

Estado Sólido Avanzado

Tarea 01: Dinámica de la Red Cristalina

Dr. Omar De la Peña Seaman

05 Septiembre 2013

Problema 1 *Linear chain with m th 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,

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

(a) Show that the originally obtained dispersion relation,

$$\omega(k) = \sqrt{\frac{2K(1 - \cos ka)}{M}} = 2\sqrt{\frac{K}{M}} \left| \sin \frac{ka}{2} \right|$$

must be generalized to

$$\omega = 2 \sqrt{\sum_{m>0} K_m \frac{\sin^2 mka/2}{M}}.$$

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

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

must be generalized to:

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

.....

Problema 2 *Diatomic linear chain*

Consider a linear chain in which alternate ions have mass M_1 and M_2 , and only nearest neighbors interact.

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

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

- (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,

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

when $M_1 \approx M_2$.

.....

Problema 3 *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,

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

- (b) Einstein model,

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

.....

Problema 4 *van Hove singularities*

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

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

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.

.....