

SPIDER-WEB NETWORKS:

- I. SELF-AVOIDING WALKS AND SELF-AVOIDING POLYGONS
 - II. HIGH-TEMPERATURE EXPANSION
 - III. VIBRATIONAL SPECTRA
-

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DISSERTATION
SUBMITTED IN PARTIAL FULFILLMENT
FINAL YEAR PROJECT
5 YEAR BS-MS DUAL DEGREE PROGRAM

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INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH (IISER), PUNE

April 2011

Certificate

This is to certify that the thesis entitled "**Spider-Web Networks: I. Self-Avoiding Walks(SAWs) and Self-Avoiding Polygons(SAPs) II. High Temperature Expansion III. Vibrational Spectra**" is the result of work carried out by Mr. Ajit C. Balram in the Department of Theoretical Physics (DTP), Tata Institute of Fundamental Research (TIFR), Mumbai, under my supervision as part of his Masters program from August, 2010 to March, 2011.

Acknowledgements

I would like to take this opportunity to express my deep sense of gratitude and thankfulness to my advisor Prof. Deepak Dhar. He has been a constant source of inspiration and it has been a privilege to work under his expert guidance. I thank Dr. Arijit Bhattacharyay for consenting to be my local advisor at IISER, Pune. I am grateful to the administration of TIFR, especially DTP, for allowing me to freely use all the facilities in TIFR, which has helped immensely in the smooth completion of this work. I wish to thank all my batchmates at IISER Pune and colleagues in DTP, who have made my stay in Pune and TIFR a pleasant and memorable one. I would also like to thank Kishore Vaigyanik Protsahan Yojana(KVPY) and TIFR for financial support. I would like to thank IISER, Pune for providing me this opportunity to do my MS thesis in TIFR. Thanks are due to my parents, brother and grandfather, who have been very much caring and understanding throughout. I express my appreciation for their immense love, patience and endurance. Finally, I wish to thank Bedartha for making this Thesis's LaTeX template.

Abstract

A $2^N \times M$ - node spider network is a set of M -layers each of which has 2^N nodes which can be represented by N -bit binary numbers. A site in layer r may be represented by an N -bit integer. The site in the r^{th} layer with the bit label $abcd\dots ij$ is connected to two sites with labels $bcd\dots ij0$ and $bc\dots ij1$ in the layer $r+1$. The layer M is connected in the same way to layer 1. We enumerate self-avoiding walks(SAWs) and self-avoiding polygons(SAPs) on a spider-web network. The high-temperature expansion of the Ising model on this network is discussed. Then we consider a spring network on this graph, with a mass m placed at each node, and for each link, there is a spring of spring constant K connecting the masses at the ends. I discuss the normal modes of this lattice.

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Chapter 1

Introduction

This project was aimed at understanding some graphical enumeration techniques in statistical physics. There are not many problems in statistical physics which can be solved exactly. A useful general technique to study these problems is series expansions which involve diagram counting. As an example of this technique we find the number of self-avoiding walks(SAWs) and self-avoiding polygons(SAPs) on a class of graphs which are called spider-web networks precisely defined later. We calculated the high temperature expansion of the Ising model on this network. We also look at the normal modes of a spring network on this graph. These networks have some very interesting properties which we will allude to in the next section.

Such networks were first seen in the telecommunications industry in the middle of the 20th century. Spider-web networks were introduced by Ikeno[[1]], though the term appears first in Feiner and Kappel[[2]]. For a sequence of such networks that is optimal, Ikeno proved that the linking probability tends to a limit and conjectured the limit is true even for spider-web networks. Takagi[[3]] showed that in a certain class of interconnection designs, the spider-web network is optimal in the sense that it has the highest linking probability. But, Chung and Hwang[[4]] showed, by giving a counter-example, that they are not optimal in the larger class of networks. Pippenger[[5]] proved, within the model of Lee[[6]] and Le Gall[[7, 8]], that they are only *asymptotically* optimal.

From the early 1940s, since the introduction of such networks in automatic telephony, their performance, in terms of the blocking probability, under various traffic conditions with different number of switches have been a source of interesting and challenging problems. Hwang[[9]] gave an efficient method to compute this probability for these networks and Pippenger[[10, 11]] later showed, as conjectured by Ikeno[[1]], that if the occupancy probability is below the threshold $2 - \sqrt{2} = 0.5857\dots$, then the blocking probability tends to zero, whereas above this threshold it tends to unity.

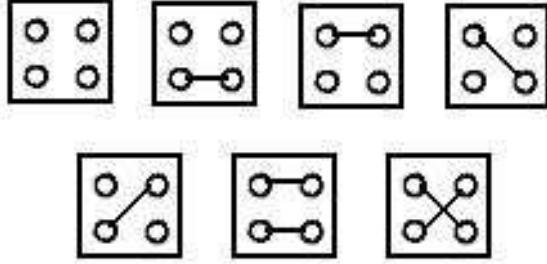


Figure 1.1: The seven configurations of a 2×2 crossbar with only one to one connections between the inlets and outlets. The two nodes on the left are the inlets and the two on the right are the outlets.

With the advent of digital electronics, these networks lost their technological interest, yet it still remains of interest to graph-theorists, probabilists and combinatoricians. We look at three problems on this network namely,

1. High-temperature expansion of the Ising model
2. The number of self-avoiding walks(SAWs) and self-avoiding polygons(SAPs)
3. Normal modes of the spring problem on this network

We'll use the word polygons and loops interchangeably. The first two problems are looked at in detail in the second chapter. We show that the free energy function has an expansion of the form:

$$F(x) = \frac{x^4}{2} + \frac{15}{4}x^8 + \mathcal{O}(x^{12}) \quad (1.1)$$

where $x = \tanh(\beta J)$ is the high temperature expansion parameter.

The third chapter is devoted to the vibrational spectra of spider networks. We obtain the entire spectrum for small values of N and also describe the qualitative features of the spectrum in the thermodynamic limit of $M \rightarrow \infty$.

1.1 Spider-web Networks[10]

The basic component of this network is a 2×2 "crossbar". A crossbar has four terminals, two inlets and two outlets. It has four simple on-off switches(the two terminals are either connected together or disconnected from each other) to establish one to one or many to one connections between some or all of the inlets and outlets. If we allow only one to one connections, then there are seven possible configurations of the crossbar. There are shown in Figure(1.1).

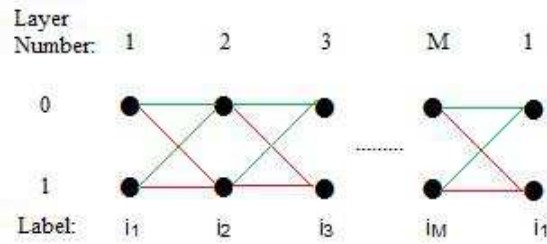


Figure 1.2: Shuffle Pattern: $ab \rightarrow b0$ (red) and $ab \rightarrow b1$ (green) where a and b are either 0 or 1

A "spider-web" has, for some integer $N \geq 3$, $2N - 1$ "layers/stages", each having 2^{N-1} crossbars. The inlets of the crossbar at the first layer are the inputs of the network. For, $1 \leq k \leq 2N - 2$, the outlets of the k^{th} layer serve as inputs for the $(k + 1)^{th}$ layer, i.e. the outlets of the crossbar at the k^{th} layer are connected by "links" to the inlets of the crossbar in the $(k + 1)^{th}$ layer according to a "shuffle" pattern. The shuffle pattern can be defined by numbering the inlets and outlets with binary representation of integers from 0 to $2^N - 1$ such that the inlets of each crossbar receive the same numbers as the outlets and these numbers differ only in their least significant bit in the binary representation. The outlets of the crossbar in the last layer are the "outputs" of the network. In a spider-web network there are 2^{N-1} paths between each input and each output.

Our network is a slight modification of the spider-web network. There is no restriction on the number of layers, it can be any integer ($\geq l$). We denote the number of layers in the network by M ($M \geq N$), where M is even. The M^{th} layer is connected back to the first layer. Hence, there is no input or output to the network. We will have two to one connections between the crossbars of the k^{th} and $(k + 1)^{th}$ layer (last layer connects back to the first layer) defined by the following two shuffle patterns: connect each outlet in the k^{th} layer to two inlets in the $(k + 1)^{th}$ whose number has the binary representation obtained by cyclically shifting one place to the left the representation of the outlet and putting a 0 or a 1 in the least significant bit.

For us, a $2^N \times M$ - node spider-web network is a set of M -layers each of which has 2^N nodes which can be represented by N -bit binary numbers. A site in layer r may be represented by an N -bit integer. The site in the r^{th} layer with the bit label $abcd...ij$ is connected to two sites with labels $bcd...ij0$ and $bcd...ij1$ in the layer $r + 1$. The layer M is connected in the same way to layer 1.

The $N = 2, M = 4$ network is shown in Figure(1.2). It is easy to see that the spider-web network is bipartite since we have an even number of layers in all. The

vertices can be grouped into two sets with the vertices of the odd layers in one and the vertices of the even ones in the other. This explicit construction of the two sets shows that the graph is bipartite. The network is locally tree-like though it does have loops of small sizes. Also, all sites in the network are exactly equivalent. We will label sites in the first layer as i_1, i_2, \dots, i_N in the second layer as i_2, i_3, \dots, i_{N+1} and so on. We will always require M such labels from i_1 to i_M to denote the sites in the lattice. Each layer is denoted by such a set of N consecutive labels and then each particular site in the layer is obtained by giving those variables values namely 0 and 1. This scheme will work if and only if $M \geq N$.

Chapter 2

Self-Avoiding Walks and Polygons and High-Temperature Expansion

2.1 Ising Model

Consider a one-dimensional lattice with N sites, labeled by integers from 1 to N . At each site i , there is a spin σ_i which can take value either $+1$ or -1 . The Hamiltonian of this system in the absence of an external magnetic field is:

$$H = - \sum_{i=1}^{N-1} J_{i,i+1} \sigma_i \sigma_{i+1} \quad (2.1)$$

For each pair, if

1. $J_{i,i+1} > 0$ the interaction is called ferromagnetic
2. $J_{i,i+1} < 0$ the interaction is called antiferromagnetic
3. $J_{i,i+1} = 0$ the spins are noninteracting

A ferromagnetic interaction tends to align spins, and an antiferromagnetic tends to antialign them. We assume the this coupling between the spins is the same for all pairs, i.e., $J_{i,i+1} = J$. Our first problem is to find the partition function which is obtained by exponentiating the Hamiltonian and summing over all the 2^N configurations:

$$Z = \sum_C e^{-\beta H} \quad (2.2)$$

The system is in contact with a heat bath at temperature T and each configuration C occurs in the *canonical ensemble*, with a probability $Prob(C) = \exp -\beta H(C)/Z$, where Z is given by Equation(12). β is $1/k_B T$, where k_B is the Boltzmann's constant and cancels whatever dimensions the Hamiltonian may have.

We do a change of variables. Define variables $\{\tau_i\}$ with $\{\tau_1\} = \sigma_1$, and $\{\tau_i\} = \sigma_{i-1} \sigma_i$, for $i > 1$. These variables are again Ising in the sense that $\tau_i = \pm 1$. Then, we get

$H = -J \sum_{i=2}^N \tau_i$. Now the summations over all configurations is easy to do in terms of the $\{\tau_i\}$. And we get,

$$\begin{aligned} Z &= \sum_{\{\tau_i\}} e^{\beta H(\{\tau_i\})} \\ &= 2 \prod_{i=2}^N 2 \cosh(\beta J) \\ &= 2^N [\cosh(\beta J)]^{N-1} \end{aligned} \quad (2.3)$$

The free energy per site in the *thermodynamic limit* of large N can be defined as $f(\beta) = \lim_{N \rightarrow \infty} = -k_B T (\log Z) / N$. Hence,

$$f(\beta) = -k_B T (\log [2 \cosh(\beta J)]) \quad (2.4)$$

From the partition function one may in principle derive all the important thermodynamical features of the physical system being modeled: magnetization, specific heat, susceptibility, internal energy and so on. Phase transitions will show up as discontinuities in f or in one of its derivatives. It is not always possible to find a closed-form, analytic expression for the function f . In these cases we resort to graphical enumeration techniques such as high and low temperature expansions. In the next section we will give the general idea of high-temperature expansion for Ising systems and work out an explicit example for the two-dimensional square lattice zero-field Ising model. The exact solution for this problem is known. The general d-dimensional hypercube lattice Ising model has the form:

$$H = - \sum_{\langle i,j \rangle} J_{i,j} \sigma_i \sigma_j \quad (2.5)$$

where $\langle i, j \rangle$ denotes nearest neighbor spins. We will use a "wrap-around" lattice, i.e., a lattice with periodic boundary conditions. As in the one-dimensional case we will set all the couplings $J_{i,j}$ to a constant J .

2.2 High-Temperature Expansion for Ising systems[12]

We shall begin by converting the partition function from exponentials into polynomials. This is based on the identity:

$$e^{\pm y} = \cosh y \pm \sinh y = \cosh y (1 \pm \tanh y) \quad (2.6)$$

Now since the variables σ_i take on the values ± 1 , we have:

$$\begin{aligned} Z &= \sum_{\pm 1} e^{\sum_{\langle i,j \rangle} \beta J \sigma_i \sigma_j} \\ &= \sum_{\pm 1} (e^{\Pi_{\langle i,j \rangle} \beta J \sigma_i \sigma_j}) \\ &= \sum_{\pm 1} (\prod_{\langle i,j \rangle} \cosh(\beta J) (1 + \sigma_i \sigma_j x)) \\ &= \cosh(\beta J)^B \sum_{\pm 1} (\prod_{\langle i,j \rangle} (1 + \sigma_i \sigma_j x)) \end{aligned} \quad (2.7)$$

where B is the number of bonds, $x = \tanh(\beta J)$. Since we are using periodic boundary conditions, $B = dN$, where $d = 1, 2, 3, \dots$ is the dimension of the model. We can now introduce the factor of 2^N which is the total number of possible configurations:

$$Z = [2 \cosh^d(\beta J)]^N \frac{1}{2^N} \sum_{\pm 1} (\prod_{\langle i,j \rangle} (1 + \sigma_i \sigma_j x)) \quad (2.8)$$

The free energy function now consists of two parts:

$$F = \lim_{N \rightarrow \infty} \frac{1}{N} \log Z = \log(2 \cosh^d(\beta J)) + \lim_{N \rightarrow \infty} \frac{1}{N} \log Z' \quad (2.9)$$

where

$$Z' = \frac{1}{2^N} \sum_{\pm 1} (\prod_{\langle i,j \rangle} (1 + \sigma_i \sigma_j x)) \quad (2.10)$$

The first part $\log(2 \cosh^d(\beta J))$, is always analytic for real values of β and J ; hence it does not exhibit any discontinuity. We will not look at "non-trivial" part Z' . Since $\sigma_i^2 = 1$ for all i , we have:

$$\prod_{\langle i,j \rangle} (1 + \sigma_i \sigma_j x) = P_0(x) + \sigma_1 P_1(x, \sigma_1, \dots, \sigma_N) + \sigma_1 P_2(x, \sigma_3, \dots, \sigma_N) + \dots + \sigma_N P_N(x) \quad (2.11)$$

for polynomials P_0, P_1, \dots, P_N . Note that P_0 is of degree dN in x . When we do the sum over all configurations, each $\sigma_l P_l$ term vanishes:

$$\begin{aligned} \sum_{\pm 1} \sigma_l P_l(x, \sigma_1 + 1, \dots, \sigma_N) &= \left(\sum_{\pm 1} \sigma_l \right) \left(\sum_{\pm 1} P_l(x, \sigma_1 + 1, \dots, \sigma_N) \right) \\ &= 0 \end{aligned} \quad (2.12)$$

This implies that the non-trivial part of the partition function is:

$$Z' = \frac{1}{2^N} \sum_{\pm 1} P_0(x) = P_0(x) \quad (2.13)$$

Since the degree of P_0 in x is dN , we can write it as:

$$P_0(x) = 1 + c(1)x + c(2)x^2 + \dots + c(dN)x^{dN} \quad (2.14)$$

where $c(i)$ are the coefficients of the polynomial. These coefficients have a simple combinatorial interpretation. If we think of the lattice as a graph with the sites being the vertices and the bonds between nearest neighbor sites being the edges, then $c(n)$ counts the number of "even" subgraphs with n edges, where by "even" we mean that each vertex has positive, *even* coordination number. This can be seen by letting the presence of absence of the bond $\langle i, j \rangle$ in a subgraph correspond to the choice of $\sigma_i \sigma_j x$ or 1 in the expansion of $\prod_{\langle i,j \rangle} (1 + \sigma_i \sigma_j x)$. Each subgraph corresponds to a term in the expansion: $\prod_{\sigma_i} \theta_i x^n$, where θ_i is the coordination number of vertex i and $n = \frac{1}{2} \sum_i \theta_i$ is the number of edges. Unless each σ_i is raised to an even power, there is no contribution of this subgraph to Z' . Therefore, only even

subgraphs contribute to the non-trivial partition function Z' .

Each connected component of an even subgraph forms a closed path in the original lattice. Now it is easy to see the solution of the one-dimensional Ising model: with periodic boundary conditions, there is one and only one close path, namely, the complete circuit of length N . Therefore, $Z' = 1 + x^N$, so that:

$$\begin{aligned} F &= \log(2 \cosh^d(\beta J)) + \lim_{N \rightarrow \infty} \log(1 + x^N) \\ &= \log(2 \cosh^d(\beta J)) \end{aligned} \tag{2.15}$$

since $|x| = \tanh(\beta J) < 1$. If we did not have periodic boundary conditions, then there are *no* closed paths, hence $\log(Z') = 0$ directly.

In dimensions 2 and 3, clearly closed paths exist, but they must be of even length unless they are long enough to make use of the wrap around. Also, the shortest paths are of length 4, so we have

$$P(x) = 1 + c(4)x^4 + c(6)x^6 + c(8)x^8 + \dots \tag{2.16}$$

if the lattice is sufficiently large. We shall show the computation of the coefficient $c(n)$ for $n = 4, 6$ and 8 for $d = 2$.

An even subgraph with $n = 4$ edges is a square. For every lattice point there is a square with a specified corner(top-right-hand) at that lattice point, so this implies that $c(4) = N$. Now, an even subgraph with $n = 6$ edges is either a 2×1 or a 1×2 rectangle, which can be located at any of the N lattice sites. Hence $c(6) = 2N$.

From $n = 8$ onwards, the subgraphs need not be connected. For $n = 8$ a disconnected subgraph has to necessarily be two disjoint squares. The "first" square maybe placed with its top-right-hand corner are any of the lattice points, while the same corner of the "second" square needs to avoid exactly nine sites(see Figure(2.1)). Hence in all there are $N(N - 9)/2$ disconnected even subgraphs with exactly eight edges. We need to divide by 2 to remove the distinction between "first" and "second".

The connected paths of length 8 are shown in Figure(2.2). These four different types, with a total of 9 orientations give $9N$ connected subgraphs with exactly 8 edges. An exhaustive enumeration of octagons shows that there are $c(8) = N(N + 9)/2$ of them.

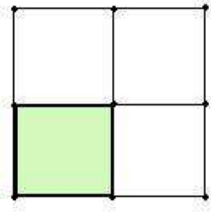


Figure 2.1:

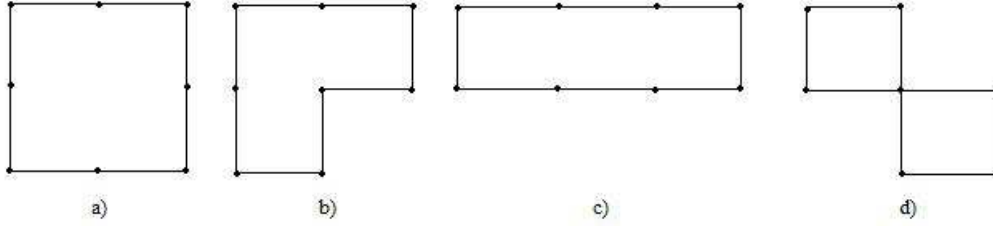


Figure 2.2: a) N of these, b) $4N$ of these since there are 4 possible orientations(\ulcorner , \lrcorner , \llcorner and \lrcorner) c) $2N$ of these for 2 orientations(horizontal and vertical)and d) $2N$ of these for two orientations(\setminus and $/$)

Knowing the first few terms in Z' allows us to compute the corresponding terms in the power series for the thermodynamic limit. We can do the formal Taylor series expansion of the logarithm,

$$\log(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots \quad (2.17)$$

Therefore,

$$\begin{aligned} \log(Z') &= \log[1 + c(4)x^4 + c(6)x^6 + c(8)x^8 + \dots] \\ &= [1 + c(4)x^4 + c(6)x^6 + c(8)x^8 + \dots] \\ &\quad - \frac{[1 + c(4)x^4 + c(6)x^6 + c(8)x^8 + \dots]^2}{2} + \dots \\ &= c(4)x^4 + c(6)x^6 + [c(8) - \frac{c(4)^2}{2}]x^8 + O(x^{10}) \end{aligned} \quad (2.18)$$

Using the value of $c(n)$ from our computations above, we get:

$$F' = \lim_{N \rightarrow \infty} \frac{\log Z'}{N} = x^4 + 2x^6 + \frac{9}{2}x^8 + \dots \quad (2.19)$$

After taking the thermodynamic limit, we get a power series for the modified(non-trivial) free energy F' . That the coefficients of F' are independent of the lattice size N is a consequence of the extensivity of the free energy.

Truncating the power series expansion for $\log(1 + x)$ and looking at only terms of small orders is going to be valid only in the limit of high-temperature, since then as $\beta \rightarrow 0$, $x \rightarrow 0$ and the contribution from higher orders becomes vanishingly small.

2.3 Self-Avoiding Walks and Polygons on Spider-web networks

To count the number of self-avoiding polygons(SAPs) and self-avoiding walks(SAWs) we use a depth first search with backtracking algorithm. Using the number of SAPs we can in turn infer the number of even subgraphs which will enable us to do the high-temperature expansion of the Ising model on the network.

Backtracking is a general algorithm for finding all (or some) solutions to a computational problem, that incrementally builds candidates to the solutions, and abandons each partial candidate c ("backtracks") as soon as it determines that c cannot possibly be completed to a valid solution. When it is applicable, however, backtracking is often much faster than brute force enumeration of all complete candidates, since it can eliminate a large number of candidates with a single test.

The famous "Eight Queens Puzzle" is an example where the depth first search with backtracking algorithm gives the most efficient way to find solutions[13].

In the spider network each node in a layer l is connected directly to four nodes, two in layer $l - 1$ and two in $l + 1$. We will call these four operators as:

1. a cyclically shifts one place to the left the representation of the node and puts a 0 in the least significant bit. Therefore, a takes a node in layer l to $l + 1$.
2. b cyclically shifts one place to the left the representation of the node and puts a 1 in the least significant bit. Therefore, b takes a node in layer l to $l + 1$.
3. c cyclically shifts one place to the right the representation of the node and puts a 0 in the most significant bit. Therefore, c takes a node in layer l to $l - 1$.
4. d cyclically shifts one place to the right the representation of the node and puts a 1 in the most significant bit. Therefore, d takes a node in layer l to $l - 1$.

Since the spider-web network is bipartite, there are no odd loops. We can start with any given node, since all nodes are equivalent. We define a preference order in the following way: $a > b > c > d$. Let the size of the even loop, the number of which we wish to count be n . A set of operators of the form $f = abdcacba\dots$ acts on a node i and forms an n -sized loop. We denote by $f(i)$ the set of nodes which occur at every step. For example: if $f = abdc$, then $abdc(i_0) = abd(i_1) = ab(i_2)i_1 = a(i_3)i_2i_1 = i_4i_3i_2i_1 = f(i_0)$, where $i_1 = c(i_0)$ and $i_2 = d(i_1)$ and so on. For a 4-loop to occur $i_0 = i_4$. Similarly for n -loop, $i_0 = i_n$. Since the operator f generates loops, the number of $a + b$ in f must match the number of $c + d$ and this number has to be necessarily equal to $n/2$, else we will not be able to return to the starting node on

Loop-size(n)	Number of SAPs per site(p_n)	$\frac{p_{n+2}}{p_n}$
4	0.5	0.000
6	0	undefined
8	4	0.000
10	0	undefined
12	32	6.000
14	192	2.333
16	448	7.142
18	3200	6.570
20	21024	5.065
22	106496	5.593
24	595712	5.966
26	3554304	-
Extrapolated Value(∞)	-	5.280

Table 2.1: The number of self-avoiding polygons per site in a spider-web network

applying f on the starting node.

Also as we are interested in SAPs, there is an additional check which needs to be added. We need to make sure that every node (other than the starting node) appears only once, i.e., none of the i_k other than i_0 should appear more than once in $f(i_0)$. For self-avoiding walks, none of the nodes including the first one should appear more than once. Using these checks, I wrote a depth first search with backtracking program in C++ to count the number of SAPs and SAWs on the spider-web network. The numbers are shown in Table(2.1) and Table(2.2) respectively.

Let us take a closer look at Tables(2.1,2.2). We will denote steps taken in the forward direction, i.e from a layer r to $r + 1$ by an F and in the backward direction by B and the loop or walk-size by n and the number of loops and walks of a given size n by p_n and c_n respectively. There are two choices each for F and B . F^k and B^k will denote k steps in the forward and backward directions respectively. Since these are polygons, the number of F is equal to the number of B is equal to half the polygon size. Due to the self-avoiding property, whenever an F and a B occur together, there is only one unique specification that can be made, i.e of the two choices only one will work. Without loss of generality we can always choose F to be the first step. Now there is one and only one polygon of size-4 which is denoted by $F B F B$. Once we choose the the first F as obtained by applying say operator a on the site, the whole polygon gets fixed. We necessarily have to choose operators $d b c$ in that order to form a 4-loop because of the above reason. Now we could have chosen c instead of a for the first step, but that gives the same 4-loop, just traversed in the opposite orientation. Hence, there is only one unique 4-loop which can be constructed starting at any arbitrary site. Now since a 4-loop has two sites in a single layer, the number of these per lattice site is $1/2$.

Walk-size(n)	Number of SAWs per site(c_n)	$\frac{c_{n+1}}{c_n}$
1	4	3.000
2	12	3.000
3	36	2.888
4	104	2.923
5	304	2.921
6	888	2.918
7	2592	2.895
8	7504	2.901
9	21776	2.921
10	63624	2.888
11	183774	2.899
12	532832	2.901
13	1545792	2.897
14	4479424	2.899
15	12986688	2.898
16	37639936	2.898
17	109109248	2.897
18	316174464	2.898
19	916331776	2.897
20	2654878208	2.897
21	7692865792	-
Extrapolated Value(∞)	-	2.897

Table 2.2: The number of self-avoiding walks per site in a spider-web network

None of the possible combinations of 3 F 's and 3 B 's lead to a 6-loop. There is only one type of 8-loop denoted by $F^2B^2F^2B^2$ and there are exactly 8-such polygons possible. The eight polygons correspond to the two choices of the three bold face steps in $F\mathbf{F}B\mathbf{B}F\mathbf{F}B\mathbf{B}$. For $n = 10$ there are no loops possible and for $n = 12$ there is exactly one loop denoted by $F^3B^3F^3B^2FB^2$ and there are 64 polygons of this type. From $n = 14$ onwards, we have more than one type of loop. For $n = 14$, there are six types of loops namely $F^3B^2F^2B^3F^2B^2$, $F^3B^2FB^2F^3B^3$, $F^3B^3F^3B^2FB^2$, $F^3B^3F^2BF^2B^3$, $F^2BF^2B^3F^3B^3$ and $F^2B^2F^3B^2F^2B^3$. There are 2^6 number of loops of each type giving a total of 384 loops. We have done this analysis for all loop-sizes till 20. We fit a function of the form $A_n\mu_{SAP}^n$ for p_n , μ_{SAP} is called the connective constant of SAPs. We find that μ_{SAP} for SAPs on a spider-web network is close to 2.298.

We do a similar analysis for walks as we did for polygons. It is straightforward to see that the number of SAWs of sizes 1, 2 and 3 are respectively 4, 12 and 36 respectively. We have 4 choices for the first step corresponding to choosing either of

a , b , c or d as the first operator and from the second step we have 3 choices. This will hold only for walk-size ≤ 4 . From $n = 4$ onwards we get loops, so we need to eliminate them while counting walks. There are 4 different walks that one can construct from a given site. This corresponds to the 4 choices of the operators. Now we need to subtract these from all possible walks of size 4. Hence, the number of SAWs of size 4 is $4 \times 3^3 - 4 = 104$. Similarly one can show that the number of SAWs of size 5 is $3 \times 104 - 8 = 304$ and so on. We fit a function of the form $B_n \mu_{SAW}^n$ for c_n , μ_{SAW} is called the connective constant of SAWs. It is trivial to see that for this network $2 < \mu_{SAW} < 3$. From the fitting function, we find that μ_{SAP} for SAPs on a spider-web network is close to 2.90. For most lattices, $\mu_{SAP} = \mu_{SAW}$, but for our lattice this is not true. Another example of a lattice where $\mu_{SAP} \neq \mu_{SAW}$ is the Bethe lattice, where you can construct SAWs of arbitrary length, but there are no loops at all.

2.4 High-Temperature Expansion of Ising Model on Spider-Web Network

An even subgraph with $n = 4$ edges is a 4-loop an example of which is shown in Figure(2.3). $c(4) = N/2$ and $c(6) = 0$ from the above table. For $c(8)$ we need to do a little more work. Other than the self-avoiding polygons(connected) which are $4N$ in number, we can now have two 4-loops which together will form an even subgraph with $n = 8$ edges. As can be inferred from Figure(2.3), the number of these would be $N(N - 2)/8$. The "first" 4-loop maybe placed with either of its left-hand corners at any of the lattice points, while the left-hand corners of the "second" square needs to avoid exactly two sites(see Figure(2.3)). Hence in all there are $\frac{N(N-2)}{2}$ disconnected even subgraphs with exactly eight edges. We need to divide by 2 to remove the distinction between "first" and "second". An exhaustive enumeration of octagons shows that there are $c(8) = 4N + N(N - 2)/8 = N(N + 30)/8$ of them.

From Table(??) we see that there are no SAPs of size 10. Also, since $c(6) = 0$, we cannot have 4-loop and a 6-loop combining to give a 10-loop as would have happened in the two-dimensional Ising model on the square lattice. Hence, $c(10) = 0$. Using Equation(2.19), we can find the free energy function as follows:

$$\begin{aligned} \log(Z') &= c(4)x^4 + c(6)x^6 + [c(8) - \frac{c(4)^2}{2}]x^8 + O(x^{10}) \\ &= \frac{N}{2}x^4 + [\frac{N(N+30)}{8} - \frac{(\frac{N}{2})^2}{2}]x^8 + O(x^{10}) \end{aligned} \quad (2.20)$$

As explained above, there will be no x^{10} term as well. Hence,

$$F' = \frac{Z'}{N} = \frac{x^4}{2} + \frac{15}{4}x^8 + \mathcal{O}(x^{12}) \quad (2.21)$$

Similarly, higher order terms can be computed.

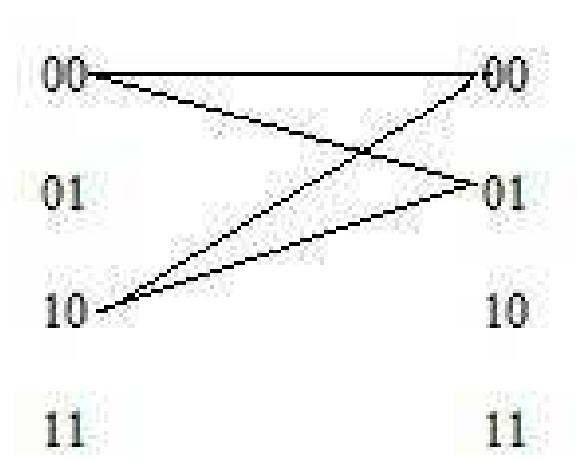


Figure 2.3: An example of a 4-loop. Two sites in a layer form one 4-loop.

Chapter 3

Vibrational Spectra of Spider-Web Networks

3.1 The Spring Problem

In the spring problem, for displacement x_i at vertex i ($i = 1$ to $N_0 = 2^N \times M$), the Hamiltonian is(Equation(3.1)):

$$\begin{aligned}
 H &= \frac{1}{2} \sum_i (dx_i/dt)^2 + \frac{1}{2} \sum_{i,j} K(x_i - x_j)^2 \\
 &= \frac{1}{2} \sum_i (dx_i/dt)^2 + \frac{1}{2} \sum_{i,j} x_i \mathbb{K}_{ij} x_j
 \end{aligned} \tag{3.1}$$

The matrix \mathbb{K} is given in terms of the Adjacency matrix of the graph. $\mathbb{K}_{i,j} = -1$ if i is directly connected to j , 0 otherwise. $\mathbb{K}_{i,i} = 4$ in our problem, for all i since there are 4 springs emanating from each site. Hence if Λ is the Adjacency matrix of this graph, then the matrix \mathbb{K} is given by(Equation(3.2)):

$$\mathbb{K}_{ij} = 4 - \Lambda_{ij} \tag{3.2}$$

Therefore, $\mathbb{K} = 4\mathbb{I} - \Lambda$ where \mathbb{I} is the $2^N \times M$ size identity operator.

The eigenvalue problem is(Equation(3.3)):

$$\mathbb{K}\psi_\alpha = E_\alpha\psi_\alpha \tag{3.3}$$

here ψ_α is the eigenvector for eigenvalue E_α .

If there is symmetry of \mathbb{K} , then there is a set of symmetry operators F_r [$r = 1, R$] such that $[F_r, F'_r] = 0$, and $[\mathbb{K}, F_r] = 0$ then \mathbb{K} and F_r can be simultaneously diagonalized. If the eigenvectors of F 's are known by other means, they must also be eigenvectors of \mathbb{K} .

For the problem of vibrational modes of a harmonic crystal, F is the translation operator, and its eigenvalues are $\exp(\iota ka)$, which then reduces it to a finite matrix diagonalization problem[[14]].

In our case, one symmetry is flipping j th bit. Call this F_j , then $F_j F_j = \mathbb{I}$. Hence eigenvalues of F_j are $+1$ and -1 . When all $F_j = +1$, then translational invariance exists. If we denote the translational operator by T , then $[F_j, T] = 0$ for all j . We can find out the eigenvalues of the translation operator using the fact that $T^M = \mathbb{I}$, hence the M eigenvalues of T are the M roots of unity denoted by $\exp(ik)$ with $k = 2\pi n/M$ with $n = 0, 1, 2, \dots, M-1$. Here we have M independent commuting operators F_1, F_2, \dots, F_M . That gives decomposition of the large \mathbb{K} matrix into $2^M \times 2^M$ blocks and several of these blocks are of zero size as will be shown below.

There are in all 2^M values for the set of operators $\{F_i\}$, since there are two choices for each F_i . But it turns out that not all of these result in non-zero values for the displacement x_i . The wavefunction at each node is labeled by two entities: 1. its layer number, the variable for which we will call as x and 2. an N -bit integer, the variable for which we will call y . Hence $\psi \equiv \psi(x, y)$. Therefore, $F_i \psi(x, y) = \pm \psi(F_i(x, y))$. We cannot set the eigenvalue of F_i and F_j both equal to -1 if $|i - j| \geq N$ since that results in identically zero amplitudes at each of the nodes.

For example, let us look at the $N = 3$ case. We will label the sites in layer 1 as $i_1 i_2 i_3$ in layer 2 as $i_2 i_3 i_4$ and so on and in the M^{th} layer as $i_M i_1 i_2$ so that it connects back to the 1^{st} layer. Let us see what happens if $F_1 = -1$ and $F_4 = -1$. Note that there is no site which has a label which has both i_1 and i_4 in it. The action of F_4 on $i_1 i_2 i_3$ is $F_4 \psi(i_1 i_2 i_3) = -\psi(F_4(i_1 i_2 i_3)) = -\psi(i_1 i_2 i_3)$ which implies that $\psi(i_1 i_2 i_3) = 0$ since $F_4 \psi(i_1 i_2 i_3)$ is just $\psi(i_1 i_2 i_3)$ as there is no i_4 . Hence F_4 will set amplitudes of all sites in which there is no i_4 to 0. Similarly, F_1 will set all amplitudes in which there is no i_1 to 0. As noted earlier we don't have any site which has both i_1 and i_4 in its label, hence the amplitudes of all sites identically vanish. From the same line of argument, if within a set of N consecutive operators, $F_i = -1$ and $F_j = -1$ such that $|i - j|$ is maximum and the rest of $M - N$ F operators have eigenvalue $+1$, then there are exactly $N - |i - j|$ modes coming from this set of F 's.

We just need to deal with the eigenvalue problem for Λ since the identity operator is anyway diagonal. Therefore, if λ_α and ψ_α is an eigenvalue and eigenvector of Λ , then the corresponding eigenvalue and eigenvector for \mathbb{K} will be $4 - \lambda_\alpha$ and ψ_α . We will have $2^N \times M$ eigenmodes for the N -bit M -layer problem. We will also set the spring constant and the mass of each atom to unity, i.e $K, m = 1$. The frequency of an eigenmode is denoted by ω_α and $\omega_\alpha^2 = E_\alpha$.

We will denote by $D(\omega_\alpha^2)$, the fractional number of times an eigenvalue ω_α^2 appears, i.e number of times the eigenvalue appears divided by $2^N \times M$ in the limit that $M \rightarrow \infty$. Hence, $0 \leq D(\omega_\alpha^2) \leq 1$. This is called the spectral density function and $D(\omega_\alpha^2) d\omega_\alpha^2$ denotes the fractional number of modes between ω_α^2 and $\omega_\alpha^2 + d\omega_\alpha^2$. We will always plot the spectrum in the limit as $M \rightarrow \infty$ since that is of interest to us.

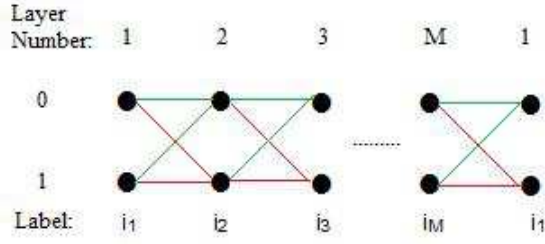


Figure 3.1: $N = 1$ spider network, Rule: $a \rightarrow 0$ (green) and $b \rightarrow 1$ (red) where a and b are either 0 or 1

3.1.1 $N=1$

There are $2M$ modes. The network looks as follows(see Figure(3.1)): Since all sites are just labeled by a single i_L , we can at max set one of the $F_p = -1$. The moment we set an $F_p = -1$, the wavefunction amplitude of all sites other than those in the layer p vanish identically. Let us now look at the sites in this p -layer. The eigenvalue equation for any site in this layer will be $\lambda_\alpha \psi_\alpha = 0$ since all the four sites to which it is connected have identically zero amplitudes. Hence $\omega_\alpha^2 = 4$. The eigenvector upto an overall multiplicative constant is $\psi_\alpha = (0, 0, 0, \dots, 1, -1, \dots, 0)$, where the first two entries are the amplitudes of the wavefunction at the first(0) and second(1) site of layer 1, the next two entries are for the sites in layer 2 and so on; 1 and -1 are the amplitudes of the two sites in the p^{th} layer. From now on we will not worry about the overall multiplicative constant. Now we have M choices for p which gives us M of the modes each of which has $\omega_\alpha^2 = 4$. We will always get these set of modes whenever we have a set of N consecutive F_p 's equal to -1 .

The other M modes come from translational invariance when we set all the $F_p = +1$. The eigenvalue equation for any site is(Equation(3.4)):

$$\begin{aligned} \lambda_\alpha \psi_\alpha &= 2(\lambda_\alpha \exp(\iota k) \psi_\alpha + \lambda_\alpha \exp(-\iota k) \psi_\alpha) \\ \lambda_\alpha &= 4 \cos k \\ k &= 2\pi n/M, n = 0, 1, 2, \dots, M-1 \end{aligned} \quad (3.4)$$

These are the other M modes with:

$$\begin{aligned} \omega_\alpha^2 &= 4 - 4 \cos k \\ &= 8 \sin^2(k/2) \end{aligned} \quad (3.5)$$

$$\begin{aligned} \omega_\alpha^2 &= 4 - 4 \cos k \\ &= 8 \sin^2(k/2) \end{aligned} \quad (3.6)$$

By equating the number of modes in k -space with that in frequency space, we

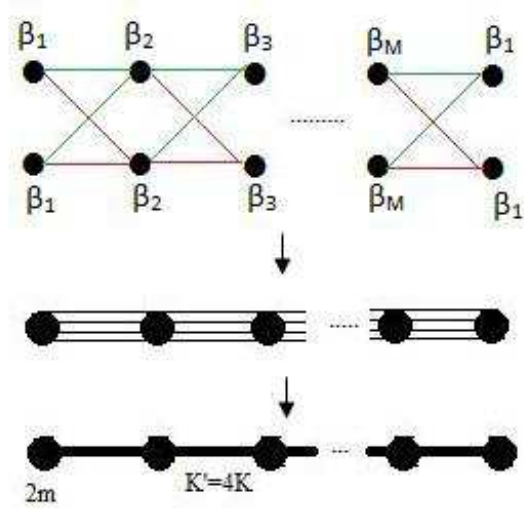


Figure 3.2: In the case of translational invariance, the problem reduces to that of finding the normal modes of a 1 – D monatomic lattice

get

$$\int \frac{dk}{2\pi} = \int D(\omega_\alpha^2) d\omega_\alpha^2$$

$$D(\omega_\alpha^2) = \frac{1}{2\pi} \left| \frac{dk}{d\omega_\alpha^2} \right|. \quad (3.7)$$

Using Equation(3.6), one can show that:

$$D(\omega_\alpha^2) = \frac{1}{2\pi [\omega_\alpha^2 (8 - \omega_\alpha^2)]^{\frac{1}{2}}} \quad (3.8)$$

The eigenvectors obtained for the first M modes were of the form $\psi_\alpha = (0, 0, 0, \dots, 1, -1, \dots, 0)$, where the 1 and -1 are the amplitudes of the two sites in the p^{th} layer for which $F_p = -1$. Now the other M modes have to be orthogonal to all these modes. Hence the most general wavefunction which satisfies this condition is of the form $(\beta_1, \beta_1, \beta_2, \beta_2, \dots, \beta_M, \beta_M)$ where the amplitude of the sites in a given layer are exactly the same. This wavefunction by construction is orthogonal to any eigenmode which we obtained by setting $F_p = -1$. Now since the amplitude of the two sites in a layer are identical, we can as well combine the two sites into one. This now reduces to the problem of finding the normal modes of a one-dimensional monatomic lattice with periodic boundary conditions. The only change is that each atom now has a mass $m' = 2m$ and is connected to its neighbours with a spring constant $K' = 4K$ (See Figure(3.2)). The eigenmodes have a frequency $\omega(k) = 2\sqrt{K'/m'} |\sin(k/2)|$ [[14]]. Plugging in the values of K' and m' we get Equation(3.6). These translational-invariant modes also exist for all N when all the $F_p = +1$. Hence, from now on we will only discuss rest of the modes other than these $2M$. Of the $2^N \times M$ modes, M of the modes are extended. These are the translationally-invariant modes. Rest of the modes can be chosen to be localized.

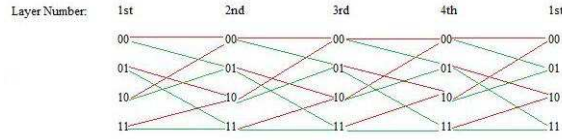


Figure 3.3: Rule: $ab \rightarrow b0$ (red) and $ab \rightarrow b1$ (green) where a and b are either 0 or 1

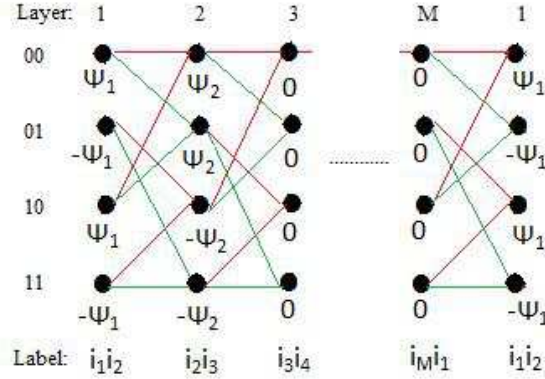


Figure 3.4: Rule: $ab \rightarrow b0$ (red) and $ab \rightarrow b1$ (green) where a and b are either 0 or 1

3.1.2 $N=2$

The network for $M = 4$ is shown in Figure(3.3). In all there are $4M$ modes, but as explained above, $2M$ of these come from translational invariance(M modes) and by setting 2 consecutive F 's equal to -1 (M modes). Hence, we just need to find out the other $2M$ modes. We can set any of the $F_p = -1$ and all other $F_r = +1 \forall r \neq p$. For example, let us set $F_2 = -1$. The wavefunction at sites in all layers other than 1 and 2 vanishes identically as explained above(3.1). The wavefunction amplitudes at sites in layers 1 and 2 will be as shown in Figure(3.4). The eigenvalue equation now becomes(Equation(3.9)):

$$\begin{aligned} \lambda\psi_1 &= 2\psi_2 \\ \lambda\psi_2 &= 2\psi_1 \end{aligned} \quad (3.9)$$

Solving this, we get two values for λ , namely -2 and $+2$. These are the other $2M$ modes corresponding the M choices for p . One can similarly work out the modes for other values of N . In the next section, we will present the general framework to deal with this problem.

3.2 General Framework for the N -bit M -layer spring problem

In all there are $2^N \times M$ modes since there are those many sites in the lattice. We know the identity(Equation(3.10)):

$$\begin{aligned} (1+x)^N &= \sum_{k=0}^N {}^N C_k x^k \\ &= {}^N C_0 x^0 + {}^N C_1 x^1 + {}^N C_2 x^2 + \dots + {}^N C_N x^N \end{aligned} \quad (3.10)$$

Setting $x = 1$ in the above equation and multiplying both sides by M we get Equation(3.11):

$$2^N \times M = ({}^N C_0 + {}^N C_1 + {}^N C_2 + \dots + {}^N C_N) \times M \quad (3.11)$$

In our context ${}^N C_k$ means that of a set of N consecutive F operators, k are such that the eigenvalues of these are -1 , the other $N - k$ have eigenvalue $+1$. Rest of the $M - N$ [F] operators have eigenvalue $+1$. Now, ${}^N C_0$ represents the case of translation symmetry, when $F_i = +1 \forall i$. Let us denote the translation operator by T . Then $T^M = \mathbb{I}$. Hence the eigenvalues of T are $\exp(2\pi i j/M)$ with $j = 0, 1, \dots, M - 1$. Call $2\pi j/M$ as θ . Then the eigenmodes have eigenvalues $\lambda = 2(\exp(i\theta) + \exp(-i\theta)) = 4\cos(\theta)$. This gives us a set of M eigenvalues which are $4\cos(\theta)$, where $\theta = 2\pi j/M$ with $j = 0, 1, 2, \dots, M - 1$. ${}^N C_N$ represents the case when a set of N consecutive F_i 's have eigenvalue -1 and all the other F_i 's have eigenvalue $+1$. This gives us M of the eigenvalues which are all 0. The other $(2^N - 2)M$ eigenvalues need to be looked at a little more carefully. Each of the other ${}^N C_k$'s are further partitioned. To fix up the notation, I'll label the symmetry operators as F_i with i going from $1, 2, \dots, M$.

3.2.1 $N = 1$

Here we have only ${}^1 C_0$ which is the case of translation symmetry and ${}^1 C_1$ in which of the M operators, for exactly one i , $F_i = -1$ and $F_j = +1 \forall j \neq i$. In the case of translation symmetry, the eigenvalues are $4\cos(\theta)$, where $\theta = 2j\pi/M$ with $j = 0, 1, 2, \dots, M - 1$ and for the other case all eigenvalues are 0. The spectrum is shown in Figure(3.5).

Since these modes exist for all other values of N as well, I have given explanation only for the rest of the $(2^N - 2) \times M$ eigenvalues.

3.2.2 $N = 2$

There are these ${}^2 C_1 \times M = 2M$ extra eigenvalues. These are such that any $F_i = -1$ and $F_j = +1 \forall j \neq i$. We get two eigenvalues for each i which are $\lambda = -2$ and

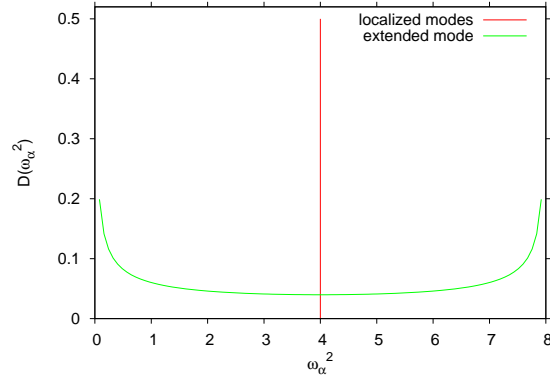


Figure 3.5: Plot of $D(\omega_\alpha^2)$ vs ω_α^2 for $N = 1$ and $M \rightarrow \infty$

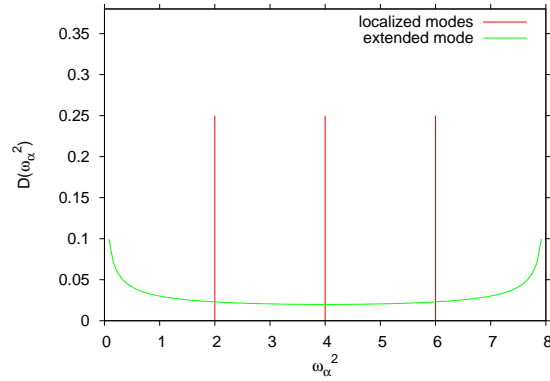


Figure 3.6: Plot of $D(\omega_\alpha^2)$ vs ω_α^2 for $N = 2$ and $M \rightarrow \infty$

$\lambda = +2$. And there are M choices for this i , hence the $2M$ eigenvalues. These are the $2M$ values which we will always get when a set of $2M$ modes are generated. Including the $2M$ eigenvalues which appeared for $N = 1$, we have the complete set of $4M$ eigenmodes. Note that 2C_2 gives us one eigenvalue which is 0. The spectrum is shown in Figure(3.6).

3.2.3 $N = 3$

Case of exactly 1 F being negative

One of the $F_i = -1$ and rest of the $F_j = +1, \forall j \neq i$. So for example we can take $F_1 = -1$ and $F_2, F_3 = +1$ and $\forall i > 3, F_i = +1$. This has 3 eigenmodes with eigenvalues $\lambda = 0, -2\sqrt{2}, +2\sqrt{2}$. These are the $3M$ values which we will always get when a set of $3M$ modes are generated. These are eigenvalues of the following

tridiagonal matrix(see Appendix(.1)): $\begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$ So this gives us $3M$ modes.

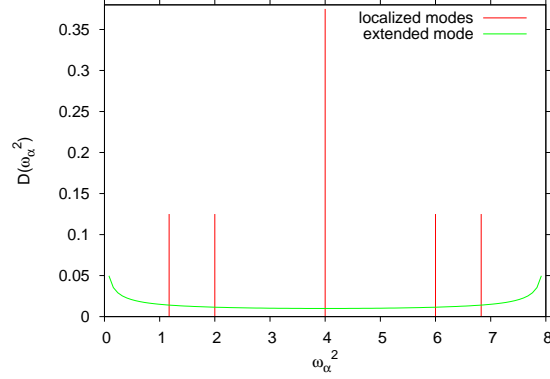


Figure 3.7: Plot of $D(\omega_\alpha^2)$ vs ω_α^2 for $N = 3$ and $M \rightarrow \infty$

Case of 2 F 's being negative

This gets divided into following 2 sets:

$F_1 = -1, F_2 = -1, F_3 = +1$ and $F_i = +1 \forall i > 3$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$. These are $2M$ in number.

$F_1 = -1, F_2 = +1, F_3 = -1$ and $F_i = +1 \forall i > 3$ This has 1 eigenmode with eigenvalue $\lambda = 0$ These are the rest of the M modes.

Including the $2M$ eigenvalues which appeared for $N = 1$, we have the complete set of $8M$ eigenmodes. Now let us look at eigenmodes obtained from 3C_3 and 3C_2 . It results in two sets of M eigenmodes and a set of $2M$ eigenmodes. The spectrum is shown in Figure(3.7).

3.2.4 $N = 4$

Case of exactly 1 F being negative

One of the $F_i = -1$ and rest of the $F_j = +1 \forall j \neq i$. So for example we can take $F_1 = -1$ and $F_2, F_3, F_4 = +1$ and $\forall i > 4, F_i = +1$. This has 4 eigenmodes with eigenvalues $\lambda = \sqrt{5} - 1, \sqrt{5} + 1, -\sqrt{5} - 1, -\sqrt{5} + 1$. These are the $4M$ values which we will always get when a set of $4M$ modes are generated. These are eigenvalues of

the following tridiagonal matrix(see Appendix(.1)):
$$\begin{pmatrix} 0 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$
 So this gives

us $4M$ modes.

Case of 2 F 's being negative

This gets divided into following 3 sets:

$F_1 = -1, F_2 = -1, F_3 = +1, F_4 = +1$ **and** $F_i = +1 \forall i > 4$ This has 3 eigenmodes with eigenvalues $\lambda = 0, -2\sqrt{2}, +2\sqrt{2}$. These are $3M$ in number.

$F_1 = -1, F_2 = +1, F_3 = -1, F_4 = +1$ **and** $F_i = +1 \forall i > 4$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$. These are $2M$ in number.

$F_1 = -1, F_2 = +1, F_3 = +1, F_4 = -1$ **and** $F_i = +1 \forall i > 4$ This has 1 eigenmode with eigenvalue $\lambda = 0$ These are M in number.

Adding up all these we get the $6M$ modes.

Case of 3 F 's being negative

This gets divided into following 3 sets:

$F_1 = -1, F_2 = -1, F_3 = -1, F_4 = +1$ **and** $F_i = +1 \forall i > 4$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$. These are $2M$ in number.

$F_1 = -1, F_2 = -1, F_3 = +1, F_4 = -1$ **and** $F_i = +1 \forall i > 4$ This has 1 eigenmode with eigenvalue $\lambda = 0$ These are M in number..

$F_1 = -1, F_2 = +1, F_3 = -1, F_4 = -1$ **and** $F_i = +1 \forall i > 4$ This has 1 eigenmode with eigenvalue $\lambda = 0$ These are M in number.

Adding up all these we get the $4M$ modes.

Now let us look at eigenmodes obtained from ${}^4C_4, {}^4C_3$ and 4C_2 . It results in four sets of M eigenmodes, two sets of $2M$ eigenmodes and a set of $3M$ eigenmodes. Including the $2M$ eigenvalues which appeared for $N = 1$, we have the complete set of $16M$ eigenmodes. The spectrum is shown in Figure(3.8).

The same analogy can be extended for higher values of N . It is evident that we can forget about M and just concentrate on any set of N consecutive symmetry operators. Without loss of generality, henceforth, we'll always choose the set F_1, F_2, \dots, F_N as our set of N consecutive operators. The number of partitions of ${}^N C_k$ is always going to be ${}^{N-1} C_{k-1}$ since we'll set $F_1 = -1$ in all cases which will leave us with a choice of $k-1$ among $N-1$ operators. I have written down $F_1 = -1$ in each of the cases just for the sake of completeness. Also set $F_i = +1 \forall i$ such that $N < i \leq M$.

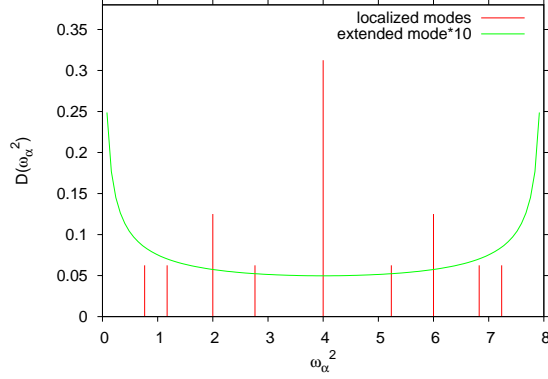


Figure 3.8: Plot of $D(\omega_\alpha^2)$ vs ω_α^2 for $N = 4$ and $M \rightarrow \infty$

3.2.5 $N = 5$

Case of exactly 1 F being negative

One of the $F_i = -1$ and rest of the $F_j = +1 \forall j \neq i$. So for example we can take $F_1 = -1$ and $F_2, F_3, F_4, F_5 = +1$. This has 5 eigenmodes. This has 5 eigenmodes with eigenvalues $\lambda = 2\sqrt{3}, 2, 0, -2, -2\sqrt{3}$. These are the $5M$ values which we will always get when a set of $5M$ modes are generated. These are eigenvalues of the

following tridiagonal matrix(see Appendix(.1)):

$$\begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 \\ 0 & 2 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & 2 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix}$$

Case of 2 F 's being negative

This gets divided into following $4(^4C_1)$ sets:

$F_1 = -1, F_2 = -1, F_3 = +1, F_4 = +1, F_5 = +1$ This has 4 eigenmodes with eigenvalues $\lambda = \sqrt{5} - 1, \sqrt{5} + 1, -\sqrt{5} - 1, -\sqrt{5} + 1$.

$F_1 = -1, F_2 = +1, F_3 = -1, F_4 = +1, F_5 = +1$ This has 3 eigenmodes with eigenvalues $\lambda = 0, -2\sqrt{2}, +2\sqrt{2}$.

$F_1 = -1, F_2 = +1, F_3 = +1, F_4 = -1, F_5 = +1$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$.

$F_1 = -1, F_2 = +1, F_3 = +1, F_4 = -1, F_5 = +1$ This has 1 eigenmode with eigenvalue $\lambda = 0$

The above add up to $10(4 + 3 + 2 + 1)$.

Case of 3 F 's being negative

This gets divided into following $6({}^4C_2)$ sets:

$F_1 = -1, F_2 = -1, F_3 = -1, F_4 = +1, F_5 = +1$ This has 3 eigenmodes with eigenvalues $\lambda = 0, -2\sqrt{2}, +2\sqrt{2}$.

$F_1 = -1, F_2 = -1, F_3 = +1, F_4 = -1, F_5 = +1$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$.

$F_1 = -1, F_2 = +1, F_3 = -1, F_4 = -1, F_5 = +1$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$.

$F_1 = -1, F_2 = -1, F_3 = +1, F_4 = +1, F_5 = -1$ This has 1 eigenmode with eigenvalue $\lambda = 0$

$F_1 = -1, F_2 = +1, F_3 = -1, F_4 = +1, F_5 = -1$ This has 1 eigenmode with eigenvalue $\lambda = 0$

$F_1 = -1, F_2 = +1, F_3 = +1, F_4 = -1, F_5 = -1$ This has 1 eigenmode with eigenvalue $\lambda = 0$

The above add up to $10(3 + 2 + 2 + 1 + 1 + 1)$.

Case of 4 F 's being negative

One of the $F_i = +1$ and rest of the $N - 1$ F_j 's have eigenvalue -1 . This gets divided into following $4({}^4C_3)$ sets:

$F_1 = -1, F_2 = -1, F_3 = -1, F_4 = -1, F_5 = +1$ This has 2 eigenmodes with eigenvalues $\lambda = -2$ and $\lambda = +2$.

$F_1 = -1, F_2 = -1, F_3 = -1, F_4 = +1, F_5 = -1$ This has 1 eigenmode with eigenvalue $\lambda = 0$

$F_1 = -1, F_2 = -1, F_3 = +1, F_4 = -1, F_5 = -1$ This has 1 eigenmode with eigenvalue $\lambda = 0$

$F_1 = -1, F_2 = +1, F_3 = -1, F_4 = -1, F_5 = -1$ This has 1 eigenmode with eigenvalue $\lambda = 0$ Adding up all these we get the $5(2 + 1 + 1 + 1)$ modes.

Now let us look at eigenmodes obtained from ${}^5C_5, {}^5C_4, {}^5C_3$ and 5C_2 . It results in $2^{5-2} = 8$ set of M eigenmodes, $2^{5-3} = 4$ set of $2M$ eigenmodes, $2^{5-4} = 2$ set of $3M$ eigenmodes and $2^{5-5} = 1$ set of $4M$ eigenmodes. Including the $2M$ eigenvalues which appeared for $N = 1$, we have the complete set of $2^5 \times M = 32M$ eigenmodes. The spectrum is shown in Figure(3.9).

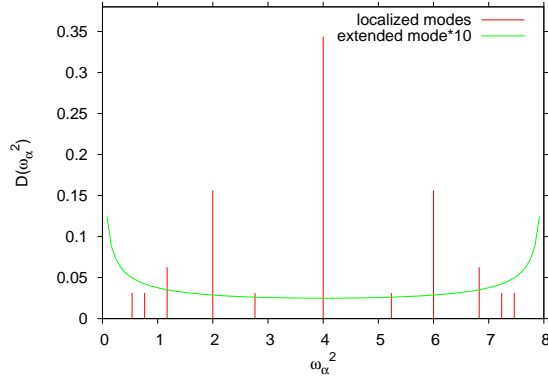


Figure 3.9: Plot of $D(\omega_\alpha^2)$ vs ω_α^2 for $N = 5$ and $M \rightarrow \infty$

We saw that there are always a set of 2^{N-2} set of M eigenmodes, 2^{N-3} set of $2M$ eigenmodes, 2^{N-4} set of $3M$ eigenmodes and 2^{N-5} set of $4M$ eigenmodes. This pattern continues for higher values of N as well. The reason for this is as follows: Let will look at the case of $N = 5$ a little more carefully. The eigenvalues of the F operators are denoted as $(f_1, f_2, f_3, f_4, f_5)$, where f_i is $+$ if eigenvalue of $F_i = +1$ and f_i is $-$ if eigenvalue of $F_i = -1$.

1) Case of all five F 's being negative:

($-$, $-$, $-$, $-$, $-$): There is exactly one possible way to do it, which gives us M modes.

2) Case of four F 's being negative:

2a) ($-$, $.$, $.$, $.$, $-$): We need to set 2 more F 's equal to -1 and we have three operators left " F_2, F_3 and F_4 ". Hence there are ${}^3C_2 = 3$ ways to do it, which gives us 3 sets of M modes.

2b) ($-$, $.$, $.$, $-$, $+$): We cannot set $F_5 = -1$ since that will again result in case 2a. We still need to set 2 more F 's equal to -1 and we have exactly two operators left " F_2 and F_3 ". Hence there are ${}^2C_2 = 1$ ways to do it, which gives us a set of $2M$ modes.

3) Case of three F 's being negative:

3a) ($-$, $.$, $.$, $.$, $-$): We need to set 1 more F equal to -1 and we have three operators left " F_2, F_3 and F_4 ". Hence there are ${}^3C_1 = 3$ ways to do it, which gives us 3 sets of M modes.

3b) ($-$, $.$, $.$, $-$, $+$): We need to set 1 more F equal to -1 and we have exactly two operators left " F_2 and F_3 ". Hence there are ${}^2C_1 = 2$ ways to do it, which gives us a 2 sets of $2M$ modes.

3c) ($-$, $.$, $-$, $+$, $+$): We need to set 1 more F equal to -1 and we have exactly one operators left namely F_2 . Hence there are ${}^1C_1 = 1$ way to do it, which gives us a set of $3M$ modes.

4) Case of two F 's being negative:

4a) ($-$, $.$, $.$, $.$, $-$): We need to set no more F 's equal to -1 . Hence, we can think of this as if there are ${}^3C_0 = 1$ way to do it, which gives us a set of M modes.

4b) ($-$, $.$, $.$, $-$, $+$): We need to set no more F 's equal to -1 . Hence, we can think of

this as if there are ${}^2C_0 = 1$ way to do it, which gives us 1 set of $2M$ modes.

4c) $(-, ., -, +, +)$: We need to set no more F 's equal to -1 . Hence, we can think of this as if there are ${}^1C_0 = 1$ way to do it, which gives us a set of $3M$ modes.

4c) $(-, -, +, +, +)$: We need to set no more F 's equal to -1 . Hence, we can think of this as if there are ${}^0C_0 = 1$ way to do it, which gives us a set of $4M$ modes.

So in all, we see that there is a set of $4M$ modes, two sets of $3M$ modes, four sets of $2M$ modes and eight sets of M modes. This put together with the modes arising from 5C_0 and 5C_1 give us the $32M$ modes. We get $(N+1) \times M$ modes from NC_0 and NC_1 . The other binomial coefficients give $\sum_{k=2}^N 2^{N-k}(k-1)M$ modes. This is an arithmetic-geometric series the sum of which is $(2^N - N + 1)M$. This when added to the $(N+1)M$ modes coming from NC_0 and NC_1 give us exactly $2^N \times M$ modes.

Note that whenever a set of mM modes are generated, we get a set of m eigenvalues which are each M fold-degenerate. These m modes are the eigenvalues of the following $m \times m$ tridiagonal matrix A(Equation(3.12)):

$$A_{ij} = \begin{cases} 2 & \text{for } |i - j| = 1 \\ 0 & \text{otherwise} \end{cases} \quad (3.12)$$

The eigenvalues of this matrix are given by(see Appendix(.1))(Equation(3.13)):

$$\lambda_s = 4\cos\left(\frac{\pi s}{m+1}\right), s = 1, 2, \dots, m \quad (3.13)$$

The sum of the eigenvalues is always 0 since $\text{trace}(A) = 0$. The eigenvalues are also symmetric about 0 since $\cos(\pi - \theta) = -\cos(\theta)$. Also note that within a set of m modes, no eigenvalue repeats. Also since $-4 \leq \lambda_s \leq 4$, $\omega_\alpha^2 \in [0, 8]$.

Whenever we have an odd set of modes, we always have $\lambda = 0$ as one of the eigenvalues by symmetry. So this eigenvalue has a degeneracy of at least $2^{N-2} + 2^{N-4} + 2^{N-6} + \dots$ (summing over all the m modes). This sum equals $2^N/3$ for large N . We say at least because we are ignoring the eigenvalues generated from NC_0 and NC_1 . Now in the limit of $N \rightarrow \infty$, we can ignore the $({}^NC_0 + {}^NC_1) = N + 1$ eigenvalues in comparison to the 2^N . Hence, $D(4) = \lim_{N \rightarrow \infty} \frac{2^N}{3 \cdot 2^N} = 1/3$.

Similarly, the eigenvalue $\lambda = +2$ and $\lambda = -2$ will occur with a degeneracy of $2^{N-3} + 2^{N-6} + 2^{N-9} + \dots$, which in the limit of large N implies that $D(6) = D(2) = 1/7$.

The other values for $D(\omega_\alpha^2)$ as follows: $D(4 - 2\sqrt{2}) = D(4 + 2\sqrt{2}) = 1/15$
 $D(3 - \sqrt{5}) = D(3 + \sqrt{5}) = D(5 - \sqrt{5}) = D(5 + \sqrt{5}) = 1/31$
 $D(4 - 2\sqrt{3}) = D(4 + 2\sqrt{3}) = 1/63$.

Hence, the spectrum in the thermodynamic limit of $N \rightarrow \infty$ (and consequently $M \rightarrow \infty$) looks like(Figure(3.10)). These set of values alone account for more than 90% of the total eigenvalues. Hence, $D(\omega_\alpha^2)$ can be written as

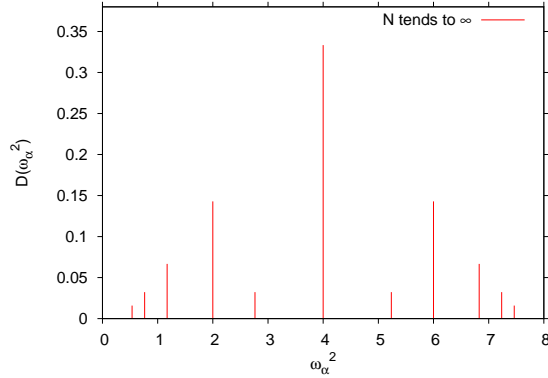


Figure 3.10: Plot of $D(\omega_\alpha^2)$ vs ω_α^2 for $N, M \rightarrow \infty$. We only show eigenvalues which have a weight $\geq 1/63$

$$D(\omega_\alpha^2) = \frac{1}{3}\delta(\omega_\alpha^2 - 4) + \frac{1}{7}\delta(\omega_\alpha^2 - 2) + \frac{1}{7}\delta(\omega_\alpha^2 - 6) + \dots \quad (3.14)$$

We can clearly see that eigenvalues coming from mM modes but not coming from kM modes where $k < m$ modes has a fractional frequency $1/(2^{m+1} - 1)$ which in the limit of large m goes to 2^{-m} .

The integral of the spectral density function D is called the cumulative distribution function F and is defined as:

$$F(\omega_\alpha^2) = \int_0^{\omega_\alpha^2} D(\omega_1^2) d\omega_1^2 \quad (3.15)$$

$F(\omega_\alpha^2)$ gives us the fractional number of modes with frequencies less than equal to ω_α^2 . We wish to know what $F(\omega_\alpha^2)$ is as $F(\omega_\alpha^2) \rightarrow 0$. If we ignore the extended modes the smallest eigenvalue from a set of mM modes is $4 - 4\cos(\frac{\pi}{m+1}) = 8\sin^2(\frac{\pi}{2(m+1)}) = \omega_0^2$. Now as explained above for the limit of large m , the fractional degeneracy of this mode is 2^{-m} and these modes will only occur for kM modes where $k \geq m$. For large m we can approximate the sine by which we get $m^2 \sim \frac{1}{\omega_0^2}$. Therefore the fractional number of eigenvalues which are less than ω_0 are given by

$$F(\omega_0^2) = \int_m^\infty 2^{-x} dx \quad (3.16)$$

Therefore, we get:

$$F(\omega_0^2) \sim 2^{-m} \sim \exp(-A\sqrt{\frac{1}{\omega_0^2}}) \quad (3.17)$$

where $A = \ln 2$. Similarly when $\omega_1^2 \approx 8$, $F(\omega_1^2)$ goes as:

$$F(\omega_1^2) \sim 1 - \exp(-A\sqrt{\frac{1}{(8 - \omega_1^2)}}) \quad (3.18)$$

Chapter 4

Summary and Conclusions

Graphical enumeration techniques such as series expansions and diagram counting are an extremely useful tool to handle problems in statistical physics. We enumerated the number of self-avoiding walks(SAWs) and self-avoiding polygons(SAPs) on a spider-web network using a depth-first search with backtracking algorithm. The series we get for the number of SAWs and SAPs are new. The High-temperature expansion of the Ising model was implemented on the same network and we calculated the expansion of the free energy up to $\mathcal{O}(x^{10})$, where $x = \tanh(\beta J)$ is the high-temperature expansion parameter. Finally, we look at the normal modes of the spring problem on this graph. An exact procedure to find the complete vibrational spectra for a finite number of sites in a layer of the lattice is illustrated. Qualitative features of the spectra in the thermodynamic limit are also discussed. The spectra has not been reported in literature.

.1 The eigenvalues of a special tridiagonal matrix[[15]]

We want to find the eigenvalues of $m \times m$ tridiagonal matrix of the form(Equation(1)):

$$A_{ij} = \begin{cases} a & \text{for } |i - j| = 1 \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

We solve the eigenvalue problem $Ax = \lambda x$, where $\lambda \in \mathbf{R}$ and $x = [x_1, x_2, \dots, x_m]^T \neq 0$. The eigenvalue problem for A results in the following difference equation:

$$\begin{aligned} ax_{j-1} + ax_{j+1} &= \lambda x_j, j = 1, \dots, m \\ x_0, x_{m+1} &= 0 \end{aligned} \quad (2)$$

We try a series solution of the form cr^j and find that the solution of such an equation can be expressed in terms of the roots of the characteristic polynomial which in this case is:

$$p(r) = ar^2 - \lambda r + a \quad (3)$$

Assume the the roots of p are given as r_1 and r_2 . Then the solution of the difference equation is:

$$x_j = c_1 r_1^j + c_2 r_2^j \quad (4)$$

for $j = 0, \dots, m + 1$. We determine the unknown coefficients by using the initial condition:

$$x_0 = c_1 + c_2 = 0 \Leftrightarrow c_2 = -c_1 \quad (5)$$

which gives

$$x_j = c_1(r_1^j - r_2^j), j = 0, \dots, m + 1 \quad (6)$$

Furthermore we have

$$x_{m+1} = c_1(r_1^{m+1} - r_2^{m+1}) = 0 \quad (7)$$

since $x \neq 0$ we need $c_1 \neq 0$, so we find that

$$r_1^{m+1} = r_2^{m+1} \Leftrightarrow \left(\frac{r_1}{r_2}\right)^{m+1} = 1 \quad (8)$$

We can eliminate r_2 from this equation using the product of roots $r_1 r_2 = 1$. Thus:

$$\left(\frac{r_1}{r_2}\right)^{m+1} = \left(\frac{r_1^2}{r_1 r_2}\right)^{m+1} = \left(\frac{r_1^2}{1}\right)^{m+1} = 1 \quad (9)$$

The roots of this quadratic polynomial are in general complex, so the above equation can be written in the form:

$$r_1^2 = e^{2\pi i \left(\frac{s}{m+1}\right)}, s = 1, \dots, m \quad (10)$$

We immediately see that the possible roots are:

$$\begin{aligned} r_{1,s} &= e^{\pi i \left(\frac{s}{m+1}\right)} \\ r_{2,s} &= e^{-\pi i \left(\frac{s}{m+1}\right)}, \end{aligned} \quad (11)$$

where $s = 1, \dots, m$. For every $s = 1, \dots, m$ there is thus an eigenvalue λ_s given by the equation (use the sum of roots):

$$\begin{aligned} r_{1,s} + r_{2,s} &= \frac{\lambda_s}{a} \\ 2\cos\left(\frac{\pi\iota s}{m+1}\right) &= \frac{\lambda_s}{a} \\ \lambda_s &= 2a\cos\left(\frac{\pi\iota s}{m+1}\right) \end{aligned} \tag{12}$$

In our case $a = 2$, hence the eigenvalues turned out to be $\lambda_s = 4\cos\left(\frac{\pi\iota s}{m+1}\right)$. The corresponding eigenvector is:

$$x_{s,j} = 2\iota c_1 \sin\left(\frac{\pi\iota j s}{m+1}\right) \tag{13}$$

i.e

$$x_s = \left[\sin\left(\frac{\pi\iota s}{m+1}\right), \sin\left(\frac{\pi\iota 2s}{m+1}\right), \dots, \sin\left(\frac{\pi\iota m s}{m+1}\right) \right] \tag{14}$$

for $s = 1, \dots, m$.

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