Estado Sólido Avanzado
Tarea 01: Dinámica de la Red Cristalina

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21 Enero 2019

Problema 1 *Linear chain with mth nearest-neighbor interactions*

Reexamine the theory of the linear chain, without making the assumption that only nearest neighbors interact, using as harmonic energy the following,

$$U^{harm} = \sum_n \sum_{m>0} \frac{1}{2} K_m \left\{ u[na] - u[(n+m)a] \right\}^2 .$$

(a) Show that the originally obtained dispersion relation,

$$\omega(k) = \sqrt{\frac{2K(1-\mathrm{Cos}\,ka)}{M}} = 2\sqrt{\frac{K}{M}} \left| \mathrm{Sen}\,\frac{ka}{2} \right|$$

must be generalized to

$$\omega = 2\sqrt{\sum_{m>0} K_m \frac{\mathrm{Sen}^2(mka/2)}{M}}.$$

(b) Show that the long-wavelenght limit of the dispersion relation

$$\omega = \left(a\sqrt{\frac{K}{M}} \right) |k|$$

must be generalized to:

$$\omega = a \left(\sum_{m>0} m^2 K_m / M \right)^{1/2} |k|.$$

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Problema 2 *Diatomic linear chain*

Consider a linear chain in which alternate ions have mass M_1 and M_2 ($M_1 \neq M_2$), and only nearest neighbors interact.

(a) Show that the dispersion relation for the normal modes is

$$\omega^2 = \frac{K}{M_1 M_2} \left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \mathrm{Cos}\,ka} \right).$$

(b) Discuss the form of the dispersion relation and the nature of the normal modes when $M_1 \gg M_2$.

(c) Compare the dispersion relation with that of the monoatomic linear chain,

$$\omega(k) = \sqrt{\frac{2K(1-\mathrm{Cos}\,ka)}{M}} = 2\sqrt{\frac{K}{M}}\left|\mathrm{Sen}\,\frac{ka}{2}\right|,$$

when $M_1 \approx M_2$.

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Problema 3 *Weakly perturbed monoatomic Bravais lattice*

Examine the dispersion relation for the one-dimensional lattice with a basis (two identical ions), in the limit in which the coupling constants K (intramolecular) and G (intermolecular) become very close,

$$K = K_0 + \Delta, \qquad G = K_0 - \Delta, \qquad \Delta \ll K_0.$$

Show that the dispersion relation differs from that of the monoatomic chain only by terms of order $(\Delta/K_0)^2$.

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Problema 4 *Specific heat for different limits of T*

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

(a) Debye model,

$$c_v = 9nk_B\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/T}\frac{x^4e^x dx}{(e^x-1)^2}$$

(b) Einstein model,

$$c_v^{opt} = pnk_B\left(\frac{\hbar\omega_E}{k_BT}\right)^2\frac{e^{\hbar\omega_E/k_BT}}{(e\hbar\omega_E/k_BT-1)^2}$$

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Problema 5 *van Hove singularities*

In a linear harmonic chain with only nearest-neighbor interactions, the normal-mode dispersion relation has the form,

$$\omega(k) = \omega_0\left|\mathrm{Sen}\frac{ka}{2}\right|,$$

where the constant ω_0 is the maximum frequency (assumed when k is on the zone boundary). Show that the density of normal modes (phonons) in this case is given by

$$g(\omega) = \frac{2}{\pi a\sqrt{\omega_0^2-\omega^2}}.$$

The singularity at $\omega = \omega_0$ is a van Hove singularity.

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