Final Exam

P555
May 15, 2024

SHOW ALL YOUR WORK TO GET FULL CREDIT!

The final has two problems. The first one is worth 50 points and the second one 30. The second problem has 2 bonus questions indicated in blue worth 10 points each. Thus, there are 100 points available, but 80 points should give 100% of the grade.

Problem 1: In the periodic table we see that the Zr atom has an electronic structure given by [Kr]$4d^2 5s^2$.

a) Use Hund rules to obtain S and L for the ground state of the Zr atom. Draw the energy levels in the relevant shells and indicate the electronic placement. (5 points)

b) What is the degeneracy of the ground state of Zr based on its L and S values? (5 points)

c) What are the allowed values of J for this atom? (5 points)

d) Provide the degeneracy for each of the values of J that you found in (c) and compare with the result you found in part (b). (5 points)

e) Now, using Hund's rules, find the value of J for the ground state of the Zr atom and, using the results you found in (a) provide the values for L, S, and J of the ground state of the atom of Zr using spectroscopic notation: ${}^{2S+1}L_J$. (Hint: remember that the spectroscopic notation for L is S, P, D, F, G, H, I, J, K, etc.) (5 points)

f) Calculate the Landé factor g for the Zr atom. (5 points)

g) What is the energy splitting ΔE linear in the magnetic field B for the ground state of a Zr atom placed in a magnetic field B? Provide the energy of each energy level as a function of B, in terms of μ_B and E_0, where μ_B is the Bohr magneton and E_0 is the energy of the degenerate ground state when $B = 0$. (5 points)

h) What is the magnetization $\mathbf{M}$ of a sample of Zr that contains N atoms in a volume V? (5 points)

i) How do you expect the magnetization $\mathbf{M}$ calculated in (h) to evolve from $kT \gg \mu_B B$ to $kT \ll \mu_B B$? Why? (5 points)

j) Now provide the actual value of the magnetization $\mathbf{M}$ calculated in (h) when $kT \gg \mu_B B$ and when $kT \ll \mu_B B$ and confirm your answer to point (i). (5 points)

Problem 2: A three-dimensional solid is made of N atoms with one atom at each point of a simple cubic Bravais lattice with lattice constant a and it has a phonon spectrum given by

$$\omega(k_x, k_y, k_z) = \omega_0[\sin^2(\frac{k_x a}{2}) + \sin^2(\frac{k_y a}{2}) + \sin^2(\frac{k_z a}{2})]^{1/2}. \tag{1}$$

Notice that the spectrum is independent of the polarization ν.

Bonus question (10 points): what is the degeneracy of this branch? Explain.

a) Consider the first Brillouin zone of this crystal centered at the origin, i.e. $\Gamma = (0, 0, 0)$, and provide its boundaries along the k_x, k_y, and k_z directions.(5 points)

b) Now in momentum space draw arrows identifying the following directions (5 points):
i) $\Gamma \to X$ where $\Gamma = (0, 0, 0)$ and $X = (\frac{\pi}{a}, 0, 0)$.
ii) $\Gamma \to K$ where $\Gamma = (0, 0, 0)$ and $K = (\frac{\pi}{a}, \frac{\pi}{a}, 0)$.
iii) $\Gamma \to L$ where $\Gamma = (0, 0, 0)$ and $L = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$.

c) Now provide an expression and sketchs of ω versus $\mathbf{k}$ along the following directions (5 points):
i) $\Gamma \to X$.

ii) $\Gamma \to K$.

iii) $\Gamma \to L$.

d) Now provide expressions for the speed of sound along each of the 3 directions for which you drew the phonon dispersions in part (c). (10 points)

e) Now in the figures you made for part (c) draw the ω versus $\mathbf{k}$ curve for the Debye approximation to the dispersion curves as dashed lines in your previous diagrams. (5 points)

Bonus: Now assuming that the speed of sound for the crystal is given by the average of the 3 speeds that you have already calculated, call it c_s, calculate the Debye frequency ω_D for this crystal. Provide your results in terms of ω_0 and N. (10 bonus points)

Useful information:

$$\mathcal{B}_J(x) = \frac{2J+1}{2J}\coth(\frac{2J+1}{2J}x) - \frac{1}{2J}\coth(\frac{x}{2J}). \tag{2}$$

$$\lim_{x\to 0}\coth(x) \approx \frac{1}{x} + \frac{x}{3} + ... \tag{3}$$