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)

Notice that the 5s-shell is filled. Thus, we need to look at the 4d-shell which is less than half-filled (see Fig. 1). We see that the total spin is $S = 1$, and $L = 3$.

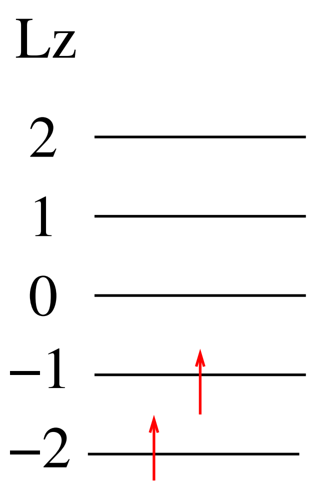

FIG. 1:

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

The degeneracy is given by

$$(2L + 1)(2S + 1) = 7 \times 3 = 21 \quad (1)$$

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

The allowed values of J go from $L + S$ to $|L - S|$ by units of 1. Then we get

$$J = 4, 3, 2. \quad (2)$$

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)

The degeneracy for each J is $2J + 1$. Thus the degeneracy in terms of J is 9, 7, and 5 for J=4, 3, and 2. The total degeneracy is 9+7+5=21, i.e., the same number as when we calculated the degeneracy in terms of L and S, as expected.

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)

We see that $J = |L - S| = 2$ since the shell is less than half-filled.
The spectroscopic notation for the ground state of the atom is:$^3F_2$.

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

$$g_{Zr} = \frac{1}{2}\frac{[3J(J+1) - L(L+1) + S(S+1)]}{J(J+1)} = \frac{1}{2}\frac{18-12+2}{6} = \frac{2}{3}. \tag{3}$$

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)

The energy splitting is given by

$$\Delta E = g\mu_B B = \frac{2}{3}\mu_B B. \tag{4}$$

The degeneracy 5 is now split and each level will have energy

$$E = E_0 + J_z g\mu_B B = E_0 + J_z\frac{2}{3}\mu_B B, \tag{5}$$

where E_0 is the energy of the degenerate level and $J_z = \pm 2, \pm 1$, and 0. Thus, $E_{-2} = E_0 - \frac{4}{3}\mu_B B$, $E_{-1} = E_0 - \frac{2}{3}\mu_B B$, $E_0 = E_0$, $E_1 = E_0 + \frac{2}{3}\mu_B B$, and $E_2 = E_0 + \frac{4}{3}\mu_B B$.

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

$$M = n\mu_B gJ\mathcal{B}_J(\beta\mu_B gJB) = \frac{N}{V}\mu_B\frac{2}{3}2\mathcal{B}_2(\frac{4}{3}\beta\mu_B B) = \frac{4}{3}\frac{N}{V}\mu_B\mathcal{B}_2(\frac{4}{3}\beta\mu_B B). \tag{6}$$

Using that

$$\mathcal{B}_J(x) = \frac{2J+1}{2J}\coth(\frac{2J+1}{2J}x) - \frac{1}{2J}\coth(\frac{x}{2J}), \tag{7}$$

we see that

$$\mathcal{B}_2(\frac{4}{3}\beta\mu_B B) = \frac{5}{4}\coth(\frac{5}{3}\beta\mu_B B) - \frac{1}{4}\coth(\frac{\beta\mu_B B}{3}). \tag{8}$$

Then,

$$M = \frac{N}{3V}\mu_B[5\coth(\frac{5}{3}\frac{\mu_B B}{kT}) - \coth(\frac{1}{3}\frac{\mu_B B}{kT})]. \tag{9}$$

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)

I expect at high T, i.e. x very small the magnetization will be zero because the spins will be disordered due to the thermal fluctuations; as the temperature starts to decrease, and x increases, the magnetization will increased linearly with x, Curie's law, and when the temperature becomes very small compared with B, i.e., when x is very large, the magnetization will reach its maximum possible value that corresponds to full polarization of the spins since the magnetic energy now prevails over the thermal energy.

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)

For $kT \gg \mu_B B$ we see that x is small and we can use the expansion of $\coth(x)$ provided in the "Useful information" section, in Eq. 9. Then,

$$\lim_{x \to 0} M = \frac{N}{V}\frac{8}{9}\frac{\mu_B^2 B}{kT}, \tag{10}$$

which vanishes when $x = 0$ ($T \to \infty$) and satisfies Curie's law. For $kT \ll \mu_B B$ we see that x is large and we can replace $\coth(x) = \frac{\cosh(x)}{\sinh(x)} \approx \frac{e^x}{e^x} \approx 1$ in Eq. 9. Then,

$$\lim_{x \to \infty} M = \frac{N}{V}\frac{4}{3}\mu_B, \tag{11}$$

which is the maximum value that the magnetization can have.

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

$$\omega(k_x, k_y, k_z) = \omega_0[\sin^2(\frac{k_x a}{2}) + \sin^2(\frac{k_y a}{2}) + \sin^2(\frac{k_z a}{2})]^{1/2}. \tag{12}$$

Notice that the spectrum is independent of the polarization ν.

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

Since the system is 3 dimensional there should be one longitudinal and two transversal modes. Thus, the degeneracy of the branch is 3.

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)

We know that the reciprocal lattice is generated by the vectors $\mathbf{b}_i = \frac{2\pi}{a}$ with $i = x$, y, and z. Thus, the FBZ is a cube of side $\frac{2\pi}{a}$. If we centered this cube at the origin we find that it is defined by

$$\frac{-\pi}{a} < k_i \leq \frac{\pi}{a}, \tag{13}$$

with $i = x$, y, and z.

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 $L = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$.

See Fig. 2.

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

$$\omega(k, 0, 0) = \omega_0 |\sin(\frac{ka}{2})|, \tag{14}$$

with $k_x = k$ for $0 \leq k \leq \frac{\pi}{a}$.
ii) $\Gamma \to K$.

$$\omega(k, k, 0) = \omega_0 \sqrt{2} |\sin(\frac{ka}{2\sqrt{2}})|. \tag{15}$$

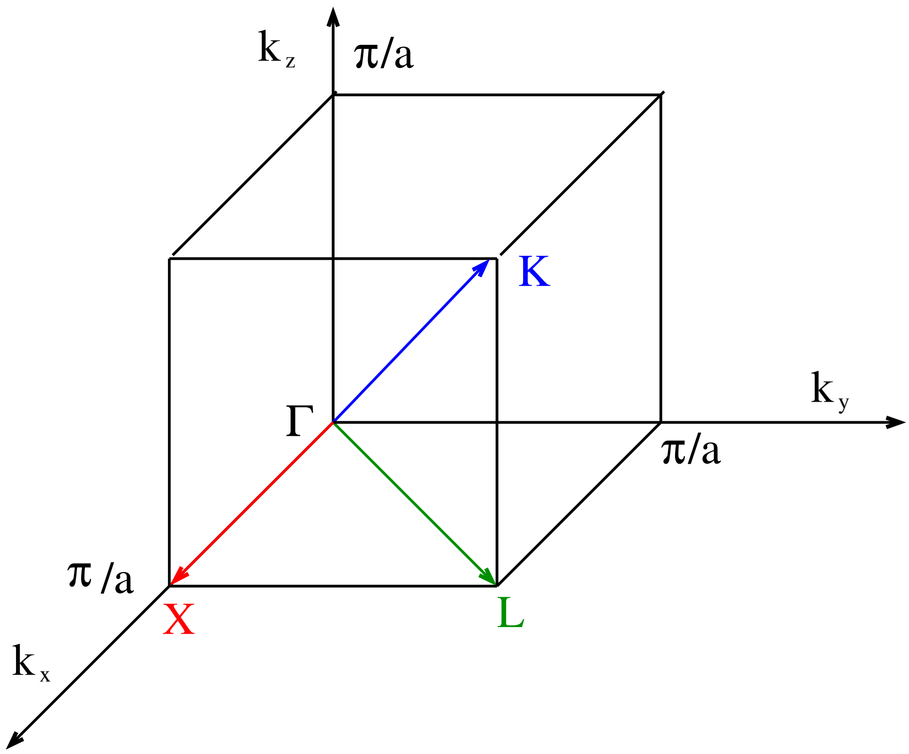

FIG. 2:

with $k_x = k_y = \frac{k}{\sqrt{2}}$ for $0 \leq k \leq \frac{\sqrt{2}\pi}{a}$.

iii) $\Gamma \to L$.

$$\omega(k,k,k) = \omega_0 \sqrt{3} |\sin(\frac{ka}{2\sqrt{3}})|. \tag{16}$$

with $k_x = k_y = k_z = \frac{k}{\sqrt{3}}$ for $0 \leq k \leq \frac{\sqrt{3}\pi}{a}$.

For the sketchs see Fig. 3.

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)

The speed of sound is given by $\frac{d\omega}{dk}$ in the limit in which $k \to 0$. Then we obtain:

i) $\Gamma \to X$.

$$\omega(k_x, 0, 0) \approx \omega_0 |\frac{ka}{2}|. \tag{17}$$

Then $C_{sX} = \omega_0 \frac{a}{2}$.

ii) $\Gamma \to K$.

$$\omega(k,k,0) \approx \omega_0 \sqrt{2} |\frac{ka}{2\sqrt{2}}|. \tag{18}$$

Then $C_{sK} = \omega_0 \frac{a}{2}$.

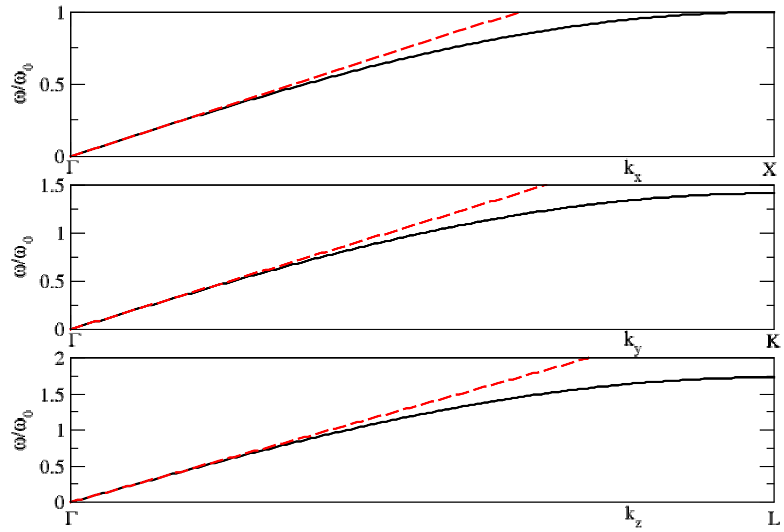

FIG. 3:

iii) $\Gamma \to L$.

$$\omega(k,k,k) \approx \omega_0\sqrt{3}|\frac{ka}{2\sqrt{3}}|. \tag{19}$$

Then $C_{sL} = \omega_0 \frac{a}{2}$.

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)

See Fig. 3.

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)

We know that

$$3N = V\int_0^{\infty} d\omega D(\omega). \tag{20}$$

In the Debye approximation in 3 dimensions

$$D(\omega) = \frac{3\omega^2}{2\pi^2 c_s^3}\Theta(\omega_D - \omega). \tag{21}$$

Then

$$3N = V\int_0^{\omega_D} d\omega \frac{3\omega^2}{2\pi^2 c_s^3} = \frac{\omega_D^3}{2\pi^2 c_s^3}. \tag{22}$$

Then, using that $V = Na^3$,

$$\omega_D = (\frac{3N2\pi^2 c_s^3}{Na^3})^{1/3} = (6\pi^2)^{1/3}\frac{\omega_0}{2}. \tag{23}$$

Useful information:

$$\mathcal{B}_J(x) = \frac{2J+1}{2J}\coth(\frac{2J+1}{2J}x) - \frac{1}{2J}\coth(\frac{x}{2J}). \tag{24}$$

$$\lim_{x\to 0}\coth(x) \approx \frac{1}{x} + \frac{x}{3} + ... \tag{25}$$