Statistical physics I

Spring 2012

Exercise 6

1. Within the realms of non-relativistic quantum mechanics, the wavefunction for N electrons can be built with the so-called Slater determinant as follows:

$$\Psi(\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_N}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(\mathbf{x_1}) & \varphi_1(\mathbf{x_2}) & \ldots & \varphi_1(\mathbf{x_N}) \\ \varphi_2(\mathbf{x_1}) & \varphi_2(\mathbf{x_2}) & \ldots & \varphi_2(\mathbf{x_N}) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_N(\mathbf{x_1}) & \varphi_N(\mathbf{x_2}) & \ldots & \varphi_N(\mathbf{x_N}) \end{vmatrix},$$

   where φ_i are one-particle wavefunctions and $\mathbf{x_i}$ the *spatial* coordinates of the electrons.

   Consider the Hamiltonian operator

$$\hat{H}_{\text{elec}} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{\alpha=1}^{M} \frac{Z_\alpha}{r_{i\alpha}} + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}},$$

   where Z_α are positive charges, $r_{i\alpha}$ distance between positive charge α and electron i and r_{ij} the distance between electron i and j (thus the system could be *e.g.* a many-electron atom, a molecule, a molecular cluster...).

   Calculate the expectation value for the ground-state energy $\langle \hat{H}_{\text{elec}} \rangle$ using the Slater determinant wavefunction.

2. Consider a classical ideal gas of N particles with a mass m. Confine the gas in an infinitely long cylindrical thermally isolated container and place the container in a gravitational field with constant acceleration of g. Assume further that the thermal equilibrium is reached.

   Calculate the partition function Z_N, the Helmholtz free energy F, the internal energy U, the enthalpy H and the heat capacities C_V and C_P.

3. The classical Hamiltonian for a N-particle system is $H(\mathbf{q}, \mathbf{p}) = K(\mathbf{p}) + U(\mathbf{q})$, where $\mathbf{q} = (\vec{q_1}, ..., \vec{q_N})$, $\mathbf{p} = (\vec{p_1}, ..., \vec{p_N})$, $K(\mathbf{p}) = \sum_{i=1}^{N} \frac{\vec{p_i}^2}{2m}$ is the kinetic energy of the particles, and $U(\mathbf{q})$ is the interparticle potential energy. Show that the distribution of particle velocities is given by the Maxwell distribution.

4. Consider a simple system of spins. Assume that each of the N spins σ_i can have discrete values $\sigma_i = \pm 1$ and that the interaction energy between the spins is $K_{ij} = {}^{-\epsilon}/_{N}$, that is, the same between all the spins. Let's further assume that the spins feel the presence of an external magnetic field B. The Hamiltonian of the system can then be written as

$$H = \frac{-\epsilon}{2N} \sum_{i,j=1}^{N} \sigma_i \sigma_j - B \sum_i \sigma_i.$$

a) Show that the energy of the system is

$$E = -N \left(\frac{\epsilon m^2}{2} + Bm \right), \text{ where } m \equiv \sum_{i=1}^{N} \frac{\sigma_i}{N} = \frac{M}{N}.$$

b) Show that the partition function

$$Z = \sum_{\{\sigma_i\}} e^{-\beta H}$$

can be written as

$$Z = \sum_M e^{-\beta F(m,B)},$$

and expand the free energy $F(m, B)$ to the fourth order in m.

c) If the external field B is turned off and the temperature decreased, spontaneous magnetization will take place. Find out the transition temperature where this happens and calculate the magnetization in the low temperature phase (use the free energy from above and find magnetization m^* which minimizes it... you can also use the result $\langle M \rangle = T \frac{\partial \ln Z}{\partial B}$).

Return your solutions *at the exercise session* on Friday the second of March in D112 starting at 12:15. If you don't want to/can't participate the session, return your solutions into the box in the 2nd floor A-lobby *by the latest 12 o'clock* on Friday the second of March.

Voit siis palauttaa ratkaisusi vasta laskuharjoitussessiossa perjantaina 02. maaliskuuta. Vaihtoehtoisesti voit palauttaa ratkaisusi laatikkoon, tällöin kalmanraja on kello 12 samaisena perjantaina. Pisteytetyt vastauspaperit palautetaan myöhemmin.