Midterm Exam for Advanced Statistical Physics: NS-370B

Date: 07-10-2014

Time : 13:15 - 14:45

The exam consists of 2 questions, total possible points is 34.
This is a closed-book exam, i.e. notes and electronic devices are not allowed.
Please start every exercise on a new sheet of paper, with your name clearly written on every page.
Exam can be written in either English or Dutch. Please write clearly!

A few formulas and information that may or may not be useful in this exam:

- The canonical partition function of a classical thermodynamic system of N particles in a volume V a temperature T is written as $Z(N,V,T) = 1/(N!h^{3N})\int d\Gamma \exp[-\beta H(\Gamma)]$, with Hamiltonian $H(\Gamma) = \sum_{i=1}^{N} \mathbf{p}_i^2/2m + \sum_{i<j}^{N} \phi(r_{ij})$, where $\mathbf{p}_i$ is the momentum of particle i, and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ the distance between the positions of particle i en j, and with $\phi(r)$ the pair potential and $\beta^{-1} = k_B T$.
- The grand partition function is $\Xi(\mu, V, T) = \sum_{N=0}^{\infty} \exp(\beta\mu N) Z(N,V,T)$, and the grand-canonical distribution is $f_g(\Gamma, N) = \exp[\beta\mu N - \beta H(\Gamma)]/[N!h^{3N}\Xi(\mu,V,T)]$, with μ the chemical potential.
- The second virial coefficient is $B_2(T) = (1/2)\int d\mathbf{r}[1 - \exp(-\beta\phi(r))]$,
- $k_B = 1.13 \times 10^{-23}$J/K, $e = 1.6 \times 10^{-19}$C, and $R = 8.31$J/K/mol.
- The binomial coefficient (i.e. m choose n, which is the number of ways n object can be choosen from m objects) is given by $\left(\frac{m!}{(m-n)!n!}\right)$.
- Stirling's approximation to order $O(N)$ is given by $\log(N!) = N\log N - N$.
- The Taylor series of $f(x)$ around $x = a$ is given by $f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots$.
- The following critical exponents for the Ising model:
  - β is associated with the *spontaneous magnetization*.
  - α is associated with the *specific heat* when the external field is zero
  - γ is associated with the *zero field susceptibility*
  - δ is associated with the *magnetization at the critical temperature*

1. (Max 20 points)
Consider a one-dimensional Ising model with both nearest neighbor and next-nearest neighbor interactions, such that the Hamiltonian reads:

$$\mathcal{H} = -J_1 \sum_{i=1}^{N} S_i S_{i+1} - J_2 \sum_{i=1}^{N} S_i S_{i+2}, \tag{1}$$

with J_1 and J_2 greater than zero. Assume the system has periodic boundary conditions, such that $S_{N+1} \equiv S_1$.

(a) Using the relation $S_i = \langle S \rangle + \delta S_i$, write down the mean-field Hamiltonian, and show that it has the form:

$$\mathcal{H} = A \langle S \rangle^2 - B \langle S \rangle \sum_{i=1}^{N} S_i, \tag{2}$$

where B is a function of J_1 and J_2 and is greater than zero.

(b) Using the mean-field Hamiltonian, show that the average magnetization m can be written:

$$m = \tanh(\alpha \beta m), \tag{3}$$

where α is a function of J_1 and J_2. If you are unsure of your solution to (a), use the Hamiltonian in Eq. 2 to solve this problem.

(c) Using the self-consistent expression derived in (b), determine the transition temperature. Note that any non-trivial solution (i.e. $m \neq 0$) can be assumed to have the lowest free energy.

(d) Write down the mean-field Helmholtz free energy as a function of the average magnetization m. Show that it has the form:

$$\beta F/N = \beta C m^2 - \log\left[2\cosh(\beta D m)\right], \tag{4}$$

with C and D functions of J_1 and J_2.

(e) Determine the Landau free energy of this system, using the mean-field free energy from part (d). Include terms up to and including order m^4 and explain what is needed to stop at this order. Determine the transition temperature using the Landau free energy. Is the phase transition continuous or discontinuous? Explain.

2. (Max 10 points)

(a) Consider a closed system of N identical particles in a volume V, and with energy U. Assume that this system has two competing phases labeled α and γ. Assume that phase α has N_α particles in a volume V_α and that phase γ has N_γ particles in a volume V_γ. Furthermore, assume that the energy of phases α and γ are U_α and U_γ, respectively.

(i) What is the first law of thermodynamics?

(ii) What does the second law of thermodynamics say about the entropy?

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(iii) Using the first and second laws of thermodynamics, derive a function which relates dS to dU, dV, and dN.

(iv) Assume that the temperatures of the phases α and γ are equal. Using the second law of thermodynamics and the expression derived in part c), show that when two phases are in coexistence the pressures in phases α and γ are equal.

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(b) (Max 4 points)
Here we are going to re-examine the percolation threshold for a square lattice. Consider a square lattice in which each cell is occupied with a probability p. Break the square lattice up into subsystems of 3x3 blocks. Assume each subsystem percolates when the majority of its cells are occupied. Determine the Renormalization Group equation and explain in words how you would use it to determine the percolation threshold.