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

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Nombre del Estudiante: ____

Problema 1 *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:

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

(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 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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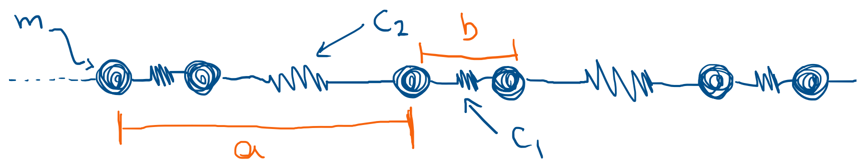
Problema 3 *Linear chain with alternating force constants*

Consider a linear chain of identical atoms, with mass M each of them, and a lattice constant a. The chain has a two-atom basis, which are separated by a distance b ($b < a/2$), and two different force constants C_1 and C_2,



For this particular system:

(a) Obtain the equations of motion.

(b) Find out the dispersion relation $\omega(k)$.

(c) Calculate the frequencies at the center ($k = 0$) and boundary ($k = \pi/a$) of the Brillouin zone.

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Problema 4 *Vibrational energy of a linear chain*

The linear chain of N atoms of mass M, which are coupled by equal interaction constant C, and has a (relaxed) separation a, shows the following dispersion relation:

$$\omega(q) = 2\sqrt{\frac{C}{M}}\left|\text{Sen}\left(\frac{qa}{2}\right)\right| \quad \forall \;\; q = -\frac{\pi}{a} + \frac{2\pi m}{Na},$$

with $m = 1, 2, \ldots, N$, so q is limited to the first Brillouin zone (IBZ): $q \in [-\pi/a, \pi/a]$.

(a) Determine the vibrational energy U and the specific heat C_V at the high-temperature limit.

(b) Describing U as an integral inside the IBZ of the q-space, calculate its behavior, as well as of C_V, at the low-temperature limit.

Hint: Remember the following functions:

$$\int_0^\infty \frac{x^{s-1}}{e^x - 1} dx = \Gamma(s)\zeta(s),$$
$$\text{with} \;\; \Gamma(s) = (s-1)! \;\; \forall \;\; s \in \mathbb{Z}^+,$$
$$\text{and} \;\; \zeta(2) = \pi^2/6, \;\; \zeta(4) = \pi^4/90, \;\; \zeta(6) = \pi^6/945.$$

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Problema 5 *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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