Department of Physics
The Ohio State University

Prof. R. Bundschuh

Sixth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important date: Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Feb 17

16. Adsorption to a surface

10 points

Consider a solid surface to be a two-dimensional lattice with M sites. Each site can be either empty or occupied with a single adsorbed atom. An adsorbed atom has a binding energy $-\varepsilon$ and we neglect any interactions between the atoms.

a) Calculate the grand canonical partition function of the adsorbed atoms as a function of temperature T, lattice size M, and chemical potential μ'. Use variables $n_i \in \{0, 1\}$ for each $i = 1, \ldots, M$ to describe if site i is empty or occupied.

b) Calculate the grand canonical potential of the adsorbed atoms as a function of temperature T, lattice size M, and chemical potential μ'.

c) Calculate the average number of adsorbed atoms N as a function of temperature T, lattice size M, and chemical potential μ'.

d) The surface is exposed to an ideal gas of the atoms at some pressure P and the same temperature T as the surface. Calculate the fraction N/M of adsorbed atoms as a function of the pressure P of the ideal gas and the temperature T of the system. (Hint: in thermodynamic equilibrium the chemical potentials of the adsorbed atoms and the atoms in the ideal gas have to be equal.)

17. Density operator

10 points

a) In a two-dimensional Hilbert space an operator $\hat{\rho}$ is given by the matrix

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 + a_1 & a_2 \\ a_3 & 1 - a_1 \end{pmatrix}.$$

Determine for which values of the three complex parameters a_1, a_2, and a_3 this operator is a density operator. For which values of the three parameters is it a pure state?

b) Prove that for a hermitian Hamiltonian $\hat{H}$ the operator $\hat{\rho} \equiv e^{-\beta \hat{H}} / \operatorname{tr} e^{-\beta \hat{H}}$ is a density operator.