Estado Sólido I
Tarea 3: Vibraciones de la Red y Propiedades Térmicas

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Nombre del Estudiante: ____

Problema 1 *Monatomic linear lattice*

Consider a longitudinal wave $u_s = u\text{Cos}(\omega t - sKa)$ 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

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

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

$$\frac{1}{4}M\omega^2u^2 + \frac{1}{2}C(1 - \text{Cos } Ka)u^2 = \frac{1}{2}M\omega^2u^2$$

where in the last step we have used the dispersion relation $\omega^2 = (4C/M)\text{Sin}^2\ (Ka/2)$. *Hint:* The time-average is calculated as $\Lambda = \tau^{-1}\int_0^\tau \Lambda dt$, for Λ as the kinetic or potential energy, and $\tau = 2\pi/\omega$ as the period.

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Problema 2 *Basis of two unlike atoms*

Consider a chain of a two unlike atom basis of mass M_1 and M_2 ($M_1 > M_2$). Let a denote the repeat distance of the lattice. Take into account waves that propagate only in the direction of the chain.

(a) Write down the equations of motion under the assumption that each atom interacts only with its nearest-neighbors (with an interaction constant C) and solve them to obtain the phonon dispersion $\omega(k)$, considering different amplitudes u and v for the atom of mass M_1 and M_2, respectively.

(b) Analyze the cases when $k \ll \pi/a$ and $k = \pi/a$ for $\omega(k)$.

(c) Sketch and discuss the vibrational patterns for the center zone ($k = 0$).

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Problema 3 *Linear chain with rigid boundary conditions*

Consider a linear chain of $N+1$ atoms of mass M, which are coupled by equal interaction constant C while in the equilibrium state (relaxed) they are separated by a distance a, and has rigid boundary conditions, i.e., the displacements $u[na]$ of the nth atom must fulfill the boundary condition $u[0] = u[Na] = 0$. That is, from the $N+1$ atoms only the $1, \ldots, N-1$ atoms can oscillate, while the 0 and N atoms can't.

(a) Write the equation of motion and solve it using the following proposal:

$$u[na, t] = A \ \mathrm{Sin}(nka) e^{i\omega t}.$$

(b) Determine the dispersion relation $\omega(k)$.

(c) Which k values are allowed, and how is defined its first Brillouin zone?

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Problema 4 *Quantum correction to the Dulong-Petit limit*

From the general expression of quantum vibrational energy in $3D$,

$$U(T) = \sum_{\mathbf{q},s} \hbar\omega_s(\mathbf{q}) \left(\frac{1}{e^{\beta\hbar\omega_s(\mathbf{q})} - 1} + \frac{1}{2} \right),$$

obtain the temperature-dependent quantum correction for the specific heat C_V at the high-temperature limit.

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