Course on "Advanced Statistical Physics"
Spring Semester (2016)
School of Nano Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
Lecturer: Ali Naji (School of Physics, IPM)
Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #4: Spin Models Due: April 19, 2016

▶ Problems (except #4) are (partly or fully) adopted from *Statistical Mechanics of Phase Transitions* by J. M. Yeomans (1992)

1: Write down a model Hamiltonian for a binary alloy comprising two different (but equal numbers of) species A and B occupying lattice sites of a body-centered cubic lattice. Assume that the site occupation state is given by a two-state spin variable, $s_i = +1$ and -1, representing occupation of site i with an A or a B atom, respectively. Further assume that the energetic coupling exists only between atoms in nearest-neighbor sites with the respective coupling constants given by J_{AA}, J_{BB} and J_{AB}. Prove that this model is equivalent to a spin-1/2 Ising model of the form

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - H\sum_i s_i + C,$$

and determine the constants J, H, and C.

2: Prove that the two-state lattice-gas model defined by the Hamiltonian

$$\mathcal{H} = -J_L\sum_{\langle ij\rangle} t_i t_j - \mu_L\sum_i s_i, \quad t_i = 0, 1$$

is equivalent to a spin-1/2 Ising model.

3: Show that the q-state Potts model defined by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle ij\rangle} \delta_{\sigma_i\sigma_j}, \quad \sigma_i = 1, \cdots q$$

has q equivalent ground states, where all spins are identical. Prove that for $q = 2$, Potts model is equivalent to a spin-1/2 Ising model.

4: Consider two electrons interacting via a two-body potential $V(r)$.

(i) Write down the most general Hamiltonian for this system in the absence of magnetic field.

(ii) Let's assume $\phi_a(r)$ is the spatial eigenfunction of the electron a in the absence of the other electron. Write down all possible eigenfunctions of the *two-electron* system in the absence of their interaction (ignore spin and exclusion principle but not indistinguishability).

(iii) Write down all possible spin states of the two spin-1/2 particles.

(iv) Using (ii) and (iii) write down all possible wavefunctions of the two non-interacting electron system considering spin and exclusion principle.

(v) Using first-order perturbation theory write the shift of energy of each of the states obtained in (iv). Call the spin-symmetric ones $\delta\varepsilon_S^{(1)}$, $\delta\varepsilon_S^{(2)}$ and $\delta\varepsilon_S^{(3)}$ and the spin-antisymmetric one $\delta\varepsilon_A$. If $V(r) > 0$, which one is the lowest?

(vi) Show that the *exchange Hamiltonian* $\hat{H} = -(J/2)\left(\mathbf{S}_1 + \mathbf{S}_2\right)^2$ has four eigenstates. Based on this, determine what J should be to produce the above energies and spin eigenstates. Note that we can shift the lowest energy to zero.

(vii) Conceptually justify why for repulsive interaction the electrons prefer to have parallel spin state in the ground state. How about attractive interactions? Give examples.

(viii) Show that $\hat{H}$ is the same as the Heisenberg Hamiltonian.

(ix) In the presence of anisotropies in a crystalline system, $\hat{H}$ turns out to be not a correct model of exchange interaction. Why?

Spring Semester (2016)
School of Nano Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
Lecturer: Ali Naji (School of Physics, IPM)
Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #4: Spin Models Due: April 19, 2016

5: Find the ground state (stable configuration at $T = 0$) of the following spin models:

(i) The one-dimensional Ising model with first and second neighbor interactions:

$$\mathcal{H} = -J_1 \sum_i s_i s_{i+1} - J_2 \sum_i s_i s_{i+2}, \quad s_i = \pm 1$$

Consider both positive and negative values of the exchange parameters.

(ii) The one-dimensional p-state chiral clock model:

$$\mathcal{H} = -J \sum_i \cos\{2\pi(n_i - n_{i+1} + \Delta)/p\}, \quad n_i = 1, 2, \cdots p$$

for $J > 0$ and all values of Δ.

(iii) The spin-1 Ising model on a simple cubic lattice:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - K \sum_{\langle ij \rangle} s_i^2 s_j^2 - D \sum_i s_i^2, \quad s_i = \pm 1, 0$$

Consider both positive and negative exchange interactions.

(iv) The antiferromagnetic spin-1/2 Ising model on a triangular lattice:

$$\mathcal{H} = J \sum_{\langle ij \rangle} s_i s_j, \quad s_i = \pm 1$$

with $J > 0$.

6: Show that on the square lattice the spin-1 Ising model, described by the following Hamiltonian:

$$\begin{aligned}\mathcal{H} = &-J \sum_{\langle ij \rangle} s_i s_j - K \sum_{\langle ij \rangle} s_i^2 s_j^2 - D \sum_i s_i^2 \\ &- L \sum_{\langle ij \rangle} \left(s_i^2 s_j + s_i s_j^2\right) - H \sum_i s_i, \quad s_i = \pm 1, 0\end{aligned}$$

has the same symmetry as the three-state Potts model,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}, \quad \sigma_i = 1, 2, 3,$$

if

$$D + 2(J + K) = 0, \quad H = 0, \quad L = 0.$$

7: The one-dimensional, p-state clock model is described by the Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos\{2\pi(n_i - n_j)/p\}, \quad n_i = 1, 2, \cdots p.$$

Show that this model is equivalent to the q-state Potts model:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}, \quad \sigma_i = 1, 2, \cdots q,$$

for $p = q = 2$ and $p = q = 3$ but not for higher values of p.

Spring Semester (2016)
School of Nano Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
Lecturer: Ali Naji (School of Physics, IPM)
Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #4: Spin Models Due: April 19, 2016

8: The Ising lattice gas is described by a Hamiltonian:

$$\mathcal{H} = -J_L \sum_{\langle ij \rangle} s_i s_j t_i t_j - K_L \sum_{\langle ij \rangle} t_i t_j - D_L \sum_i t_i$$
$$s_i = \pm 1, \quad t_i = 0, 1.$$

Find a transformation which demonstrates the equivalence of this model to the spin-1 Ising model given by the Hamiltonian in problem 6 with $H = L = 0$.