Final Exam

P555

May 11, 2023

SHOW ALL YOUR WORK TO GET FULL CREDIT!

The final has 18 questions worth 5 points each. You only need to answer 12 of the 18 questions to get full credit. Thus, the additional 6 questions that you may have time to address will give you extra credit.

Problem 1: In the periodic table we see that the Pr atom has an electronic structure given by $4f^3 5d^0 6s^2$.

a) Use Hund rules to obtain S, L, and J for the ground state of the Pr atom. Draw the energy levels in the relevant shells and indicate the electronic placement. Provide your final result 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)

b) What is the degeneracy of the ground state of Pr? (5 points)

c) Calculate the Landé factor g for the Pr atom. (5 points)

d) What is the energy splitting ΔE linear in the magnetic field B for the ground state of a Pr 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)

e) When the Pr atom is ionized the first electrons being lost are the ones in the 6s shell. Knowing this, provide the electronic structre of the ion Pr^{3+}. (5 points)

f) Use Hund rules to obtain S, L, and J for the ground state of the Pr^{3+} ion. Draw the energy levels in the relevant shells and indicate the electronic placement. Provide your final result 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)

g) Calculate the Landé factor g for the Pr^{3+} ion. (5 points)

h) What is the degeneracy of the ground state of Pr^{3+}? (5 points)

i) Is the separation between energy levels at a given field B larger in Pr or in Pr^{3+}? Why? (5 points)

j) What is the magnetization $\mathbf{M}$ of a sample of Pr^{3+} that contains N atoms in a volume V? (5 points)

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

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

Problem 2: A one-dimensional solid made of N atoms with one atom at each point of the Bravais lattice with lattice constant a has a phonon density of states given by

$$D_D(\omega) = \frac{1}{\pi c}\Theta(\omega - \omega_D), \quad (1)$$

in the Debye approximation, with c the speed of sound, $\omega_D = \pi c n$ is the Debye frequency, $n = N/L$ is the atomic density ($L = Na$), and Θ is the Heaviside function.

a) Explain Debye's approximation and why it is important. What progress in our understanding of the heat capacity did it allow? (5 points)

b) Write an expression for the heat capacity C of the one dimensional material in the Debye's approximation. (5 points)

c) What should be the heat capacity of the 1D material at very high temperature? Why? (5 points)

d) Now provide an expression for C when $T \to \infty$ and verify your answer to part (c). (5 points)

e) How do you expect the heat capacity to evolve as a function of the temperature from $T = 0$ to $T \to \infty$? Why? (5 points)

f) Now provide an expression for C when $T \to 0$ and verify your answer to part (e). Hint: you can express your results in terms of an integral that does not depend on the temperature. (5 points)

Useful information:

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

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

Heat capacity in 3D:

$$C_V = V\int_0^\infty d\omega D(\omega)\frac{\partial}{\partial T}\frac{\hbar\omega}{(e^{\beta\hbar\omega} - 1)}. \tag{4}$$