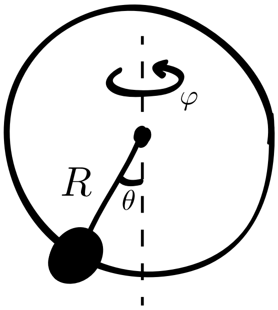
Exercise 1. ***Free Rotors***

We consider N independent free rotors (fixed on a lattice) which are free to point in any direction in space, with the moment of inertia $I = mR^2$ (see figure).



(a) Classical rotors: we use the Hamiltonian for each independent rotor expressed by mometa in spherical coordinates,

$$\mathcal{H} = \frac{1}{2I}\left(p_\theta^2 + \frac{p_\varphi^2}{\sin^2\theta}\right) . \tag{1}$$

Calculate the (canonical) partition function, the internal energy and the heat capacity.

(b) Quantum rotors: we use the equivalent Hamiltonian for the free rotors expressed by the angular momentum,

$$H = \frac{\mathbf{L}^2}{2mR^2} = \frac{\mathbf{L}^2}{2I} . \tag{2}$$

Calculate the (canonical) partition function. Determine the entropy, the internal energy, and the heat capacity. Calculate the average value of the magnitude of the angular momentum, $\langle \mathbf{L}^2 \rangle$ and the z-axis component, $\langle L_z \rangle$. Compute them numerically and study the high and low temperature limits. It is useful to define θ_{rot} by $k_B\theta_{\text{rot}} = 1/I$.

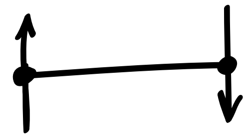
Hint. *If $f^{(n)}(\infty) \to 0, \forall n \in \mathbb{N}$ then the Euler–Maclaurin formula could be simplified to:*

$$\sum_{l=0}^{\infty} f(l) = \int_0^\infty dl f(l) + \frac{1}{2}f(0) - \sum_{k=2}^{\infty} \frac{(-1)^k b_k}{(k)!} f^{k-1}(0) + R_\infty \tag{3}$$

where R_∞ is a small correction and b_k are the Bernoulli numbers $b_2 = 1/6, b_3 = 0, b_4 = -1/30, \cdots$.
http://people.csail.mit.edu/kuat/courses/euler-maclaurin.pdf

Exercise 2. ***Independent Dimers in a Magnetic Field. Quantum vs Ising.***

We consider a system of N independent dimers of two spins, $s = 1/2$, described by the Hamiltonian



$$\mathcal{H}_0^{\text{quantum}} = J \sum_i \left(\vec{S}_{i,1} \cdot \vec{S}_{i,2} \right), \tag{4}$$

where i is the dimer index. $\vec{S}_{i,1}$ and $\vec{S}_{i,2}$ are the spin operators of the first and second particle of the dimer, respectively. Both spins have size $s = 1/2$. For simplicity, we use $\hbar = 1$. To this quantum system corresponds a classical Ising dimer, described by:

$$\mathcal{H}_0^{\text{Ising}} = \frac{1}{2} J \sum_i \left(\sigma_{i,1} \cdot \sigma_{i,2} - \frac{1}{2} \right), \tag{5}$$

where $\sigma_{i,m} = \pm 1$. The spins are aligned along the z axis. We will use eigenstates and eigenenergies to denote also the classical states and energies.

(a) What are the eigenstates and the eigenenergies of a single dimer for the two cases?

(b) For both cases consider the macroscopic system and determine the Helmholtz free energy, the entropy, the internal energy and the specific heat as a function of temperature and N. Discuss the limit $T \to 0$ and $T \to \infty$ for both signs of J (antiferromagnetic and ferromagnetic case).

(c*) We now apply a magnetic field along z direction leading to an additional term in the Hamiltonian,

$$\mathcal{H}_{\text{mag}}^{\text{quantum}} = -g\mu_B H \sum_{i,m} S_{i,m}^z \tag{6a}$$

$$\mathcal{H}_{\text{mag}}^{\text{Ising}} = -g\mu_B H \sum_{i,m} \frac{\sigma_{i,m}}{2}. \tag{6b}$$

How do the eigenenergies change? Sketch the energies with respect to the applied field H, the partition functions and determine the ground state for both cases. For the antiferromagnetic case you should notice a critical field. What differences do you notice between the classical and quantum system when the the critical field is reached? For the quantum case discuss in this context the entropy per dimer in the limit $T \to 0$.

(d*) Calculate the magnetization m for the two cases. In which limit are they the same? Moreover compute the magnetic susceptibility χ for the quantum case and discuss its dependence on H for different temperatures.

Office Hours: Monday, October 20, 8-10 AM (Lea Krämer, HIT K 32.2).