# Selection Rejection in Ising Spin systems with an exponential distribution of Spins

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ABSTRACT

## 1. INTRODUCTION

We consider an Ising spin system where the spins have a Gaussian distribution about their equilibrium state. Such a model can be used as reasonable approximation for bonds of polymers which are known to exist to fluctuate about the t, g, $g^+$ states. We note that Sherrington and Kirkpatrick [12] have studied the spin-glass state with the spin-spin interaction being given by an exponential distribution. As the model proposed here is similar to the SK model we expect to see
spin glass states in the system. In fact spin glass states have in fact been observed in polymers [11-12].

We first examine the statistical mechanics of an Ising system with the spins having an exponential distribution. The Edwards-Anderson order parameter (q) is computed for this model. It is shown that a spin glass state is possible in this model.

## 2. Sherrington Kirkpatrick Model

The Hamiltonian for the Sherrignton-Kirkpatrick model [12-13] is given by

$$H = \sum_{\langle\ \rangle} J_{ij} S_i S_j \quad ij \tag{1}$$

where the interaction constant $J_{ij}$ is given by

$$J_{ij} = \prod_{\langle ij \rangle} \frac{1}{\sqrt{2\pi J^2}} e^{-J^2/} \tag{2}$$

Here
$$S_i, S_j = \pm 1 \tag{3}$$

Further
$$\overline{J}_{ij} = 0 \tag{4}$$

In the high temperature phase one has

$$\langle \sigma_i \rangle = 0 \tag{5}$$

However at low temperatures one has

$$\langle \sigma_i \rangle \neq 0 \tag{6}$$

Further in the Spin Glass phase the magnetization is given by

$$M = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle = 0 \tag{7}$$

The Edwards-Anderson parameter is similarly given by

$$q = \frac{1}{N} \sum_{i} \langle \sigma_i \rangle^2 \neq 0 \tag{8}$$

## 3. Spin Glass model of Biopolymers

The spin glass model of biopolymers is the same as (1) with the difference that the spins have an Gaussian distribution about an equilibrium point. The interaction constant $J_{ij}$ is a constant and does not have an exponential distribution unlike the SK model. In this picture one has

$$H = \sum_{<ij>} J_{ij} S_i S_j e^{-(\theta - \theta)^2} \; e^{-\frac{1}{2}(\theta_i - \theta_j)^2} \tag{9}$$

For ease of calculation we put $\theta_i = \theta_j$ and $\theta_1 = \theta_2 = \theta_0$. This approximation implies that we are treating all moieties in the biopolymer as the same and hence they have identical Gaussian fluctuations about the equilibrium. The Hamiltonian now becomes

$$H = \sum_{<ij>} J_{ij} e^{-(\theta - \theta_0)^2} S_i S_j \tag{10}$$

The Hamiltonian (12) is exactly similar to the Hamiltonian of SK [12-13] and hence admits spin glass states. Experimental evidence of Spin Glass states in fact have been found in Biopolymers via x-ray diffraction [10] and Mossbauer studies [11] thus justifying our conjecture of moieties of biopolymers having Gaussian distributions about their equilibrium positions. We note that spin glass states are very different from other states normally dealt with in Statistical Mechanics. In the spin glass state each state is frozen or quenched into one configuration [1-9]. Thus

different states do not interact with each other and interchange energy as happens in gases. The partition function is written as

$$Z \quad \frac{(e^{-\beta E})^{n}}{n} - 1 \tag{11}$$

where $n$ is the number of replicas. The number of replicas has to be more than 1. (Hence the -1 ).

## 4. Overlaps

One feature of spin glass states is that there are overlaps between spin glass states. Replicas by definition do not interact: they are simply replicas of one another. However the fluctuations and consequent overlaps are the symmetry breaking aspect of replicas. In Biopolymers this effect is most pronounced. The hydrogen bonds are one of the most important intra- and Intermolecular interactions in biological macromolecules [1], and are responsible for the structural and functional differences in RNA and DNA. The use of the overlap population, as a quantum

Selection criterion presents the advantage that offers the possibility of the evaluation of the

Relative strength of different H-bonds, and also of the detection not only of the weaker H-bonds

Induced Magnetization due to Overlaps The induced magnetization due to overlaps in spin glass states has been calculated by M. Mezard, G. Parisi, and M. A. Virasoro [16]. Here we present a physical basis. Any overlap between states $\alpha$, $\beta$ due to a fluctuation induces magnetization. The induced magnetization is given by

$$M = N\,\mu tanh(\beta\mu B) \tag{12}$$

The induced magnetic field $B$ is proportional to the spins and due to (8) we have

$$B \quad \propto \sqrt{q} \tag{13}$$

The total magnetization due to both states $\alpha$ and $\beta$ is

$$M = N\,\mu tanh^{2}(\beta\mu Jz\sqrt{q}) \tag{14}$$

The overlap between the two states is given by error function. Hence one obtains

$$m = N\mu \int_{-\infty}^{\infty} dz e^{\frac{-z^{2}}{2}} tanh^{2}(\beta\mu Jz\sqrt{q}) \tag{15}$$

## 5. Applications

Differentiating (17) one obtains

$$\frac{dm}{dz} = e^{-\frac{z^2}{2}} \tanh^2(\beta\mu Jz\sqrt{q}) \tag{16}$$

The exponential pre-factor simply localizes the allowed values of z. We therefore neglect the pre factor and incorporate its effect by evaluating the integral at specific values of z. We thus have to solve

$$\frac{dm}{dz} = \tanh^2(\beta\mu Jz\sqrt{q}) \tag{17}$$

Using

$$y = \beta\mu Jz\sqrt{q} \tag{18}$$

One obtains

$$\frac{dm}{dy} = \frac{\tanh^2(y)}{\beta\mu J\sqrt{q}} \tag{19}$$

The solution of (21) is

$$m = \frac{1}{\beta\mu J\sqrt{q}}(y - \tanh(y)) \tag{20}$$

The first term in (22) is the baseline term. Neglecting this term we plot m as function of y as shown in fig. 1.

## 6. Conclusion

Our conjecture of Gaussian distribution of moieties about their equilibrium positions of biopolymers leads to spin glass states of biopolymers. The spin glass states of biopolymers has been verified via x-ray [10] and Mossbauer experiments [11] thus verifying our conjecture. Spin glass states are characterized by varying degrees of overlap. In biopolymers this is due to differing affinities of Hydrogen bonds [14], amino acid interactions [15]. This leads to differing levels of interaction between moieties in biopolymers.

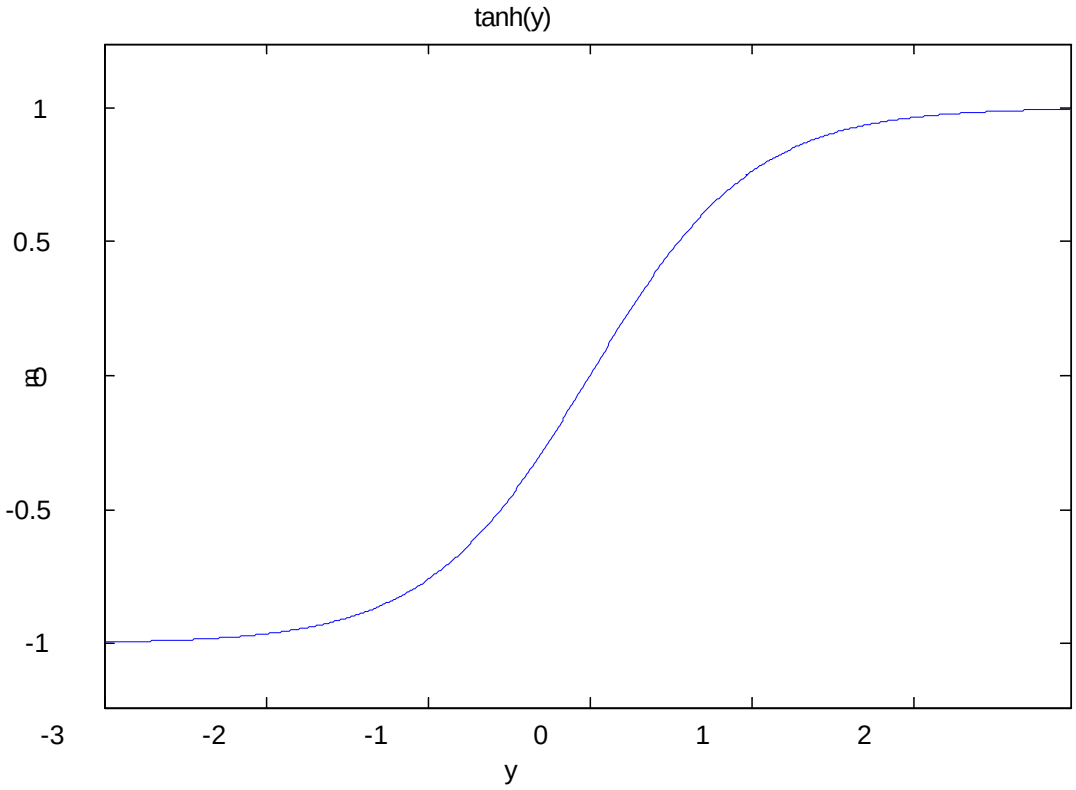


Fig. 1

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