ADVANCED TOPICS IN STATISTICAL PHYSICS

Spring term 2013

EXERCISES

Note: All undefined notation is the same as employed in class.

Exercise 1301. Quantum spin chains

a. Show that the 1D Heisenberg and XY Hamiltonians commute with the magnetic field operator $\mathcal{M} = \sum_j \sigma_j^z$.

b. Why is it not possible to diagonalize the 1D Heisenberg model by means of the Jordan-Wigner transformation?

c. Express $\mathcal{M}$ in terms of the fermion operators.

d. Show, neglecting boundary effects, that

$$\mathcal{H}_{\mathrm{XY}} = -4J \sum_q \cos q \;\; \eta_q^\dagger \eta_q \,. \tag{1}$$

For a chain of N sites q runs through an appropriate set of N wavenumbers determined by the boundary conditions. Assuming that these are equally spaced and symmetric about $q = 0$, calculate the ground state energy e_0 per site in the thermodynamic limit. [*Answer*: $e_0 = -4J/\pi$.] What is the ground state magnetization? We just remark here that the ground state itself is a complicated ("entangled") superposition of spin states.

e. Can the one-dimensional XY Hamiltonian still be diagonalized
(i) if the xx and yy spin couplings are unequal ($J_x \neq J_y$) ?
(ii) if a magnetic field term $-H \sum_j \sigma_j^z$ is added to the Hamiltonian?
(iii) if a next-nearest neighbor coupling $-J_2 \sum_j [\sigma_j^x \sigma_{j+2}^x + \sigma_j^y \sigma_{j+2}^y]$ is added to it?

Exercise 1302. Operator algebras related to quantum spin chains

a. Consider a periodic chain of N sites on each of which a spin one-half is located. Characterize the Lie algebra generated by the set of operators $\sigma_j^x \sigma_{j+1}^x$ and $\sigma_j^y \sigma_{j+1}^y$ for $j = 1, 2, \ldots, N$. A definition good enough here is the following: if A and B belong to a Lie algebra, then so does their commutator $[A, B]$.

b. What changes if
(i) the operators σ_j^z for $j = 1, 2, \ldots, N$ are included in the initial set?
(ii) the operators $\sigma_j^z \sigma_{j+1}^z$ for $j = 1, 2, \ldots, N$ are included in the initial set?

Exercise 1303. Transfer matrix for the 2D Ising model

One of the earliest uses of the Pauli spin matrices outside of quantum mechanics was by Lars Onsager in his solution of the two-dimensional Ising model. In this exercice we will see the starting point of his method.

a. Consider the one-dimensional Ising model

$$\mathcal{H}_{N1} = -J \sum_{i=1}^{N} s_i s_{i+1} \tag{2}$$

with the periodic boundary condition $s_N + 1 = s_1$. Show that the canonical partition function Z_{1N} at inverse temperature β may be expressed as

$$Z_{N1} = \mathrm{e}^{NG} \operatorname{Tr} T_1^N \tag{3}$$

where T_1 is the transfer matrix

$$T_1 = \mathrm{e}^{K^* \sigma^x}. \tag{4}$$

Find G and K^* in terms of $K \equiv \beta J$ and determine Z_{N1} from (3).

b. Now consider the Ising model on the ladder lattice,

$$\mathcal{H}_{N2} = -J \sum_{i=1}^{N} \left[s_{i,1} s_{i,2} + s_{i,1} s_{i+1,1} + s_{i,2} s_{i+1,2} \right], \tag{5}$$

with periodic boundary conditions $s_{N+1,j} = s_{1,j}$ for $j = 1, 2$. Show that

$$Z_{N2} = \mathrm{e}^{2NG} \operatorname{Tr} T_2^N \tag{6}$$

in which the 4×4 transfer matrix T_2 may be written as

$$T_2 = U_2 V_2, \quad U_2 = \mathrm{e}^{K \sigma_1^z \sigma_2^z}, \quad V_2 = \mathrm{e}^{K^* (\sigma_1^x + \sigma_2^x)}. \tag{7}$$

Do U_2 and V_2 commute? Can you write them as a single exponential of spin operators?

c. Next consider the Ising model on the $N \times M$ square lattice,

$$\mathcal{H}_{NM} = -J \sum_{i=1}^{N} \sum_{j=1}^{M} \left[s_{i,j} s_{i+1,j} + s_{i,j} s_{i,j+1} \right], \tag{8}$$

with the periodic boundary conditions $s_{N+1,j} = s_{1,j}$ and $s_{i,M+1} = s_{i,1}$. Show that

$$Z_{NM} = \mathrm{e}^{NMG} \operatorname{Tr} T_M^N \tag{9}$$

in which the $2^M \times 2^M$ transfer matrix T_M^N may be written as

$$T_M = U_M V_M, \quad U_M = \mathrm{e}^{\mathcal{U}_M}, \quad V_M = \mathrm{e}^{\mathcal{V}_M}, \tag{10}$$

where $\mathcal{U}_\mathcal{M}$ and $\mathcal{V}_M$ are expressions in terms of the spin matrices $\sigma_1^z, \ldots, \sigma_M^z$ and $\sigma_1^x, \ldots, \sigma_M^x$, respectively. Find these expressions.

d. Let $f(\beta)$ be the free energy per site of the square Ising lattice in the thermodynamic limit, at inverse temperature β. Using (9) we therefore have

$$-\beta f(\beta) = G + \lim_{N,M\to\infty} \frac{1}{NM} \log \sum_{\alpha=1}^{2^M} \lambda_{M,\alpha}^N \tag{11}$$

where the $\lambda_{M,\alpha}$ are the eigenvalues of T_M.

If we managed to write $T_M = \mathrm{e}^{\mathcal{T}_M}$, then it would suffice to find the eigenvalues of $\mathcal{T}_M$. One may attempt to find $\mathcal{T}_M$ by using the Campbell-Baker-Hausdorff formula

$$\mathrm{e}^A \mathrm{e}^B = \mathrm{e}^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]+\frac{1}{12}[[A,B],B]+\ldots}, \tag{12}$$

where the dot terms are a linear expression in the operators generated from A and B by multiple commutation. We will not pursue this here but merely ask the following question:

For the particular case of $\mathcal{U}_M$ and $\mathcal{V}_M$, characterize the Lie algebra L_M of operators generated by this commutation procedure. How does $|\mathsf{L}_M|$ depend on M? What changes if one adds to $\mathcal{H}_{NM}$ a magnetic field term $-H\sum_{i,j} s_{i,j}$?

Remark. To find out how the transfer matrix calculation of Z_{NM} may be completed and $f(\beta)$ calculated explicitly, see Onsager's original work or see the article by Schultz, Mattis, and Lieb.

- L. Onsager, *Phys. Rev.* **65** (1944) 117. Method: transfer matrix and operator algebra.
- T.D. Schultz, D.C. Mattis, and E.H. Lieb, *Rev. Mod. Phys.* **36** (1964) 856. Method: transfer matrix expressed in fermions.

Here is a list of a few solutions of the two-dimensional Ising model by other methods.

- B. Kaufmann, *Phys. Rev.* **76** (1949) 1232. Method: simplification of Onsager's.
- R.B. Potts and J.C. Ward, *Progr. Theoret. Phys.* **13** (1955) 38. Combinatorial method.
- B. McCoy and F.Y. Wu, *The two-dimensional Ising Model,* (Harvard U.P., Cambridge, Mass., 1973). Method: Pfaffian. This method was developed by P. Kasteleyn, *Physica* **27** (1961) 1209; *J. Math. Phys.* **4** (1963) 287.
- M. Kac and J.C. Ward, *Phys. Rev.* **88** (1952)1332. Combinatorial method, leading to a determinant.
- C.A. Hurst and H.S. Green, *J. Chem. Phys.* **33** (1960) 1059. Method: Pfaffian, related to Kac-Ward determinant.
- N.V. Vdovichenko, *Zh. Eksp. Teor. Fiz.* **47** (1964) 715, English translation *Soviet Phys. JETP* **21** (1965) 350. Method: combinatorial, counting of random loops.

• H.J. Hilhorst, M. Schick, and J.M.J. van Leeuwen, *Phys. Rev. Lett.* **40** (1978) 1605; *Phys.Rev. B* **19** (1979) 2749. Method: exact renormalization based on the star-triangle transformation.

• R.J. Baxter and I.G. Enting, *399th solution of the Ising model, J. Phys. A* **11** (1978) 2463. Method: star-triangle transformation.

• M.-C. Wu and C.-K. Hu, *J. Phys. A* **35** (2002) 5189. Method: Grassmann variables.

• V.N. Plechko, *Theoretical and Mathematical Physics* **64** (1985) 748. Method: Grassmann variables.

• B. Kastening, *Phys. Rev. B* **66** (2002) 057103. Simplified transfer matric method.

• S.N. Vergeles, *500th solution of the 2D Ising model* `arXiv:0805.0225`.

Note: A relation with the "complexity classes" of the theory of computation is claimed by S. Istrail and others. See
http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.119.1820
or `cs.brown.edu/ sorin/pdfs/Ising-paper.pdf`

Exercise 1304. Interface in the 2D Ising model

We consider the low-temperature regime of the 2D Ising model. A simplified model for the interface between two coexisting phases is obtained as follows. On a square lattice shaped as a strip of width L in which a region of spins up (to the left) is separated from a region of spins down (to the right) by a boundary that may run only east, west and south without intersecting itself.

a. Draw a figure.

b. Find the partition function $Z_{\rm int}(\beta)$ of this interface and from there, dealing appropriately with the thermodynamic limit, the free energy $f_{\rm int}(\beta)$ per unit length of the interface.

c. Show that there is a critical temperature and determine the behavior of $f_{\rm int}(\beta)$ in its vicinity. Draw conclusions.

d. In the 3D Ising model the interface between two coexisting phases is two-dimensional. Extending the above simplification to 3D leads to the Hamiltonian

$$\mathcal{H}_{\rm SOS} = J \sum_{\langle i,j \rangle} |h_i - h_j|, \qquad (13)$$

in which i and j are two-dimensional lattice vectors. Interpret the variables h_i. Expression (13) is called the *Solid-On-Solid* Hamiltonian. Explain this name. Although there is no known way of calculating the associated canonical partition function $Z_{\rm SOS}$ analytically, many of its properties are known. We will return to these later in this course.

Exercise 1305. Duality and defect free energies

a. Verify that the duality transformation shown in class is still possible when each bond $\langle i, j\rangle$ has its own coupling $K_{i,j}$.

b. Redo the duality transformation for the case of a *negative* bond $K_{ij} < 0$. Show that, apart from inessential factors, it leads to the replacement (with the notation defined in class)

$$\mathrm{e}^{K_{ij}s_is_j} \quad \mapsto \quad t_k t_\ell\, \mathrm{e}^{K^*_{ij}t_kt_l} \tag{14}$$

and express K^*_{ij} in terms of K_{ij}. We will refer to the prefactor t_kt_ℓ in (14) as an *insertion*.

c. Consider an Ising model with bonds $K_{ij} = \epsilon_{ij}K$ where $\epsilon_{ij} = \pm 1$. State the conditions that allow to eliminate the ϵ_{ij} by a redefinition of the spin variables. When these conditions are satisfied, what are the consequences for the duality transformation in terms of the insertions that appear?

Let $\mathcal{S}$ be the set of bonds for which $\epsilon_{ij} = -1$. We may interpret this set of bonds as a defect. Let $Z(\mathcal{S})$ be the corresponding partition function.

d. Write

$$\frac{Z(\mathcal{S})}{Z(\emptyset)} = \mathrm{e}^{-\beta\Delta F_{\mathcal{S}}(\beta)} \tag{15}$$

and justify the name *defect free energy* given to $\Delta F_{\mathcal{S}}(\beta)$.

We are now interested in the pair correlation function $g(r) = \langle s_0 s_r\rangle$, where r is an arbitrary lattice site.

e. Write $g(r)$ as the ratio of two partition functions of which one with an insertion, $g(r) = Z(\mathcal{R})/Z$. Apply the duality transformation to both numerator and denominator. Interpret $g(r)$ in terms of a defect free energy $\Delta F_{\mathcal{R}}$ and characterize the defect $\mathcal{R}$.

f. Under plausible assumptions about ΔF_r find the behavior of $g(r)$ in the limit of large $|r|$ in the two cases $T > T_\mathrm{c}$ and $T < T_\mathrm{c}$.

Exercise 1306. Star-triangle transformation

Consider a star of three Ising spins s_1, s_2, and s_3 connected to a central spin s_0 as shown in figure 1. Each of the three spins may interact with an arbitrary number of other spins, but s_0 may not.

a. Show that one can relate the K_i to the p_i in such a way that the system to the left has the same partition function as the one to the right up to a factor e^G. Determine G and show that the relation between the K_i and the p_i may be written as

$$\mathrm{e}^{4K_i} = \frac{\cosh(p_i + p_j + p_k)\cosh(p_i - p_j - p_k)}{\cosh(p_i - p_j + p_k)\cosh(p_i + p_j - p_k)}\,, \tag{16}$$

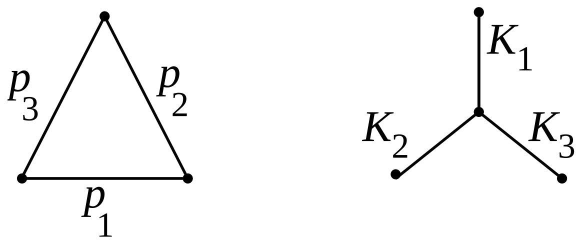

Figure 1: The star-triangle transformation.

where i, j, k are all different. These relations are called the *star-triangle transformation,* or sometimes the *$Y\Delta$ transform.* With some effort one may rewrite them in several more elegant ways and invert them.

b. Find an equation for the critical coupling of the triangular lattice with uniform coupling K, and of the hexagonal lattice with uniform coupling p. Compare the numerical values of the critical couplings of the triangular, the square, and the hexagonal 2D Ising model.

c. We define the Hamiltonian $\mathcal{H}$ of the Gaussian model with uniform coupling J by the expression

$$\mathcal{H}_{\mathrm{G}} = \frac{1}{2}\sum_i S_i^2 - J\sum_{\langle i,j\rangle} S_i S_j\,. \tag{17}$$

Show that this model has a star-triangle transformation and that, using similar notation as above, we may express this transformation and its inverse as

$$p_i = \frac{K_j K_k}{[K_1K_2K_3 + K_1K_2 + K_2K_3 + K_3K_1]^{1/2}}\,, \tag{18}$$

$$K_i = \frac{p_j p_k}{1 - p_1^2 - p_2^2 - p_3^2}\,. \tag{19}$$

The star-triangle transformation has an analog in electrical circuit theory. As is well-known, in any circuit one may replace two resistances R_1 and R_2 by a single resistance R given by $R = R_1 + R_2$ when the two are in series, and $R^{-1} = R_1^{-1} + R_2^{-1}$ when the two are in parallel (Kirchhoff's first and second law). Kirchhoff's third law says that similarly in any circuit a "star" of three resistances r_i may be replaced with a triangle of resistances R_i given by

$$R_i = \frac{r_1r_2 + r_2r_3 + r_3r_1}{r_i}\,. \tag{20}$$

This relation was exploited by H. Taitelbaum and E. Havlin, *J. Phys. A: Math. Gen.* **21** (1988) 2265, to calculate the resistance of a Sierpinski gasket with random resistances.

d. Show how to obtain Kirchhoff's first and second law from (20).

Note 1: The Yang-Baxter equations, essential in the theory of exactly soluble models, are a generalization of the star-triangle equations. See for example J.H.H. Perk and H. Au-Yang, `arXiv math-ph/0606053`, published in Encyclopedia of Mathematical Physics, eds. J.-P. Françoise, G.L. Naber and S.T. Tsou, Oxford: Elsevier, 2006, volume 5, pages 465-473.
Note 2: The star-triangle relation has recently been of interest on so-called *isoradial* graphs.

Exercise 1307. Lower critical dimension in the Ising model

a. Using Kadanoff's "bond moving scheme" find an approximate renormalization equation for the Ising model on a d-dimensional hypercubic lattice. Set $d = 1 + \epsilon$ and find the critical temperature $T_{\rm c}(d)$ by an expansion in ϵ. What does this calculation suggest about the lower critical dimension of the Ising model?

b. Find another argument showing that for the Ising model $d_\ell = 1$.

Exercise 1308. High temperature expansion of the correlation function

Show that at sufficiently high temperature the correlation function $g(r) = \langle s_0 s_r \rangle$ of the 2D Ising model must decrease exponentially for $|r| \to \infty$.

Exercise 1309. Correlation function by transfer matrix

On the example of the 1D Ising model, show how the correlation function $g(\ell) = \langle s_k s_{k+\ell} \rangle$ may be expressed in terms of the ratio of the two eigenvalues of the transfer matrix.

Exercise 1310. Crossed bonds

Find the transfer matrix $\mathcal{T}$ in terms of Pauli spin operators
(i) for the Ising model on a ladder with crossed bonds;
(ii) for the 2D Ising model with crossed bonds.
Make any relevant comments.

Exercise 1311. Random sequential filling

Each site $j = 0, \pm 1, \pm 2, \dots$ of a one-dimensional lattice may be empty or occupied. We associate with these states the "spin" variables $s_j = 1$ and $s_j = -1$, respectively. At time $t = 0$ all sites are empty. The time evolution rule is as follows. Each empty site having two neighboring empty sites is filled at a rate γ. This is known as the *Random Sequential Adsorption (RSA)* or *random* *sequential filling* problem. The main question is to calculate the fraction $\phi(t)$ of occupied sites, and in particular the asymptotic filling fraction $\phi^* \equiv \phi(\infty)$.

a. Express the time evolution operator for this problem in terms of spin operators.

b. Examine the Lie algebra of operators generated. Explain why you think this problem is or is not exactly solvable.

c. Examine the same problem on the ladder lattice.

Note 1: The problem on the 1D lattice was solved long ago, see B. Widom, *J. Chem. Phys.* **58** (1973) 4043. The problem on the ladder lattice may also be solved. The results are

$$\begin{aligned} \phi^* &= \tfrac{1}{2}(1-\mathrm{e}^{-2}) = 0.4323..., && \text{1D lattice,} \\ \phi^* &= \tfrac{1}{4}(2-\mathrm{e}^{-1}) = 0.4080..., && \text{ladder lattice.} \end{aligned} \tag{21}$$

Working out the operator method may well lead to some new results; I am not aware of anyone who has done this.
Note 2. The same problem may be solved in continuous 1D space for the adsorption of hard rods of unit length on the axis. This problem was formulated and solved by Rényi, *Publ. Math. Inst. Hung. Acad. Sci.* **3** (1958) 109, English translation in *Selected Transl. Math. Stat. Prob.* **4** (1963) 203.

Exercice 1312. The 1D kinetic Ising model

a. We consider the operator $\hat{\mathcal{W}}$ for Glauber model on a one-dimensional lattice of N sites with periodic boundary conditions. Find the time evolution equations for
(i) the magnetization $m_i(t) \equiv \langle\sigma_i\rangle_t$
(ii) the pair correlation $g_{i,j}(t) \equiv \langle\sigma_i\sigma_j\rangle_t$

b. Find the spectrum of relaxation times of the magnetization. Interpret the largest relaxation time.

c. Starting from the set of equations (ii) and letting $N \to \infty$, find the expression for the pair correlation function in equilibrium. Hint: Use that in equilibrium g depends only on the difference $|i-j|$.

d. Discuss the structure of the time evolution equations for the four-point correlations $\langle\sigma_i\sigma_j\sigma_k\sigma_\ell\rangle_t$. Do you see a way of solving these equations?

e. Consider now the 1D kinetic Ising model in which Glauber's transition rates W are replaced with

$$W'(s^{(j)}|s) = \mathrm{e}^{\beta J s_j(s_{j-1}+s_{j+1})}. \tag{22}$$

Construct the corresponding operator $\hat{\mathcal{W}}'$. Find again the time evolution equations for $m_i(t)$. Make any relevant comments.