

Spring Semester (2016)

School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

Lecturer: Ali Naji (School of Physics, IPM)

Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #3: Spin Models

Due: March 1, 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

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

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* $\hat{H} = -(J/2)(\mathbf{S}_1 + \mathbf{S}_2)^2$ 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 Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

Lecturer: Ali Naji (School of Physics, IPM)

Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #3: Spin Models

Due: March 1, 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:

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

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:

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

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:

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

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

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

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

Spring Semester (2016)

School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

Lecturer: Ali Naji (School of Physics, IPM)

Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #3: Spin Models

Due: March 1, 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 $H = L = 0$.