{5}(\varepsilon_F + 2k_B T)^{5/2} - \frac{A}{5}(\varepsilon_F - 2k_B T)^{5/2} - \frac{2A}{7(4k_B T)}$$

$$\left(\varepsilon_F + 2k_B T\right)^{7/2} - \frac{2A}{7(4k_B T)}(\varepsilon_F - 2k_B T)^{7/2} + \frac{2A\varepsilon_F}{5(4k_B T)}\left[\frac{(\varepsilon_F + 2k_B T)^{5/2}}{(\varepsilon_F - 2k_B T)^{5/2}}\right]$$

$$= \frac{2A}{5}(\varepsilon_F - 2k_B T)^{5/2}\left\{1 - \left(\frac{1}{2} + \frac{\varepsilon_F}{4k_B T}\right) - \frac{5}{7}\cdot\frac{1}{4k_B T}(\varepsilon_F - 2k_B T)\right\} +$$

$$\frac{2A}{5}(\varepsilon_F + 2k_B T)^{5/2}\left\{\left(\frac{1}{2} + \frac{\varepsilon_F}{4k_B T}\right) + \frac{5}{7}\cdot\frac{1}{4k_B T}(\varepsilon_F + 2k_B T)\right\}$$

$$= \frac{2A}{5}\left\{(\varepsilon_F - 2k_B T)^{5/2}\left(\frac{6}{7} - \frac{12}{7}\frac{\varepsilon_F}{4k_B T}\right)\right\} + \frac{2A}{5}(\varepsilon_F + 2k_B T)^{5/2}\left\{\frac{6}{7} + \frac{12}{7}\frac{\varepsilon_F}{4k_B T}\right\}$$

$$= \frac{2A}{5}\left\{\varepsilon_F^{5/2}\left(1 - \frac{2k_B T}{\varepsilon_F}\right)^{5/2}\left(\frac{6}{7} - \frac{12}{7}\frac{\varepsilon_F}{4k_B T}\right)\right\} + \frac{2A}{5}\left\{\varepsilon_F^{5/2}\left(1 + \frac{2k_B T}{\varepsilon_F}\right)^{5/2}\left(\frac{6}{7} + \frac{12\varepsilon_F}{7\,4k_B T}\right)\right\}$$

$$= \frac{2A}{5}\left\{\varepsilon_F^{5/2}\left(1 - \frac{10k_B T}{2\varepsilon_F}\right)\left(6 - 12\frac{\varepsilon_F}{4k_B T}\right)\right\} + \frac{2A}{5}\left\{\frac{\varepsilon_F^{5/2}}{7}\left(1 + \frac{10 k_B T}{2\varepsilon_F}\right)\left(6 + 12\frac{\varepsilon_F}{4k_B T}\right)\right\}$$

$$U = \frac{2A}{5}\frac{\varepsilon_F^{5/2}}{7}\left[6 - 12\frac{\varepsilon_F}{4k_B T} - \frac{30k_B T}{\varepsilon_F} + \frac{10}{2}\times\frac{12}{4} + 6 + 12\frac{\varepsilon_F}{4k_B T} + \frac{30k_B T}{\varepsilon_F} + \frac{10}{2}\times\frac{12}{4}\right]$$

$$U = \frac{2A}{5}\frac{\varepsilon_F^{3/2}}{7}\left[12 - 2\times\frac{10}{4}\right]$$

$$U = \frac{2A}{5}\frac{\varepsilon_F^{5/2}}{7}[7]$$

$$U = \frac{2A}{5}\varepsilon_F^{5/2} \qquad \text{(Independent of } T\text{)}$$

$$c_v = \frac{\partial U}{\partial T} = 0 \qquad \text{Ans}$$

2.9 Problem: Debye Frequency

A monoatomic, cubic material has lattice spacing of a. The sound velocity for longitudinal and transverse phonons is approximately equal, $c_T = c_L = c$, is isotropic, and the highest phonon frequency is ω^*. What is the Debye frequency?

[6] This Ansatz is suggested by Ibach and Lüth [4] p. 61.

2.9 Solution: Debye Frequency

The Debye frequency is determined by two conditions:

− the total number of modes
− the sound velocity.

From the total number of modes we obtain the Debye wavenumber, k_D,

$$\frac{4\pi}{3} k_D^3 \left(\frac{L}{2\pi}\right)^3 = N \quad \Longrightarrow \quad k_D = (6\pi^2 n)^{1/3}, \qquad (\text{II.2.41})$$

where n is the number of modes per unit volume ($n = \frac{N}{L^3}$).

The sound velocity converts the Debye wavenumber to the Debye frequency,

$$\omega_D = c k_D = c(6\pi^2 n)^{1/3}. \qquad (\text{II.2.42})$$

Although ω^* and ω_D are typically of the same order of magnitude, there is no firm relationship between the two quantities, and $\omega^* = \omega_D$ happens only by accident.

1. *Monatomic linear lattice.* Consider a longitudinal wave

$$u_s = u \cos(\omega t - sKa)$$

which propagates in a monatomic linear lattice of atoms of mass M, spacing a, and nearest-neighbor interaction C.

(a) Show that the total energy of the wave is

$$E = \tfrac{1}{2} M \sum_s (du_s/dt)^2 + \tfrac{1}{2} C \sum_s (u_s - u_{s+1})^2 .$$

where s runs over all atoms.

(b) By substitution of u_s in this expression, show that the time-average total energy per atom is

$$\tfrac{1}{4} M\omega^2 u^2 + \tfrac{1}{2} C(1 - \cos Ka)u^2 = \tfrac{1}{2} M\omega^2 u^2 ,$$

where in the last step we have used the dispersion relation (

1a. The kinetic energy is the sum of the individual kinetic energies each of the form $\frac{1}{2} M u_s^2$. The force between atoms s and s+1 is $-C(u_s - u_{s+1})$; the potential energy associated with the stretching of this bond is $\frac{1}{2} C(u_s - u_{s+1})^2$, and we sum over all bonds to obtain the total potential energy.

b. The time average of $\frac{1}{2} M u_s^2$ is $\frac{1}{4} M\omega^2 u^2$. In the potential energy we have

$$u_{s+1} = u \cos[\omega t - (s+1)Ka] = u\{\cos(\omega t - sKa)\cdot \cos Ka$$
$$+ \sin(\omega t - sKa)\cdot \sin Ka\}.$$

Then $u_s - u_{s+1} = u\{\cos(\omega t - sKa)\cdot(1 - \cos Ka)$
$- \sin(\omega t - sKa)\cdot \sin Ka\}.$

We square and use the mean values over time:

$$<\cos^2> = <\sin^2> = \frac{1}{2} ; <\cos \sin> = 0.$$

Thus the square of u{} above is

$$\frac{1}{2} u^2[1 - 2\cos Ka + \cos^2 Ka + \sin^2 Ka] = u^2(1 - \cos Ka).$$

The potential energy per bond is $\frac{1}{2} Cu^2(1 - \cos Ka)$, and by the dispersion relation $\omega^2 = (2C/M)(1 - \cos Ka)$ this is equal to $\frac{1}{4} M\omega^2 u^2$. Just as for a simple harmonic oscillator, the time average potential energy is equal to the time-average kinetic energy.

Continuum wave equation. Show that for long wavelengths the equation of motion (2) reduces to the continuum elastic wave equation

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \quad,$$

where v is the velocity of sound.

2. We expand in a Taylor series

$$u(s+p) = u(s) + pa\left(\frac{\partial u}{\partial x}\right)_s + \frac{1}{2}p^2 a^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_s + \cdots ;$$

On substitution in the equation of motion (16a) we have

$$M\frac{\partial^2 u}{\partial t^2} = \left(\sum_{p>0} p^2 a^2 C_p\right)\frac{\partial^2 u}{\partial x^2} \quad,$$

which is of the form of the continuum elastic wave equation with

4-1

$$v^2 = M^{-1} \sum_{p>0} p^2 a^2 C_p.$$

Atomic vibrations in a metal. Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $3/4\pi R^3$, which defines R. (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2/MR^3)^{1/2}$. (b) Estimate the value of this frequency for sodium, roughly. (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in the metal.

PS: F = ma = mω^2r, and coulomb force

(a)

The restoring force is given by Coulomb's law:

$$F = \frac{kq_1q_2}{r^2}$$

Explanation:

where:

- F is the restoring force
- k is Coulomb's constant
- q_1 is the charge of the ion
- q_2 is the charge of the conduction electrons
- r is the distance between the ion and the center of the sphere

In this case, the charge of the conduction electrons is negative, so the restoring force is positive.

This means that the ion will be pulled back to its equilibrium position.

The equation of motion for the ion is:

$$ma = \frac{-kq_1 \times q_2}{r^2}$$

where m is the mass of the ion and a is the acceleration of the ion.

Assuming that the ion is oscillating about its mean position, then linearizing the equation of motion:

$$ma = \frac{-kq_1 \times q_2}{r^0}$$

where r^0 is the mean distance between the center of the sphere and the ion.

The angular frequency of the oscillation:

$$\omega = \sqrt{\frac{kq_1q_2}{mr^0}}$$

Substituting the given values,

$$\omega = \sqrt{\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{e(-e)}{MR^3}}$$

$$\omega = \sqrt{\frac{e^2}{4\pi\varepsilon_0 MR^3}}$$

$$\omega = \left(\frac{e^2}{MR^3}\right)^{\frac{1}{2}}$$

Therefore, the frequency of the ion is:

$$\omega = \left(\frac{e^2}{MR^3}\right)^{\frac{1}{2}}$$

Explanation:

This gives the frequency of the ion.

(b)

The mass of a sodium ion is 22.99 amu. The number density of sodium ions is 2.65×10^{28} ions/m³.

Substituting these values into the equation for the frequency,

$$\omega = \sqrt{\left(\frac{e^2}{4\pi\varepsilon_0 22.99 \text{ amu} 2.65 \times 10^{28}\text{ions/m}^3}\right)^{\frac{1}{2}}}$$

$$\omega = 1.6 \times 10^{12}\text{Hz}$$

Explanation:

Therefore, the frequency of the sodium ion is approximately 1.6 terahertz.

(c)

The velocity of sound in a metal is given by the following equation:

$$v_s = \sqrt{\frac{K}{\rho}}$$

where:

- v_s is the velocity of sound
- K is the bulk modulus
- Invalid Math is the density of the metal

The bulk modulus is a measure of the stiffness of the material. It is given by the following equation:

$$K = 9B$$

where B is the bulk modulus.

The bulk modulus of sodium is 7.0GPa.

Substituting these values into the equation for the velocity of sound,

$$v_s = \sqrt{\frac{9 \times 7.0\text{GPa}}{971\text{kg/m}^3}}$$

$$v_s = = 3.5\text{km/s}$$

Explanation:

Therefore, the order of magnitude of the velocity of sound in sodium is 3.5 kilometers per second.

Diatomic chain. Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.
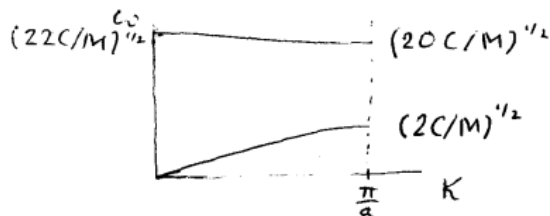
5. By analogy with Eq. (18),

$$Md^2u_s/dt^2 = C_1(v_s - u_s) + C_2(v_{s-1} - u_s);$$
$$Md^2v_s/dt^2 = C_1(u_s - v_s) + C_2(u_{s+1} - v_s), \quad \text{whence}$$
$$-\omega^2 Mu = C_1(v - u) + C_2(ve^{-iKa} - u);$$
$$-\omega^2 Mv = C_1(u - v) + C_2(ue^{iKa} - v), \quad \text{and}$$

$$\begin{vmatrix} (C_1 + C_2) - M\omega^2 & -(C_1 + C_2 e^{-iKa}) \\ -(C_1 + C_2 e^{iKa}) & (C_1 + C_2) - M\omega^2 \end{vmatrix} = 0$$

For $Ka = 0$, $\omega^2 = 0$ and $2(C_1 + C_2)/M$.

For $Ka = \pi$, $\omega^2 = 2C_1/M$ and $2C_2/M$.

6. (a) The Coulomb force on an ion displaced a distance r from the center of a sphere of static or rigid conduction electron sea is $- e^2 n(r)/r^2$, where the number of electrons within a sphere of radius r is $(3/4 \pi R^3)(4\pi r^3/3)$. Thus the force is $-e^2 r/R^2$, and the

force constant is e^2/R^3. The oscillation frequency ω_D is (force constant/mass)$^{1/2}$, or $(e^2/MR^3)^{1/2}$. (b) For sodium $M \simeq 4 \times 10^{-23}$ g and $R \simeq 2 \times 10^{-8}$ cm; thus $\omega_D \simeq (5 \times 10^{-10})(3 \times 10^{-46})^{1/2}$ $\simeq 3 \times 10^{13}$ s^{-1} (c) The maximum phonon wavevector is of the order of 10^8 cm^{-1}. If we suppose that ω_0 is associated with this maximum wavevector, the velocity defined by $\omega_0/K_{max} \approx 3 \times 10^5$ cm s^{-1}, generally a reasonable order of magnitude.

Kohn anomaly. We suppose that the interplanar force constant C_p between planes s and $s + p$ is of the form

$$C_p = A \frac{\sin p k_0 a}{pa} \ ,$$

where A and k_0 are constants and p runs over all integers. Such a form is expected in metals. Use this and Eq. (16a) to find an expression for ω^2 and also for $\partial\omega^2/\partial K$. Prove that $\partial\omega^2/\partial K$ is infinite when $K = k_0$. Thus a plot of ω^2 versus K or of ω versus K has a vertical tangent at k_0: there is a kink at k_0 in the phonon dispersion relation $\omega(K)$.

4. $\qquad \omega^2 = \frac{2}{M} A \sum_{p>0} \frac{\sin p k_0 a}{pa} (1 - \cos pKa) \ ;$

$$\frac{\partial\omega^2}{\partial K} = \frac{2A}{M} \sum_{p>0} \sin p k_0 a \ \sin pKa$$

$$= \sum_{p>0} \frac{1}{2} (\cos (k_0 - K) pa - \cos (k_0 + K) pa)$$

When $K = k_0$,

$$\frac{\partial\omega^2}{\partial K} = \frac{A}{M} \sum_{p>0} (1 - \cos 2 k_0 pa) \ ,$$

which in general will diverge because $\sum_p 1 \to \infty$.

Basis of two unlike atoms. For the problem treated by (18) to (26), find the amplitude ratios u/v for the two branches at $K_{max} = \pi/a$. Show that at this value of K the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

At $K_{max} = \pm\pi/a$ the roots are

$$\omega^2 = 2C/M_1 \; ; \qquad \omega^2 = 2C/M_2 \; .$$

$$-\omega^2 M_1 u = Cv[1 + \exp(-iKa)] - 2Cu \; ;$$
$$-\omega^2 M_2 v = Cu[\exp(iKa) + 1] - 2Cv \; .$$

3. From Eq. (20) evaluated at $K = \pi/a$, the zone boundary, we have

$$-\omega^2 M_1 u = -2Cu \; ;$$
$$-\omega^2 M_2 v = -2Cv \; .$$

Thus the two lattices are decoupled from one another; each moves independently. At $\omega^2 = 2C/M_2$ the motion is in the lattice described by the displacement v; at $\omega^2 = 2C/M_1$ the u lattice moves.