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

Dr. Omar De la Peña Seaman

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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

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

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 $\omega^2 = (4C/M)\text{Sin}^2\ (Ka/2)$.

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**Problema 2** *Continuum wave equation*

Show that for long wavelengths the equation of motion

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

reduces to the continuum elastic wave equation

$$\frac{\partial^2 u}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2},$$

where $v$ is the velocity of sound.

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## **Problema 3** *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 considering different amplitudes $u$ and $v$ for the different atoms.

(b) Analize the case when $qa \ll 1$ and $q = \pm\pi/a$ for the frequencies and the $u/v$ ratio.

(c) Discuss the vibrational patterns for the center zone ($q = 0$) and the boundary ($q = \pi/a$).

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## **Problema 4** *Kohn anomaly*

We suppose that the interplanar force constant $C_p$ between planes $s$ and $s+p$ is of the form

$$C_p = A\frac{\text{Sin } pq_0a}{pa},$$

where $A$ and and $q_0$ are constants and $p$ runs over all integers. Such form is expected in metals. Using this and the following equation,

$$\omega^2 = (2/M)\Sigma_{p>0}C_p(1 - \text{Cos } pqa),$$

to find an expression for $\omega^2$ and also for $\partial\omega^2/\partial q$. Prove that $\partial\omega^2/\partial q$ is infinite when $q = q_0$. Thus a plot of $\omega^2$ versus $q$ or of $\omega$ versus $q$ has a vertical tangent at $q_0$: there is a kink at $q_0$ in the phonon dispersion relation $\omega(q)$.

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## **Problema 5** *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,

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

(b) Einstein model,

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

*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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