M.Phys Option in Theoretical Physics: C6. Problem Sheet 2 HT2018

Question 9. A lattice model for non-ideal gas is defined as follows. The sites *i* of a lattice may be empty or occupied by at most one atom, and the variable n_i takes the values $n_i = 0$ and $n_i = 1$ in the two cases. There is an attractive interaction energy *J* between atoms that occupy neighbouring sites, and a chemical potential μ . The model Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i \,, \tag{1}$$

where $\sum_{\langle ij \rangle}$ is a sum over neighbouring pairs of sites.

(a) Describe briefly how the *transfer matrix method* may be used to calculate the statistical-mechanical properties of one-dimensional lattice models with short range interactions. Illustrate your answer by explaining how the partition function for a one-dimensional version of the lattice gas, Eq. (1), defined on a lattice of N sites with periodic boundary conditions, may be evaluated using the matrix

$$\mathbf{T} = \begin{pmatrix} 1 & \mathrm{e}^{\beta\mu/2} \\ \mathrm{e}^{\beta\mu/2} & \mathrm{e}^{\beta(J+\mu)} \end{pmatrix} \,.$$

(b) Derive an expression for $\langle n_i \rangle$ in the limit $N \to \infty$, in terms of elements of the eigenvectors of this matrix. (c) Show that

$$\langle n_i \rangle = \frac{1}{1 + \mathrm{e}^{-2\theta}} \,,$$

where

$$\sinh(\theta) = \exp(\beta J/2) \sinh(\beta [J+\mu]/2)$$

Sketch $\langle n_i \rangle$ as a function of μ for $\beta J \gg 1$, and comment on the physical significance of your result.

Question 10. The one-dimensional 3-state Potts model is defined as follows. At lattice sites i = 0, 1, ..., L "spin" variables σ_i take integer values $\sigma_i = 1, 2, 3$. The Hamiltonian is then given by

$$H = -J \sum_{i=0}^{L-1} \delta_{\sigma_i, \sigma_{i+1}},$$

where $\delta_{a,b}$ is the Kronecker delta, J > 0.

(a) What are the ground states and first excited states for this model?

(b) Write down the transfer matrix for (2). Derive an expression for the free energy per site f in the limit of large L in terms of the transfer matrix eigenvalues. Show that vectors of the form $(1, z, z^2)$ with $z^3 = 1$ are eigenvectors, and hence find the corresponding eigenvalues. Show that at temperature T (with $\beta = 1/k_BT$) and in the limit $L \to \infty$

$$f = -k_B T \ln \left(3 + e^{\beta J} - 1\right).$$

(c) The boundary variable σ_0 is fixed in the state $\sigma_0 = 1$. Derive an expression (for large *L*), that the variable at site $\ell \gg 1$ is in the same state, in terms of the transfer matrix eigenvalues and eigenvectors. Show that your result has the form

$$\langle \delta_{\sigma_{\ell},1} \rangle = \frac{1}{3} + \frac{2}{3} e^{-\ell/\xi}.$$

How does ξ behave in the low and high temperature limits?

Question 11. Consider a one dimensional Ising model on an open chain with N sites, where N is odd. On all even sites a magnetic field 2h is applied, see Fig. 1. The energy is

$$E = -J \sum_{j=1}^{N-1} \sigma_j \sigma_{j+1} + 2h \sum_{j=1}^{(N-1)/2} \sigma_{2j}.$$
 (2)

(a) Show that the partition function can be written in the form



Figure 1: Open Ising chain with magnetic field applied to all even sites.

$$Z = \langle u | T^{(N-1)/2} | v \rangle \,.$$

where T is an appropriately constructed transfer matrix, and $|u\rangle$ and $|v\rangle$ two dimensional vectors. Give explicit expressions for T, $|u\rangle$ and $|v\rangle$.

(b) Calculate Z for the case h = 0.

Question 12. Consider a Landau expansion of the free energy of the form

$$F = \frac{a}{2}m^2 + \frac{b}{4}m^4 + \frac{c}{6}m^6$$

with c > 0. Examine the phase diagram in the a-b plane, and show that there is a line of critical transitions a = 0, b > 0 which joins a line of first order transitions $b = -4(ca/3)^{1/2}$ at a point a = b = 0 known as a tricritical point.

Supposing that a varies linearly with temperature and that b is independent of temperature, compare the value of the exponent β at the tricritical point with its value on the critical line.

From Yeomans, Statistical Mechanics of Phase Transitions

Question 13.

(a) Discuss how an order parameter may be used to characterise symmetry breaking at a phase transition.
(b) Argue that the uniaxial ferromagnet-paramagnet transition can be described by by a Landau free energy of the form

$$F = \int d^3 \mathbf{r} \left[\frac{1}{2} |\nabla \phi(\mathbf{r})|^2 - h\phi(\mathbf{r}) + \alpha_2 \phi^2(\mathbf{r}) + \alpha_3 \phi^3(\mathbf{r}) + \alpha_4 \phi^4(\mathbf{r}) \right].$$

What can you say about α_4 ?

(c) What is the nature of the transition for h = 0 if $\alpha_3 \neq 0$? Explain your answer.

(d) Now assume that $\alpha_3 = h = 0$. Argue that close to the critical point

$$\alpha_2 = At$$
, $t = \frac{T - T_c}{T_c}$ and $A > 0$

(e) Derive the equation characterizing the saddle point solution for $\alpha_3 = h = 0$. What are the configurations ϕ with the lowest free energy for h = 0, at $T > T_c$ and at $T < T_c$? Why are these **r** independent?

(f) Now consider more general solutions to the saddle point equation in the low-temperature phase. With suitable boundary conditions the saddle point solutions for the order parameter are functions of x only, i.e. $\phi = \phi(x)$. Show that in this case

$$E = \frac{1}{2} \left[\frac{d\phi(x)}{dx} \right]^2 - \alpha_2 \phi^2 - \alpha_4 \phi^4$$

is independent of x. Construct a solution $\phi(x)$ such that

$$\lim_{x \to \infty} \phi(x) = \phi_1 , \quad \lim_{x \to -\infty} \phi(x) = \phi_2,$$

where $\phi_{1,2}$ are the solutions found in (d). Hint: determine E for such solutions first.

Question 14. A system with a real, two-component order parameter $(\phi_1(\mathbf{r}), \phi_2(\mathbf{r}))$ has a free energy

$$F = \int d^{d}\mathbf{r} \left[\frac{1}{2} |\nabla \phi_{1}(\mathbf{r})|^{2} + \frac{1}{2} |\nabla \phi_{2}(\mathbf{r})|^{2} - \frac{1}{2} \left(\phi_{1}^{2}(\mathbf{r}) + \phi_{2}^{2}(\mathbf{r}) \right) + \frac{1}{4} \left(\phi_{1}^{2}(\mathbf{r}) + \phi_{2}^{2}(\mathbf{r}) \right)^{2} \right] .$$

Find the order-parameter values Φ_1, Φ_2 that minimise this free energy. Consider small fluctuations around such state, with $(\phi_1(\mathbf{r}), \phi_2(\mathbf{r})) = (\Phi_1 + \varphi_1(\mathbf{r}), \Phi_2 + \varphi_2(\mathbf{r}))$ and expand F to second order in φ .

Assuming that the statistical weight of thermal fluctuations is proportional to $\exp(-F)$, calculate approximately the correlation function

$$\langle \varphi_1(\mathbf{r})\varphi_1(\mathbf{0})+\varphi_2(\mathbf{r})\varphi_2(\mathbf{0})\rangle$$

by evaluating a Gaussian functional integral. How does your result depend on the dimensionality d of the system?