

Understanding Spin Glass systems

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by

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Certificate

This is to certify that this dissertation entitled Understanding Spin Glass systems towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research, Pune represents study/work carried out by Soham Mukund Chandak at Indian Institute of Science Education and Research under my supervision during the academic year 2023-2024.



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This thesis is dedicated to all the teachers in my life

Declaration

I hereby declare that the matter embodied in the report entitled Understanding Spin Glass systems are the results of the work carried out by me at the Department of Physics, Indian Institute of Science Education and Research, Pune, under the supervision of Deepak Dhar and the same has not been submitted elsewhere for any other degree. Wherever others contribute, every effort is made to indicate this clearly, with due reference to the literature and acknowledgement of collaborative research and discussions.



Soham Mukund Chandak

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Abstract

In this thesis we estimate the average ground state energy of a spin glass model. Despite decades of study, there have been no exact explicit calculations for a mean field model of spin glass with finite ranged interactions. In the first part of the thesis we attempt to estimate the average ground state energy of the Sherrington Kirkpatrick model and the spin glass model on a random regular graph by numerical and analytic methods. We attempt to find the ground state energy by several methods such as Greedy algorithm, using Eigenvector ansatz, the cluster flip algorithm and subsequently make improvements on it. We also study the spectral properties of random regular graphs using Random Layered locally Tree like Lattice (RLTL) and compare the results to the predictions from random matrix theory.

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Chapter 1

Introduction

A lot of materials found around us are examples of disordered systems, in fact very few materials have a perfect crystal structure, since some amount of impurities are bound to be present. The spin glass is a prototypical example of a disordered system. In spin glass systems, below the transition temperature the spin degrees of freedom ‘freeze’ into a disordered state. This means that the magnetization given by $\mathbf{m} = \frac{1}{N} \sum_{i=1}^N \langle S_i \rangle_T$, or more generally the staggered magnetization given by $\mathbf{m}_{\mathbf{k}} = \frac{1}{N} \sum_{i=1}^N \langle S_i \rangle_T e^{i\mathbf{k}\cdot\mathbf{r}_i} = 0$, for $\mathbf{k} \neq 0$, where the sum runs over all the magnetic moments and $\langle \cdot \rangle_T$ represents thermal average. Yet, the local magnetization at a site given by $m_i = \langle S_i \rangle_T$ is non-zero.

Spin glass states are quite ubiquitous, examples of systems in which spin glass states can be found include non-magnetic metal hosts doped with magnetic metallic impurities, magnetic insulators, amorphous alloys. Spin glass states are also found in systems with the spin degrees of freedom being electric instead of magnetic such as ferroelectric-antiferroelectric mixtures. Thus, understanding the physics of such disordered systems is an important problem.

Historically, the study of spin glass systems began in the 1970s when a series of measurements on the susceptibility of non-magnetic metal hosts doped with magnetic metallic impurities at different temperatures revealed cusps at particular temperature [1]. Cusps in susceptibility measurements are indicative of second order phase transition. However, curiously, magnetization measurements revealed no net magnetization and checking for antiferromagnetic ordering by neutron scattering experiments revealed no such ordering.

These observations can be explained as follows: The magnetic moments due to the im-

purities in the non-magnetic host metal are coupled to each other via the itinerant electrons inside the host metal. This indirect exchange interaction is known as the RKKY interaction (Ruderman-Kittel-Kasuya-Yoshida) [2, 3, 4]. The RKKY interaction goes as:

$$J_{ij} \propto \frac{\cos(2k_f r_{ij})}{r_{ij}^3}$$

Here k_f is the momentum at the Fermi level. The sign of the interaction is oscillatory in nature. Sam Edwards and Paul Anderson guessed that since the spin glass phase can be observed in many other systems too, the exact details of the interaction J_{ij} and the exact locations of the spin degrees of freedom in the crystal do not play a role and proposed the EA model. The Edwards-Anderson (EA) model is a simple model which shows a spin glass phase with the Hamiltonian:

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j \quad (1.1)$$

where the Ising spins S_i lie on a regular lattice and the sum runs over all pairs of neighbouring spins. J_{ij} is are independent random variables with a fixed probability distribution function $P(J_{ij})$.

It is important to define statistical averaging for disordered systems. For instance, since the set of couplings $\mathbf{J} = \{J_{ij}\}$ will be different for each sample, the partition function $Z_N(\beta, \mathbf{J})$, β is the inverse temperature, for the EA model would be different for each sample. But, the physical properties of the system such as the Helmholtz free energy per spin (f) are nearly same, with small fluctuations for a very large number of particles. Thus,

$$f = \lim_{N \rightarrow \infty} -\frac{1}{N} \cdot \frac{1}{\beta} [\ln Z_N(\beta, \mathbf{J})]_{av} = f_\infty(\beta) \quad (1.2)$$

where $[\cdot]_{av}$ is called as disorder averaging defined as

$$[A]_{av} = \int d\mathbf{J} P(\mathbf{J}) A(\mathbf{J}) \quad (1.3)$$

Quantities which have a well defined average under disorder averaging in the thermodynamic limit ($N \rightarrow \infty$) are called as self averaging quantities. Self averaging requires that the variance of the distribution for the quantity go to 0 as $N \rightarrow \infty$. For example, the internal energy of the system per particle, the free energy per particle are self averaging whereas the partition function is not. Thus for disordered models, it is more appropriate to use the terms average ground state energy/ average free energy rather than simply the ground state

energy/free energy.

Exact calculation of the thermodynamic quantities such as free energy, internal energy is a difficult problem for most of the models in statistical physics. Instead one often resorts to mean-field models which capture the physics correctly away from the critical point and for models in high enough dimensions, even close to the critical point. Mean-field models thus serve as a first attempt at a much harder problem. In 1975, David Sherrington and Scott Kirkpatrick proposed a mean-field model of the EA model, now known as the Sherrington-Kirkpatrick (SK) model [18]:

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} S_i S_j \quad (1.4)$$

where J_{ij} is a random variable with a fixed probability distribution $P(J_{ij})$. The difference from the EA model is that now the sum runs over all spins and not just neighboring pairs of spins.

The SK model is not very realistic, since the interaction is independent of the distance between the spins. A step in the direction to extend our understanding of the EA model would be by considering a mean-field model with a finite range of interaction. For the ferromagnetic Ising model, the mean-field solution is identical to the exact solution for the ferromagnetic Ising model (with only nearest neighbor interactions) on a Bethe lattice. Thus, one can make a similar attempt at solving the random interaction Ising model on the Bethe lattice in the hopes of obtaining a more accurate mean-field description of the EA model.

However, the Bethe lattice is not accessible to numerical methods. Furthermore, dealing with the boundary conditions for the spin glass Ising model is a highly non-trivial problem. Thus, instead we resort to solving the spin glass Ising model on a random regular graph.

As of date solving the mean-field models for the spin glass model has turned out to be a hard problem. The best known solution by Parisi [5, 6] attempts to solve the problem by replica symmetry breaking. While the solution is correct at high temperatures and near the spin glass transition temperature, at lower temperatures, the validity of the solution is not known. In particular, it has not been possible to calculate exactly the average ground state energy of the model. Even numerically, it is not easy to determine the exact average ground state energy by simulated annealing because the presence of several metastable states. The system gets stuck in such metastable states.

In this thesis we will try to understand the ground state energy of the SK model and the spin glass Ising model on a random regular graph (with degree 3) better. The rest of

the thesis is organized as follows: in Chapter 2, I will attempt to find ground state energy using methods such as Greedy algorithm, eigenvector ansatz. In particular, in section 2.1 I will estimate the free energy of SK model by a high temperature expansion, in section 2.2 we discuss the minimised energy obtained by using a Greedy algorithm for the SK model, section 2.3 discusses an improved attempt at finding the ground state energy for the SK model using eigenvectors as an ansatz. In section 2.4 we switch to the problem of finding ground state energy for the the random bond Ising model on random regular graph and discuss the construction of Random Layered locally Tree like Lattice (RLTL) which is expected to behave like the Bethe lattice but does not suffer from strong surface effects. Sections 2.5 and 2.6 discuss ground state energy obtained for spin glass on a random regular graph using Greedy algorithm, eigenvector ansatz and other methods. In the problem of spin glass on a random regular graph, the structure of the graph plays an important role in determining the properties of the model and in fact leads to lower bounds on the ground state energy of the model. In Chapter 3 we analyze the spectral properties of random regular graphs and explain the small variance in the density of states using random walks. We also explore the spectrum of non-backtracking random walks on the graph.

Chapter 2

Bounds on the ground state energy of Ising spin glass models

In 1975 Sherrington and Kirkpatrick gave a solution to the SK model, while the solution is correct for high temperature phase of the model, the solution is incorrect below the spin glass transition temperature T_{sg} . This solution is also known as replica symmetric solution. In the following years several people including Mézard, Thouless, Parisi made significant contributions to solving the model (calculating the free energy of the model). In 1980 Parisi gave the solution to the SK model with replica symmetry breaking, which is believed to be correct. A rigorous proof of the solution was given only as recent as 2006 by Talagrand [23], yet the calculation of free energy using this method at lower temperatures involves increasingly complicated patterns of replica symmetry breaking and at 0 temperature requires infinite step replica symmetry breaking and thus, an exact analytic expression for the ground state energy of the SK model is not known.

The Hamiltonian for the Sherrington Kirkpatrick model is:

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} S_i S_j \quad (2.1)$$

where the sum is over all spins, J_{ij} are *i.i.d.* random variables with the probability density function $P(J_{ij})$. For simplicity we will consider the cases:

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{J_{ij}^2}{2\sigma^2}}$$

with $\sigma^2 = \frac{J^2}{N}$ where J is a constant. This scaling ensures that the free energy is extensive.

We wish to find the average ground state energy for these models. Note that for different set of couplings $\{J_{ij}\}$ we obtain different ground state energies. Thus for disordered averaging, we will calculate the minimized energy for several set of couplings and average over them to obtain the average minimized energy. We will describe some analytic and computational approaches to estimate the average ground state energy in the following sections.

2.1 High Temperature expansion for the SK model

We will consider the Hamiltonian

$$H = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} S_i S_j \quad (2.2)$$

with

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{J_{ij}^2}{2\sigma^2}}$$

and all J_{ij} 's being independently and identically distributed. To have extensive free energy, we will require that $\sigma^2 = \frac{J^2}{N}$, where, N is the number of spins and J is a constant. Then the partition function \mathcal{Z} for a particular set of couplings $\{J_{ij}\}$

$$\mathcal{Z} = \sum_{\{S_i\}} \prod_{\langle ij \rangle} e^{-\beta J_{ij} S_i S_j} = \sum_{\{S_i\}} \prod_{\langle ij \rangle} \cosh(\beta J_{ij}) (1 + X(J_{ij}) S_i S_j) \quad (2.3)$$

Here $X(J_{ij}) = \tanh(\beta J_{ij})$

$$\mathcal{Z} = \left(\prod_{\langle ij \rangle} \cosh(\beta J_{ij}) \right) \left(\sum_{\{S_i\}} \left(1 + \sum_{i<j} X(J_{ij}) S_i S_j + \sum_{i<j,k<l} X(J_{ij}) X(J_{kl}) S_i S_j S_k S_l + \dots \right) \right) \quad (2.4)$$

Note that by summing over all possible spin configurations, the only terms that will survive are those that can form 'closed loops'. Thus, we will have

$$\mathcal{Z} = 2^N \cdot \left(\prod_{\langle ij \rangle} \cosh(\beta J_{ij}) \right) \cdot (1 + T(3) + T(4) + T(5) + T(6) + \dots) \quad (2.5)$$

where we denote by $T(n)$

$$T(n) = \sum_{i_1 < i_2 \dots < i_n} X(J_{i_1 i_2}) X(J_{i_2 i_3}) \dots X(J_{i_{n-1} i_n}) \quad (2.6)$$

$$\ln \mathcal{Z} = N \ln 2 + \sum_{i < j}^N \ln \cosh(\beta J_{ij}) + \ln(1 + T(3) + T(4) + T(5) + T(6) + \dots)$$

The free energy per spin f is given by:

$$f = f_\infty(\beta) = \lim_{N \rightarrow \infty} -\frac{1}{N} \cdot \frac{[\ln \mathcal{Z}]_{av}}{\beta}$$

where $[\cdot]_{av}$ indicates disorder averaging. Thus,

$$f = \lim_{N \rightarrow \infty} -\frac{\ln 2}{\beta} - \frac{1}{N\beta} \sum_{i < j}^N [\ln \cosh \beta J_{ij}]_{av} - \frac{[\ln(1 + T(3) + T(4) + T(5) + T(6) + \dots)]_{av}}{\beta N} \quad (2.7)$$

For rest of the calculation, we will assume $\beta \ll 1$. The terms that will survive in the thermodynamic limit ($N \rightarrow \infty$), for $\beta < 1$ are the ones with power of $N > 0$. First consider the term with $\ln \cosh(\beta J_{ij})$, since all J_{ij} are i.i.d. random variables

$$\sum_{i < j}^N [\ln \cosh(\beta J_{ij})]_{av} = \frac{N(N-1)}{2} [\ln \cosh(\beta J_{12})]_{av}$$

Now,

$$\ln \cosh(x) = \frac{x^2}{2} - \frac{x^4}{12} + \frac{x^6}{45} - \dots$$

Thus,

$$[\ln \cosh(\beta J')]_{av} = \frac{1}{2\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \beta^2 J'^2 e^{-J'^2/2\sigma^2} dJ' - \frac{1}{12\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \beta^4 J'^4 e^{-J'^2/2\sigma^2} dJ' + \dots$$

$$[\ln \cosh(\beta J')]_{av} = \frac{\beta^2 J^2}{2N} - \frac{\beta^4 J^4}{4N^2} + \dots$$

At higher orders, powers of $N > 1$ will be in the denominator and thus terms beyond 2nd order don't survive the thermodynamic limit. Thus,

$$\lim_{N \rightarrow \infty} \frac{1}{N\beta} \sum_{i < j}^N [\ln \cosh \beta J_{ij}]_{av} = \frac{\beta J^2}{4} \quad (2.8)$$

Now, $\ln(1+x) = x - x^2/2 + \dots$ and $\tanh(x) = x - x^3/3$. Thus for the $[\ln(1 + T(3) + \dots)]_{av}$ term, the ones that survive disorder averaging are smaller than $O(N)$.

$$\lim_{N \rightarrow \infty} \frac{[\ln(1 + T(3) + T(4) + T(5) + T(6) + \dots)]_{av}}{\beta N} = 0 \quad (2.9)$$

Putting together equations 2.7, 2.8 and 2.9

$$f = -\frac{\ln 2}{\beta} - \frac{\beta J^2}{4} \quad (2.10)$$

In fact, the free energy obtained is the same as the replica symmetric solution obtained by Sherrington and Kirkpatrick [18] for the model. However, while the solution is correct for temperatures above the spin glass transition temperature, the solution is incorrect below it as $T \rightarrow 0 \implies \beta \rightarrow \infty$ and thus even terms with $\frac{1}{N}$ dependence may not go to 0.

2.2 Greedy Algorithm for energy minimization of SK model

We can try a very simplified computational approach to find the ground state energy in the following way: For a given set of couplings, initialize the values of the spins $\{S_i\}$ in a random fashion. Then, calculate the 'mean-field' $\sum_{j \neq i} J_{ij} S_j$ experienced by a spin S_i . Make a list $L_{non-align}$ of all the spins that are not aligned correctly to minimize the energy, i.e. the spin is not aligned with the local 'mean-field' experienced by that spin. Randomly choose a spin from the list L and then flip it to align it with its local mean-field. Update the list to include any new spins whose orientation is not aligned with local field and discard any spins which are now aligned with their local field. This process is continued until there are no more spins remaining to flip.

Repeat the above process for several different initial configurations of spins $\{S_i\}$ and take the minimum energy $E_{gs \text{ min}}$ obtained from all the minimum energy configurations obtained. Then average of these $E_{gs \text{ min}}$ minimum energies is an upper bound for the average ground state energy. i.e. $[E_{gs}] \leq [E_{gs \text{ min}}]$. The resulting energies are plotted in figure 2.1

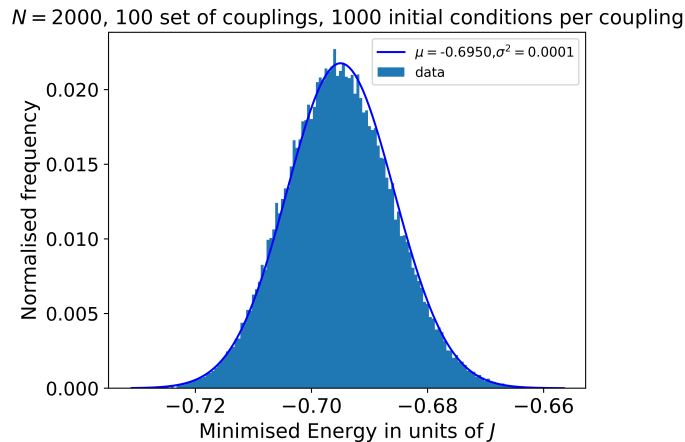
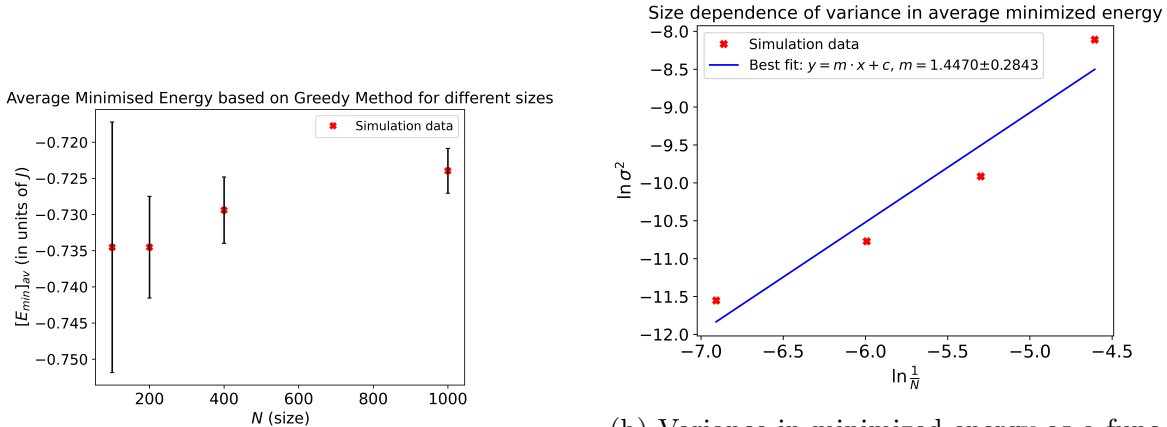


Figure 2.1: Histogram plot of Minimized Energy for random initial configuration of spins for several different sets of couplings via Greedy algorithm for the SK model. $N = 2000$ spins.



(a) Average minimized energy per spin using basic cluster flip algorithm.

(b) Variance in minimized energy as a function of size. Here the variance $\sigma^2 \sim 1/N^m$, m is the slope of the best fit line.

Figure 2.2: Results for the SK model from the Greedy algorithm. Disordered averaging over 10^3 systems for each size.

The expectation value from of the energy obtained by the simulation, in the large N limit, can be estimated analytically to obtain an upper bound on the energy obtained from

the simulations. The idea is as follows: When the spins are initialized, the mean-field experienced by each spin can be considered as a sum of several random variables with mean $\mu = 0$ and variance $\sigma^2 = J^2/N$ as the mean-field is given by $\sum_{j \neq i} J_{ij} S_j$. Thus in the limit $N \rightarrow \infty$, the mean-field experienced converges in distribution to a Gaussian Random variable with mean 0 and variance 1.

In the initial state, the mean-field for different spins are uncorrelated random variables. However, as the spin flips are performed, these variables get correlated in some complicated way, hence the above calculation will only lead to an upper bound on the numerically obtained value. This (upper bound) is given by:

$$E_{bound} = -\frac{J}{2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |h| e^{-h^2/2} dh = -\frac{J}{\sqrt{2\pi}} \approx -0.398942 J \quad (2.11)$$

This is much higher from estimated true average ground state energy obtained computationally as we have completely ignored the fact that after performing spin flips, the mean-field values for different spins become strongly correlated.

Such class of algorithms where the energy of the system is obtained by local minimization of the energy are called as Greedy Algorithms. In this case the algorithm leads to a state which is stable to a single spin flip i.e. the energy cannot be minimized further by flipping just one spin. For further improvement, instead of minimizing energy for a single spin, we can consider the minimum energy configuration for larger clusters with 2, 3, ... spins. However, as the cluster size increases, the amount of time required to cycle through all possible states increases as $N^{\text{cluster size}}$ and the program becomes very slow.

2.3 Improvement on the Greedy algorithm: Eigenvector method

Alternatively, to estimate the ground state energy, we can utilize the eigenvectors of the coupling matrix obtained by rewriting the SK Hamiltonian in a matrix form:

$$2E = \Psi_s^\dagger \mathbf{H} \Psi_s \quad (2.12)$$

Where,

$$\mathbf{\Psi}_s = \begin{bmatrix} S_1 \\ S_2 \\ \vdots \\ S_N \end{bmatrix}$$

and

$$\mathbf{H} = \begin{bmatrix} 0 & -J_{12} & -J_{13} & \cdots & -J_{1n} \\ -J_{21} & 0 & -J_{23} & \cdots & -J_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -J_{N1} & -J_{N2} & -J_{N3} & \cdots & 0 \end{bmatrix}$$

Suppose for the moment, we allow S_i to take any real value (instead of ± 1), then we can find the eigenvectors corresponding of \mathbf{H} . Suppose we find the normalized eigenvectors of \mathbf{H} , then as \mathbf{H} is real and symmetric, we can find a orthonormal eigenbasis of \mathbf{H} , $\{\psi_{\lambda_i}\}$ with eigenvalues $\{\lambda_i\}$. Thus we can express any $\mathbf{\Psi}_s$ as

$$\mathbf{\Psi}_s = \sum_i c_i \psi_{\lambda_i} \quad (2.13)$$

Suppose the smallest eigenvalue value is λ_{min} with corresponding eigenvector $\psi_{\lambda_{min}}$. Then we have that

$$\frac{\mathbf{\Psi}_s^\dagger \mathbf{H} \mathbf{\Psi}_s}{\mathbf{\Psi}_s^\dagger \mathbf{\Psi}_s} = \sum_{i=1}^N c_i^2 \lambda_i \geq \lambda_{min} \quad (2.14)$$

A good choice to begin for the search of minimum energy is in the state Ψ with its entries defined by $[\Psi]_i = \text{sgn}([\psi_{\lambda_{min}}]_i)$, where $\text{sgn}(x)$ is the function defined by $\text{sgn}(x) = 1$ for $x > 0$ and $\text{sgn}(x) = -1$ for $x < 0$. We begin in this state and apply the Greedy Algorithm as before. This also helps us obtain a lower bound for the average ground state energy as we will have for any Ising spin configuration $\mathbf{\Psi}_s$:

$$\frac{\mathbf{\Psi}_s^\dagger \mathbf{H} \mathbf{\Psi}_s}{\mathbf{\Psi}_s^\dagger \mathbf{\Psi}_s} \geq \lambda_{min} \implies \frac{2E}{N} \geq \lambda_{min}$$

this follows from equation 2.12 and the fact that $\mathbf{\Psi}_s^\dagger \mathbf{\Psi}_s = N$ for an Ising spin configuration. Thus,

$$\text{Average ground state energy per spin} = \frac{[E]_{av}}{N} \geq \frac{[\lambda_{min}]_{av}}{2} \quad (2.15)$$

For the SK model, thus we obtain

Numerical results for the eigenvector method are in figures 2.3 and 2.4

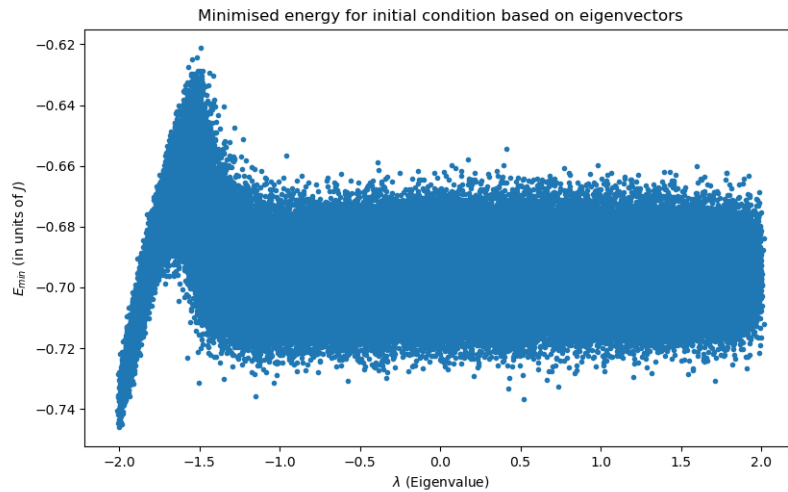


Figure 2.3: Minimised energy versus eigenvalue for eigenvector method

Average Minimised Energy based on Eigenvector Ansatz for different sizes

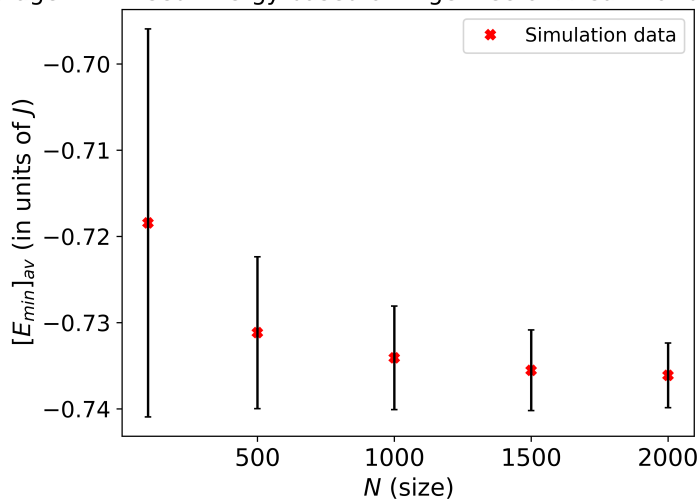


Figure 2.4: Average minimum energy for different sizes using eigenvector method

Next we analyze the random coupling Ising model in a finite interaction range setting. In particular we analyze the random coupling Ising model with only nearest neighbor interaction on a 3 co-ordinated random regular graph. The Hamiltonian for the model is given by:

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j \quad (2.16)$$

where the sum is over all pairs of nearest neighbors on a random regular graph and for

simplicity, we consider the case with

$$P(J_{ij}) = \frac{1}{2}[\delta(J + J_{ij}) + \delta(J - J_{ij})]$$

with J a constant.

First, let us note that the average ground state energy per spin for a fully ferromagnetic model on the same lattice will be $-1.5 J$. Clearly, for the spin-glass model this quantity will be greater than $-1.5 J$ because of frustration. The frustration arises because of the randomness in the couplings and the presence of loops in the lattice. However, random regular graphs have a locally tree like structure and the probability that a loop of size smaller than $O(\log N)$ passes through a site goes as $\frac{1}{N}$. Thus, there are only $O(1)$ loops of small size present in a typical random regular graph. More details about properties of random regular graphs can be found in [19, 20]. Spectral properties of these graphs are explored in Chapter 3.

The spin glass Ising model on a Bethe lattice has been studied extensively in the past, however, even after four decades, the model is not well understood at low temperatures. For instance, [9, 10] estimate the average ground state energy per spin from free energy calculations to be $-1.2778 J$ which equal to the value given by the replica symmetric solution to the problem. However in [8] the value is $-1.1790 J$ and in [7] it is $-1.3581 J$. Using cavity method upto 1 step replica symmetry breaking (RSB), Parisi [13, 14] has estimated the average ground state energy per spin to be $-1.2723 J$. It is conjectured that full replica symmetry breaking will give the correct solution to the problem, however as of date there have been no explicit calculations beyond the 1 RSB solution.

In numerical studies, the average ground state energy per spin has been estimated using extremal optimization heuristic in [21], the energy is estimated as $-1.2716 J$ but note that this is not an exact calculation of ground state energy. Using simulated annealing, the average minimum energy for the ferromagnetic Ising model with zero magnetization is calculated to be $-1.26 J$ in [26, 27]. The exact ground state energy for random regular graphs (of degree 4 and higher) using the branch and cut method has been estimated for small system sizes in [22].

A particular model of the 3 co-ordinated random regular graph is a Random Layered Locally Tree like Lattice (RLTL). The construction of the RLTL is explained in the following section.

2.4 Construction of RLTL

A random regular graph is a graph where all vertices of the graph have the same degree. Two methods to construct a random regular graph are given in this section. The spins are located on the vertices of the graph and the vertices corresponding to nearest neighbor spins have an edge between them.

2.4.1 Method 1

Consider a graph G_{ini} consisting of 2 rings of n sites each, $n \in \mathbb{N}$. Let us call the rings G_{C1} and G_{C2} and the vertex sets for these graphs as $V_1 = \{1, 2, \dots, n\}$ and $V_2 = \{1', 2', \dots, n'\}$.

Now add an edge between a vertex in G_{C1} and a vertex in G_{C2} as follows: Perform a random permutation P on V_2 and then add an edge between the vertices i and $P(i')$, $\forall i \in V_1$.

A Random Regular graph with degree 3 at each vertex and order $2n$ has been generated.

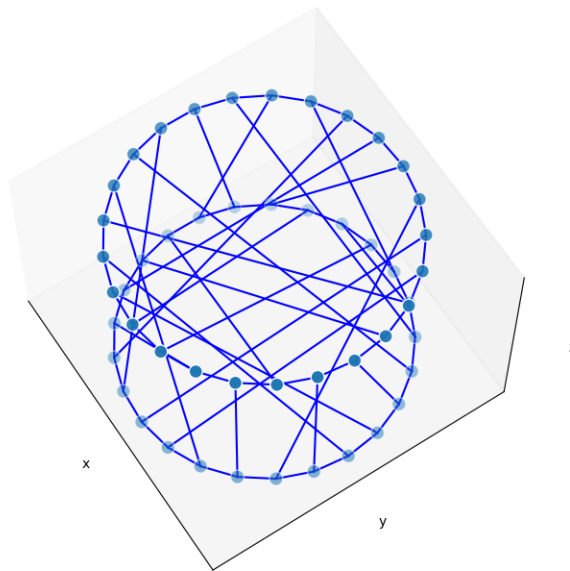


Figure 2.5: An example of Random regular graph generated by Method 1 of size 50

2.4.2 Method 2

Consider a cycle graph C_{2n} , $n \in \mathbb{N}$ with vertices $V = \{1, 2, \dots, 2n\}$. Clearly the graph is bipartite where we can partition the vertices into $U = \{1, 3, \dots, 2n-1\}$ and $W = \{2, 4, \dots, 2n\}$ so that all elements in U have edges connecting with elements in W only.

Now we add an edge between a vertex in W and a vertex in U as follows: Perform a random permutation P on U . We reject the permutation if $|P(i) - i| = 2$ for any $i \in U$ and retry till we get a permutation which satisfies $|P(i) - i| \neq 2 \forall i \in U$.

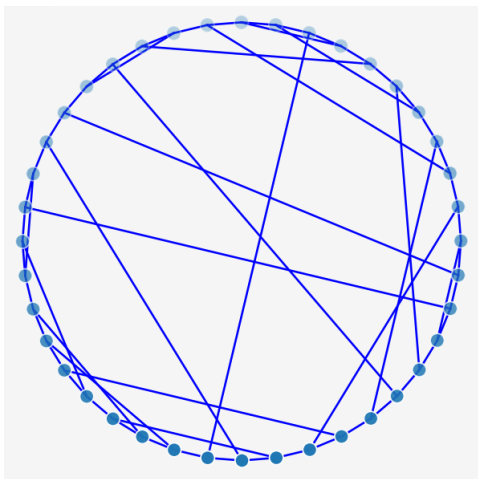


Figure 2.6: An example of Random Regular graph of size 40 generated by Method 2.

2.5 Greedy Algorithm for energy minimization of Ising spin glass model on a random regular graph

The Hamiltonian for the problem is:

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j \quad (2.17)$$

where $P(J_{ij}) = \frac{1}{2}[\delta(J + J_{ij}) + \delta(J - J_{ij})]$, J is a constant.

Then, just like for the SK model, we can implement a Greedy algorithm where the spins are initialised to a random initial condition and then we choose a random spin to flip among the spins not aligned with their local mean-field. We repeat this procedure till there are no sites where a single spin flip will lead to a decrease in the energy.

2.5.1 Connection between Greedy algorithm and Dimer problem

We now show that the Greedy algorithm for the Spin Glass on a 3 co-ordinated random regular graph is similar to the Dimer problem at zero temperature on the same lattice.

For a given configuration of spins and couplings, we introduce the terminology:

A ‘**bond**’ between two spins is said to be satisfied if the configuration of spins is such that it is the minimised energy configuration for the two spins, given the coupling between the spins. We will denote such a bond by a **blue** bond. Similarly, a bond between two spins is said to be unsatisfied if the configuration of spins is such that it is **not** the minimised energy configuration for the two spins, given the coupling between the spins. We will denote such a bond by a **red** bond.

The Hamiltonian is invariant under the following transformation:

$$S_i \rightarrow \sigma_i S_i, \quad J_{ij} \rightarrow \sigma_i \sigma_j J_{ij} \quad (2.18)$$

where $\sigma_i \in \{\pm 1\}$.

$$H' = - \sum_{\langle ij \rangle} (\sigma_i \sigma_j J_{ij}) (\sigma_i S_i) (\sigma_j S_j) = - \sum_{\langle ij \rangle} J_{ij} S_i S_j = H \quad (2.19)$$

as $\sigma_i^2 = 1$. Thus, the Hamiltonian is gauge invariant under the gauge transformation given by equation 2.18 and all the information about the energy of the system is fully contained in the bonds [25].

The **red** bonds can be thought of as dimers on the lattice formed by the vertices of the graph. The Greedy algorithm simply ensures that no two dimers ‘touch’ each other. Then it is possible to estimate the average energy obtained by the Greedy algorithm by assuming: (i) For every possible dimer configuration there exists a corresponding configuration of spins which has **red** bonds in place of dimers and (ii) All possible dimer configurations are sampled with a weight proportional to their Boltzmann weight (the dimer configuration being the configuration obtained at the end of the Greedy algorithm), then the Greedy algorithm is the same as the Dimer problem at $T = 0$.

The partition function for the Dimer problem is given by:

$$\Omega(z) = \sum_{r=0}^{max} N_r \cdot z^r \quad (2.20)$$

where $z = e^{-\beta E_{bond}}$ is the Boltzmann weight and N_r is the number of configurations with r red bonds satisfying the condition that no two red bonds have end at a common site. For our case $z = 1$. We wish to estimate the average energy obtained by the Greedy algorithm. As the number of possible dimer tilings $W(N_D)$ with N_D dimers grows exponentially with the size of the lattice, the number of dimers (i.e. **red** bonds) in a typical configuration $\overline{N_D}$ must be the value that maximizes W . Thus by estimating $\overline{N_D}$ we can obtain the average energy of a configuration generated by the Greedy algorithm.

Denote by $\mathcal{Z}_N(z; 0)$ the partition function for the Cayley tree with N layers with the top site not occupied by a dimer and similarly, by $\mathcal{Z}_N(z; 1)$ the partition function for the case of the top site occupied by a dimer. Then we have the recursions:

$$\mathcal{Z}_{N+1}(0) = [\mathcal{Z}_N(0) + \mathcal{Z}_N(1)] \cdot [\mathcal{Z}_N(0) + \mathcal{Z}_N(1)] \quad (2.21)$$

and

$$\mathcal{Z}_{N+1}(1) = 2z\mathcal{Z}_N(0)[\mathcal{Z}_N(0) + \mathcal{Z}_N(1)] \quad (2.22)$$

Now, define

$$f_N = \frac{\mathcal{Z}_N(1)}{\mathcal{Z}_N(0)} \quad (2.23)$$

and thus,

$$f_{N+1} = \frac{2z}{1 + f_N} \quad (2.24)$$

Thus,

$$\lim_{N \rightarrow \infty} f_N = f^*, f^* = \frac{2z}{1 + f^*}$$

Thus,

$$f^* = \frac{-1 + \sqrt{1 + 8z}}{2} \quad (2.25)$$

Now, the average energy of a Dimer configuration is given by

$$E_{avg} = -1.5 \left(1 - \frac{2p}{3}\right) J \quad (2.26)$$

where p is the probability of a site being occupied by a dimer. Now,

$$p = \frac{N(\text{occupied})}{N(\text{unoccupied}) + N(\text{occupied})}$$

Thus,

$$p = \lim_{N \rightarrow \infty} \frac{3z \mathcal{Z}_N(0) [\mathcal{Z}_N(0) + \mathcal{Z}_N(1)]^2}{3z \mathcal{Z}_N(0) [\mathcal{Z}_N(0) + \mathcal{Z}_N(1)]^2 + [\mathcal{Z}_N(0) + \mathcal{Z}_N(1)]^3} \quad (2.27)$$

and hence,

$$p = \frac{3z}{3z + 1 + f^*} \implies E_{avg} = -0.9 J \quad (2.28)$$

2.5.2 Numerical results

The results from the numerical approach are in figure 2.7

The results from the simulation disagree with the analytic calculation for Dimer problem because assumption (i) is invalid as the only Dimer configurations that will be allowed are the ones which satisfy the frustration constraints due to the large loops of order $\log N$ present in the system. These frustration constraints have a non-trivial effect even in the thermodynamic limit.

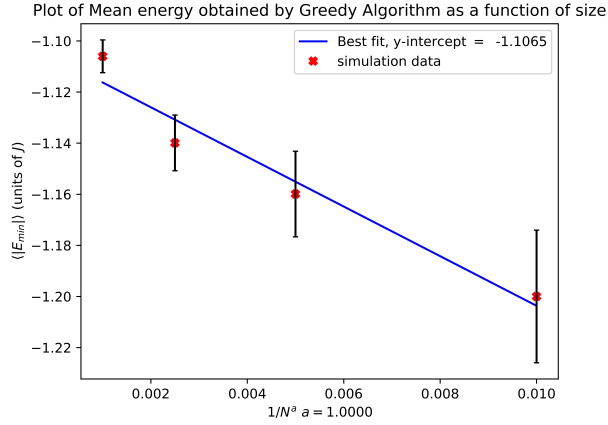


Figure 2.7: Size relation of the average minimum energy obtained by Greedy Algorithm

2.5.3 3 Spin cluster Calculation

We want to calculate the average energy per spin for the ensemble of dimer configurations in which 2 blinkers are not adjacent on a Cayley tree, assuming all final configurations are equally likely. Refer to figure 2.8 for notations. Following similar notation as in previous section and from the figure 2.8, we have the recursions:

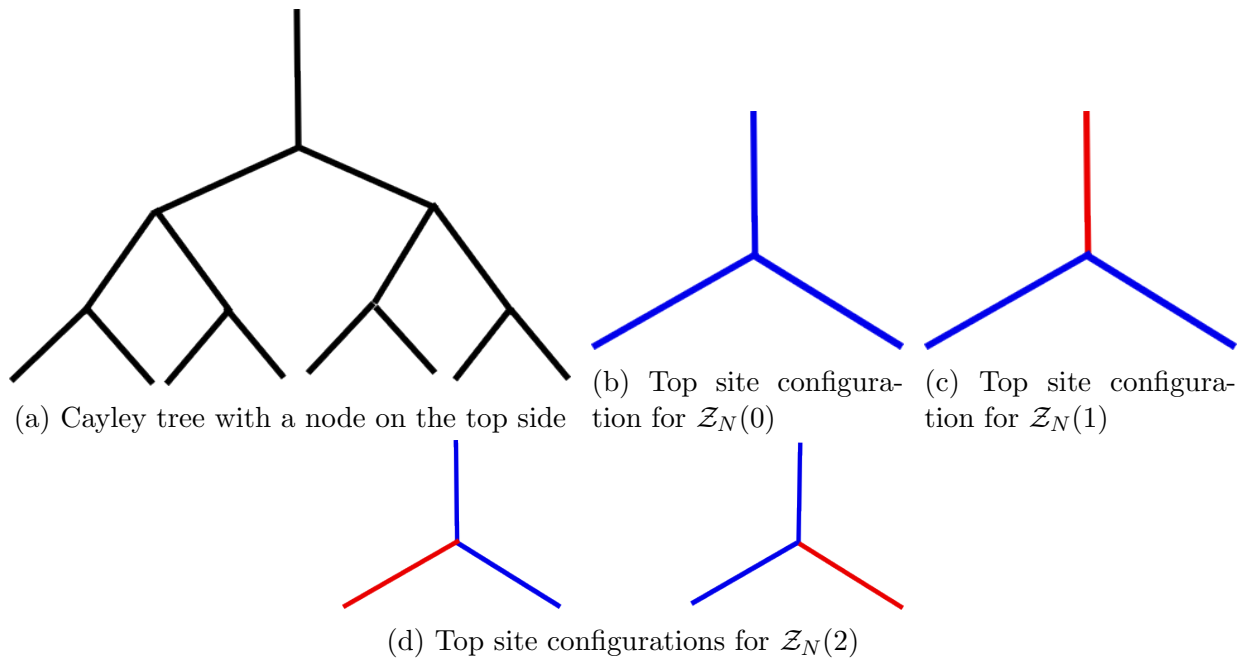


Figure 2.8: For the 3 spin cluster calculation Calculation

$$\mathcal{Z}_{N+1}(0) = 4[\mathcal{Z}_N(0) + \mathcal{Z}_N(2)]^2 \cdot [\mathcal{Z}_N(0) + 2\mathcal{Z}_N(1) + \mathcal{Z}_N(2)] \quad (2.29)$$

$$\mathcal{Z}_{N+1}(1) = z[\mathcal{Z}_N(0) + \mathcal{Z}_N(2)]^2 \cdot [(\mathcal{Z}_N(0) + \mathcal{Z}_N(2))^2 + 4\mathcal{Z}_N(1)\mathcal{Z}_N(0)] \quad (2.30)$$

$$\mathcal{Z}_{N+1}(2) = 2z[\mathcal{Z}_N(0) + \mathcal{Z}_N(2)]^2 \cdot [(\mathcal{Z}_N(0) + \mathcal{Z}_N(2))^2 + 2\mathcal{Z}_N(1)\mathcal{Z}_N(0)] \quad (2.31)$$

Define

$$f_N = \frac{\mathcal{Z}_N(1)}{\mathcal{Z}_N(0)}, \quad g_N = \frac{\mathcal{Z}_N(2)}{\mathcal{Z}_N(0)} \quad (2.32)$$

Then from the recursions, we have

$$f_{N+1} = \frac{z[(1 + g_N)^2 + 4f_N]}{4(1 + 2f_N + g_N)^2}, \quad g_{N+1} = \frac{z[(1 + g_N)^2 + 2f_N]}{2(1 + 2f_N + g_N)^2} \quad (2.33)$$

Deep inside the Cayley tree let the probability of a site being occupied be p , then,

$$p = \frac{3z\mathcal{Z}_N(1) \cdot [\mathcal{Z}_N^2(0) + 2\mathcal{Z}_N(0)\mathcal{Z}_N(2)]}{3z\mathcal{Z}_N(1) \cdot [\mathcal{Z}_N^2(0) + 2\mathcal{Z}_N(0)\mathcal{Z}_N(2)] + [\mathcal{Z}_N(0) + \mathcal{Z}_N(2)]^3} = \lim_{N \rightarrow \infty} \frac{3zf^*[1 + 2g^*]}{3zf^*[1 + 2g^*] + (1 + g^*)^3} \quad (2.34)$$

Where

$$f^* = \frac{z(1 + g^*)^2 + 4f^*}{4(1 + 2f^* + g^*)^2}, \quad g^* = \frac{z(1 + g^*)^2 + 2f^*}{2(1 + 2f^* + g^*)^2}$$

Solving for f^*, g^* numerically to obtain p , we get

$$E_{avg} = -1.196315 J \quad (2.35)$$

for the stability of 3 spin clusters.

2.6 Improvements on the Greedy algorithm

In this section, we will look at a better approach to find the average ground state energy for the spin glass on a random regular graph. The key idea is to identify clusters of spins that can be flipped to obtain a lower energy. We will then add on improvements in it. Unless specified otherwise, all results are for RLTLs generated using method 1.

2.6.1 Basic cluster flip algorithm

We will discuss the method considering the structure to be the RLTL constructed using the 1st method as it is analytically tractable to some extent. The lattice has two large rings of size N . It is always possible to set the spins on a ring in a configuration so that at the most one bond is red: Pick orientation of the first spin at random. Then moving along the ring, for all the spins that follow, set their orientation so that the bond with the spin just prior is satisfied. Then only the bond between spins S_N and S_1 might remain unsatisfied.

In the first step of the algorithm, we set the initial orientation of the spins such that at most one of the bonds along the ring is unsatisfied. To keep the discussion simple, we will simply set the coupling between spins S_N and S_1 so that the bond between them is satisfied (this introduces a correction of $O(1/N)$). Thus, all the bonds on the rings are satisfied. Each inter-ring bond is equally likely to be satisfied or unsatisfied independently of other inter-ring bonds. Note that this initial state is already stable to single spin flips and the average energy in this state is $-J$. We note that even at this level, the ground state energy estimate is substantially better than the Greedy algorithm estimate.

Now, we identify clusters of spins which can be flipped to give a state of a lower energy.

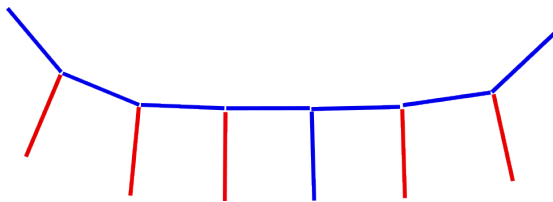


Figure 2.9: Initial configuration of bonds

This is done as follows: Starting from S_1 in the upper ring, we note the status of inter-ring bonds associated with each spin on the upper ring and denote a unsatisfied bond with the letter **R** and a satisfied bond with the letter **B**. In the readout of the inter-ring bonds along the upper ring, if there are two or more adjacent **R**s then the spins corresponding those bonds can be flipped to get a state equivalent or lower energy. Each such cluster reduced the number of **red** bonds by $r - 2$ where r is the size of the cluster because 2 **red** bonds are introduced in the ring at the ends of the cluster by such a process. We flip all such clusters.

For the next step, we note that when we perform the above flips, it is possible that we introduce adjacent **red** bonds in the ring. The spin common to the adjacent red bonds can be flipped to reduce the number of **red** bonds by 1. We flip all such spins where there are two adjacent **red** bonds. The above two steps can be repeated in the same order on the lower

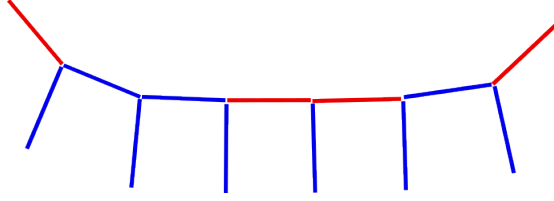


Figure 2.10: Configuration of bonds after flipping inter-ring bonds

ring. And all these steps can be performed repetitively till the energy cannot be lowered any further.

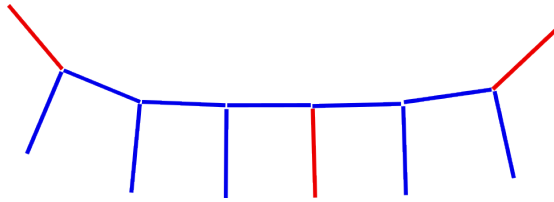


Figure 2.11: Configuration of bonds after flipping intra-ring bonds

Theoretical calculation for bound on the Ground State Energy:

In our method, we begin in the configuration where all the bonds in the ring are satisfied. For the bonds in the inter-ring layer, initially, it is equiprobable that the bonds are Unsatisfied (**R**) or Satisfied (**B**). However, we will still make the calculation for the general case that the probability of the Unsatisfied bonds in the inter ring layer is p . This will be used later. Consider the sequence of bonds in the inter ring layer read beginning on a spin in the upper layer :

BRBBRRRRRBRBB...

Now probability (or number $\mathcal{N}_r(p)$) of a clusters of length r is

$$(1-p)p^r(1-p) \text{ or } N(1-p)p^r(1-p)$$

In our first step, we flip all the spins associated with a **R** bond in a cluster of size greater than 1. Thus, the number of **R** bonds in the inter ring layer after the first step is just the number of clusters of length 1.

$$N(1) = Np(1-p)[1-p]$$

and the number of intra-ring **R** bonds is

$$2N \times P(r > 1) = Np(1-p)[2p]$$

The average energy per spin at this step is

$$E_1 = -\frac{J}{2N}[3N - 2Np(1-p)(1+p)] = [-1.5 + p(1-p^2)]J = -1.125 J$$

for $p = 0.5$. This matches with the simulation.

Now we perform the set of flips in the the upper ring. For this, we can have two adjacent **R** bonds only if initially there were two clusters of length $r > 1$ side by side. The probability for this occurring is given by

$$S = \sum_{r_1, r_2=2}^{\infty} (1-p)p^{r_1}(1-p)p^{r_2}(1-p) = p(1-p)(p^3)$$

This introduces NS **R** bonds in the inter-ring layer and reduces the number of intra-ring **R** bonds by $2NS$. Thus, at the end of this step, the number of inter ring **R** bonds and the number of intra ring **R** bonds is:

$$\mathcal{N}_{inter} = Np(1-p)[p^3 - p + 1] = N\mathcal{F}_{I1}(p) \quad (2.36)$$

and

$$\mathcal{N}_{intra} = Np(1-p)[2p - 2p^3] = N\mathcal{F}_{R1}(p) \quad (2.37)$$

respectively The average energy per spin at this step is given by

$$E_2 = -\frac{J}{2N}[3N - 2Np(1-p)(1+p-p^3)] = [-1.5 + p(1-p)(1+p-p^3)]J = -1.15625 J \quad (2.38)$$

for $p = 0.5$. Again this matches well with the simulation.

If we repeat the above steps for lower ring, this time, we can say that we are in a similar situation as in the beginning, except that the probability for a **R** bond now is $\mathcal{F}_{I1}(p)$. Thus,

$$E_4 = -\frac{J}{2N}[3N - 2N(\mathcal{F}_{I2}(p) + \mathcal{F}_{R2}(p) + \mathcal{F}_{R1}(p))] = -\frac{38942187}{32^5}J = -1.1605676115 J \quad (2.39)$$

for $p = 0.5$ where,

$$\mathcal{F}_{I_2}(p) = \mathcal{F}_{I_1}^2(p) \quad \text{and} \quad \mathcal{F}_{R_2} = \mathcal{F}_{R_1}(\mathcal{F}_{I_1}(p))$$

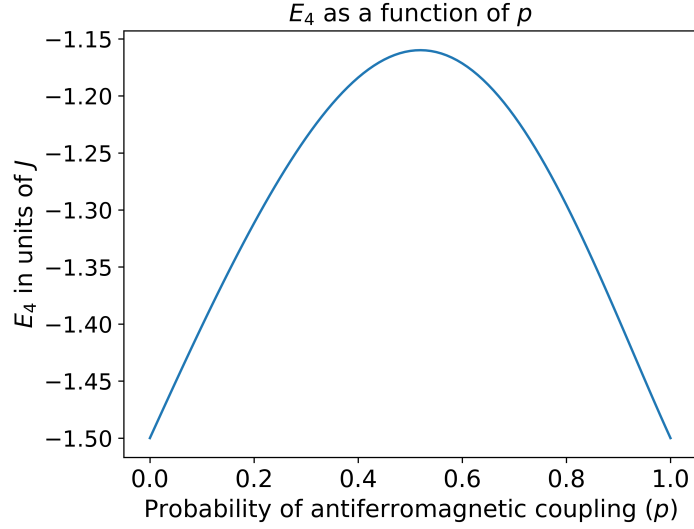


Figure 2.12: E_4 as a function of probability of antiferromagnetic coupling. Refer to equation 2.39

From simulation, we obtained the following values for the fraction of \mathbf{R} bonds considering a system size of $N = 100001$ and averaging over 1000 different initializations:

- $\frac{\mathcal{N}_{intra}}{N} = 0.11174441255587443$
- $\frac{\mathcal{N}_{URing}}{N} = 0.1875352346476535$
- $\frac{\mathcal{N}_{LRing}}{N} = 0.04018434815651844$
- $E_{numerical} = -1.1605746 J$

Compare these with the theoretically obtained values:

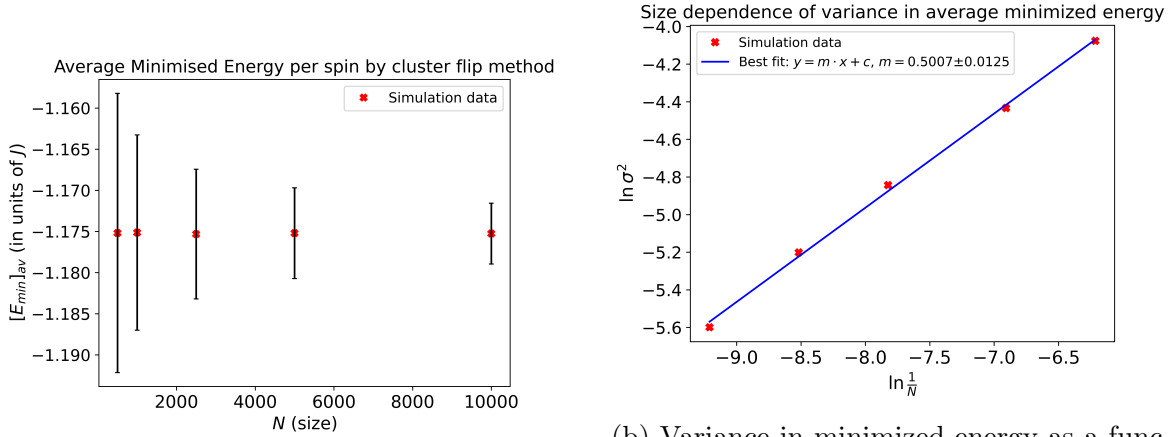
- $\mathcal{F}_{I_2}(0.5) = \frac{1857893}{16627005} = 0.111739486456$
- $\mathcal{F}_{R_1}(0.5) = \frac{3}{16} = 0.1875$

- $\mathcal{F}_{R2}(0.5) = \frac{89011}{2214595} = 0.0401929020882$
- $E_4 = -1.1605676115 J$

Thus, there is agreement in the theoretically obtained and values obtained by simulation upto 4 digits after decimal.

Numerical simulation results:

1. In the first step on flipping clusters of size 1 too, it lowers the energy further in later steps if the lattice is generated by using *1st* method. If instead the lattice is generated using the *2nd* method, it increases energy. Results in figures 2.13a and 2.13b for graphs generated using *1st* method.



(a) Average minimized energy per spin using basic cluster flip algorithm.

(b) Variance in minimized energy as a function of size. Here the variance $\sigma^2 \sim 1/N^m$, m is the slope of the best fit line.

Figure 2.13: Results for basic cluster flip algorithm, with clusters of size 1 also flipped as it reduces energy further. Disordered averaging over 10^3 systems for each size.

2.6.2 Improvement estimate of ground state energy by identifying flippable spin clusters of size 3

In order to identify all spin clusters of size 3 that can be flipped to reduce energy, first we identify all ‘blinker’ structures. Blinkers are defined as follows: Spin clusters of size 2 that have 2 red bonds with the bond between the two spins being blue. We will associate the term ‘blinker bond’ with the bond joining 2 such spins. See figure 2.14 for types of blinkers.

After performing the spin flips in the algorithm in the previous subsection, we obtain

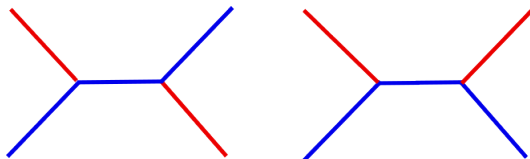


Figure 2.14: Types of blinker configurations

a state that is stable (neutrally) to 2 spin flips. Thus, all cluster of size 3 configuration whose energy can be minimized have a similar structure: See figure 2.15. We simply need to identify all such clusters and flip them to obtain the minimum energy.

Alternatively, if two blinker bonds are adjacent to each other, the spins associated with the blinker bonds are a cluster of 3 spins that can be flipped to reduce energy. Thus, in our algorithm we identify all adjacent blinkers and perform the necessary spin flips. Note that by the structure of random regular graph of co-ordination number 3, if a state is stable to 3 spin flips, then it is also stable (neutrally) to 4 spin flips.

Results for this are presented in figures 2.16a and 2.16b. The average minimized energy obtained for large sizes this way is about $-1.185 J$ quite close to the energy obtained in the 3 spin cluster stable calculation 2.35, $-1.196315 J$. Note that the numerical results for this give a **Lower average Ground State energy** than in [8], where the average ground state energy per spin is $-1.1790 J$.

2.6.3 Improvement: Identifying flippable pairs of blinkers

Let us define the ‘distance’ between blinker bonds as follows: A blinker bond is at a distance 0 from itself, blinker bonds adjacent to each other have a distance of 1 between them, blinker bonds adjacent to a common bond but not adjacent to each other are at a distance 2 and so

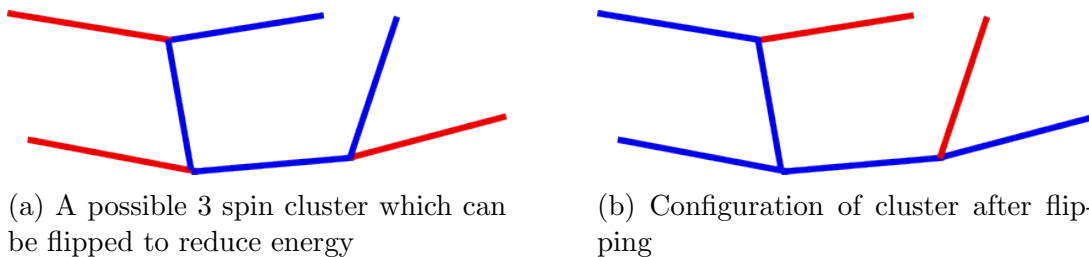


Figure 2.15: How 3 spin clusters can be flipped to reduce energy

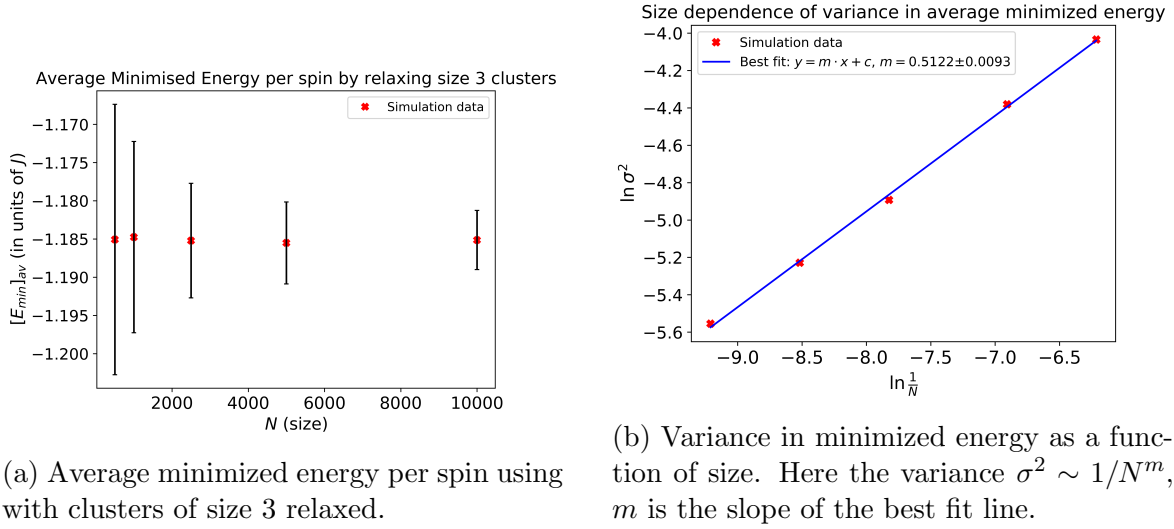


Figure 2.16: Average minimized energy after basic cluster flip algorithm and relaxing all spin clusters of size 3. Disordered averaging over 10^3 systems for each size.

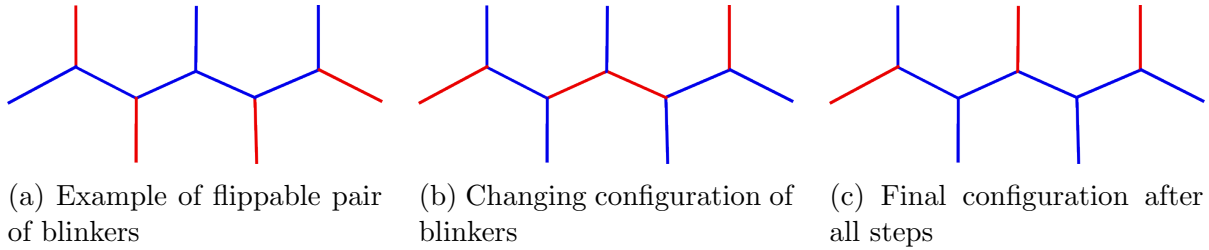


Figure 2.17: Steps to identify and reduce energy using flippable pairs of blinkers

on. Then, if 2 blinker bonds are at a distance 3, then it is possible to identify a cluster of 5 spins that can be flipped to reduce energy. Refer to figure 2.17 for reference.

Since blinkers can be flipped with 0 energy cost to another state, it is possible to introduce 2 red bonds at the site connecting the two blinkers. If the spin associated with the site is then flipped, we reduce the number of red bonds by 1. The numerical results for this algorithm can be found in figures 2.18a and 2.13b. We obtain average minimized energy of $-1.192 J$ per spin after this step.

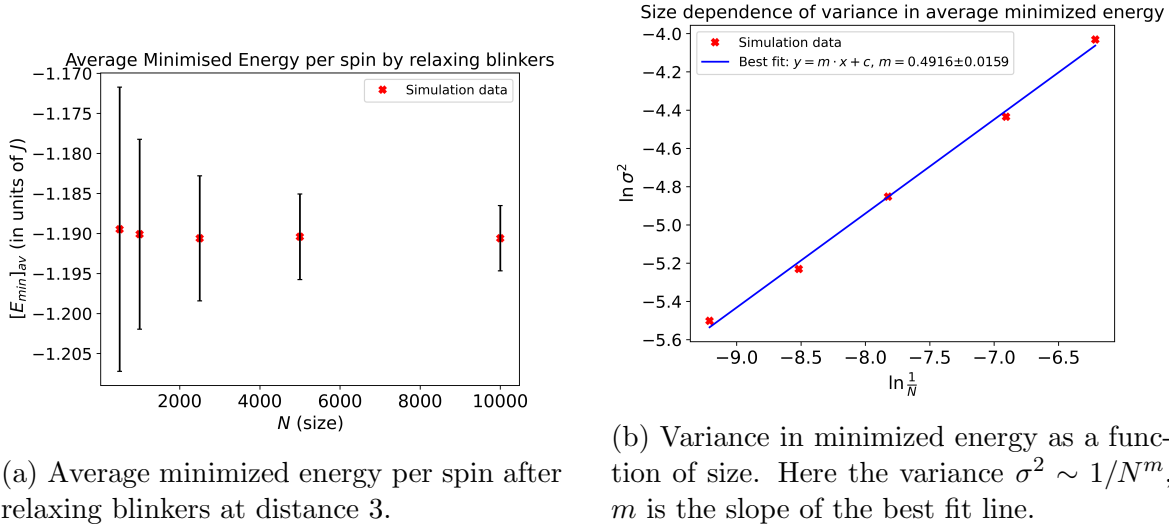


Figure 2.18: Results after relaxing blinkers at distance 3. Note that more spin clusters of size 3 that can be relaxed after such a procedure, so the algorithm for relaxing spin clusters of size 3 is called twice: Once before relaxing blinkers at distance 3 and once after. Disordered averaging over 10^3 systems for each size.

2.6.4 Eigenvector ansatz

Just like for the SK model in the previous chapter, we can use the eigenvectors of the coupling matrix as an ansatz to find the ground state configuration. Once we get the configuration using eigenvector, we can then apply the methods in the previous subsections to reduce the energy of the configuration even further. The results for this are indicated in 2.19.

From equation 2.15 we have

$$\frac{[E]_{av}}{N} \geq \frac{[\lambda_{min}]_{av}}{2}$$

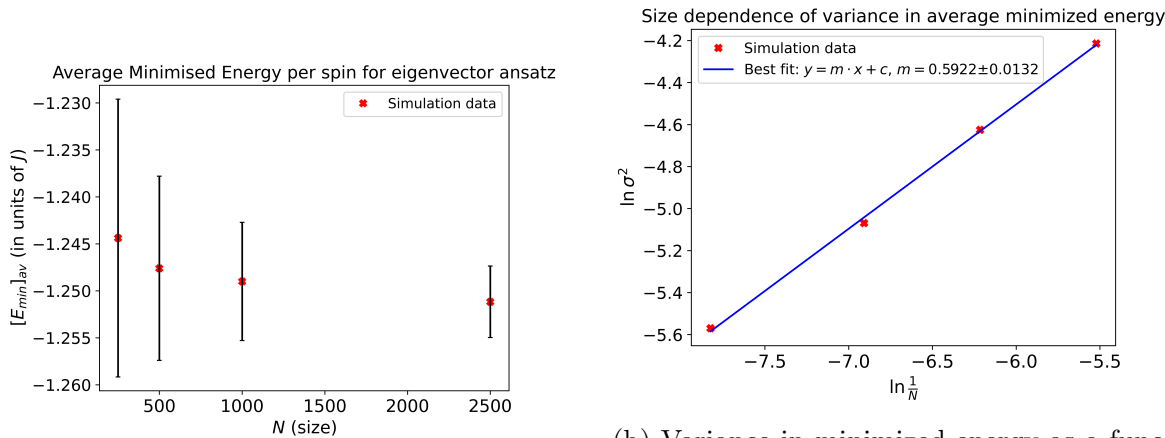
From random matrix theory, we know that

$$[\lambda_{min}]_{av} = 2\sqrt{2} \implies \text{Average ground state energy per spin} \geq \sqrt{2} J \approx -1.4142 J \quad (2.40)$$

Note that after combining all the methods so far, we obtain an average ground state energy of about $-1.25 J$ per spin. Parisi solution using Cavity method gives an average ground state energy per spin of $-1.2723 J$ and previous numerical results using extremal

optimization gives $-1.2716 J$. Thus, from the results presented in this thesis so far, we have

$$-1.25 J \geq [E_{min}]_{av} \geq -1.141 J \quad (2.41)$$



(a) Average minimized energy per spin using eigenvector ansatz.

(b) Variance in minimized energy as a function of size. Here the variance $\sigma^2 \sim 1/N^m$, m is the slope of the best fit line.

Figure 2.19: Results for eigenvector ansatz after performing relaxation of blinkers at distance 3 and obtaining a 4 spin flip stable state on the eigenvector ansatz. Disordered averaging over 10^3 systems for each size.

2.7 Ground state energy for unequal $\pm J$ couplings

Numerical estimation of the ground state energy for different proportions of anti-ferromagnetic coupling in the system indicate that the average minimized energy per spin is locally flat as a function of probability of anti-ferromagnetic bonds near $p = 0.5$, where $P(J_{ij}) = p\delta(J + J_{ij}) + (1 - p)\delta(J - J_{ij})$.

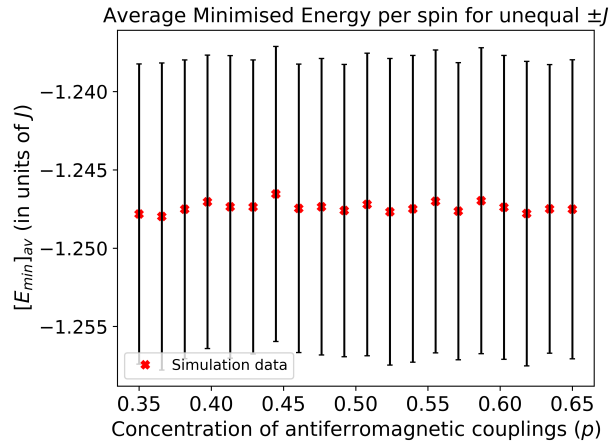


Figure 2.20: Average minimized energy as a function of probability of anti-ferromagnetic coupling. Size of system $N = 500$. For each value of probability, the averaging is performed over 1000 systems.

Chapter 3

Spectral properties of Random Regular Graphs

The structure of the underlying lattice plays an important role in the properties of the spin glass model. For instance, equation (2.40) was used to give lower bounds on the average ground state energy per spin. This result actually arises from the properties of the graph. In this chapter, we will study spectral properties of random regular graphs to gain insight into the structure of these graphs. The key question we will address is differentiating between random regular graphs of same size. Since all random regular graphs have a structure that is locally tree like, it is non-trivial to differentiate between two random regular graphs of the same size. We will use the following terminology for the rest of the chapter:

1. By the ensemble of random regular graphs (of a fixed size) we refer to the ensemble of random regular graphs where each graph is sampled with equal probability. However, for numerical results, we will generate the graphs according to the method described in Section 2.4. The assumption is that the ensemble of RLTL and the ensemble of random regular graph are equivalent for calculation of thermodynamic quantities.

2. We will denote by V and E the set of vertices of the graph and the set of edges of the graph respectively.

3. We will denote by \mathbf{A} the adjacency matrix of a graph defined by $\mathbf{A}_{ij} = 1$ if \exists an edge between the vertices i and j and $\mathbf{A}_{ij} = 0$ otherwise. \mathbf{D} denotes the degree matrix of the graph, which is diagonal with $\mathbf{D}_{ii} = d_i$, where d_i is the degree of the vertex i . Thus, $\mathbf{D} = d\mathbf{I}$ for random regular graphs, where d is the degree of the graph and \mathbf{I} is the Identity matrix.

The matrix defined by $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is called as the Laplacian of the graph.

4. We define the spectral density of a matrix \mathbf{Q} with the list of eigenvalues denoted by $\lambda(\mathbf{Q})$ as

$$\rho(\mu) \equiv \frac{1}{N} \sum_{\mu_Q \in \lambda(\mathbf{Q})} \delta(\mu - \mu_Q) \quad (3.1)$$

where N is the number of eigenvalues of \mathbf{Q} .

3.1 Spectrum of random regular graphs

Consider the following system: Place a mass $m = 1$ at each vertex of a random regular graph. Two masses are connected with a spring of spring constant $k = 1$ only if an edge exists between the vertices at which the masses are placed.

The frequencies of the normal modes of such a system can then be found by diagonalizing the matrix $\mathbf{M} = 3\omega\mathbf{I} - \omega\mathbf{A}$, where $\omega = \sqrt{\frac{k}{m}} = 1$ and \mathbf{I}, \mathbf{A} are the Identity matrix and Adjacency matrix of the graph respectively.

The eigenvalues of the \mathbf{M} matrix will be equal to the square of the frequencies of the normal modes. The set of eigenvalues of \mathbf{M} is called as the ‘spectrum’ of the graph.

Since $\omega^2 \geq 0$, the smallest possible eigenvalue is 0 and this eigenvalue corresponds to the normal mode in which there is no relative displacement between any of the masses. Thus, $\omega^2 = 0$ is an eigenvalue.

Similarly, the largest possible eigenvalue for a Bipartite graph will correspond to the mode in which the masses on belonging to different partition sets displace completely out of phase with each other. This enables us to write the equation of motion as $\ddot{x}_i = \sum_{neighbours} -2x_i \forall i$ where x_i is the displacement of the i th mass with respect to its equilibrium position $\implies -\omega^2 = -6$ as each vertex has 3 neighbors. Thus, the largest eigenvalue will be equal to 6.

Thus, the eigenvalues for the \mathbf{M} , λ will lie between 0 and 6, with both 0 and 6 as possible eigenvalues. As $\mathbf{M} = 3\mathbf{I} - \mathbf{A}$, their eigenvalues are related by $\lambda_A^{(i)} = 3 - \lambda_M^{(i)}$. Furthermore, if graph is bipartite, the matrix \mathbf{A} will have a off-diagonal block structure as follows:

$$\mathbf{A} = \begin{bmatrix} 0 & \mathbf{B} \\ \mathbf{B}^T & 0 \end{bmatrix} \quad (3.2)$$

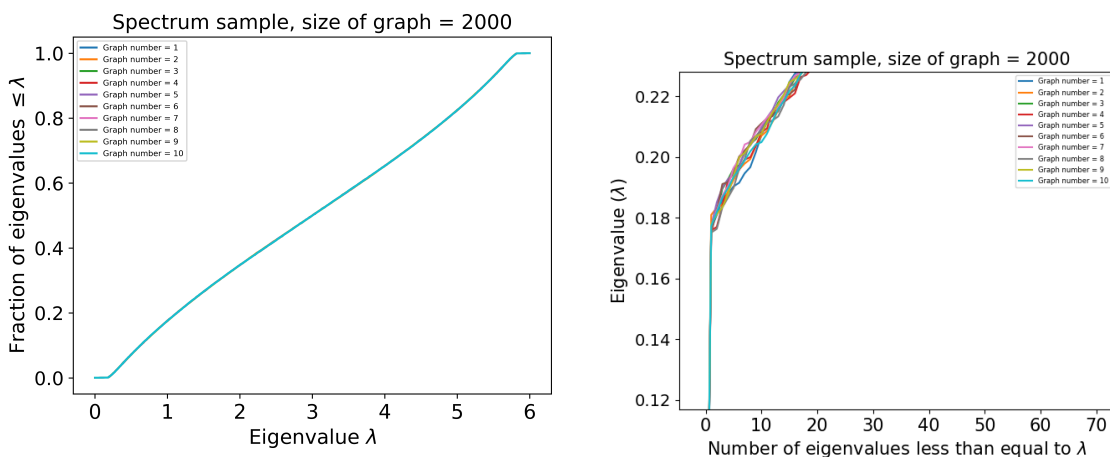
Then, the eigenvalue equation can be written as:

$$\det(\mathbf{M} - \lambda_M \mathbf{I}) = 0 \implies \det((3 - \lambda_M)^2 \mathbf{I} - \mathbf{B}\mathbf{B}^T) = 0 \quad (3.3)$$

Thus, the eigenvalues come in pairs: $\lambda_M = 3 \pm \alpha, 0 < \alpha \leq 3$.

The spectrum of the graphs looks as follows:

1. For the random regular graph generated using 2nd method (Bipartite): Spectrum of the \mathbf{M} matrix is plotted for 10 graphs in figure 3.1



(a) Size of graphs is 2000. There is a gap in the spectrum at 0 (and hence at 6 due to bipartite nature of the graph).

(b) Same figure as on the left but with the x and y axis inverted and zoomed in to show the difference in eigenvalues

Figure 3.1: Spectrum of 10 bipartite random regular graphs generated using method 2.

2. For the random regular graphs generated using 1st method: Spectrum is plotted for 10 graphs in figure 3.2.

In non-bipartite graphs, the largest eigenvalue is strictly less than 6 because the graph is not bipartite.

From the plots, we observe that the eigenvalues for different random graphs are quite close. This can be explained by considering random walks on random regular graph.

The adjacency matrix can be thought of (upto a constant) as the transition matrix \mathbf{W} for a Markov process in which a particle jumps from a site to any neighbouring site with equal

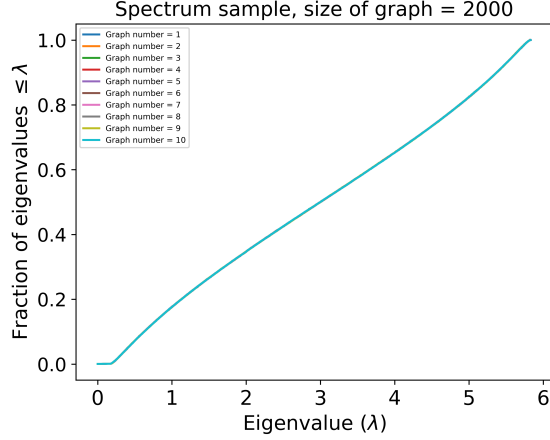


Figure 3.2: Spectrum of 10 non-bipartite random regular graphs generated using method 1. Size of graphs is 2000.

probability for all the neighbouring sites. Thus, $\mathbf{W}_{ij} = 1/3$ (for a 3 co-ordinated random regular graph) if sites i and j are connected by an edge and $\mathbf{W}_{ij} = 0$ otherwise. Also, let us denote by $|1_i\rangle$ the vector $(\underbrace{0, 0, \dots}_{i-1 \text{ zeros}}, 1, 0, \dots)^T$, which is the initial state of a particle at site i .

Now we can calculate the probability that a particle performing such a Markov process will return to it's starting point in $2, 4, 6, \dots, 2n$ steps, n is some natural number. Let us denote by $p_{2k}^{(i)}$ the probability of returning to site i in $2k$ steps. Then,

$$p_2^{(i)} = \langle 1_i | \mathbf{W}^2 | 1_i \rangle = \frac{1}{3} \implies \text{Tr}[\mathbf{W}^2] = N/3 \quad (3.4)$$

In general we have

$$\sum_{i=1}^N \lambda_i^{2n} = \text{Tr}[\mathbf{M}^{2n}] = \text{Tr}[(3\mathbf{I} - \mathbf{A})^{2n}] = \sum_{k=0}^{2n} \binom{2n}{k} 3^{2n-k} (-1)^k \text{Tr}[\mathbf{A}^k]$$

Where N is the number of sites in the graph and λ_i 's are the eigenvalues of \mathbf{M} . As $\mathbf{A} = 3\mathbf{W}$

$$\frac{1}{N} \sum_{i=1}^N \lambda_i^{2n} = \frac{1}{N} \sum_{k=0}^n (-1)^k \binom{2n}{k} 3^{2n} \text{Tr}[\mathbf{W}^k]$$

Now,

$$\text{Tr}[\mathbf{W}^k] = \sum_{i=1}^N p_k^{(i)} = \frac{n_k^{(i)}}{3^k} \quad (3.5)$$

where $n_k^{(i)}$ denotes the number of walks beginning at site i that return to site i after k steps. Thus, for a graph in which no cycles upto order $2n$ are present

$$\frac{1}{N} \sum_{i=1}^N n_{2k}^{(i)} = n_{2k}, \quad \text{The number is same for all sites} \quad (3.6)$$

There are no odd length walks (upto length $2n$) that return because of the locally tree like structure. Hence,

$$\frac{1}{N} \sum_{i=1}^N \lambda_i^{2n} = \sum_{k=0}^n \binom{2n}{2k} \cdot 3^{2n-2k} \cdot n_{2k} \quad (3.7)$$

Where n_{2k} are the number of walks of length $2k$ that return to the starting site.

If no cycles of length $4, 6, 8, \dots, 2n$ are present in the graph, then the 2nd, 4th, ... $2n$ th moments of the eigenvalues are fixed. This constrains the eigenvalues and in fact with enough number of constraints, the eigenvalues would be completely determined for a finite graph. However, in the graphs that are generated, there are small cycles of order $4, 6, \dots$ present in numbers $\ll N$ (the number of sites in the graph) and the correction in the moments is only $O(1/N)$. Thus, one expects the eigenvalues of two typical random regular graphs of same size to be quite close to each other in value and thus the variance in $f(\lambda)$, the fraction of eigenvalues less than λ , is low. Results for numerical investigation of density of states and variance in $f(\lambda)$ are in figures 3.3 and 3.4.

It is possible to calculate the density of states for a Bethe lattice [15, 16]. The derivation given below is identical to the one in [15]:

Define $P_{x,0}(N)$ as the probability of being at site x in N steps starting from site 0. Define the generating function of $\tilde{P}_{x,0}(\lambda)$ as

$$\tilde{P}_{x,0}(\lambda) = \sum_{N=0}^{\infty} \lambda^N P_{x,0}(N) \quad (3.8)$$

Then, $\tilde{P}_{x,0}(\lambda)$ satisfies

$$\tilde{P}_{0,0}(\lambda) = \lambda \tilde{P}_{1,0}(\lambda) + 1 \quad (3.9)$$

and

$$\tilde{P}_{N,0}(\lambda) = \frac{\lambda}{z} \tilde{P}_{n-1,0}(\lambda) + \frac{\lambda(z-1)}{z} \tilde{P}_{N+1,0}(\lambda) \quad (3.10)$$

Where z is the co-ordination number of the Bethe Lattice. Now, in deep inside the lattice,

the ratio

$$p_N = \frac{\tilde{P}_{N+1,0}(\lambda)}{\tilde{P}_{N,0}(\lambda)} \quad (3.11)$$

is independent of N . Thus, we get a quadratic equation in p_N from the previous equations.

On solving, we get

$$\tilde{P}_{0,0}(\lambda) = \frac{2(z-1)/z}{(z-2)/z + \sqrt{1 - (4\lambda^2(z-1)/z^2)}} \quad (3.12)$$

The Laplace transform of the return probability is related to generating function $\tilde{P}_{x,0}(\lambda)$ by

$$\tilde{P}_{0,0}(\omega) = \lambda \tilde{P}_{0,0}(\lambda)|_{\lambda=1/(1+\omega)} \quad (3.13)$$

And the density of states (for \mathbf{M}) is given by the analytic continuation of the Laplace transform

$$\rho_M(\epsilon) = -\frac{1}{\pi} \text{Im} \tilde{P}_{0,0}(-\epsilon + i0^+) \quad (3.14)$$

Using this, for $z = 3$, we have

$$\rho_M(\epsilon) = \frac{3}{2\pi} \frac{\sqrt{2\epsilon - \epsilon^2 - 1/9}}{2\epsilon - \epsilon^2} \quad (3.15)$$

3.15 gives the density of states for \mathbf{M} , thus, the density of states for \mathbf{A} is given by

$$\rho_A(\mu) = \frac{3}{2\pi} \frac{\sqrt{8 - \mu^2}}{9 - \mu^2}, \quad |\mu| < 2\sqrt{2} \quad (3.16)$$

In fact, Kesten and McKay (cite Kesten and McKay) showed that for random regular graphs with degree d the spectral density for

$$\lim_{N \rightarrow \infty} \langle \rho_A(\mu) \rangle = \frac{d}{2\pi} \frac{\sqrt{4(d-1) - \mu^2}}{d^2 - \mu^2}, \quad |\mu| < 2\sqrt{(d-1)} \quad (3.17)$$

where $\langle \cdot \rangle$ denotes averaging over random regular graph ensemble. This matches well with the numerical evidence in figure 3.3.

The plots for Variance in fraction of eigenvalues less than the eigenvalue are in figure 3.4

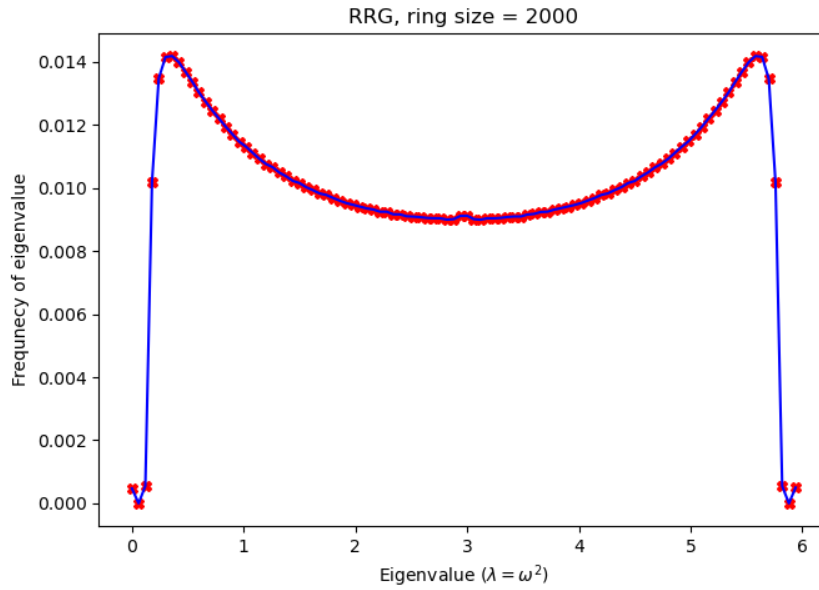


Figure 3.3: Plot of average density of states as a function of eigenvalue obtained numerically for 1000 graphs of size 2000. Number of bins = 100.

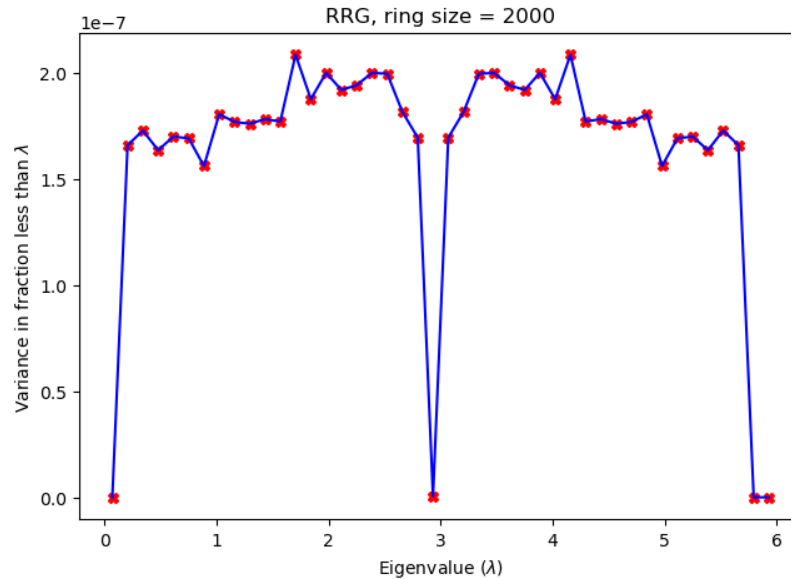


Figure 3.4: Plot for variance in fraction of eigenvalues less than a given eigenvalue obtained numerically for 1000 graphs of size 2000. Number of bins = 45

3.2 Variance of Top Eigenvalue

A quantity of interest in Random Matrix Theory is the variance of the extreme eigenvalues as a function of the size of the matrix [17]. According to random matrix theory prediction

for the Gaussian Orthogonal Ensemble (GOE), the variance of the largest eigenvalue scales as $N^{-\frac{2}{3}}$. In the plot in the figure 3.5 we have compared the scaling of variance of largest non-trivial eigenvalue for a random regular graph with the size. While the random regular graph ensemble is not completely identical to the GOE, it is expected that some general properties of the ensemble follow the random matrix theory prediction. The numerical evidence indicates that the scaling is within the prediction of random matrix theory for the GOE.

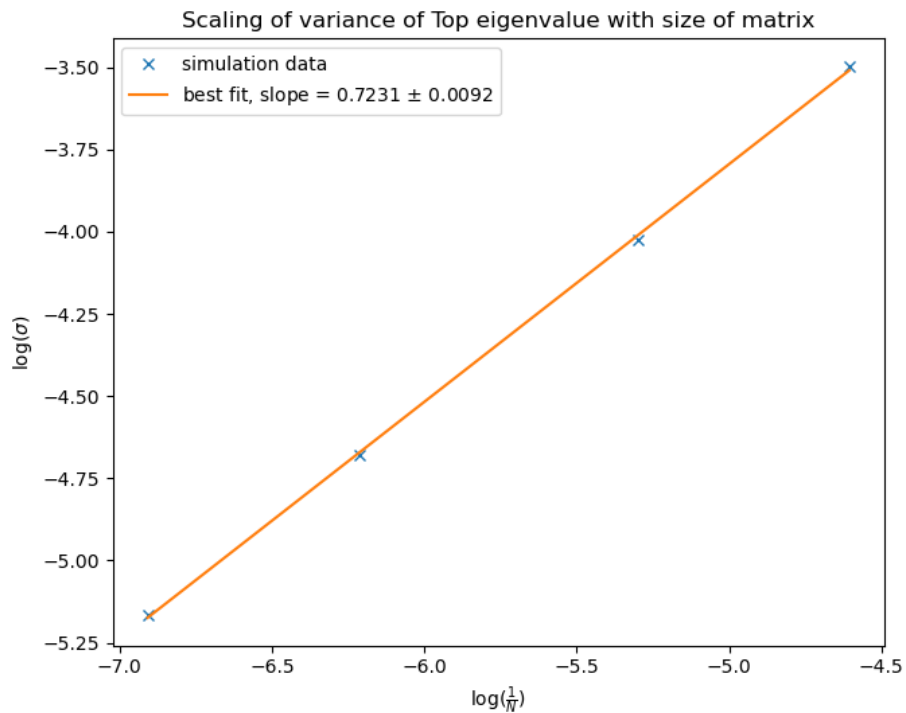


Figure 3.5: Scaling of the standard deviation of largest non-trivial eigenvalue in the spectrum of a Random Regular graph

3.3 Non-backtracking random walk on RLTL

Next, we will consider the problem of a non-backtracking random walk (NBRW) on the random regular graph. In NBRW, at each step, a particle has equal probability to hop to any neighboring site subject to the constraint that it cannot jump to a site visited in the step just before the current step. This type of random walk problem too can be reformulated

as a Markov process on the random regular graph. We can think of the each site having 3 states determined by which neighbor the particle arrives from at the present site.

Alternatively, we can consider the edges of the graph to be directed edges $e(i, j)$ with the origin $o(e) = i$ and terminus $t(e) = j$. In this notation $e(i, j) \neq \hat{e}(j, i)$. Consider the $3N \times 3N$ matrices \mathbf{B} (transmission matrix) defined by $\mathbf{B}_{e,e'} = \delta_{t(e),o(e')}$ and \mathbf{J} (back scattering matrix) defined by $\mathbf{J}_{e,e'} = \delta_{\hat{e},e'}$. Then, NBRW is the Markov process defined by the matrix $\mathbf{Y} = \mathbf{B} - \mathbf{J}$.

We wish to find out the spectrum of \mathbf{Y} . In fact, it is possible to calculate the eigenvalues of \mathbf{Y} can be expressed as a function of the eigenvalues of \mathbf{A} . The derivation closely follows the papers [30, 31] The Bartholdi Identity applied to random regular graphs of degree 3 gives

$$\det(\mathbf{I}_{3N \times 3N} - s(\mathbf{B} - w\mathbf{J})) = (1 - w^2s^2)^{N/2} \det(\mathbf{I}_{N \times N}(1 + w(3 - w)s^2) - s\mathbf{A}) \quad (3.18)$$

Setting $w = 1$, we get

$$\det(\mathbf{I}_{3N \times 3N} - s\mathbf{Y}) = (1 - s^2)^{N/2} \det(\mathbf{I}_{N \times N}(1 + 2s^2) - s\mathbf{A}) \quad (3.19)$$

Thus,

$$\prod_{i=1}^{3N} (1 - s\lambda_i^Y) = (1 - s^2)^{N/2} \prod_{j=1}^N (1 + 2s^2 - s\lambda_j^A) \quad (3.20)$$

Thus, the list of eigenvalues of \mathbf{Y} is given by:

- ± 2 (-2 for Bipartite graphs only)
- $+1$, with degeneracy $N/2$
- -1 , with degeneracy $N/2$
- $\sqrt{2}e^{\pm i\phi_k}$, where $\phi_k = \cos^{-1}\left(\frac{\lambda_k^A}{2\sqrt{2}}\right)$

Numerically determined eigenvalues for the matrix describing the Markov process of non-backtracking random walk can be seen in figure 3.6

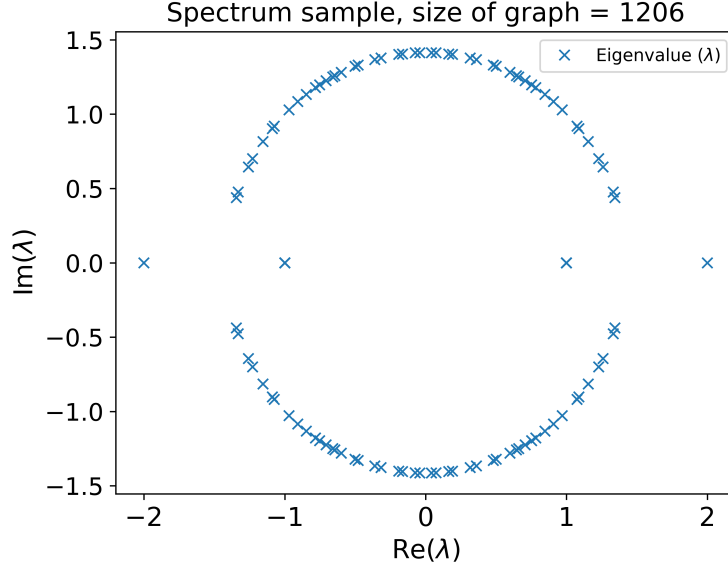


Figure 3.6: Spectrum for non-backtracking random walk on a bipartite random regular graph of size 1206. Note that there is a large degeneracy of eigenvalues at ± 1 .

3.4 Spherical model on RLTL

It is useful to study some soluble models to study how much thermodynamic quantities are affected by the sample to sample fluctuations in the RLTL. These thermodynamic quantities can be used to differentiate between different random regular graphs of same size. The spherical model is an important example of such a solvable model of ferromagnetism. It was first solved by Kac and Berlin [32]. This model exhibits a second order transition at temperature in $D > 2$, D is the dimension of the lattice. We will follow the procedure from [33]. The Hamiltonian is given by:

$$H = -J \sum_{\langle ij \rangle} S_i S_j, \text{ subject to the constraint } \sum_{i=1}^N S_i^2 = N \quad (3.21)$$

where S_i are real numbers and the sum is over nearest neighbors. Then the partition function of the system $\mathcal{Z}(\beta)$, β is the inverse temperature, is given by:

$$\mathcal{Z} = \int \cdots \int dS_1 \cdots dS_N e^{\frac{\beta}{2} \sum_{i,j} S_i S_j} \delta\left[\sum_{i=1}^N S_i^2 - N\right] \quad (3.22)$$

where the sum in the integral is over nearest neighbors and the Dirac delta function $\delta[\sum_{i=1}^N S_i^2 - N]$ enforces the constraint $\sum_{i=1}^N S_i^2 = N$. Using the identity

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk \quad (3.23)$$

Thus, rewriting the Dirac delta as an integral over k and exchanging the orders of S_i and k integrals, we can express \mathcal{Z} as

$$\mathcal{Z} = \int_{-\infty}^{\infty} dk \int \cdots \int dS_i \cdots dS_N e^{ikN} \cdot e^{\frac{\beta J}{2} \sum_{i,j} S_i S_j - ik \sum_{i=1}^N S_i^2} \quad (3.24)$$

Note that the expression in the second exponential is bilinear in S_i and thus can be expressed in the form

$$-\frac{1}{2} S^T \mathbf{V} S = \frac{\beta J}{2} \sum_{i,j} S_i S_j - ik \sum_{i=1}^N S_i^2 \quad (3.25)$$

Thus,

$$\mathbf{V} = 2ik\mathbf{I} - \beta J\mathbf{A} \quad (3.26)$$

If a change of variables is made to the basis so that \mathbf{V} is diagonal, the S_i integrals will become a product of gaussian integrals and since the transformation is an orthogonal transformation, the Jacobian for the transformation is unity. Thus, we obtain

$$\mathcal{Z} = \left(\int_{-\infty}^{\infty} dk e^{ikN} \right) \cdot \frac{(2\pi)^{\frac{N}{2}}}{(\det[\mathbf{V}])^{\frac{1}{2}}} = (2\pi)^{\frac{N}{2}} \int_{-i\infty}^{i\infty} du e^{uN} \frac{1}{\prod_{i=1}^N (2u - \beta J\lambda_i)^{\frac{1}{2}}} \quad (3.27)$$

Where $u = ik$. And hence,

$$\mathcal{Z} = (2\pi)^{\frac{N}{2}} \int_{-\infty}^{\infty} du e^{N(u - \frac{1}{2N} \sum_{i=1}^N \ln(2u - \beta J\lambda_i))} = (2\pi)^{\frac{N}{2}} \int_{-\infty}^{\infty} du e^{N\phi(u)} \quad (3.28)$$

In the large N limit, the integral can be approximated by the method of steepest descent. Note that the free energy per spin is given by $f(\beta) = -\frac{1}{N\beta} \ln \mathcal{Z}$. Thus, we expect non-trivial behavior for the free energy when $\phi'(u) = 0$. This is the saddle point equation will allow us to estimate the critical temperature. Below the critical temperature we see that the order parameter given by $m = \frac{1}{N} \sum_{i=1}^N S_i$ becomes non-zero and we have a second order phase

transition. The saddle point equation is

$$N = \sum_{i=1}^N \frac{1}{u - \beta J \lambda_i} \quad (3.29)$$

At the critical point, $u = 0$. Thus,

$$k_B T_c = N \cdot \left(\sum_{i=1}^N \frac{1}{J \lambda_i} \right)^{-1} \quad (3.30)$$

Chapter 4

Summary

Spin glass models are prototypical examples of disordered systems. For most of the models in Statistical physics, exact analytic calculation of the partition function or thermodynamic quantities is a hard problem and instead one often resorts to mean-field models of the problem which capture the essential physics and are easier to solve. However, for the spin glass models, solving even the mean-field models has proven to be a challenge. While previous work by Parisi has provided us with a method to solve the problem, an explicit calculation of thermodynamic quantities at low temperatures involves an increasingly higher step replica symmetry breaking. In particular, despite being studied for over four decades, an exact analytic expression for the ground state energy of such models has not been calculated. In this thesis we have attempted to understand better the average ground state energy for the Sherrington Kirkpatrick (SK) model and the Ising spin glass model on a Random Layered locally Tree like Lattice (RLTL), which is a variation of random regular graph, by numerical and analytic methods.

In Chapter 2 we first attempt to find the average ground state energy for the Sherrington Kirkpatrick model. We first attempt this by a Greedy algorithm which minimizes energy based on the mean-field experienced by each spin. We then improve our attempt by making a guess for the configuration of spins based on eigenvectors of the coupling matrix that describes the Hamiltonian of the system. This method gives an average minimized energy per spin as $-0.742 J$. For comparison, the solution by Parisi predicts the average minimized energy per spin as $-0.763 J$ for the SK model.

Next in Chapter 2, we attempt to find the average ground state energy per spin for the

Ising spin glass model on a random regular graph. Like for the SK model, we first attempt to minimize energy using a Greedy algorithm and estimate an analytic calculation of the minimized energy from the Greedy algorithm by relating the algorithm to the Dimer problem on the lattice. The analytic prediction from this calculation fails to match the numerical data, indicating that constraints due to presence of loops in the lattice persist even in the thermodynamic limit. We then improved methods to minimize the energy by identifying clusters of spins that can be flipped to minimize energy and obtain a state stable upto 4 spin flips. Finally, we use eigenvectors of the coupling matrix in combination with the cluster flip algorithm to obtain average minimized energy per spin of $-1.25 J$. For comparison, the 1 step Replica Symmetry Breaking solution gives an average ground state energy per spin of $-1.2723 J$ and numerical studies of average ground state energy per spin of $-1.2716 J$ using heuristic optimization. From analysis of the eigenvalues, we obtain a lower bound for the average ground state energy of $-\sqrt{2} J \approx -1.4142 J$.

In Chapter 3 we investigate the spectrum of random regular graph by analyzing random walks on the graph. We obtain an exact expression for the Density of states on the Bethe lattice. We also analyze the spectrum of the Markov process by defining non-backtracking random walks on the random regular graph. We obtain the spectrum in terms of the eigenvalues of the Adjacency matrix of the graph and find a large degeneracy in the eigenvalues ± 1 . This analysis allows us to obtain the average smallest eigenvalue for the coupling matrix. Next, we address the question of using a thermodynamic quantity to differentiate between different random regular graphs of same size. We show that the critical temperature, related to the eigenvalues of the Adjacency matrix for the spherical model on the random regular graph, is a suitable quantity for distinguishing between random regular graphs of same size.

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