

HW6, PHYS 3113

P1 (6.22) In most paramagnetic materials, the individual magnetic particles have more than two independent states (orientations). The number of independent states depends on the particle's angular momentum "quantum number" j , which must be a multiple of $1/2$. For $j = 1/2$ there are just two independent states. More generally, the allowed values of the z component of a particle's magnetic moment are

$$\mu_z = -j\delta_\mu, (-j+1)\delta_\mu, \dots, (j-1)\delta_\mu, j\delta_\mu,$$

where δ_μ is a constant, equal to the difference in μ_z between one state and the next. (When the particle's angular momentum comes entirely from electron spins, δ_μ equals twice the Bohr magneton. When orbital angular momentum also contributes, δ_μ is somewhat different but comparable in magnitude. For an atomic nucleus, δ_μ is roughly a thousand times smaller.) Thus the number of states is $2j+1$. In the presence of a magnetic field B pointing in the z direction, the particle's magnetic energy (neglecting interactions between dipoles) is $-\mu_z B$.

(a) Prove the following identity for the sum of a finite geometric series:

$$1 + x + x^2 + \dots + x^n = \frac{1 - x^{n+1}}{1 - x}.$$

(b) Show that the partition function of a single magnetic particle is

$$Z = \frac{\sinh \left[b \left(j + \frac{1}{2} \right) \right]}{\sinh \frac{b}{2}},$$

where $b = \beta\delta_\mu B$.

(c) Show that the total magnetization of a system of N such particles is

$$M = N\delta_\mu \left[\left(j + \frac{1}{2} \right) \coth \left[b \left(j + \frac{1}{2} \right) \right] - \frac{1}{2} \coth \frac{b}{2} \right],$$

where $\coth x$ is the hyperbolic cotangent, equal to $\cosh x / \sinh x$. Plot the quantity $M/N\delta_\mu$ for a few different values of j .

P2 (6.30) The constant ϵ for ordinary hydrogen, H_2 , is 0.0076 eV. Only half of the terms in the rotational partition function

$$Z_{\text{rot}} = \sum_{j=0}^{\infty} (2j + 1) e^{-j(j+1)\epsilon/kT}$$

contribute for any given molecule. More precisely, the set of allowed j values is determined by the spin configuration of the two atomic nuclei. There are four independent spin configurations, classified as a single “singlet” state and three “triplet” states. The time required for a molecule to convert between the singlet and triplet configurations is ordinarily quite long, so the properties of the two types of molecules can be studied independently. The singlet molecules are known as **parahydrogen** while the triplet molecules are known as **orthohydrogen**.

- (a) For parahydrogen, only the rotational states with even values of j are allowed. Use a computer to calculate the rotational partition function, average energy, and heat capacity of a parahydrogen molecule. Plot the heat capacity as a function of kT/ϵ .
- (b) For orthohydrogen, only the rotational states with odd values of j are allowed. Repeat part (a) for orthohydrogen.
- (c) At high temperature, where the number of accessible even- j states is essentially the same as the number of accessible odd- j states, a sample of hydrogen gas will ordinarily consist of a mixture of 1/4 parahydrogen and 3/4 orthohydrogen. A mixture with these proportions is called **normal hydrogen**. Suppose that normal hydrogen is cooled to low temperature without allowing the spin configurations of the molecules to change. Plot the rotational heat capacity of this mixture as a function of temperature. At what temperature does the rotational heat capacity fall to half its high temperature value (i.e., to $k/2$ per molecule)?