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 and solve them to obtain the phonon dispersion $\omega(k)$, considering different amplitudes u and v for the different atoms.

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

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

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Problema 3 *Linear chain with an impurity*

Consider a chain of atoms of mass m with nearest-neighbor interaction C, and spacing a between them. Additionally, at the center position of the chain ($n = 0$) there is an impurity atom of mass M.

(a) Obtain the equations of motion of the chain for $u[na]$, and for the impurity with $u[0] = u_0$, considering that each atom interacts only with its nearest-neighbors.

(b) Due to the impurity there are damping effects on all the atoms of the chain, which can be taken into account by the following proposal of displacement:

$$u(\zeta a, t) = A_\zeta e^{-\alpha|\zeta|a} e^{ik\zeta a - i\omega t} \quad \forall \quad A_\zeta = \text{cte.},$$

where ζ is the position of the atom on the chain ($\zeta = \ldots -1, 0, 1, \ldots, n, n+1, \ldots$). Demonstrate that the normal-mode's frequency of the system at the zone boundary ($k = \pi/a$) is given by:

$$\omega = 2\sqrt{\frac{C}{M}}\sqrt{\frac{m}{2m - M}}.$$

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Problema 4 *Specific heat for different limits of T*

Derive the behaviour of C_v for both regimes, the low− and high−temperature, under the following approaches:

(a) Debye model,

$$C_v = 9Nk_B\left(\frac{T}{\Theta_D}\right)^3 \int_0^{x_D} \frac{x^4 e^x}{(e^x - 1)^2} dx \;\; \forall \;\; x_D = \Theta_D/T$$

(b) Einstein model,

$$C_v = 3Nk_B\left(\frac{\hbar\omega_E}{k_B T}\right)^2 \frac{e^{\beta\hbar\omega_E}}{(e^{\beta\hbar\omega_E} - 1)^2}.$$

Hint:

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \Gamma(4)\zeta(4) = \frac{\pi^4}{15},$$

where $\Gamma(z)$ and $\zeta(z)$ are the Gamma and zeta-Riemann functions, respectively.

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