PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #2

(1) Consider a d-dimensional ideal gas with dispersion $\varepsilon(\boldsymbol{p}) = A|\boldsymbol{p}|^\alpha$, with $\alpha > 0$. Find the density of states $D(E)$, the statistical entropy $S(E)$, the equation of state $p = p(N, V, T)$, the heat capacity at constant volume $C_V(N, V, T)$, and the heat capacity at constant pressure $C_p(N, V, T)$.

(2) Find the velocity distribution $f(\boldsymbol{v})$ for the particles in problem (1). Compute the most probable speed, mean speed, and root-mean-square velocity.

(3) A spin-1 Ising magnet is described by the noninteracting Hamiltonian

$$H = -\mu_0 \mathsf{H} \sum_{i=1}^{\mathsf{N}} \sigma_i \ ,$$

where $\sigma_i = -1, 0, +1$.

(a) Find the entropy $S(\mathsf{H}, T, \mathsf{N})$.

(b) Suppose the system starts off at a temperature $T = 10\,\mathrm{mK}$ and a field $\mathsf{H} = 20\,\mathrm{T}$. The field is then lowered adiabatically to $\mathsf{H} = 1\,\mathrm{T}$. What is the final temperature of the system?

(4) Consider an adsorption model where each of N sites on a surface can accommodate either one or two adsorbate molecules. When one molecule is present the energy is $\varepsilon = -\Delta$, but when two are present the energy is $\varepsilon = -2\Delta + U$, where U models the local interaction of two adsorbate molecules at the same site. You should think of there being two possible binding locations within each adsorption site, so there are four possible states per site: unoccupied (1 possibility), singly occupied (2 possibilities), and doubly occupied (1 possibility). The surface is in equilibrium with a gas at temperature T and number density n.

(a) Find the surface partition function.

(b) Find the fraction f_j which contain j adsorbate molecules, where $j = 0, 1, 2$.

(5) Consider a system of dipoles with the Hamiltonian

$$H = \sum_{i<j} J_{ij}^{\alpha\beta}\, m_i^\alpha\, m_j^\beta - \mu_0 \sum_i \mathsf{H}_i^\alpha\, m_i^\alpha \ ,$$

where

$$J_{ij}^{\alpha\beta} = \frac{J}{R_{ij}^3} \left(\delta^{\alpha\beta} - 3\, \hat{R}_{ij}^\alpha\, \hat{R}_{ij}^\beta \right) .$$

Here $\boldsymbol{R}_i$ is the spatial position of the dipole $\boldsymbol{m}_i$, and $\boldsymbol{R}_{ij} = \boldsymbol{R}_i - \boldsymbol{R}_j$ with $\hat{R}_{ij}^\alpha \equiv R_{ij}^\alpha / R_{ij}$ the unit direction vector from j to i. The dipole vectors m_i^α are three-dimensional unit vectors. H_i^α is the local magnetic field.

(a) Find an expression for the free energy $F\big(T, \{\vec{\mathsf{H}}_i\}\big)$ valid to order β^2, where $\beta = 1/k_{\rm B}T$.

(b) Obtain an expression for the uniform field magnetic susceptibility tensor $\chi_{\alpha\beta}$.

(c) An experimentalist plots the quantity $T\chi_{\alpha\beta}$ *versus* T^{-1} for large temperatures. What should the data resemble if the dipoles are arranged in a cubic lattice structure? How about if they are arranged in a square lattice in the (x, y) plane? (You'll need to separately consider the various cases for the indices α and β. You will also need to numerically evaluate certain lattice sums.)

(6) The general form of the kinetic energy for a rotating body is

$$T = \tfrac{1}{2} I_1 \big(\dot\phi\,\sin\theta\sin\psi + \dot\theta\cos\psi\big)^2 + \tfrac{1}{2} I_2\,\big(\dot\phi\,\sin\theta\cos\psi - \dot\theta\,\sin\psi\big)^2 + \tfrac{1}{2} I_3\,\big(\dot\phi\cos\theta + \dot\psi\big)^2\ ,$$

where (ϕ, θ, ψ) are the Euler angles.

(a) Find the Hamiltonian $H(p_\phi, p_\theta, p_\psi)$ for a free asymmetric rigid body.

(b) Compute the rotational partition function,

$$\xi_{\rm rot}(T) = \frac{1}{h^3}\int\limits_{-\infty}^{\infty} dp_\phi \int\limits_{-\infty}^{\infty} dp_\theta \int\limits_{-\infty}^{\infty} dp_\psi \int\limits_0^{2\pi} d\phi \int\limits_0^{\pi} d\theta \int\limits_0^{2\pi} d\psi\; e^{-H(p_\phi, p_\theta, p_\psi)/k_{\rm B}T}$$

and show that you recover eqn. 3.288 in the notes.

(7) For polyatomic molecules, the full internal partition function is written as the product

$$\xi(T) = \frac{g_{\rm el}\cdot g_{\rm nuc}}{g_{\rm sym}} \cdot \xi_{\rm vib}(T)\cdot \xi_{\rm rot}(T)\ ,$$

where $g_{\rm el}$ is the degeneracy of the lowest electronic state[1], $g_{\rm nuc} = \prod_j (2I_j + 1)$ is the total nuclear spin degeneracy, $\xi_{\rm vib}(T)$ is the vibrational partition function, and $\xi_{\rm rot}(T)$ is the rotational partition function[2]. The integer $g_{\rm sym}$ is the *symmetry factor* of the molecule, which is defined to be the number of identical configurations of a given molecule which are realized by rotations when the molecule contains identical nuclei. Evaluate $g_{\rm nuc}$ and $g_{\rm sym}$ for the molecules CH_4 (methane), CH_3D, CH_2D_2, CHD_3, and CD_4. Discuss how the successive deuteration of methane will affect the vibrational and rotational partition functions. For the vibrations your discussion can be qualitative, but for the rotations note that all one needs, from eqn. 3.288 of the notes, is the product $I_1 I_2 I_3$ of the moments of inertia, which is the determinant of the inertia tensor $I_{\alpha\beta}$ *in a body-fixed center-of-mass frame*. Using the parallel axis theorem, one has

$$I_{\alpha\beta} = \sum_j m_j\big(\boldsymbol{r}_j^2\,\delta_{\alpha\beta} - r_j^\alpha\, r_j^\beta\big) + M\big(\boldsymbol{R}^2\,\delta_{\alpha\beta} - R^\alpha R^\beta\big)$$

[1] We assume the temperature is low enough that we can ignore electronic excitations.

[2] Note that for linear polyatomic molecules such as CO_2 and HCN, we must treat the molecule as a rotor, *i.e.* we use eqn. 3.278 of the notes.

where $M = \sum_j m_j$ and $\boldsymbol{R} = M^{-1} \sum_j m_j \boldsymbol{r}_j$. Recall that methane is structurally a tetrahedron of hydrogen atoms with a carbon atom at the center, so we can take $\boldsymbol{r}_1 = (0, 0, 0)$ to be the location of the carbon atom and $\boldsymbol{r}_{2,3,4,5} = (1, 1, 1)\,, (1, -1, -1)\,, (-1, 1, -1)\,, (-1, -1, 1)$ to be the location of the hydrogen atoms, with all distances in units of $\frac{1}{\sqrt{3}}$ times the $\mathrm{C} - \mathrm{H}$ separation.