

PHYS 6107 homework 5, due Monday 03/09 5pm

- Exercise 7.9. Stat. Mech. can be used to calculate not only macroscopic thermodynamic quantities (energy, entropy, specific heat,..), but also averaged microscopic quantities. For example, the averaged relative momenta $|\vec{p}_i - \vec{p}_k|$ between particles i and k in an ideal gas can be calculated. Using the probability distribution for this relative momenta:

$$f_{ik}(p) = \langle \delta(p - |\vec{p}_i - \vec{p}_k|) \rangle,$$

calculate the mean $\langle |\vec{p}_i - \vec{p}_k| \rangle$ for an ideal gas of N particles at temperature T .

- Read section 7.5 and derive expression Eq. (7.133) for the probability density function of a system energy near the mean value $\langle E \rangle$. (it's a Gaussian as we learned from Chapter 2 on probability theory).
- Section 8.2: *Quantum magnetic dipoles* (In class we studied paramagnetism of a classical magnetic dipoles) : The energy of magnetic dipoles with total angular momentum \vec{j} in a magnetic field H is $E = -\vec{\mu} \cdot \vec{H} = -g\mu_B Hm$, where g, μ_B are the gyromagnetic ratio and magneton Bohr correspondingly (they're constants), $m = -j, -(j-1), -(j-2), \dots, (j-1), j$, is the component of \vec{j} along the magnetic field direction (for $j=1/2$, m would either be $-1/2$ or $+1/2$). Write down the single particle partition function. Calculate the free energy, entropy, energy, mean total magnetic moment, magnetic susceptibility, specific heat of a system of N such dipoles.

- Gas of classical rotors.* The Hamiltonian of a symmetric 3D rotor has the following form:

$$H = \frac{p^2}{2m} + \frac{p_\theta^2}{2I_1} + \frac{p_\psi^2}{2I_3} + \frac{(p_\varphi - p_\psi \cos\theta)^2}{2I_1 \sin^2\theta}$$

p is the momentum conjugate to the position of the center of mass of the rotor. $p_{\theta, \psi, \varphi}$ are the momentums conjugate to the corresponding rotational angles θ, ψ , and φ ,

$\theta \in [0, \pi]; \psi, \varphi \in [0, 2\pi]$. A gas of N such rotors is in contact with a heat reservoir at temperature T . Calculate the partition function, free energy, entropy, heat capacity of the gas. How is the heat capacity behave at small, large temperature ?

- Consider an adsorbent surface having N sites, each of which can adsorb one gas molecule. This surface is in contact with an ideal gas with chemical potential m (determined by the pressure p and the temperature T). Assuming that the adsorbed molecule has energy $-\varepsilon_0$ compared to one in a free state
 - find the grand canonical partition function and
 - calculate the covering ratio θ , i.e. the ratio of adsorbed molecules to adsorbing sites on the surface.

$$\text{Hint : } (1+x)^N = \sum_{k=0}^N x^k \frac{N!}{k!(N-k)!}.$$

- Calculate the partition function, internal energy, pressure, heat capacity of an ideal gas of N molecules with kinetic energy $H = \sum_{i=1}^N A |\vec{p}_i|^\alpha$, A and α are constants. Do this using canonical ensemble. (Notice how the equipartition theorem is changed for non-harmonic gas.).
- Do problem 6 using grand-canonical ensemble.