Theoretical Physics VI: Statistical Physics - Theory of Heat

Problem Set 5

due: 21. 11. 2007, 10:15 am

Problem 5.1 *Distinguishable vs. indistinguishable particles* (5 pts.)
An ideal gas is composed of N 'red' atoms, N 'blue' atoms and N 'green' atoms. All atoms are of mass m, and atoms of the same color are indistinguishable, while atoms of different colors are distinguishable (different color may correspond to e.g. different spin states of otherwise identical atoms).
(a) Use the canonical ensemble to compute the entropy of this gas.
(b) Compute the entropy of an ideal gas of $3N$ red atoms of mass m. Does it differ from that of the mixture? If so, by how much?

Problem 5.2 *Simplified model for adsorption on a surface* (8 pts.)
An ideal gas acts as a temperature and particle reservoir for an adsorbing surface. To construct a simple model for adsorption, assume that either two, one or no particles can adsorb at M sites of the surface. Denote the energy at these sites by ϵ_2, ϵ_1, and $\epsilon_0 = 0$, respectively. The interaction between atoms at different sites is so small that it can be neglected.
(a) Calculate the grand partition function of the adsorbed molecules.
(b) Compute the grand potential, the average number of adsorbed particles and the mean energy.
(c) Given the pressure p and the temperature T of the ideal gas, calculate the number of adsorbed particles. Discuss the number of adsorbed particles in the limit of high and low temperature, assuming $\epsilon_1, \epsilon_2 < 0$.
Hint: Use the Sackur-Tetrode equation for the ideal gas,

$$S(E, V, N) = Nk_B \left[\ln\left(\frac{V}{N}\right) + \frac{3}{2}\ln\left(\frac{4\pi mE}{3Nh^2}\right) + \frac{5}{2} \right] .$$

Problem 5.3 *Atoms in a lattice* (5 pts.)
A lattice contains N normal sites and N interstitial sites. The lattice sites are all distinguishable. N identical atoms sit on the lattice, M on the interstitial sites, $N - M$ on the normal sites ($N \gg M \gg 1$). If an atoms occupies a normal site, it has energy $E = 0$. If an atoms occupies an interstitial site, it has energy $E = \epsilon$.
Compute the internal energy and the heat capacity as a function of temperature for this lattice.

Problem 5.4 *Density operator* (4 pts.)
For a spin-1 system, the angular momentum operator $\hat{\mathbf{J}}_z$ has eigenvalues $+1$, 0, -1. Denote its eigenbasis by $\{|m_i\rangle\}$. A matrix representation of the density operator is given in this basis,

$$\langle m_j|\hat{\boldsymbol{\rho}}|m_i\rangle = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} . \tag{1}$$

(a) Show that Eq. (1) fulfills indeed the definition of a density operator (Hermicity, positive-semidefiniteness, and $\mathsf{Tr}(\hat{\boldsymbol{\rho}}) = 1$).
(b) Does $\hat{\boldsymbol{\rho}}$ correspond to a pure or to a mixed state?
(c) What are the mean and the variance of $\hat{\mathbf{J}}_z$ of the state described by $\hat{\boldsymbol{\rho}}$?

Problem 5.5 *Purity* (2 pts.)
Show that $\mathsf{Tr}(\hat{\boldsymbol{\rho}}^2) \leq 1$ in general and $\mathsf{Tr}(\hat{\boldsymbol{\rho}}^2) = 1$ for a pure state.