One Dimensional Random Field Ising Model

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We consider one dimensional random field Ising model (RFIM) in the context of protein folding problem. Using replica technique, we attempt to obtain the phase diagram for the RFIM model. Finally, we compare replica method predictions to the simulation of chain with 30 spins.

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I. INTRODUCTION

The systems with quenched disorder have been intensively studied for more than thirty years. The examples of these systems include: hopping conductivity in the semiconductors, pinning of magnetic vortices on defects in superconductors, random-bond interfaces, and spin glasses. The distinguishing feature of systems with quenched disorder is that the characteristic time on which the random parameters of the systems change is much larger than the time scale characterizing the changes of internal degrees of freedom. This is opposite to the systems with annealed disorder, where the random variables are allowed to evolve.

There exist several exactly solvable models with quenched disorder. Edwards-Anderson (EA) and Sherrington–Kirkpatrick (SK) are the most known models of spin glasses [1], [2]. Both models consider Ising like spins with randomly distributed ferromagnetic and antiferromagnetic bonds J_{ik}:

$$-\beta\mathcal{H}_J = \sum_{ik} J_{ik} s_i s_k. \tag{1}$$

In EA model, the sum runs only over nearest neighbors $\langle ij\rangle$, whereas SK model considers infinite-ranged interactions and the sum is taken over all spins such that $i \neq j$. Using replica technique, Edwards and Anderson found that in system described by Hamiltonian (1) has a phase transition: below the critical temperature there exist a preferred orientation of spins, called "spin-glass" phase. Following the same approach, Sherrington and Kirkpatrick obtained the phase diagram for random infinite-ranged Ising model. They found that depending on relation between temperature and disorder both "spin-glass" and ferromagnetic phases occur.

Another exactly solved model of system with quenched disorder is RFIM with constant infinite-ranged interactions [3]:

$$-\beta\mathcal{H}_h = J\sum_{ik} s_i s_k + \sum_{i}^{N} h_i s_i \tag{2}$$

where J is greater than zero and local magnetic fields $h = \{h_1, h_2, ..., h_N\}$ are independently distributed according to

$$P(h) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{h^2}{2\sigma^2}}. \tag{3}$$

If $2J/N\sigma^2 > \sqrt{\pi/2}$, then this system exhibit a phase transition between ferromagnetic phase and the phase where all spins are independent and at low temperatures align according to the local random fields. In case of weak coupling between spins, $2J/N\sigma^2 < \sqrt{\pi/2}$, there is no phase transition and at all temperatures the system is in independent spin phase.

Remarkably, the same kind of Hamiltonian can be applied to problem from a different realm. In this paper we argue that, if polymeric (elastic) and hydrophobic effects are the main driving forces of protein structure, then problem of protein folding can be studied within the framework of random field and random bond Ising models. Studying the behavior of the heat capacity in the RFIM with nearest neighbor interactions, we estimate at what value of the ratio between randomness of a field σ^2 and bond constant J the crossover between different regimes occurs.

II. PROTEIN FOLDING MODEL

It is well known that in globular proteins the side chains of hydrophobic amino acids are buried inside the core of the protein, whereas hydrophilic amino acids tend to be near the surface of the globule. One can assume that the sequence of the protein produces a certain hydrophobicity pattern, which has an effect of external potential that determines protein structure. Indeed, the phenomenological model that takes into account only hydrophobic and polymeric effects was proposed by J. England [4]. Within the framework of this model he was able to compute couplings between different parts of protein chain and, thus, to explain allostery in a group of proteins. It is intuitively clear that one of the important parameters in this model is the relative strength between sequence-dependent external field and the stiffness of the polymer chain. In the limit of large field the structure of a protein is completely determined by hydrophobicity pattern and different parts of a protein are decoupled. In contrast, in case of small field, different parts of a protein should be correlated.

It is worth noting, that the Hamiltonian (2) with nearest neighbor interaction incorporates the same physics as the burial trace model proposed by England. In particular, the configuration of the protein is given by a list $\{s_i\}$, where $s_i = \pm 1$ denotes whether the residue

i is on the surface or in the core of the protein. The first term in Hamiltonian (2) can be understood as a penalty for neighboring residues to be apart from each other, thus, the constant J plays the role of polymer stiffness. The second term, in turn, describes the hydrophobic effect. As a result of similarities between proteins and one-dimensional RFIM, by studying the properties of RFIM we can quantitatively estimate the importance of hydrophobic effect in protein folding.

III. QUENCHED AVERAGES AND REPLICAS

In the systems with quenched disorder we are interested in calculation of the average of free energy density

$$f = \sum_h P(h) f_h = \overline{f_h} \tag{4}$$

where f_h is free energy density of a system for given realization of disorder h. In many problems to simplify the calculation of f it is common to use the replica method, whose idea can be described as follows: one starts with calculation of

$$Z_n = \sum_h P(h)(Z_h)^n = \overline{(Z_h^n)}$$

$$f_n = -\frac{k_B T}{nN} \ln Z_n, \tag{5}$$

for any integer number of replicas n and then finds the average value of free energy density by analytic continuation $f = \lim_{n\to 0} f_n$. Here we will follow the same procedure to calculate thermodynamic quantities for one dimensional RFIM with nearest neighbor interactions.

For given disorder h we can introduce n non-interacting replicas of the system

$$Z_h^n = \sum_{\{a^1\}} ... \sum_{\{a^n\}} \exp\{-\sum_{a=1}^{n} \beta \mathcal{H}_h[s^a]\}. \tag{6}$$

If we assume that $h = \{h_1, h_2, ..., h_N\}$ are independent random variables distributed according to (3), then equation (6) averaged over random fields h takes the form

$$Z_n = \sum_{\{a^1\}} ... \sum_{\{a^n\}} \exp\left\{ J \sum_{i,a} s_i^a s_{i+1}^a + \frac{\sigma^2}{2} \sum_i \left(\sum_a s_i^a \right)^2 \right\}. \tag{7}$$

This equation introduces anisotropic two dimensional system where in "space direction" only neighboring spins interact with each other, while in "replica direction" there is an infinite-ranged interaction. The Hamiltonian for this system can be written as

$$-\beta \mathcal{H}_n = J \sum_{i,a} s_i^a s_{i+1}^a + \frac{\sigma^2}{2} \sum_{i,a\neq b} s_i^a s_i^b + \frac{Nn\sigma^2}{2}. \tag{8}$$

Because of the different form of interaction in "replica" and "space" directions, we cannot use Gaussian integrals to eliminate quadratic terms in Hamiltonian and obtain analytical expression for Z_n as it was done in [3]. Therefore, we decided to use transfer matrix approach. That is for any finite number of replicas n we can construct $2^n \times 2^n$ transfer matrix T_n between neighboring sites in "space" direction. Then for given temperature $1/\beta$ and ratio J/σ^2 we can diagonalize transfer matrix T_n and find averaged free energy density f_n numerically. The results of this calculation are shown on Fig.(1,2). One can see that the ordering of replicas at low and high temperatures is different. However, it is no clear how to analytically extrapolate these graphs for $n = 0$; therefore, it is hard to interpret the predictions of replica method.

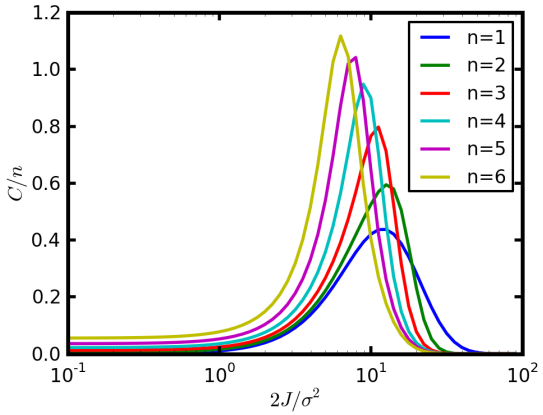

FIG. 1: Heat capacity for different number of replicas. Inverse temperature $\beta\sigma^2 = 0.1$.

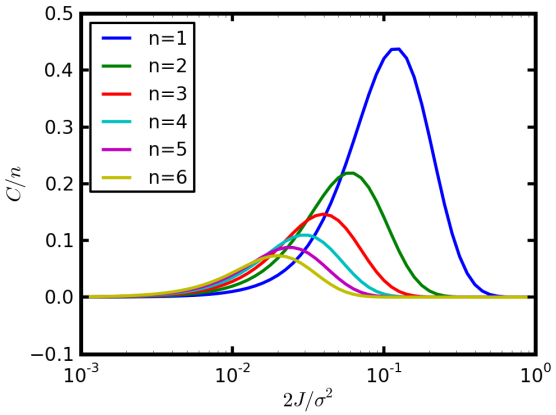

FIG. 2: Heat capacity for different number of replicas. Inverse temperature $\beta\sigma^2 = 10$.

To understand to what extent the numerical results of replica method are correct, we performed a brute force simulation for the chain with $N = 30$ spins. Just as in replica method, for fixed ratio J/σ^2 we generated 1000 samples (realizations of random fields). For each sample we computed free energy and heat capacity using transfer matrices. Then we averaged heat capacity over

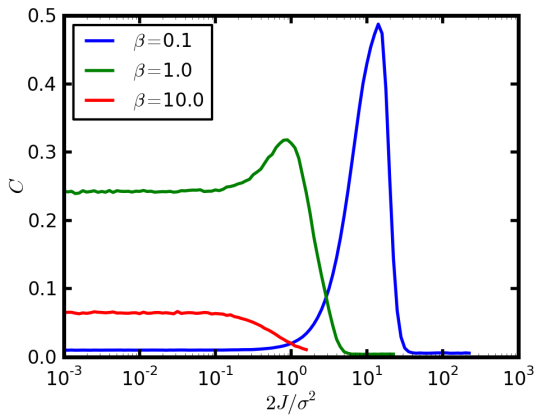

FIG. 3: Heat capacity calculated by averaging over 1000 samples. Different curves correspond to different temperatures.

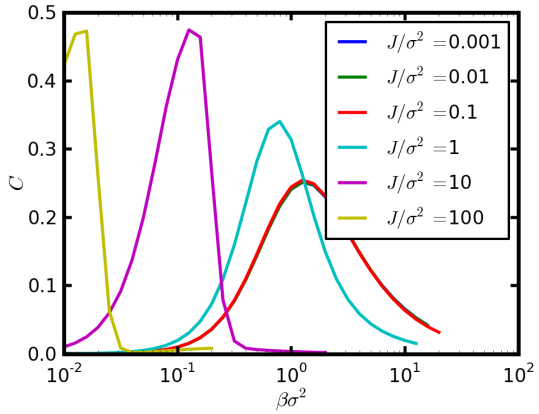

FIG. 4: Heat capacity as function of temperature calculated by averaging over 1000 samples. Different curves correspond to different values of J/σ^2.

all samples and obtained the behavior of heat capacity C as a function of ratio J/σ^2 and temperature, which is shown on Fig.(3, 4). As can be seen from these figures, if $J/\sigma^2 < 1$, then the heat capacity is completely determined by the random field. One can also notice that for high temperature $\beta\sigma^2 = 0.1$ the shape of the curve $C(J/\sigma^2)$, calculated by averaging over 1000 samples Fig.(3), is similar the shape of the curves, calculated for different number of replicas Fig.(1). In low temperature limit, $\beta\sigma^2 = 10$, the situation is different: the curves $C(J/\sigma^2)$ on Fig.(2) are qualitatively different from that of on Fig.(3). These facts might indicate that the predictions of replica method are valid only at high temperatures.

IV. CONCLUSIONS

To summarize, we showed how one dimensional random field Ising model (RFIM) can be applied to protein folding problem. Using replica technique, we numerically calculated the behavior of heat capacity as a function of temperature and the ratio of coupling between spins to the variance of the random field for different number of replicas. In the limit of high temperatures, we found that the predictions of replica method qualitatively agree with the results of simulation for the chain with 30 spins.

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