Física del Estado Sólido
Tarea 01: Enlace Químico, Vibraciones de la Red y Propiedades Térmicas

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17 Febrero 2015

Problema 1 *van der Waals interaction*

As a simple quantum mechanical model for the van der Waals interaction consider two identical harmonic oscillators (oscillating dipoles) at a separation R. Each dipole consists of a pair of opposite charges whose separations are x_1 and x_2, respectively, for the two dipoles. A restoring force f acts between each pair of charges ($f = -kx$).

(a) Write down the Hamiltonian H_0 for the two oscillators without taking into account electrostatic interaction between the charges.

(b) Determine the interaction energy H_1 of the four charges.

(c) Assuming $|x_1| \ll R$, $|x_2| \ll R$ approximate H_1 as follows

$$H_1 \approx -\frac{2e^2 x_1 x_2}{R^3},$$

(d) Show that tranformation to normal coordinates $x_s = (x_1 + x_2)/\sqrt{2}$, $x_a = (x_1 - x_2)/\sqrt{2}$, decouples the total energy $H = H_0 + H_1$ into a symmetric and an antisymmetric contribution.

(e) Calculate the frequencies ω_s and ω_a of the symmetric and antisymmetric normal vibration modes. Evaluate the frequencies ω_s and ω_a as Taylor series in $2e^2/(kR^3)$ and truncate the expansions after second order terms.

(f) The energy of the complete system of two interacting oscillators can be expressed as $U = -\hbar(\omega_s + \omega_a)/2$. Derive an expression for the energy of the isolated ocillators and show that this is decreased by an amount c/R^6 when mutual interaction (bonding) occurs.

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Problema 2 *Cohesive energy of bcc and fcc neon*

Using the Lennard-Jonnes potential, calculate the ratio of the cohesive energies of Neon (Ne) in the bcc and fcc structures. The lattice sums for the bcc are:

$$\Sigma_j' p_{ij}^{-12} = 9.11418; \quad \Sigma_j' p_{ij}^{-6} = 12.2533.$$

and for the fcc are:

$$\Sigma_j' p_{ij}^{-12} = 12.13188; \quad \Sigma_j' p_{ij}^{-6} = 14.45392.$$

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Problema 3 *Linear ionic crystal*

Consider a line of $2N$ ions of alternating charge $\pm q$ with a repulsive potential energy A/R^n between nearest neighbors.

(a) Show that at the equilibrium separation

$$U(R_0) = -\frac{2Nq^2 \ln 2}{R_0}\left(1 - \frac{1}{n}\right).$$

(b) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$. Show that the work done in compressing a unit lengh of the crystal has the leading term $C\delta^2/2$, where

$$C = \frac{(n-1)q^2 \ln 2}{R_0}.$$

Hint: the expressions are in CGS units. To obrain results in SI, replace q^2 by $q^2/4\pi\epsilon_0$.

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Problema 4 *Monatomic linear lattice*

Consider a longitudinal wave $u_s = u\mathrm{Cos}(\omega t - sKa)$ 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

$$\frac{1}{4}M\omega^2 u^2 + \frac{1}{2}C(1 - \mathrm{Cos}\ Ka)u^2 = \frac{1}{2}M\omega^2 u^2$$

where in the last step we have used the dispersion relation $\omega^2 = (4C/M)\mathrm{Sin}^2\ (Ka/2)$.

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Problema 5 *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 6 *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 in each case.

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Problema 7 *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,

$$\omega^2 = (2/M)\Sigma_{p>0}C_p(1 - \text{Cos } pq_0a),$$

to find an expression for ω^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 ω^2 versus q or of ω 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 8 *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,

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

(b) Einstein model,

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

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