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Taller II, Estado Sólido

Capítulo III

1. **Quantum solid.** In a quantum solid the dominant repulsive energy is the zero-point energy of the atoms. Consider a crude one-dimensional model of crystalline He⁴ with each He atom confined to a line segment of length L. In the ground state the wave function within each segment is taken as a half wavelength of a free particle. Find the zero-point kinetic energy per particle.

Estado Sólido Taller #2: Juan Diego Figueroa Hernández

Capítulo 3

1) Aunque el modelo es de un sólido cuántico, si se consideran solo el aporte cinético de los partículas, estas tienen la misma energía de una partícula libre. Además, la función de onda forma la mitad de la longitud de onda y se confina en un segmento L, por lo tanto:

$$L = \frac{\lambda}{2} \quad \text{y} \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{2\pi}{\lambda}\right)^2 = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2$$

entonces

$$E = \left(\frac{\hbar \pi}{L}\right)^2 \times \frac{1}{2m}$$

2. **Cohesive energy of bcc and fcc neon.** Using the Lennard-Jones potential, calculate the ratio of the cohesive energies of neon in the bcc and fcc structures (Ans. 0.958). The lattice sums for the bcc structures are

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

2) El potencial de Lennard-Jones viene dado por:

$$U_{T_{\text{LJ}}} \approx N \epsilon \left[\sum_j' \left(\frac{\sigma}{r_{ij}} \right)^{12} - \sum_j' \left(\frac{\sigma}{r_{ij}} \right)^6 \right],$$

pero sabemos que $\sum_j' \frac{1}{r_{ij}^{12}} = 9.11418$ y $\sum_j' \frac{1}{r_{ij}^6} = 12.2533$

$$\therefore U_{T_{\text{LJ}}} \approx N \epsilon \left[9.11418 \left(\frac{\sigma}{R} \right)^{12} - 12.2533 \left(\frac{\sigma}{R} \right)^6 \right]$$

se busca el mínimo $\frac{dU_T}{dR} = 0 = -2N\epsilon \left[2 \cdot 9.11418 \frac{\sigma^{12}}{R^3} - 6 \cdot 12.2533 \frac{\sigma^6}{R^7} \right]$

asi que $2 \cdot 9.11418 \frac{\sigma^{12}}{R^3} = 6 \cdot 12.2533 \frac{\sigma^6}{R^7} \Rightarrow \left(\frac{\sigma}{R} \right)^6 = \frac{12.2533}{9.11418} \times \frac{1}{2}$

$$\frac{\sigma}{R} = 0.9359 \Rightarrow R = 1.0684$$
$$\therefore U_{T_{\text{bcc}}} = 2N\epsilon \left[9.11418 \left(0.9346 \right)^{12} - 12.2533 \left(0.9346 \right)^6 \right]$$
$$U_{T_{\text{bcc}}} = 2N\epsilon (-4.1183)$$

análogamente para $U_{T_{\text{fcc}}}$ se tiene $\frac{\sigma}{R} = 0.9174$

$$\text{y } U_{T_{\text{fcc}}} = 2N\epsilon \left[12.13182 \left(0.9174 \right)^{12} - 14.4539 \left(0.9174 \right)^6 \right]$$

Q) $U_{TFcc} = 2N\epsilon(-4,30508)$, así que

$$\frac{U_{TBcc}}{U_{Fcc}} = \frac{4,11839}{4,30508} = 0,957$$

3. **Solid molecular hydrogen.** For H₂ one finds from measurements on the gas that the Lennard-Jones parameters are $\epsilon = 50 \times 10^{-16}$ erg and $\sigma = 2.96 \text{ \AA}$. Find the cohesive energy in kJ per mole of H₂; do the calculation for an fcc structure. Treat each H₂ molecule as a sphere. The observed value of the cohesive energy is 0.751 kJ/mol, much less than we calculated; thus, quantum corrections must be very important.

3) $N_A = \frac{N}{mol}$, $U_{TFcc} = 2N\epsilon \left[12,13188 \cdot \left(\frac{\alpha}{r} \right)^6 - 14,4539 \left(\frac{\alpha}{r} \right)^{12} \right]$
 y de $\frac{dU_{Fcc}}{dr} = 0$ se llega a $\left(\frac{\alpha}{r} \right)^6 = \frac{3}{2\alpha}$

Como en el inciso anterior, así que

$$U_{TF} = 2N\epsilon \left[\frac{9}{4\alpha^2} - \frac{3}{2\alpha} \right] = 2N\epsilon \left[-\frac{3}{4\alpha} \right] = -\frac{N\epsilon\beta^2}{2\alpha}$$

así que en este caso

Q) $U_{TFcc} = \frac{(6,02 \times 10^{23})(50 \times 10^{-16}) \cdot (14,4539)^2}{2 \times 12,13188} = -2,5929 \times 10^{10} \left[\frac{\text{erg}}{\text{mol}} \right]$

$$U_{TFcc} = -2,59 \left[\frac{\text{kJ}}{\text{mol}} \right]$$

4. Possibility of ionic crystals $\mathbf{R}^+\mathbf{R}^-$. Imagine a crystal that exploits for binding the coulomb attraction of the positive and negative ions of the same atom or molecule R. This is believed to occur with certain organic molecules, but it is not found when R is a single atom. Use the data in Tables 5 and 6 to evaluate the stability of such a form of Na in the NaCl structure relative to normal metallic sodium. Evaluate the energy at the observed interatomic distance in metallic sodium, and use 0.78 eV as the electron affinity of Na.

4) Energía de ionización | Afinidad electrónica
 $\text{Na} \rightarrow \text{Na}^+ + \text{e}^- - 5,14 \text{ [eV]}$; $\text{Na} + \text{e}^- \rightarrow \text{Na}^- + 0,78 \text{ [eV]}$

La energía del enlace está dada por la energía de molido: $V = \frac{k_e^2}{R} = \frac{1,75(4,8 \times 10^{-10} \text{ [eV]})^2}{3,66 \times 10^{-8}} = 11 \times 10^{-12} \text{ [ergios]}$

$V = 6,8 \text{ [eV]}$, así que la energía de Na^+Na^- es: $E = [6,8 + 0,78 - 5,14] = 2,4 \text{ [eV]}$

así que por atomo se tiene $E' = 1,2 \text{ [eV]}$

5. 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

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

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

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

To obtain the results in SI, replace q^2 by $q^2/4\pi\epsilon_0$. Note: We should not expect to obtain this result from the expression for $U(R_0)$, but we must use the complete expression for $U(R)$.

$$U(r) = \underbrace{q_1 + q_2 + \dots + q_n}_{= N}$$

$$U(r) = \begin{cases} \frac{A}{r^n} - \frac{q^2}{r} & \Rightarrow \text{Vecinos próximos} \\ \frac{A}{r^n} + \frac{q^2}{r} & \Rightarrow \text{Otro caso} \end{cases}$$

para lo tanto la energía total será:

$$U_T = \frac{1}{2} (2N) \left[\sum_j \frac{A}{P_{ij} R^n} + \sum_i (-1)^{P_{ij}} q^2 \right]$$

$$\text{donde } r_{ij} = P_{ij} R, \quad \alpha = \sum_j \frac{(-1)^{P_{ij}}}{P_{ij}}$$

$$\text{en el equilibrio } \frac{\partial U_T}{\partial R} = 0 \Rightarrow N \left[\sum_i \frac{(-1)^{P_{ij}} A}{P_{ij} R^{n+1}} + \sum_i \frac{(-1)^{P_{ij}} q^2}{P_{ij} R^2} \right] = 0$$

$$\therefore \sum_i \frac{A}{P_{ij} R^{n+1}} = - \sum_i \frac{(-1)^{P_{ij}} q^2}{P_{ij} R^2}$$

$$\Rightarrow \frac{A}{R^n} = - \frac{\sum_i (-1)^{P_{ij}} / P_{ij}}{\sum_i 1 / P_{ij}} \left(\frac{q^2}{R^2} \right)$$

$$\therefore U_T = N \left[- \sum_j \frac{1}{P_{ij}} \times \frac{\sum_i (-1)^{P_{ij}} / P_{ij}}{\sum_i 1 / P_{ij}} \left(\frac{q^2}{R^2} \right) + \sum_i \frac{(-1)^{P_{ij}} q^2}{P_{ij} R^2} \right]$$

$$= N \left(\frac{q^2}{R^2} \right) \left[- \sum_j \frac{(-1)^{P_{ij}}}{n P_{ij}} + \sum_i \frac{(-1)^{P_{ij}}}{P_{ij}} \right]$$

$$= N \frac{q^2}{R^2} \times \left(1 - \frac{1}{n} \right), \quad \text{para } \alpha = [-1 + \frac{1}{2} - \frac{1}{3} \dots]$$

$$\text{si } q \ll 1 \quad U_T = -2N \frac{q^2}{R^2} \ln(2) \left(1 - \frac{1}{n} \right) \quad \text{para } \alpha = -2 \ln 2$$

$$b) W = \Delta U \Rightarrow W = U_{(R_0)} - U_{(R_0 - R_0 \delta)}$$

$$W = -h \left(\frac{1}{R_0} - \frac{1}{R_0(1-\delta)} \right), \quad h = q^2 N l_n(\gamma) \left(1 - \frac{1}{n} \right)$$

$$W = -h \left(1 - 1 - \delta - \delta^2 - \delta^3 - \dots \right) = \frac{h}{R_0} \left(f + \delta^2 + \dots \right)$$

En aproximación armónica nos quedan entonces:

$$W \approx \frac{h}{R_0} \delta^2 = \frac{N q^2 l_n(\gamma) \left(1 - \frac{1}{n} \right)}{R_0} \delta^2$$

$$\text{el trabajo por etapa es} \Rightarrow W = \frac{W}{2N} = \frac{q^2 l_n(\gamma) \left(1 - \frac{1}{n} \right) \delta^2}{2R_0}$$

$$\text{pero } W = \frac{1}{2} C \delta^2 \quad \therefore C = \frac{q^2 l_n(\gamma) \left(1 - \frac{1}{n} \right)}{R_0} = \frac{q^2 l_n(\gamma) (n-1)}{n R_0}$$

6. Cubic ZnS structure. Using λ and ρ from Table 7 and the Madelung constants given in the text, calculate the cohesive energy of KCl in the cubic ZnS structure described in Chapter 1. Compare with the value calculated for KCl in the NaCl structure.

Handwritten notes for problem 6:

$$U = -\frac{q^2}{R_0} \left(1 - \frac{\delta}{R_0} \right)$$

$$\frac{U}{q^2} = -\frac{1}{R_0} \left(1 - \frac{\delta}{R_0} \right) \text{ force } \propto 1,638 \text{ N}$$

$$\delta = 0.326 \times 10^{-10}$$

$$\therefore \frac{U}{q^2} = -\frac{1,638}{R_0} \left(1 - 0.326 \times 10^{-10} \right) \text{ to be considered at equilibrium distance}$$

$$R_0 \approx 9.2 \rightarrow R_0 \approx 3 \text{ Å}$$

$$\therefore U = q^2 \left[-\frac{1,638}{3 \text{ Å}} \left(1 - \frac{0.326 \times 10^{-10}}{3 \times 10^{-10}} \right) \right]$$

$$= -0.489 \text{ J}$$

7. Divalent ionic crystals. Barium oxide has the NaCl structure. Estimate the cohesive energies per molecule of the hypothetical crystals Ba^+O^- and $\text{Ba}^{++}\text{O}^{--}$ referred to separated neutral atoms. The observed nearest-neighbor internuclear distance is $R_0 = 2.76 \text{ Å}$; the first and second ionization potentials of Ba are 5.19 and 9.96 eV; and the electron affinities of the first and second electrons added to the neutral oxygen atom are 1.5 and -9.0 eV. The first electron affinity of the

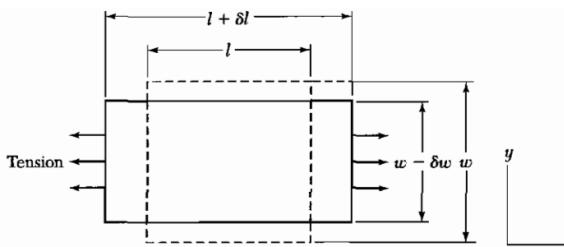


Figure 21 Young's modulus is defined as stress/strain for a tensile stress acting in one direction, with the specimen sides left free. Poisson's ratio is defined as $(\delta w/w)/(\delta l/l)$ for this situation.

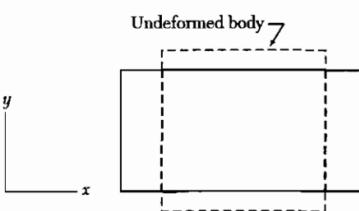


Figure 22 This deformation is compounded from the two shears $e_{xx} = -e_{yy}$.

neutral oxygen atom is the energy released in the reaction $\text{O} + e \rightarrow \text{O}^-$. The second electron affinity is the energy released in the reaction $\text{O}^- + e \rightarrow \text{O}^{--}$. Which valence state do you predict will occur? Assume R_0 is the same for both forms, and neglect the repulsive energy.

7) La energía rebotante por molécula está dada por la energía de molidlung, existen tres posibilidades:

$$q = e \quad o \quad q = z e, \text{ en general } q = a e^{\gamma} \text{ con } \gamma = 1, 2$$

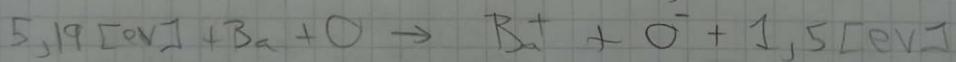
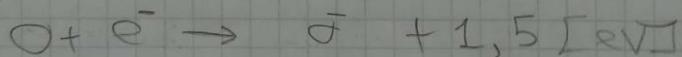
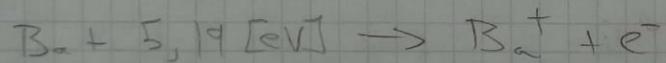
$$\frac{U}{N} = -\frac{\alpha e^2}{R_0} = -\frac{1,747565}{2,576} a e^2$$

$$\left. \frac{U}{N} \right|_{\alpha=1} = -1,46 \times 10^{-19} [\text{eV}]$$

$$\left. \frac{U}{N} \right|_{\alpha=2} = -5,84 \times 10^{-19} [\text{eV}]$$

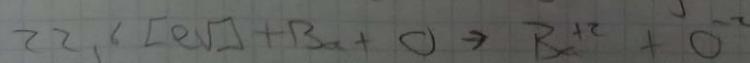
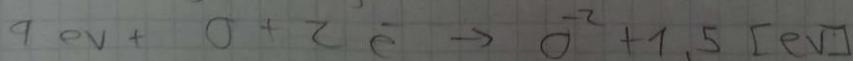
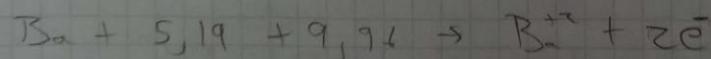
Respecto a la predicción del estado de valencia, el estado BaO^+ es más favorable que el BaO^{+2} ya que la energía es función de la carga, se genera un crecimiento 4 veces mayor y por lo tanto, es 4 veces más estable al incrementar la carga.

○ Estado Ba^{+1}O^- :



$$\therefore E_1 = 9,11 - 1,5 + 5,19 = 5,42 [\text{eV}]$$

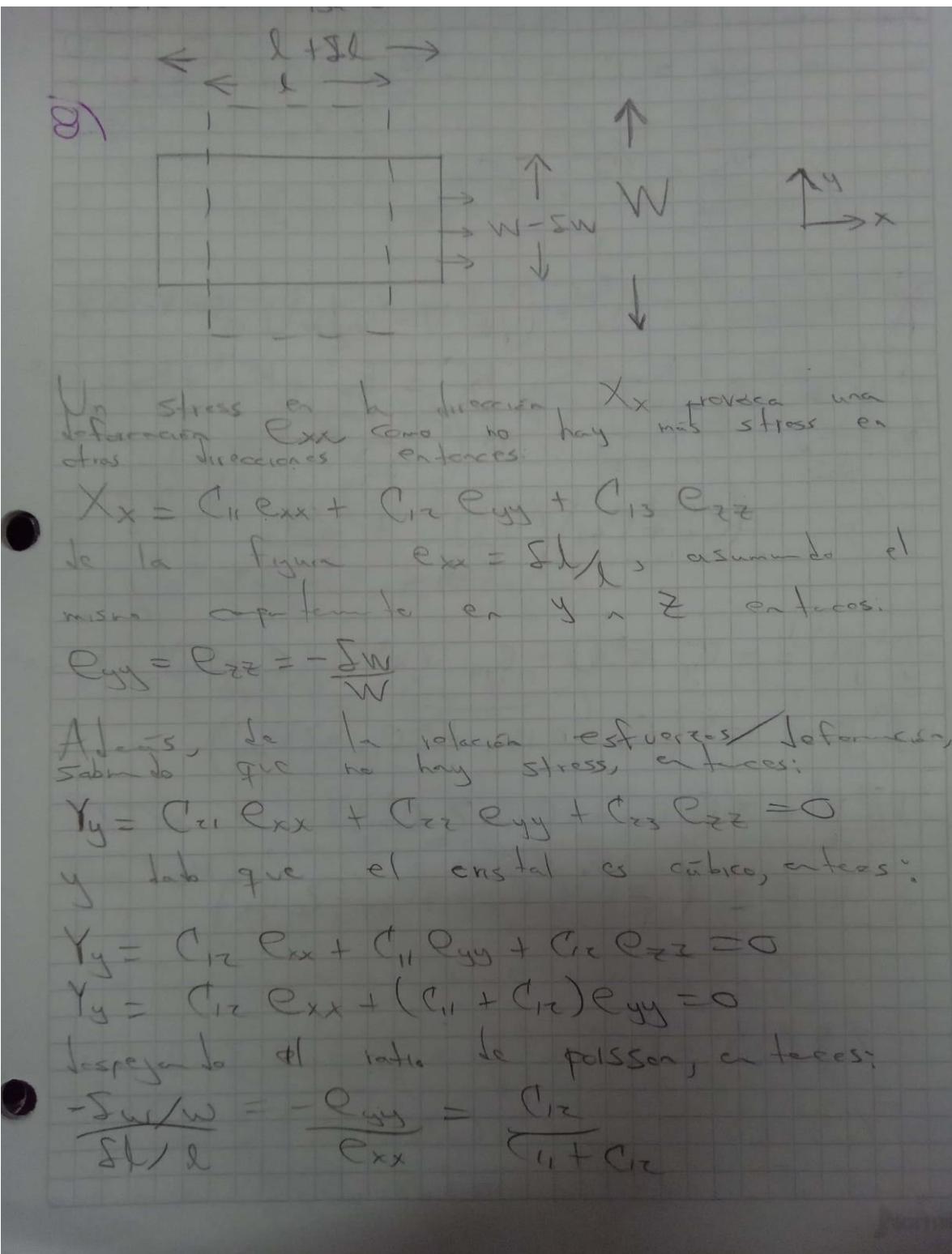
○ Estado $\text{Ba}^{+2}\text{O}^{+2}$:



$$\therefore E_2 = 31,44 - 22,56 = 13,79 [\text{eV}]$$

Por tanto, $\text{Ba}^{+2}\text{O}^{+2}$ que $E_2 > E_1$, el estado más estable es $\text{Ba}^{+2}\text{O}^{+2}$.

8. Young's modulus and Poisson's ratio. A cubic crystal is subject to tension in the [100] direction. Find expressions in terms of the elastic stiffnesses for Young's modulus and Poisson's ratio as defined in Fig. 21.



Para el módulo de Young se tendrá $\left(\frac{X_x}{E_{xx}}\right)$

$$X_x = C_{11} E_{xx} + 2C_{12} E_{yy}$$

$$\text{entonces } \frac{X_x}{E_{xx}} = C_{11} + 2C_{12} \frac{E_{yy}}{E_{xx}} = C_{11} - 2C_{12} \frac{C_{12}}{C_{11} + C_{12}}$$

$$\frac{X_x}{E_{xx}} = C_{11} - \frac{2C_{12}}{C_{11} + C_{12}}$$

- 9. Longitudinal wave velocity.** Show that the velocity of a longitudinal wave in the [111] direction of a cubic crystal is given by $v_x = [\frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})/\rho]^{1/2}$. Hint: For such a wave $u = v = w$. Let $u = u_0 e^{iK(x+y+z)/\sqrt{3}} e^{-i\omega t}$, and use Eq. (57a).

$$\cancel{\text{P} \rightarrow \text{f} \rightarrow \text{J} \rightarrow \text{U} = V = W = U_0 e^{i(K \cdot \mathbf{r} - \omega t)}}$$

$$\cancel{K_y = K_x = K_z = K, \quad K'^2 = K_x^2 + K_y^2 + K_z^2 = 3K^2}$$

$$\cancel{f \cancel{\frac{\partial U}{\partial t}} = C_{11} \frac{\partial^2 U}{\partial x^2} + C_{44} \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 U}{\partial x \partial y} + \frac{\partial^2 U}{\partial x \partial z} \right)}$$

$$-f^2 p U = -C_{11} K^2 U - C_{44} \cdot 2K^2 U - (C_{12} + C_{44}) U (K^2 + K^2)$$

$$f^2 p = K^2 (C_{11} + 2C_{44} + 2C_{12} + 2C_{44})$$

$$\cancel{f^2 p = 3(C_{11} + 4C_{44} + 2C_{12})}$$

$$V_s = \frac{K^2}{K} \left(\frac{3}{p} \right)^{1/2} (C_{11} + 4C_{44} + 2C_{12})^{1/2}$$

- 10. Transverse wave velocity.** Show that the velocity of transverse waves in the [111] direction of a cubic crystal is given by $v_s = [\frac{1}{3}(C_{11} - C_{12} + C_{44}/\rho)]^{1/2}$. Hint: See Problem 9.

10) A) Sea una onda transversal en la dirección [111]. Consideremos $U = \text{cte}$ y sea $\omega = \text{cte}$. Entonces $\nabla U = 0$. La ecuación de onda para V es:

$$\frac{\partial^2 V}{\partial t^2} = C_{11} \frac{\partial^2 V}{\partial x^2} + C_{44} \left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 U}{\partial x \partial y} + \frac{\partial^2 W}{\partial y \partial z} \right)$$

$$-\rho \gamma^2 V = -\frac{C_{11} K^2 V}{3} - \frac{2}{3} C_{44} K^2 V - \frac{(C_{11} + C_{44})}{3} K^2 W$$

$$-\rho \gamma^2 V = -\frac{C_{11} K^2 V}{3} - \frac{2}{3} C_{44} K^2 V + \frac{(C_{12} + C_{44})}{3} K^2 V$$

$$\therefore \rho \gamma^2 V = \frac{K^2 V}{3} (C_{11} + 2C_{44} - C_{12} C_{44})$$

$$\rho \gamma^2 = \frac{K^2}{3} (C_{11} - C_{12} + C_{44})$$

$$V_s = \frac{\gamma}{K} = \left(\frac{C_{11} - C_{12} + C_{44}}{3\rho} \right)^{1/2}$$

11. **Effective shear constant.** Show that the shear constant $\frac{1}{2}(C_{11} - C_{12})$ in a cubic crystal is defined by setting $e_{xx} = -e_{yy} = \frac{1}{2}e$ and all other strains equal to zero, as in Fig. 22. Hint: Consider the energy density (43); look for a C' such that $U = \frac{1}{2}C'e^2$.

11) De la teoría de energía en un cristal cúbico deformando $e_{xx} = -e_{yy} = \frac{e}{2}$ y todas las demás deformaciones son nulas

$$U = \frac{1}{2}C_{11}(e_{xx}^2 + e_{yy}^2 + e_{zz}^2) + \frac{1}{2}C_{44}(e_{yz}^2 + e_{zx}^2 + e_{xy}^2) + C_{12}(e_{yy}e_{zz} + e_{zz}e_{xx} + e_{xx}e_{yy})$$

$$\therefore U = \frac{1}{2}C_{11}\left(\frac{e^2}{4} + \frac{e^2}{4}\right) + C_{12}\left(\frac{e}{2}(-\frac{1}{2})\frac{e}{2}\right)$$

$$U = \frac{1}{2}(C_{11} - C_{12})e^2 = \frac{1}{2}\left[\frac{1}{2}(C_{11} - C_{12})\right]e^2$$

así que $\frac{1}{2}(C_{11} - C_{12})$ es la constante efectiva

12. **Determinantal approach.** It is known that an R -dimensional square matrix with all elements equal to unity has roots R and 0, with the R occurring once and the zero occurring $R - 1$ times. If all elements have the value p , then the roots are Rp and 0. (a) Show that if the diagonal elements are q and all other elements are p , then there is one root equal to $(R - 1)p + q$ and $R - 1$ roots equal to $q - p$. (b) Show from the elastic equation (57) for a wave in the [111] direction of a cubic crystal that the determinantal equation which gives ω^2 as a function of K is

$$\begin{vmatrix} q - \omega^2 p & p & p \\ p & q - \omega^2 p & p \\ p & p & q - \omega^2 p \end{vmatrix} = 0 ,$$

where $q = \frac{1}{3}K^2(C_{11} + 2C_{44})$ and $p = \frac{1}{3}K^2(C_{12} + C_{44})$. This expresses the condition that three linear homogeneous algebraic equations for the three displacement components u, v, w have a solution. Use the result of part (a) to find the three roots of ω^2 ; check with the results given for Problems 9 and 10.

12. @ Veras la matriz A de la siguiente manera:

$$A = \begin{pmatrix} q & p & \cdots & p \\ p & q & \cdots & \\ \vdots & & \ddots & q \\ p & & & \end{pmatrix} = \begin{pmatrix} p & p & \cdots & p \\ p & q & \cdots & \\ \vdots & & \ddots & p \\ p & & & \end{pmatrix} \begin{pmatrix} q-p & 0 & \cdots & 0 \\ 0 & q-p & \cdots & \\ \vdots & & \ddots & q-p \\ 0 & & & q-p \end{pmatrix}$$

$A = P + I(q-p)$, las raíces de $\det(A) = 0$ corresponden al producto de sus autovalores (como se mostró en el punto 13), así que:

$$\det(A - \lambda I) = 0$$

$$\det(P + I(q-p) - \lambda I) = 0$$

$$\det(P + I(q-p-\lambda)) = 0$$

Sabemos que de P se tienen raíces y por tanto R autovalores:

$\lambda_i^* = R_p$ (multiplicidad 1), $\lambda_i^* = 0$ (multiplicidad $R-1$), en términos de λ .

$$R_p = \lambda - q + p \rightarrow \lambda = R_p - p + q$$

$$\lambda = q + p(R-1)$$

$$0 = \lambda - q + p \rightarrow \lambda = p - q$$

Como son raíces $|I|$ ivamente, y teniendo en cuenta la multiplicidad se tiene:

$$[q + p(R-1)](p-q)^{R-1} = 0$$

b) En la dirección [111] se tiene

$$|\mathbf{r}_{(11)}| = (U_0\hat{i} + V_0\hat{j} + W_0\hat{k}) e^{i(\frac{\pi}{3} + \frac{q}{2} + \frac{r}{2}) - \gamma t}$$

$$-\rho \gamma^2 U = -\frac{C_{11}}{3} K^2 U - \frac{K^2 C_{44}}{3} (2V) - \frac{K^2}{3} (C_{11} + C_{44})(W)$$

$$-\rho \gamma^2 V = -\frac{C_{11}}{3} K^2 V - \frac{K^2 C_{44}}{3} (2U) - \frac{K^2}{3} (C_{11} + C_{44})(U + W)$$

$$-\rho \gamma^2 W = -\frac{C_{11}}{3} K^2 W - \frac{K^2 C_{44}}{3} (2U) - \frac{K^2}{3} (C_{11} + C_{44})(U + V)$$

Realizando: tenemos que:

$$\rightarrow U\left(\frac{K^2}{3}[C_{11} + 2C_{44}] - \rho \gamma^2\right) + V\frac{K^2}{3}(C_{11} + C_{44})$$

$$+ W\frac{K^2}{3}(C_{11} + C_{44}) = 0$$

$$\rightarrow U\left(\frac{K^2}{3}[C_{11} + 2C_{44}] - \rho \gamma^2\right) + V\left(\frac{K^2}{3}[C_{11} + 2C_{44}] - \rho \gamma^2\right)$$

$$+ W\frac{K^2}{3}(C_{11} + C_{44}) = 0$$

$$\rightarrow U\left(\frac{K^2}{3}[C_{11} + 2C_{44}] - \rho \gamma^2\right) + V\left(\frac{K^2}{3}[C_{11} + 2C_{44}] - \rho \gamma^2\right) + W\left(\frac{K^2}{3}[C_{11} + 2C_{44}] - \rho \gamma^2\right) = 0$$

realizamos el siguiente cambio de variables:

$$q = \frac{1}{2}K^2(C_{11} + 2C_{44}), \quad p = \frac{1}{3}K^2(C_{11} + C_{44}) \quad \therefore$$

$$U(q - \rho \gamma^2) + pV + Wp = 0$$

$$Up + (q - \rho \gamma^2)V + Wp = 0$$

$$Up + pV + W(q - \rho \gamma^2) = 0$$

Para los cuadros para bases solares en triángulos
se impone un determinante igual a cero;

$$\begin{vmatrix} q - p\gamma^2 & p & p \\ p & q - p\gamma^2 & p \\ p & p & q - p\gamma^2 \end{vmatrix} = 0$$

La cuadra es análoga a la ecuación
 $|A - \lambda I| = 0$ donde el elemento $p\gamma^2$ es
autovalor, y como se ha visto en 3, entonces:

$$\lambda_1 = \underbrace{2p+q}_{p\gamma^2}, \quad \lambda_{2,3} = q-p, \quad \gamma^2 = q-p$$

$$\gamma^2 = \frac{k^2}{3p} (2C_{12} + C_{11} + 4C_{44}), \quad \gamma^2 = \frac{k^2}{3p} (C_{11} + C_{44} - C_{12})$$

13. **General propagation direction.** (a) By substitution in (57) find the determinantal equation which expresses the condition that the displacement

$$\mathbf{R}(\mathbf{r}) = [u_0 \hat{\mathbf{x}} + v_0 \hat{\mathbf{y}} + w_0 \hat{\mathbf{z}}] \exp[i(\mathbf{K} \cdot \mathbf{r} - wt)]$$

be a solution of the elastic wave equations in a cubic crystal. (b) The sum of the roots of a determinantal equation is equal to the sum of the diagonal elements a_{ii} . Show from part (a) that the sum of the squares of the three elastic wave velocities in any direction in a cubic crystal is equal to $(C_{11} + 2C_{44})/\rho$. Recall that $v_s^2 = \omega^2/K^2$.

③ ④ ⑤

De la ecuación de onda para U, V, W

$$\rho \frac{\partial^2 U}{\partial t^2} = C_{11} \frac{\partial^2 U}{\partial x^2} + C_{44} \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 V}{\partial x \partial y} + \frac{\partial^2 W}{\partial x \partial z} \right)$$

$$\rho \frac{\partial^2 V}{\partial t^2} = C_{11} \frac{\partial^2 V}{\partial y^2} + C_{44} \left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 U}{\partial y \partial x} + \frac{\partial^2 W}{\partial y \partial z} \right)$$

$$\rho \frac{\partial^2 W}{\partial t^2} = C_{11} \frac{\partial^2 W}{\partial z^2} + C_{44} \left(\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} \right) + (C_{11} + C_{44}) \left(\frac{\partial^2 U}{\partial z \partial x} + \frac{\partial^2 V}{\partial z \partial y} \right)$$

para lo tanto se propone la siguiente solución vectorial

$$\mathbf{R}(t) = (V_0 \hat{i} + V_0 \hat{j} + W_0 \hat{k}) e^{i[\mathbf{K}^2 t + f t]}, \text{ así que se tiene}$$

$$-\mathbf{f} \mathbf{P} \mathbf{U} = -C_{11} K_x^2 U - C_{44} (K_y^2 + K_z^2) U \\ - (C_{12} + C_{44}) (K_x K_y V + K_x K_z W)$$

$$-\mathbf{f} \mathbf{P} \mathbf{V} = -C_{11} K_y^2 V - C_{44} (K_x^2 + K_z^2) V \\ - (C_{12} + C_{44}) (K_y K_z W + K_y K_x U)$$

$$-\mathbf{f} \mathbf{P} \mathbf{W} = -C_{11} K_z^2 W - C_{44} (K_x^2 + K_y^2) W \\ - (C_{12} + C_{44}) (K_z K_x U + K_z K_y V)$$

→ Expressas pues las anteriores ecuaciones en su forma matricial:

$$(C_{11} K_x^2 + C_{44} (K_y^2 + K_z^2) - f g) (C_{11} + C_{44} K_x K_y) (C_{12} + C_{44}) K_x K_z$$

$$(C_{12} + C_{44}) K_y K_x \quad C_{11} K_y^2 + C_{44} (K_z^2 + K_x^2) - f g \quad (C_{12} + C_{44}) K_y K_z$$

$$(C_{11} + C_{44}) K_z K_x \quad (C_{12} + C_{44}) K_z K_y \quad C_{11} K_z^2 + C_{44} (K_x^2 + K_y^2) - f g$$

$$x \begin{pmatrix} U \\ V \\ W \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{⑥} \quad \text{La matriz dada es simétrica de la forma } A = \begin{pmatrix} a & b & c \\ b & d & f \\ c & f & e \end{pmatrix}, \text{ así que}$$

matriz de los autovalores de A y P son de autovectores. Sabemos que

$$\text{Tr}\{AB\} = \text{Tr}\{BA\} \quad \text{y} \quad \det(AB) = \det(A) \det(B)$$

así pues $\text{Tr}(A) = \text{Tr}(P^{-1}TP) = \text{Tr}(TPT^{-1}) = \text{Tr}(T)$

$$\text{Tr}(A) = \text{Tr}(T) = a + b + c \quad \therefore \text{Se tiene que}$$

la suma de la diagonal principal de A es
 justo la suma de los autovalores de A ,
 alonso $\det A = \det(P^T + P) = 1 \times \det T \times \det P$
 $\therefore \det A = \det T = \prod a_{ii} = a \cdot b \cdot c$. Así que cada
 elemento a_{ii} es autovalor de A , y si
 $\det A = 0$ se tienen tres raíces a, b, c .

(C) Al sumar las tres diagonales, se tiene

$$c_{11}(k_x^2 + k_y^2 + k_z^2) + c_{44}(2)(k_x^2 + k_y^2 + k_z^2)$$

$$= 3F^2 P, \quad \frac{c_{11} + 2c_{44}}{P} = \frac{3F^2}{k^2} = 3V_i^2 = V_i^2, \quad i = \{1, 2, 3\}$$

14. **Stability criteria.** The criterion that a cubic crystal with one atom in the primitive cell be stable against small homogeneous deformations is that the energy density (43) be positive for all combinations of strain components. What restrictions are thereby imposed on the elastic stiffness constants? (In mathematical language the problem is to find the conditions that a real symmetric quadratic form should be positive definite. The solution is given in books on algebra; see also Korn and Korn, *Mathematical Handbook*, McGraw-Hill, 1961, Sec. 13.5-6.) Ans. $C_{44} > 0$, $C_{11} > 0$, $C_{11}^2 - C_{12}^2 > 0$, and $C_{11} + 2C_{12} > 0$. For an example of the instability which results when $C_{11} \approx C_{12}$, see L. R. Testardi et al., Phys. Rev. Letters **15**, 250 (1965).

P Sabemos que la matriz de rigidez viene dada por:

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{13} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

La matriz debe tener autovalores positivos para que sea definida y los reales sean:

$$\lambda_{1,2} = C_{11} - C_{12} > 0 \quad * \star$$

$$\lambda_3 = C_{11} + 2C_{12} > 0 \quad * \star$$

$$\lambda_{4,5} = C_{44} > 0 \quad * \star$$

De acuerdo se tiene $C_{11} - 2C_{12} > 0 \Rightarrow C_{11} + 2C_{12} > 0$
 $3C_{11} > 0 \Rightarrow C_{11} > 0 \Rightarrow C_{11} > C_{12} \Rightarrow C_{11}^2 - C_{12}^2 > 0$
 Luego se cumplen las condiciones $C_{44} > 0$, $C_{11} > 0$, $C_{11}^2 - C_{12}^2 > 0$

Capítulo IV

-
1. **Monatomic linear lattice.** Consider a longitudinal wave

$$u_s = u \cos(\omega t - sKa)$$

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

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

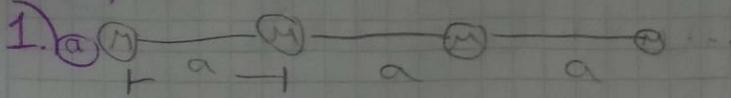
where s runs over all atoms.

- (b) By substitution of u_s in this expression, show that the time-average total energy per atom is

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

where in the last step we have used the dispersion relation (9) for this problem.

Capítulo 4



Como uno de los átomos presenta trayectoria cinética ($\frac{1}{2} M \dot{u}_s^2$) y energía potencial dada por la interacción con los vecinos cercanos dada por:

$\frac{1}{2} C (u_s - u_{s+1})^2$, al sumar para todos los átomos se tiene:

$$E = \frac{1}{2} M \sum_s \dot{u}_s^2 + \frac{1}{2} C \sum_s (u_s - u_{s+1})^2$$

① al reemplazar u_s en E se tiene:

$$E = \frac{1}{2} M \omega^2 w^2 \sum_s (\omega t - k a s)^2 + \frac{1}{2} C \left[w^2 \cos^2(\omega t - k a s) - 2 w^2 \cos(\omega t - k a s) \cos(\omega t - k a (s+1)) + w^2 \cos^2(\omega t - k a (s+1)) \right]$$

$$\therefore \langle E \rangle = \frac{1}{2} M \omega^2 w^2 \frac{1}{\pi} + \frac{1}{2} C \omega \left(\frac{1 + 1}{\pi} \right)$$

$$= w^2 C \left(\frac{1}{\pi} \left[\cos(2\omega t - 2k a s - k a) + \cos(k a) \right] \right) \rightarrow 0$$

$$\therefore \langle E \rangle = \frac{1}{4} M \omega^2 w^2 + \frac{1}{2} C \omega^2 (1 - \cos(k a)),$$

$$\text{para } w^2 = \frac{C}{M} (1 - \cos(k a)) \rightarrow 1 - \cos(k a) = \frac{w^2 M}{2 C}$$

$$\langle E \rangle = \frac{1}{4} M \omega^2 w^2 + \frac{1}{2} C \omega^2 \frac{w^2 M}{2 C} = \frac{1}{4} M \omega^2 w^2 + \frac{1}{4} M \omega^2 w^2$$

$$\langle E \rangle = \frac{1}{2} M \omega^2 w^2$$

2. Continuum wave equation. Show that for long wavelengths the equation of motion (2) 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.

2. A partir de la ecuación (2) se tiene:

$$\frac{M \ddot{u}_{ss}}{\Delta t^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

$$\therefore \frac{\ddot{u}_{ss}}{\Delta t^2} = \frac{C a^2}{M} \times u_{s+1} + u_{s-1} - 2u_s$$

teniendo el límite de ondas ($\omega \gg 1$)
el cambio en u es muy grande respecto
a "a", la distancia entre placas, es decir:

$$\frac{\ddot{u}_{ss}}{\Delta t^2} = \frac{C a^2}{M} \lim_{a \rightarrow 0} \frac{u_{s+1} - u_s - u_{s-1} + u_s}{a}$$

pero al hacer la definición de segunda derivada

$$\frac{\ddot{u}_{ss}}{\Delta t^2} = \frac{C a^2}{M} \frac{\partial^2 u}{\partial x^2} = V^2 \frac{\partial^2 u}{\partial x^2}, \quad V^2 = \frac{C a^2}{M}$$

que es finita de onda larga

$$(K a \ll 1) \quad \omega^2 = \frac{C K^2 a^2}{M} \rightarrow V^2 = \frac{\omega^2}{K^2} = \frac{C a^2}{M}$$

Lo anterior implica que para ondas largas
es decir, en la aproximación de continua se
reproducen los resultados de una ecuación de onda

3. Basis of two unlike atoms. For the problem treated by (18) to (26), find the amplitude ratios u/v for the two branches at $K_{\max} = \pi/a$. Show that at this value of K the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

3 Sabemos que en $k = K_{\max} = \frac{\pi}{a}$ los lobos acústicos y ópticos (1 y 2) son a $\omega_1^2 = \frac{C}{M_1}$, $\omega_2^2 = \frac{C}{M_2}$, al sustituir en una de las ecuaciones del sistema se tiene:

$$-\omega^2 M_1 u = C(1 + e^{ikx}) - 2Cu$$

$$-\omega^2 M_2 \frac{u}{v} = C(1 + e^{-ikx}) - 2Cv$$

$$\therefore \frac{u}{v} = \frac{C(1 + e^{-ikx})}{2C - \omega^2 M_2} = 0$$

es decir si $\omega = \omega_2$, el cociente está bien definido.

Lo cual implica que u está "estático" respecto a v . Análogamente, con la otra ecuación se obtiene:

$$-\omega^2 M_2 v = Cu(1 + e^{ikx}) - 2Cv$$

$$\therefore \frac{v}{u} = \frac{C(1 + e^{ikx})}{2C - \omega^2 M_1} = 0.$$

Por lo tanto, si $\omega = \omega_1$, v es fijo "quiere" respecto a u , es decir, uno de la red ocurre mientras que el otro no. Lo anterior es análogo a la aproximación del continuo $K \ll 1$, sólo que así como $\frac{v}{u} = 0 \Rightarrow \frac{ku}{v} = 0$, es decir $K \ll kv$.

En síntesis un desplazamiento en el espacio periódico para v es infinitesimal respecto a u .

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

$$C_p = A \frac{\sin pk_0 a}{pa} ,$$

where A and k_0 are constants and p runs over all integers. Such a form is expected in metals. Use this and Eq. (16a) to find an expression for ω^2 and also for $\partial\omega^2/\partial K$. Prove that $\partial\omega^2/\partial K$ is infinite when $K = k_0$. Thus a plot of ω^2 versus K or of ω versus K has a vertical tangent at k_0 : there is a kink at k_0 in the phonon dispersion relation $\omega(K)$.

4. $\omega^2 = \sum_M \sum_{p>0} C_p (1 - \cos(pk_0 a)) ,$

$$\omega^2 = \sum_M \sum_{p>0} \frac{A \sin(pk_0 a)}{pa} (1 - \cos(pk_0 a))$$

$$\frac{\partial \omega^2}{\partial K^2} = \frac{2A}{M} \sum_{p>0} \frac{\sin(pk_0 a) \sin(k_0 pa)}{pa}$$

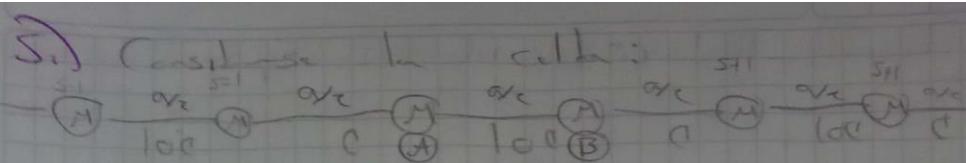
$$\text{Si } K=k_0 \Rightarrow \frac{\partial \omega^2}{\partial K^2} = \frac{2A}{M} \sum_{p>0} \sum_{k=1}^{\infty} \frac{(pk_0 a)^2}{pa}$$

$$\frac{\partial \omega^2}{\partial K^2} = \frac{2A}{M} \sum_{p>0} \frac{1}{2} (1 - \cos(2pk_0 a))$$

→ Pense que $1 \geq |\cos| & \theta \rightarrow$ la serie

$$\sum_{p=1}^{\infty} \sum_{k=1}^{\infty} \frac{1}{2} (1 - \cos(2pk_0 a)) \Big|_{K=k_0}$$

5. Diatomic chain. Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2 .



V_s ≡ desplazamientos de la masa A

V_b ≡ desplazamientos de la masa B.

Las ecuaciones de movimiento son:

$$(A) \Rightarrow M\ddot{V}_s = 10C(V_{s+1} - V_s) + C(V_s - V_b)$$

desplazamiento (\rightarrow) hacia la izquierda de la masa B hacia la A

desplazamiento (\rightarrow) hacia la derecha de la masa B hacia la A

$$(B) \Rightarrow M\ddot{V}_b = 10C(V_s - V_{s+1}) + C(V_s - V_b)$$

Se plantean soluciones de ondas planas para V_s, V_b

$$V_s = V e^{i(Ksa - \omega t)}, \quad V_b = V e^{i(Ksa - \omega t)}$$

al aplicarlas en las ecuaciones anteriores se obtiene:

$$(11C - M\omega^2)V_s = C(10e^{-ika} + 1)V_b$$

$$(11C - M\omega^2)V_b = C(10e^{ika} + 1)V_s$$

Expresas en forma $Ax = 0$, imponeas $\det A = 0$ para tener sol. no trivial, y obtenemos:

$$\begin{vmatrix} 11C - M\omega^2 & -C(10e^{-ika} + 1) \\ -C(10e^{ika} + 1) & 11C - M\omega^2 \end{vmatrix} = 0$$

$$\therefore (11C)^2 - 22CM\omega^2 + M^2\omega^4 - C^2[10^2 + 10e^{-ika} + 1 + 10e^{ika}] = 0$$

$$\therefore \omega^2 = \frac{22CM^2 \pm \sqrt{(22^2 C^2 M^2 - 4M^2 C^2)(1 - \cos ka)}}{2M^2}$$

$$\text{entonces } \omega^2 = \left(11C \pm C\sqrt{11^2 - r_0(1 - \cos\theta)}\right)/M$$

donde la parte positiva corresponde al modo óptico y la negativa al acústico.

Para $k_a = 0$

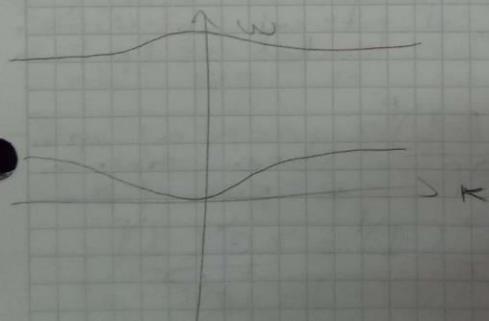
$$\omega^2 = \frac{11C \pm 11C}{M} \rightarrow \omega = \sqrt{\frac{22C}{M}} \text{ óptico}$$

$$\omega = 0 \text{ acústico}$$

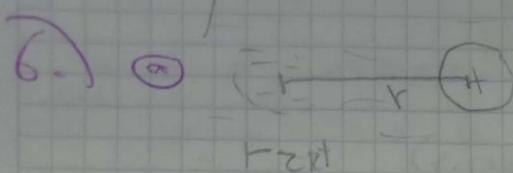
para $k_a = \pi$.

$$\omega^2 = \frac{11C \pm 9C}{M} \rightarrow \omega = \sqrt{\frac{20C}{M}} \text{ óptico}$$

$$\omega^2 = \frac{11C \pm 9C}{M} \rightarrow \omega = \sqrt{\frac{2C}{M}} \text{ acústico}$$



- 6. Atomic vibrations in a metal.** Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $3/4\pi R^3$, which defines R .
- (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2/MR^3)^{1/2}$.
 - (b) Estimate the value of this frequency for sodium, roughly.
 - (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in the metal.



al moverse el ion que tiene carga positiva, deja un espacio que se llena con carga negativa.

Esta carga provoca una fuerza eléctrica en el ion que por la ley de gauss tiene la forma:

$$\vec{E} = -\frac{q}{4\pi\epsilon_0 r^3} \hat{r} \quad \therefore \vec{P} = -\frac{q}{4\pi\epsilon_0 r^3} \hat{r}$$

Sabiendo que $\vec{F} = m\ddot{\vec{r}}$ se tiene un oscilador armónico en la forma:

$$m\ddot{r} + \frac{q}{4\pi\epsilon_0 r^3} \dot{r} = 0 \quad \text{con frecuencia } \omega = \left(\frac{q}{4\pi\epsilon_0 m} \right)^{1/2}$$

(b) Para el caso de sodio $m \sim 3 \times 10^{-23} \text{ [kg]}$ se tiene

$$R \sim 3,7 \times 10^{-10} \text{ [m]}, \text{ reemplazando } \omega \sim 1,1 \times 10^{13} \text{ [rad/seg]}$$

(c) Si la longitud de onda λ es de 5 nm, la velocidad del sonido en el sodio es de $v_s = \frac{\lambda}{T}$ y para el radio:

$$v_s \approx \frac{1,1 \times 10^{13}}{2\pi} \times 3,7 \times 10^{-10} \approx 647 \frac{\text{m}}{\text{seg}}$$

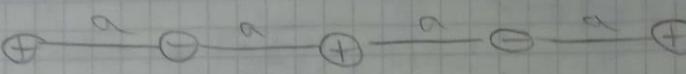
- *7. **Soft phonon modes.** Consider a line of ions of equal mass but alternating in charge, with $e_p = e(-1)^p$ as the charge on the p th ion. The interatomic potential is

*This problem is rather difficult.

the sum of two contributions: (1) a short-range interaction of force constant $C_{1R} = \gamma$ that acts between nearest neighbors only, and (2) a coulomb interaction between all ions. (a) Show that the contribution of the coulomb interaction to the atomic force constants is $C_{pC} = 2(-1)^p e^2/p^3 a^3$, where a is the equilibrium nearest-neighbor distance. (b) From (16a) show that the dispersion relation may be written as

$$\omega^2/\omega_0^2 - \sin^2 \frac{1}{2} Ka + \sigma \sum_{p=1}^{\infty} (-1)^p (1 - \cos pKa) p^{-3},$$

where $\omega_0^2 \equiv 4\gamma/M$ and $\sigma = e^2/\gamma a^3$. (c) Show that ω^2 is negative (unstable mode) at the zone boundary $Ka = \pi$ if $\sigma > 0.475$ or $4/7\zeta(3)$, where ζ is a Riemann zeta function. Show further that the speed of sound at small Ka is imaginary if $\sigma > (2 \ln 2)^{-1} = 0.721$. Thus ω^2 goes to zero and the lattice is unstable for some value of Ka in the interval $(0, \pi)$ if $0.475 < \sigma < 0.721$. Notice that the phonon spectrum is not that of a diatomic lattice because the interaction of any ion with its neighbors is the same as that of any other ion.

7. (a) 

Considerando esta cadena, el potencial interatómico debido a la interacción de Coulomb es (p cuenta el número de cellos):

$$U_p = \frac{ke^2(-1)^p}{rp} = \frac{ke^2(-1)^p}{ap} \quad \text{aprox en apariencia se sabe que:}$$

$$C_p = \frac{d^2 U_p}{dr_p^2} = \frac{(-1)(-2)e^2(-1)^p}{ap^3} = \frac{2e^2(-1)^p}{ap^3}$$

(b) De la relación de dispersion se tiene:

$$\omega^2 = \frac{M}{\mu} \sum_{p=0}^{\infty} C_p (1 - \cos(pr/a))$$

Existen dos casos para C_p :

D) Interacción de Coulomb:

$$C_p = \frac{2e^2(-1)^p}{ap^3}, \quad \forall p > 0$$

II) Considerar la fuerza a corto alcance:

$$C_p = \gamma, \quad p=1.$$

Si se consideran ambos simultáneamente se obtiene:

$$\omega^2 = \omega_0^2 \operatorname{sen}^2\left(\frac{\pi a}{2}\right) + \sum_{p=0}^{\infty} \frac{2 \operatorname{sen}^2(p)}{M} (-1)^p (1 - \cos(p\pi))$$

$$\omega^2 = \omega_0^2 \operatorname{sen}^2\left(\frac{\pi a}{2}\right) + \sum_{p=0}^{\infty} \frac{2(-1)^p}{a^2 p^2} \cdot 2 \operatorname{sen}\left(\frac{p\pi a}{2}\right)$$

$$\frac{\omega^2}{\omega_0^2} - \operatorname{sen}^2\left(\frac{\pi a}{2}\right) - 2 \sum_{p=0}^{\infty} \frac{(-1)^p \operatorname{sen}^2\left(\frac{p\pi a}{2}\right)}{p^2} = 0$$

C) $\omega < 0$ en $ka = \pi$, si $\sigma > 0$, 475.

Del punto b) vs ve que $\operatorname{sen}\left(\frac{p\pi a}{2}\right) \approx 0$.
Siendo pares se tiene $\operatorname{sen}\left(\frac{p\pi a}{2}\right) = 0$.

Para f impares se tendrá $\operatorname{sen}\left(\frac{p\pi a}{2}\right) = (-1)^{p-1}$

así que $\frac{\omega^2}{\omega_0^2} - 1 - 2 \sum_{p=0}^{\infty} \frac{(-1)^p}{p^2} = 0$
impares

$$\text{y } \frac{\omega^2}{\omega_0^2} - 1 - 2 \sum_{\substack{p=1 \\ \text{impar}}}^{\infty} (-1)^{p+1} (2p+1)^{-2} = 0$$

→ Hacemos uso de la software como Wolfram Mathematica
se aprecia que la serie converge.

$$\therefore \frac{\omega^2}{\omega_0^2} = \left(1 - \frac{14}{8} \varepsilon(3)\right),$$

$$s_1 > \frac{4}{7\varepsilon(3)} \Rightarrow \omega^2 < \omega_0^2 \left(1 - \underbrace{\frac{4}{7\varepsilon(3)} \cdot \frac{14\varepsilon(3)}{8}}_1\right)$$

∴ $\omega < 0 \Rightarrow$ la velocidad del sonido es negativa

Para la parte si $\sigma > \frac{1}{2\varepsilon(3)} = 0,721$ en $ka < 1$ y
partiendo del inciso b) puede aproximarse $\operatorname{sen} x \approx x$

$$y \text{ para } k = \frac{\pi}{2} \quad \omega^2 - \omega_m^2 - \left(\frac{\pi}{2} \right)^2 = (-1)^k p^{-3} S_m \left(\frac{\pi}{2} \right) = 0$$

$$\omega = \sqrt{\omega_m^2 S_m \left(\frac{\pi}{2} \right) + \left(\frac{\pi}{2} \right)^2 + (-1)^k p^{-3} S_m \left(\frac{\pi}{2} \right)}$$

$$V = \frac{1}{4k} \left(S_m \left(\frac{\pi}{2} \right) + (-1)^k p^{-3} S_m \left(\frac{\pi}{2} \right) \right)^{-1/2}$$

$$= \left(2 \sin \left(\frac{\pi}{2} \right) \cos \left(\frac{\pi}{2} \right) \alpha + 4 \sin \left(\frac{\pi}{2} \right) p^{-3} \sin \left(\frac{\pi}{2} \right) \alpha \right)^{-1/2}$$

$$\text{así que } V \approx \frac{\omega_m}{2} \left(\left(\frac{\pi}{2} \right)^2 - \frac{k^2 \alpha^2}{4} \right)^{-1/2} \left(\frac{\pi}{2} - \frac{\alpha k}{4} \right)$$

$$\text{ahora } \alpha > \frac{1}{2k} \Rightarrow \alpha = \frac{1}{2k}, \quad k > 1$$

$$y \quad V \leq \frac{\omega_m}{2} \left(\left(\frac{\pi}{2} \right)^2 - \frac{k^2 \alpha^2}{4} \right)^{-1/2} \left(\frac{\pi}{2} - \frac{\alpha k}{4} \right)$$

para los términos el término de la forma que sea menor que cero, así que la $V \in \mathbb{C}$

Capítulo V

- 1. Singularity in density of states.** (a) From the dispersion relation derived in Chapter 4 for a monatomic linear lattice of N atoms with nearest-neighbor interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{(\omega_m^2 - \omega^2)^{1/2}}.$$

where ω_m is the maximum frequency. (b) Suppose that an optical phonon branch has the form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $D(\omega) = (L/2\pi)^3 (2\pi/A^{3/2}) (\omega_0 - \omega)^{1/2}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

Capítulo 5.

7.1 a) De $w = \left(\frac{4C}{m}\right)^{\frac{1}{2}} \sin\left(\frac{ka}{2}\right) = w_0 \sin\left(\frac{ka}{2}\right)$,

la velocidad de grupo es:

$$v = \frac{1}{T} \omega = \frac{w_0 a \cos\left(\frac{ka}{2}\right)}{\pi}, \text{ y la densidad de estados es:}$$

$$D(\omega) = \frac{L}{2\pi} \cdot \left(\frac{dw}{dk}\right)^{-1} = \frac{L}{\pi w_0 a \cos\left(\frac{ka}{2}\right)} = \frac{L}{\pi w_0 a \sqrt{1 - \sin^2\left(\frac{ka}{2}\right)}}$$

$$D(\omega) = \frac{L}{\pi w_0 a \sqrt{1 - \frac{w^2}{w_0^2}}} = \frac{L}{\pi a \sqrt{w_0^2 - w^2}}$$

Sabemos ahora que "L" es la longitud analizada y "a" la longitud característica

$$N = \frac{L}{a}, \quad D(\omega) = \frac{N}{\pi a \sqrt{w_0^2 - w^2}}$$

b) Si $w(1R) = w_0 - AK^2 \rightarrow k = \left(\frac{w_0 - w}{A}\right)^{\frac{1}{2}}$

$$\therefore D(\omega) = \left| \frac{\sqrt{N}}{1\omega} \right| = \frac{1}{1\omega} \left(\left(\frac{L}{2\pi}\right)^3 \frac{4}{3} \pi K^3 \right)$$

$$= \left[\frac{L}{2\pi} \right]^3 \frac{4}{3} \pi \times \frac{3}{2} \left(\frac{w_0 - w}{A} \right)^{\frac{3}{2}} \times \left(\frac{1}{A} \right),$$

$$D(\omega) = \left(\frac{L}{2\pi} \right)^3 \times \frac{2\pi}{A^{\frac{3}{2}}} \times (w_0 - w)^{\frac{3}{2}}.$$

Por otra parte, la relación de suspensión implica que $w_0 > w \neq K$ (para que la frecuencia sea positiva, asumiendo $A > 0$) por lo tanto, estados donde $w < w_0$ no son permitidos que $D(\omega) = 0 \neq w_0$ esas mareas que $w_0 > w$ que $D(\omega)$ es el resultado anteriormente obtenido.

2. Rms thermal dilation of crystal cell. (a) Estimate for 300 K the root mean square thermal dilation $\Delta V/V$ for a primitive cell of sodium. Take the bulk modulus as 7×10^{10} erg cm⁻³. Note that the Debye temperature 158 K is less than 300 K, so that the thermal energy is of the order of $k_B T$. (b) Use this result to estimate the root mean square thermal fluctuation $\Delta a/a$ of the lattice parameter.

2)

a) La definición del módulo de Bulk es:

$$B = V \frac{dP}{dV} = V \frac{\partial U}{\partial V}, \text{ considerando el cambio de}$$

Variable:

$$V = V_0 (1+x) \rightarrow \frac{dV}{dx} = V_0 x \quad \text{donde } x = \frac{V - V_0}{V_0} = \frac{\Delta V}{V_0}$$

$$B = V \frac{d}{dV} \left(\frac{\partial U}{\partial V} \right) = V \frac{d}{dV} \left(\frac{\partial U}{\partial x} \right) = V \frac{\partial^2 U}{\partial x^2}$$

$$\therefore \frac{\partial^2 U}{\partial x^2} = BV_0 \rightarrow \frac{\partial U}{\partial x} = B V_0 \ln(1+x)$$

Luego approximando para series de Taylor a pequeños cambios fraccionales de volumen ($x \ll 1$):

$$\frac{\partial U}{\partial x} = BV_0 x \rightarrow U = \frac{1}{2} BV_0 x^2 = \frac{1}{2} BV_0 \left(\frac{\Delta V}{V_0} \right)^2$$

El volumen inicial de N celdas primarias de sodio es $V_0 = N a^3$, donde a es el parámetro de red, la energía por celda es

$$\bar{U} = \frac{1}{2} B a^3 x^2 \quad \text{y por fuerza de equilibrio}$$

Sabiendo que $\langle \bar{U} \rangle = \frac{1}{2} k_B T$ ($T < \Theta_D$)

igualando términos se tendrá que:

$$\frac{1}{2} B a^3 x^2 = \frac{1}{2} k_B T \Rightarrow x = \sqrt{\frac{k_B T}{B a^3}}$$

b) Dado que la celda es cúbica y despreciamos términos de orden superior

$$\frac{\Delta V}{V} = \frac{\Delta V_x}{x} + \frac{\Delta V_y}{y} + \frac{\Delta V_z}{z} = \frac{\Delta a}{a} + \frac{\Delta a}{a} + \frac{\Delta a}{a} = \frac{3 \Delta a}{a}$$

∴ La fluctuación térmica en a/a es

$$\frac{\Delta a}{a} = \frac{1}{3} \frac{\Delta V}{V} = \frac{1}{3} x = \frac{1}{3} \left(\frac{k_B T}{B a^3} \right)^{1/2}$$

- 3. Zero point lattice displacement and strain.** (a) In the Debye approximation, show that the mean square displacement of an atom at absolute zero is $\langle R^2 \rangle = 3\hbar\omega_D^2/8\pi^2\rho v^3$, where v is the velocity of sound. Start from the result (4.29) summed over the independent lattice modes: $\langle R^2 \rangle = (\hbar/2\rho V)\sum\omega^{-1}$. We have included a factor of $\frac{1}{2}$ to go from mean square amplitude to mean square displacement. (b) Show that $\sum\omega^{-1}$ and $\langle R^2 \rangle$ diverge for a one-dimensional lattice, but that the mean square strain is finite. Consider $\langle(\partial R/\partial x)^2\rangle = \frac{1}{2}\sum K^2 u_0^2$ as the mean square strain, and show that it is equal to $\hbar\omega_D^2 L/4MNv^3$ for a line of N atoms each of mass M , counting longitudinal modes only. The divergence of R^2 is not significant for any physical measurement.

3. @ $\langle R^2 \rangle = \frac{1}{2\rho V} \sum \omega^{-1}$.

En formando la densidad de estados

$$\langle R^2 \rangle = \frac{1}{2\rho V} \int \frac{D(\omega) \omega}{\omega} d\omega$$

$$D(\omega) = \frac{\sqrt{k^2}}{2\pi^2} \frac{dk}{d\omega} = \frac{\sqrt{\omega^2}}{2\pi^2(Vv)} \times \frac{1}{(Vv)} , \quad Vv \equiv V$$

$$\text{i. } \langle R^2 \rangle = \frac{1}{2\pi V} \int \frac{V w^2}{(2\pi)^2 V^2} dw = \frac{1}{2\pi V} \int w^2 dw$$

$$\langle R^2 \rangle = \frac{\hbar w_0^2}{4\pi^2 V^3 P} \Rightarrow \text{Lo cual corresponde para un modo normal para 3 modos}$$

↓ el factor 3 se divide por 3

$$\langle R^2 \rangle = \frac{3\hbar w_0^2}{8\pi^2 P V^3}$$

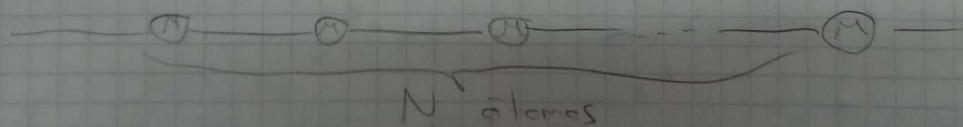
b) $\sum \tilde{w}^{-1}$ y $\langle R^2 \rangle$ divergen en una red 1D, en cesta se tiene $D(\omega) = \frac{3L}{2\pi} \frac{1}{\omega}$

$$\langle R^2 \rangle = \frac{1}{2\pi V} \int_0^{w_0} \frac{D(\omega)}{\omega} dw,$$

$$\langle R^2 \rangle = \frac{1}{2\pi V} \int_0^{w_0} \frac{3L}{2\pi V} \frac{dw}{\omega} = \frac{3\hbar L}{4\pi^2 P V} \ln(\omega) \Big|_0^{w_0}$$

Asi que tanto $\langle R^2 \rangle$ como $\sum \tilde{w}^{-1}$ (la cual esta en $\langle R^2 \rangle$) divergen: debido a la presencia del termino $\ln(\omega) \rightarrow -\infty$.

$$\text{Algo al considerar } \left\langle \left(\frac{\partial R}{\partial x} \right)^2 \right\rangle = \sum \frac{1}{2} K U_0^2 = \frac{\hbar w_0^2 L}{4 M N V^3}$$



$$\text{Y usando } U_0 = \frac{4(n+1)k}{P V W} \hbar \rightarrow U_0 = \sum_{n=0}^{\infty} \frac{k}{P V W}$$

$$\begin{aligned} \sum \frac{1}{2} k U_0^2 &= \frac{1}{P V} \sum \frac{k^2}{\omega} = \frac{1}{P V} \int_0^{w_0} D(\omega) \frac{K^2}{\omega} dw \\ &= \frac{1}{P V} \int_0^{w_0} \frac{3L}{2\pi V} \frac{K^2}{\omega} dw = \frac{3\hbar L}{P V^2 \pi V} \int_0^{w_0} \frac{1}{\omega} dw \end{aligned}$$

$$= \frac{L^2}{P V^2 \pi V^3} \frac{w_0^2}{2} = \frac{\hbar w_0^2 L}{M N 4\pi V^3}$$

4. Heat capacity of layer lattice. (a) Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^3 .

(b) Suppose instead, as in many layer structures, that adjacent layers are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures?

4.

a) Al considerarse una de las láminas el sistema pasa a ser de 2 dimensiones, por lo tanto.

$$N = \left(\frac{L}{2\pi}\right)^2, A = \frac{L^2}{4\pi^2} \pi K^2 = \frac{L^2 K^2}{4\pi^2}$$

$$D(\omega) = \frac{1}{\omega} N = \frac{1}{\omega} \frac{L^2 K^2}{4\pi^2} = \frac{L^2 K^2}{2\pi^2 \omega}$$

La energía viene dada por:

$$U = \int D(\omega) \langle \ln \omega \rangle \hbar \omega d\omega$$

$$U = \int \frac{L^2 K^2}{2\pi^2 \omega^2} \cdot \frac{1}{e^{\frac{\hbar \omega}{k_B T}} - 1} \hbar \omega d\omega$$

$$U = \frac{L^2 K^2}{2\pi^2} \int \frac{\omega^2 d\omega}{e^{\frac{\hbar \omega}{k_B T}} - 1} = \frac{L^2 (k_B T)^3}{2\pi^2 \hbar^2 c^2} \int_{x_0}^{\infty} \frac{x^2 dx}{e^x - 1}$$

Tomando $x = \frac{\hbar \omega}{k_B T} \rightarrow \omega = \frac{k_B T}{\hbar} x$

$$\therefore U = \frac{L^2 K^2}{2\pi^2 \hbar^2 c^2} \int_{x_0}^{\infty} \frac{x^2 \frac{k_B T}{\hbar} x dx}{e^x - 1} \Rightarrow C_V = 4 \times T^2$$

Finalmente

$$\alpha = \frac{L^2 K^2}{2\pi^2 \hbar^2 c^2} \int_{x_0}^{\infty} \frac{x^2 \frac{k_B T}{\hbar} x dx}{e^x - 1} \Rightarrow \alpha \text{ es constante y no depende de } T \text{ y la freq. a bajas temperaturas } x_0 \rightarrow \infty$$

b) Si las capas comienzan a interactuar debidamente, el sistema debe considerarse como tridimensional, así, la dependencia de los estados consideraría un volumen lo cual implica una dependencia de C_V en función de V , haciendo un cambio de variable simple de T^4 para V se reobtendrá con la dimensionalidad del sistema.

- *5. **Grüneisen constant.** (a) Show that the free energy of a phonon mode of frequency ω is $k_B T \ln [2 \sinh (\hbar\omega/2k_B T)]$. It is necessary to retain the zero-point energy $\frac{1}{2}\hbar\omega$ to obtain this result. (b) If Δ is the fractional volume change, then the free energy of the crystal may be written as

$$F(\Delta, T) = \frac{1}{2}B\Delta^2 + k_B T \sum \ln [2 \sinh (\hbar\omega_{\mathbf{k}}/2k_B T)] ,$$

where B is the bulk modulus. Assume that the volume dependence of $\omega_{\mathbf{k}}$ is $\delta\omega/\omega = -\gamma\Delta$, where γ is known as the Grüneisen constant. If γ is taken as independent of the mode \mathbf{k} , show that F is a minimum with respect to Δ when $B\Delta = \gamma \sum \frac{1}{2}\hbar\omega \coth (\hbar\omega/2k_B T)$, and show that this may be written in terms of the thermal energy density as $\Delta = \gamma U(T)/B$. (c) Show that on the Debye model $\gamma = -\partial \ln \theta / \partial \ln V$. Note: Many approximations are involved in this theory: the result (a) is valid only if ω is independent of temperature; γ may be quite different for different modes.

S.

@ La energía libre de Helmholtz viene dada por:
 $f = -k_B T \ln Z$, con $Z = \sum_n e^{-E_n / k_B T} = \sum_n e^{-E_n \beta}$

Para un fóton de frecuencia ω , la energía del n -ésimo modo es:

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega \text{ con } \frac{\hbar \omega}{k_B} \equiv \text{la energía base.}$$

$$\text{Así: } Z = \sum_n e^{\exp[-(n + \chi_c) \hbar \omega \beta]}$$

$$Z = \sum_{n=0}^{\infty} e^{-n \hbar \omega \beta} e^{-\chi_c \hbar \omega \beta} \quad] \text{ haciendo el cambio de variable } x = \hbar \omega \beta, \text{ entonces:}$$

$$Z = \sum_{n=0}^{\infty} \underbrace{e^{-nx}}_{\text{variable } x} \underbrace{e^{-\chi_c}}_{\text{constante}} = e^{-\chi_c} \sum_{n=0}^{\infty} e^{-nx}$$
$$\left(\frac{1}{e^x}\right)^n = \frac{1}{1 - e^{-x}} \rightarrow \text{Suponiendo } e^{-x} < 1$$

$$\therefore Z = \frac{e^{-\chi_c}}{1 - e^{-x}} = \left[2 \operatorname{senh} \left(\frac{x}{2} \right) \right]^{-1} \quad] \text{ al reemplazar } x \text{ en la energía base se resuelve la sustitución se obtiene:}$$

$$F = k_B T \ln \left[2 \operatorname{senh} \left(\frac{\hbar \omega}{k_B T} \right) \right]$$

$$\textcircled{1} \quad F(\Delta, T) = \frac{1}{2} B\Delta^2 + k_B T \sum_i \ln \left[e^{\frac{h\nu_i}{k_B T}} + e^{-\frac{h\nu_i}{k_B T}} \right]$$

Sabes al os que $\frac{\partial W}{W} = \gamma \Delta$

$\therefore W_K = W_0 - W\gamma\Delta$, imp - 1. $\frac{\partial f}{\partial \Delta} = 0$ entonces:

$$\frac{\partial F}{\partial \Delta} = B\Delta + k_B T \sum_i \left[\frac{1}{2} \tanh \left(\frac{h(\nu_i - W_K)}{2k_B T} \right) \right] \left[\cosh \left(\frac{h(\nu_i - W_K)}{2k_B T} \right) \right] \left(\frac{-h\nu_i}{2k_B T} \right)$$

$$\therefore B\Delta = \gamma \sum_i \frac{1}{2} \tanh \left(\frac{h(\nu_i - W_K)}{2k_B T} \right)$$

Por otra parte, la distorsión de planck

$$\langle n \rangle = \frac{1}{e^{h\nu/k_B T} - 1} = \frac{1}{e^u - 1} \quad \text{implica que}$$

$$\begin{aligned} \langle n \rangle + \frac{1}{2} &= \frac{1}{e^u - 1} + \frac{1}{2} = \frac{2 + e^u - 1}{2(e^u - 1)} = \frac{e^u + 1}{2(e^u - 1)} \\ &= \frac{1}{2} \coth \left(\frac{u}{2} \right) \\ &= \frac{1}{2} \coth \left(\frac{h\nu_K}{2k_B T} \right) \end{aligned}$$

y la energía es $U_{GW} = g \langle n \rangle + \frac{1}{2} h\nu = \frac{1}{2} h\nu \coth \left(\frac{h\nu_K}{2k_B T} \right)$

al reemplazar en la ecuación de $B\Delta$ nos queda:

$$B\Delta = \gamma \sum_i \frac{1}{2} h\nu \coth \left(\frac{h\nu_K}{2k_B T} \right) \quad \text{con } W_K = (W_0 - W)\gamma\Delta$$

$$\therefore B\Delta = \gamma U_{GW} \Rightarrow \Delta \propto U_{GW}/\gamma$$

⑦ Como se mencionó anteriormente $\frac{\delta w}{w} = -\gamma \Delta$

con $\Delta = \frac{\partial V}{V}$ $\therefore \frac{\delta w}{w} = -\gamma \frac{\partial V}{V}$

y sabemos que $\gamma(\ln x) = \frac{1}{x} \gamma x$

$\therefore \gamma(\ln w) = -\gamma \gamma(\ln V)$. Considerando que en la aproximación de Debye $\frac{\delta w}{w} = \frac{\Theta}{T} \Rightarrow w_0 = \frac{k_B \Theta}{h}$

Esto es $w_0 \propto \Theta$ así que:

$$\gamma(\ln(w)) = \gamma(\ln \Theta) \Rightarrow \gamma = -\frac{\gamma(\ln w)}{\gamma(\ln V)}$$

$$\gamma = -\frac{\gamma(\ln \Theta)}{\gamma(\ln V)}$$

FIN