Statistical Mechanics

Worksheet 9

June 15th, 2023

1 Fermion gas mixture

An ideal gas consists of a mixture of *green* and *red* spin-$\frac{1}{2}$ particles. All particles have mass m. A magnetic field, B, is applied to the system. The *green* particles have magnetic moment γ_G, and the *red* particles have magnetic moment γ_R, where $\gamma_R < \gamma_G$. Assume that temperature is high enough that Fermi statistics can be neglected. The system will be in equilibrium if chemical potentials the the *red* and the *green* gases are equal. Compute the ratio N_R/N_G, where N_R is the number of *red* atoms and N_G is the number of *red* particles. Use the canonical ensemble

2 Molecular oxygen

The molecular oxygen has a net magnetic spin $\vec{S}$ of unity, that is, S^z is quantized to -1, 0, or $+1$. The Hamiltonian for an ideal gas of N such molecules in a magnetic field $\vec{B} \parallel \hat{z}$ is

$$\mathcal{H} = \sum_{i+1}^{N} \left[\frac{p_i^2}{2m} - \mu B S_i^z \right], \tag{1}$$

where $\{\vec{p}_i\}$ are the center of mass momenta of the molecules. The corresponding coordinates $\{\vec{q}_i\}$ are confined to a volume V. (Ignore all other degrees of freedom.)

1. Treating $\{\vec{p}_i, \vec{q}_i\}$ classically, but the spin degrees of freedom as quantized, calculate the partition function, $\tilde{Z}(T, N, V, B)$.

2. What are the probabilities for S_i^z of a specific molecule to take on values of -1, 0, $+1$ at a temperature T?

3. Find the average magnetic dipole moment, $\langle M \rangle / V$, where $M = \mu \sum_{i=1}^{N} S_i^z$

4. Calculate the zero field susceptibility $\chi = \partial \langle M \rangle / partial B|_B = 0$.

3 Polar rods

Consider rod-shaped molecules with moment of inertia I, and a dipole moment mu. The contribution of the rotational degrees of freedom to the Hamiltonian is given by

$$\mathcal{H}_{\text{rot}} = \frac{1}{2I} \left(p_\theta^2 + \frac{p_p hi^2}{\sin^2 \theta} \right) - \mu E \cos \theta, \tag{2}$$

where E is an external electric field. ($\phi \in [0, 2\pi], \theta \in [0, \pi]$ are the azimuthal and polar angles, and p_ϕ, p_theta are their conjugate momenta.)

1. Calculate the contribution of the rotational degrees of freedom of each dipole to the classical partition function.

2. Obtain the mean polarization $P = \langle \mu \cos\theta \rangle$ of each dipole.

3. Find the zero-field polarizability
$$\chi_T = \left.\frac{\partial P}{\partial E}\right|_{E=0} \tag{3}$$

4. Calculate the rotational energy per particle (at finite E), and comment on its high- and low-temperature limits.

5. Sketch the rotational heat capacity per dipole.

4 Rotation of diatomic molecules

In our first look at the ideal gas we considered only the translational energy of the particles. But molecules can rotate, Problems with kinetic energy. The rotational motion is quantized; and the energy levels of a diatomic molecule are of the form

$$\epsilon(j) = j(j+1)\epsilon_0 \tag{4}$$

where j is any positive integer including zero: $j = 0, 1, 2, \cdots$. The multiplicity of each rotational level is $g(1) = 2j + 1$.

1. Find the partition function $Z_R(T)$ for the rotational states of one molecule. Remember that Z is a sum over all states, not over all levels (this makes a difference).

2. Evaluate $Z_R(r)$ approximately for $k_BT \gg \epsilon_0$, by converting the sum to an integral.

3. Do the same for $k_BT \ll \epsilon_0$, by truncating the sum after the second term.

4. Give expressions for the energy U and the heat capacity C, as functions of T, in both limits. Observe that the rotational contribution to the heat capacity of a diatomic molecule approaches k_B when $k_bT \gg \epsilon_0$

5. Sketch the behavior of $U(T)$ and $C(T)$, showing the limiting behaviors for $T \to \infty$ and $T \to 0$.

5 Zipper problem

A zipper has N links; each link has a state in which it is closed with energy 0 and a state in which it is open with energy ϵ. We require, however, that the zipper can only unzip from the left end, and that the link numbers can only open if all links to the left $(1, 2, ..., s-1)$ are already open.

1. Show that the partition function can be summed in the form

$$Z = \frac{1 - \exp\left[-\beta(N+1)\right]}{1 - \exp(-\beta\epsilon)} \tag{5}$$

2. In the limit $\epsilon \gg k_B T$, find the average number of open links. The model is a very simplified model of the unwinding of two-stranded DNA molecules-see C. Kittel, *Amer. J. Physics* **37**, 917 (1969).