IIT BOMBAY

DIMER MODEL

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Chapter 1

Introduction

In Statistical Mechanics, a quasi-crystalline model is defined as a regular lattice of points (sites or vertices) connected by bonds such that the lattice is fully covered with monomers and polymers. If the energy of mixing is zero, the thermodynamic properties of this system can be calculated from the "combinatorial factor", i.e. the number of ways of arranging given numbers of monomers and polymers on the lattice.

In this report, we will deal with a very special case of the quasi-crystalline model, the Dimer Model. In the Dimer Model, a planar bipartite lattice is considered such that each lattice site is covered by exactly one dimer. There are no interactions other than "hard core" infinite repulsive forces between dimers, the problem reduces to the determination of the number configurations of the lattice, which provides us the partition function using which we can derive all the thermodynamic properties of the system.

The dimer Model occurs experimentally when a diatomic gas is adsorbed onto a crystalline substrate [1]. We will see that the Dimer Problem is equivalent to the Domino Tiling Problem which arises in the cell-cluster theory of the liquid state [2]. Recent generalizations of the problem include quantum dimer models with applications to pseudo-gap metals and superconductors [3].

Definitions

We consider a graph $G = (V, E)$ where V is the set of vertices and E is the set of edges. A dimer covering of a perfect matching C on G is a subset of edges which covers all the vertices, and where no overlap occurs between two edges. We will be deal only with bipartite planar graphs, in which each vertex (except those at boundaries) have 4 edges.

In the physical system, these vertices corresponds to lattice sites on a square planar graph, and dimers are present at the edges.
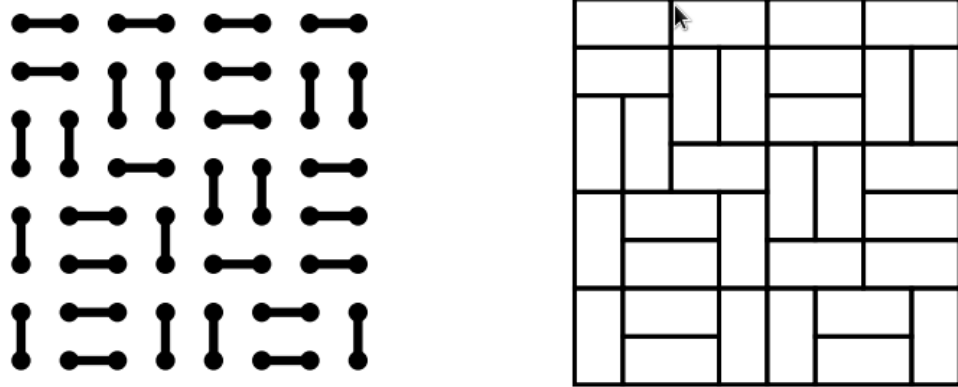

FIGURE 1.1: a dimer configuration and corresponding domino tiling(Fig 1 from [9])

The Dimer Problem on square lattice is equivalent to the Domino Tiling Problem, in which one considers the possible configurations of tiling a square grid with 2 1 rectangles.

Chapter 2

Combinatorial Approach

In this chapter, we will look at the exact calculations in Dimer model. Most of the work presented here has been done by Kasteleyn[4,5] and Fisher[6,7]. We will first consider the free boundary conditions and later look at the partition function for periodic boundary conditions(torus).

2.1   Kastelyn Theory

Let us consider a rectangular lattice with n rows and m coulmns. The lattice poitns are labelled by cartesian coordinates (r, s) where $r \in 1, 2, ..., m, s \in 1, 2, ..., n$. The toal number of the vertices is $N = mn$. If x, y are the activities of horizontal dimers and vertical dimers respectively, we can define the partition function as

$$Z = \sum_{N_x + N_y = (N/2)} g_{mn}(N_x, N_y) x^{N_x} y^{N_y} \tag{2.1}$$

where $g_{mn}(N_x, N_y)$ is the number of configuration with N_x horizontal and N_y vertical dimers. To get the number of configurations, we can put $x = y = 1$.

We number the lattice points by $k = k(r, s)$ where the value of k runs from 1 to N on the lattice points. Let $k = k(r, s)$ and $k' = k(r', s')$. We further define an anti-symmetric adjacency matrix A given by

$$A_{kk'} == \begin{cases} \alpha_{rs}x & r' = r+1, s' = s \\ \beta_{rs}y & r' = r, s' = s+1 \\ 0 & |r - r'| = |s - s'| \\ 0 & |r - r'| > 1 \, or \, |s - s'| > 1 \end{cases}$$

The elements of A for which $r' = r - 1, s' = s$ and $r' = r, s' = s - 1$ are fixed due to anti-symmetry of A. By definition of pfaffian, we have

$$pf(A) = \frac{1}{(\frac{N}{2})!2^{(\frac{N}{2})}} \sum_\sigma sgn(\sigma) A_{k_{1\sigma}k_{2\sigma}} A_{k_{3\sigma}k_{4\sigma}}...A_{k_{(N-1)\sigma}k_{N\sigma}} \quad (2.2)$$

where $(k_{1\sigma}, k_{2\sigma}, k_{3\sigma}...., k_{N\sigma}) = \sigma(1, 2, 3...., N)$ is the permutation of $(1, 2, 3...., N)$ and $sgn(\sigma)$ is the 'signature' of σ.

Each non-zero term in the expansion of $pf(A)$ denotes a possible configuration as each non-zero $A_{k_{i\sigma}k_{j\sigma}}$ denotes a presence of the bond between $k_{i\sigma}$ $k_{j\sigma}$ and all k are distinct.

However, there are several permutations which gives the same dimer configurations. These are those in which positions of different A_{ij} are interchanged, or in which i and j of A_{ij} are interchanged. The first type of interchange results in $(\frac{N}{2})!$ similar terms and the second type of interchange results in $2^{(\frac{N}{2})}$ similar terms. Hence, for each dimer configuration, there are $(\frac{N}{2})!2^{(\frac{N}{2})}$ terms in the expansion of $pf(A)$. Fortunately, we can show that all these terms have same sign.

In first type of interchange, suppose A_{ij} gets interchanged with A_{lm}. Then $sgn(\sigma)$ remains fixed as $\sigma' = (il)(jm)\sigma$. In the second type, suppose A_{ij} becomes A_{ji}. Since $A_{ji} = -A_{ij}$ and $\sigma' = (ij)\sigma$ there are two sign changes which cancels out. Therefore, the terms representing same configurations in $pf(A)$ have same sign and we can sum them up.

We will consider the mappings $k(r, s)$ such that all the even or black sites ($r + s$ even) have even k and all the odd or white sites ($r + s$ odd) have odd k. Then, using the fact that A_{ij} is non-zero if i, j have opposite parity, we can express the pfaffian in terms of distinct configurations as

$$pf(A) = \sum_\sigma sgn(\sigma) A_{k_{1\sigma}2} A_{k_{3\sigma}4}...A_{k_{(N-1)\sigma}N} \quad (2.3)$$

where $(k_{1\sigma}, k_{3\sigma}, k_{5\sigma}...., k_{(N-1)\sigma}) = \sigma(1, 3, 5...., N-1)$ and N is odd.

We want to assign signs to elements of A such that each term in equation 2.3 has the same sign. For this, we define a Kasteleyn's orientation on the square lattice in which each edge is assigned a direction. If k, k' are two adjacent vertices on the graph, then $A_{kk'}$ is positive if the edge is oriented from k to k', and negative if the edge is oriented from k' to k. The construction of such an orientation is given below.
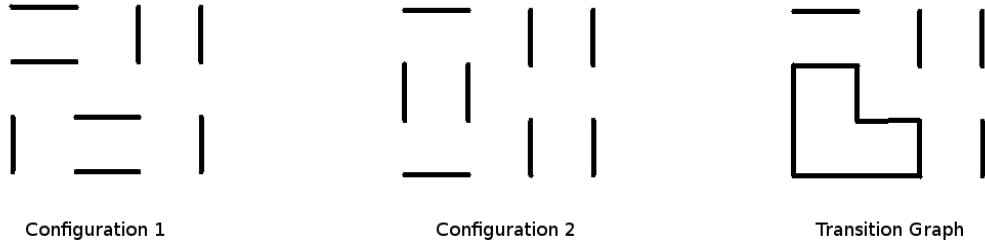

FIGURE 2.1: Two Dimer coverings and their transition graph.

Consider 2 distinct dimer coverings Γ_1 and Γ_1. If we superimpose the two coverings as shown in fig 2.1, the dimers will either coincide or form a closed loop. Therefore, the terms in the expansion of $pf(A)$ vary only for the dimers on the loop. Now, suppose Γ_1, Γ_2 differ only on one cycle C. If we prove that the terms for Γ_1, Γ_2 have same sign for any C, we can say that all terms have same sign.

Let $\sigma\Gamma_1 = \Gamma_2$ and $2s$ be the length of C. We can decompose $C = C_1 + C_2$ such that C_1 consists of dimers in configuration Γ_1 while C_2 consists of dimers in configuration Γ_2. We know that $sgn(\sigma) = (-1)^{s+1}$ and therefore we want the following condition to be satisfied-

$$\text{Product of signs in } C_1 = (-1)^{s+1} * \text{ Product of signs in } C_2$$

Where "Product of Signs" mean the product of signs of the elements of A encountered while moving anticlockwise on the cycle C. Or equivalently,

$$\text{Product of signs in } C = (-1)^{s+1}$$

Using the fact that each cycle encloses even number of points(each enclosed point is on a common dimer or on a closed cycle of even length), it is easy to prove that the orientation given in figure 2.2 satisfy the required condition for every cycle. It must be mentioned that Kasteleyn orientation is not unique.

For the convention $k = r + (s - 1) * m$, using the

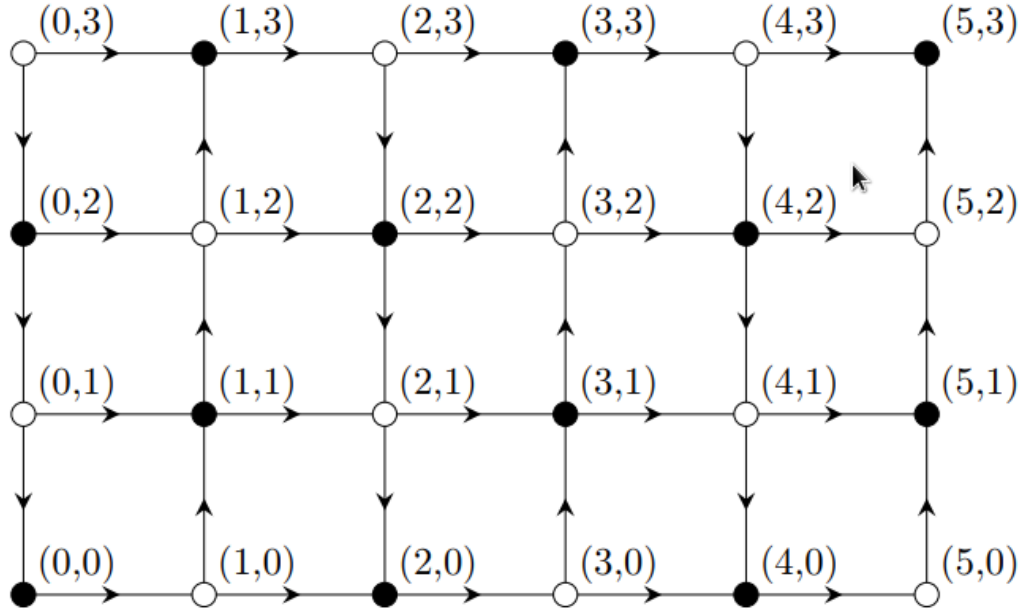$$\alpha_{rs} = 1, \beta_{rs} = (-1)^r \tag{2.4}$$

FIGURE 2.2: Kasteleyn's orientation.

Since all the terms have save sign, we have the partition function given by

$$Z = |pf(A)| \tag{2.5}$$

To get the number of configurations, set $x = y = 1$ in equation 2.5.

2.2   Kasteleyn's matrix

Let us look at a specific convention to define the Adjacency matrix which allows us to perform computations more easily. For this, we break up the lattice in odd points and even points, and number the odd points by $1, 2, 3, ..., (N/2)$ and even points by $1', 2', 3', ..., (N/2)'$ as shown in the figure. We define a $N/2 \times N/2$ kasteleyn's matrix K such that the element K_{ij} corresponds to dimer from i to j'.

We set K by

$$K_{ij} == \begin{cases} 1 & \text{(i,j') is a horizontal dimer} \\ i & \text{(i,j') is a vertical dimer} \\ 0 & \text{i and j' is not connected by a dimer} \end{cases}$$

It is easy to see that

■ 1   ■ 1'   ■ 2   ■ 1

■ 3   ■ 3'   ■ 4   ■ 4'

■ 5   ■ 5'   ■ 6   ■ 6'

■ 7   ■ 7'   ■ 8   ■ 8'

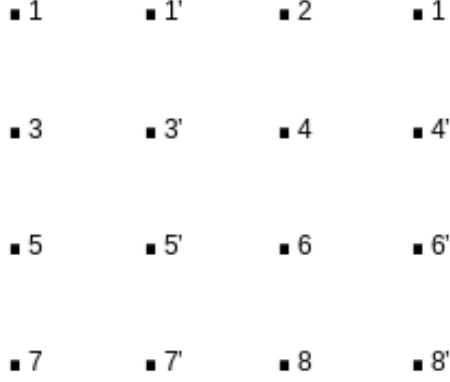FIGURE 2.3: Numbering of Lattice points.

$$det(K) = \sum_{\sigma} sgn(\sigma) K_{1,\sigma_1} K_{2,\sigma_2} ... K_{(N/2),\sigma_{(N/2)}} \tag{2.6}$$

where $(\sigma_1, \sigma_2, ..., \sigma_{(N/2)}) = \sigma(1, 2, ..., (N/2))$. Each non zero term in the expansion of $det(K)$ uniquely corresponds to a dimer configurations. Again, we need to prove that each term has the same sign. For the proof, I will use the following lemma which can be easily proved using induction-

Lemma *Given a cycle of length $2s$ enclosing n points, the alternating product of signs around this cycle is $(-1)^{1+s+n}$.*

Again considering two configurations Γ_1, Γ_2 differing only at a single cycle C and using the fact that $sgn(\sigma) = (-1)^{s+1}$ along with the stated lemma, we get the net change of sign between Γ_1 and Γ_2 is $(-1)^{s+1} * (-1)^{s+n+1}$. But since the number of points inside any closed loop is even, Γ_1 and Γ_2 have same sign in the expansion of $det(K)$. Therefore the number of configurations is given by $Z = |det(K)|$.

2.2.1 Explicit Computation for Rectangular Lattice

We now compute Z explicitly using the Kasteleyn matrix. First, we define the adjacency matrix A by

$$A = \begin{bmatrix} 0 & K^T \\ K & 0 \end{bmatrix} \tag{2.7}$$

If we renumber the white points such that $i' \rightarrow (N/2) + i$, then the elements of A are given by

$$A_{ij} == \begin{cases} 1 & \text{(i,j) is a horizontal dimer} \\ i & \text{(i,j) is a vertical dimer} \\ 0 & \text{i and j is not connected by a dimer} \end{cases}$$

Let $k = k(r, s)$ be the enumeration of the lattice points. The vectors $v^{ab} \in \mathbb{C}^N$ defined by

$$v_k^{ab} = \sin \frac{\pi r a}{m+1} \sin \frac{\pi s b}{n+1}$$

are the eigenvectors of A with eigenvalues given by

$$\lambda^{ab} = 2 \cos \frac{\pi a}{m+1} + 2i \cos \frac{\pi b}{n+1} \tag{2.8}$$

The set of eigenvectors v^{ab} where $a \in 1, 2, ..., m, b \in 1, 2, ..., n$ are orthogonal and therefore spans the eigenbasis for A. The matrix A is a normal matrix while $KK^\dagger$ is a real symmetric matrix. Therefore,

$$Z_{mn} = |pf(A)| = |det(K)| = |\prod_{a=1}^{m} \prod_{b=1}^{n} \lambda^{ab}| = \left| \prod_{a=1}^{m} \prod_{b=1}^{n} 2 \left(\cos \frac{\pi a}{m+1} + i \cos \frac{\pi b}{n+1} \right) \right| \tag{2.9}$$

Using this, the number of domino tilings of the chessboard can be found to be $Z_{8,8} = 12988816$. For large m, n,

$$\lim_{\substack{m \to \infty \\ n \to \infty}} \frac{1}{mn} \log Z_{mn} = \frac{1}{2\pi^2} \int_0^\pi \int_0^\pi log(2 \cos \theta + 2i \cos \phi) d\theta d\phi = \frac{G}{\pi}$$

where $G \approx 0.916$ is the Catalan's constant. The *Molecular freedom* or number of configurations per dimer is then given by $exp(2G/\pi)$.

2.3   Probability

Let us look at the number of configurations with a dimer between two specified points j and k'. The number of such configurations is given by $|det(K')|$ where matrix K is formed by putting all elements row j and column k except K_{jk} to be equal to zero. But then $det(K')$ is equal to C_{jk} (Cofactor). Therefore, the probability of occurance of the dimer is given by

$$P((j,k')) = \frac{|C_{jk}|}{|det(K)|} = |K_{kj}^{-1}| \tag{2.10}$$

It is possible to extend this approach to obtain the probability of having dimers on a set of given edges. Let the set of edged be $S = (j_1, k_1'), (j_2, k_2'), ..(j_p, k_p')$. Therefore, the number of configurations is equal to $|det(K_S')|$ where K_S' is the matrix formed by removing the rows $j_1, j_2...j_p$ and columns $k_1, k_2...k_p$ from A. Let K_S^{-1} be the matrix formed by taking only the rows $k_1, k_2...k_p$ and columns $j_1, j_2...j_p$ in K^{-1}. We can then write the probability of having the dimers at set S to be

$$P(S) = \left| \frac{det(K_S')}{det(K)} \right| = |det K_S^{-1}| \tag{2.11}$$

where the last equality is a mathematical identity.

Considering two dimers at (j_1, k_1') and (j_2, k_2') we get the conditional probability of presence of dimer 2 if dimer 1 is already present as

$$P(2|1) = \frac{P(2,1)}{P(1)} = \left| \frac{K_{k_1 j_1}^{-1} K_{k_2 j_2}^{-1} - K_{k_1 j_2}^{-1} K_{k_2 j_1}^{-1}}{K_{k_1 j_1}^{-1}} \right|$$

2.4 Simulation Result

For various lattices, the Probabilities were computed using Kasteleyn theory. Various plots are shown here for the lattice of size $11 * 12$ dimensions. To make it easier to visualize, the lattice was rotated by $45°$ and grid was made so that each edge will lie in 1 box. The lattice after rotation is shown below.

Let us label the reference edge by y (shown in plots by green color). The following quantities were computed for all the other edges labelled by x.

Probability of occupancy of single dimer

Joint probability of two dimers($P(x,y)$)

Conditional Probability of second dimer if 1 is already present($P(x|y)$)

Normalised Joint Probability $(\frac{P(x,y)}{P(x)P(y)})$
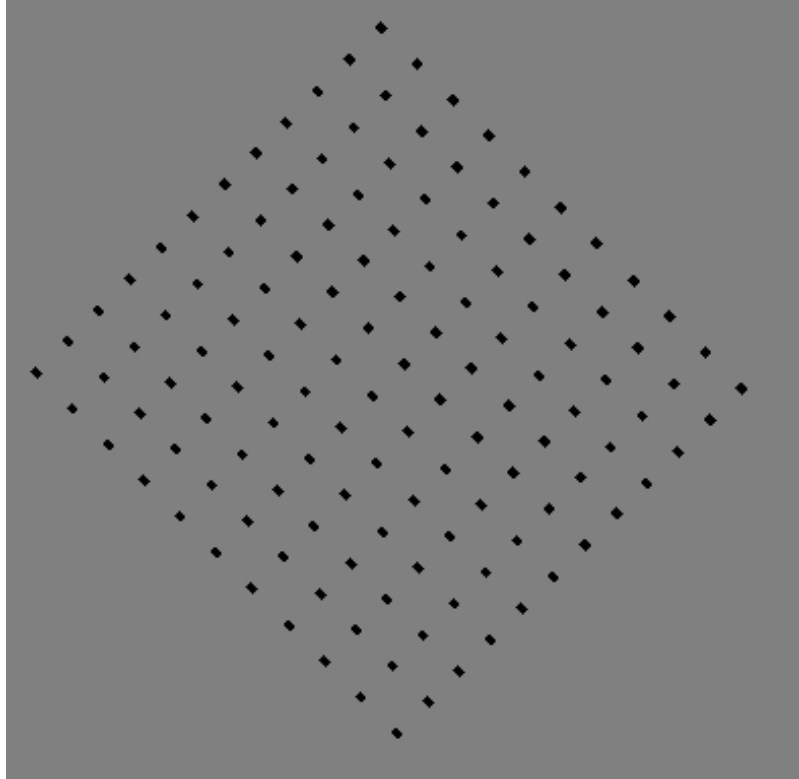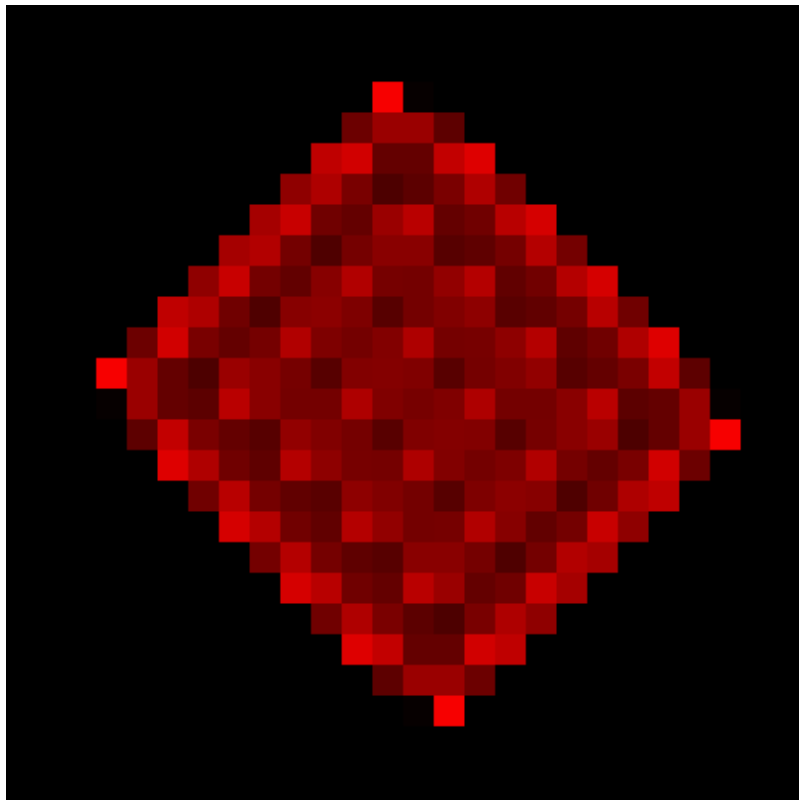
Correlation $(P(x,y) - P(x)P(y))$

FIGURE 2.4: 11*12 lattice

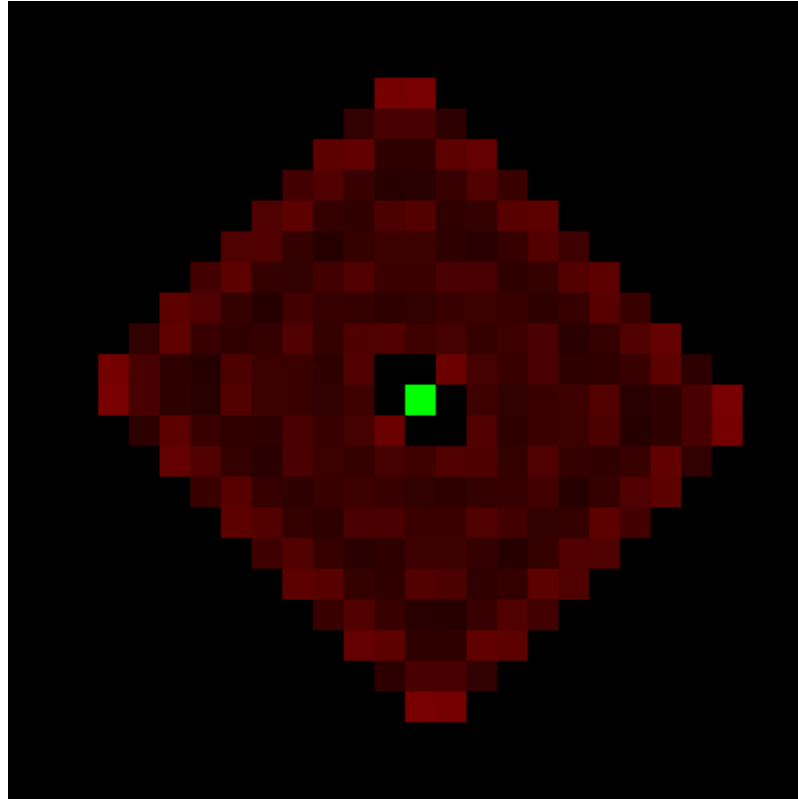FIGURE 2.5: Probability of occupancy of single dimer $(P(x))$

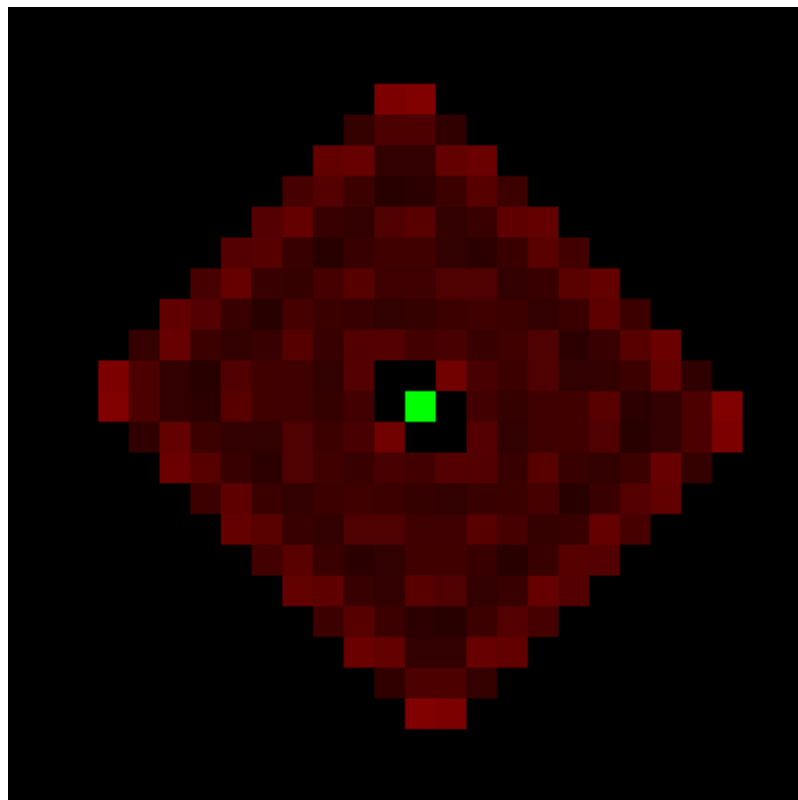FIGURE 2.6: Joint probability of two dimers($P(x,y)$)

FIGURE 2.7: Conditional Probability of second dimer if 1 is already present($P(x|y)$)
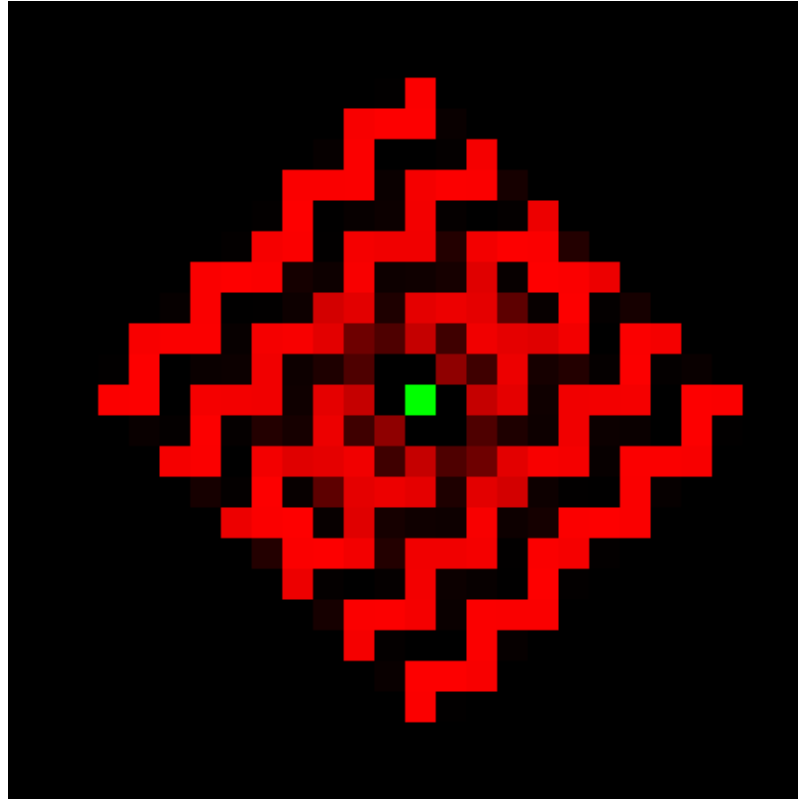
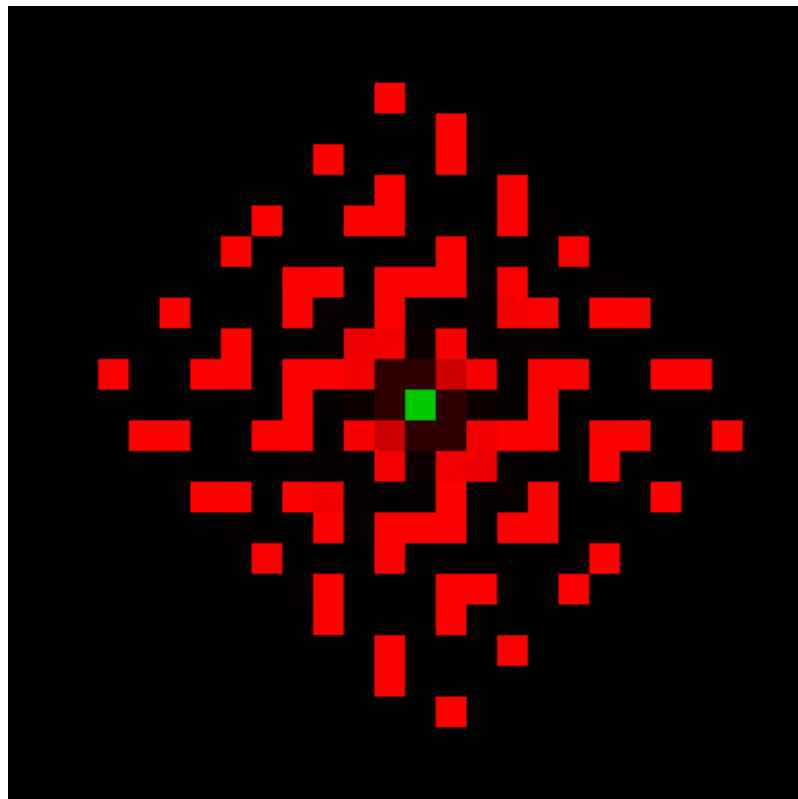FIGURE 2.8: Normalised Joint Probability ($\frac{P(x,y)}{P(x)P(y)}$)

FIGURE 2.9: Correlation ($P(x,y) - P(x)P(y)$)

In the plots shown above, the intensity of red color is directly proportional to the computed quantity for that plot. The maximum and minimum values for a $11 * 12$ lattice and for $101 * 102$ lattice are tabulated below.

Parameter	Max Value(11×12)	Max Value(101×102)
$P(x)$	0.515	0.500
$P(x,y)$	0.119	0.130
$P(x\|y)$	0.508	0.500
$\frac{P(x,y)}{P(x)P(y)}$	2.572	1.955
$P(x,y) - P(x)P(y)$	0.061(Min: -0.064)	0.068(Min: -0.062)

2.5   Torus

We have been looking only in the scenario of free boundary conditions till now. Let us shift the focus to the case of Periodic boundary conditions. The Kasteleyn theory is not applicable as the transition graph can now wind across the lattice. In particular, there does not exist a Kasteleyn orientation of the graph. Fortunately, Kasteleyn[4] developed a theory for Torus in which the partition function Z can be expressed as combination of 4 determinants.

Let us consider the four different orientations of the lattice as shown in Figure 2.9 and define their corresponding "Adjacency Matrices" given by D_{++}, D_{+-}, D_{-+} and D_{--}. The first orientation D_{++} is just the Kasteleyn orientation endowed with periodic boundary conditions while The other three orientations are obtained by applying anti-periodic boundary conditions in one or both directions.
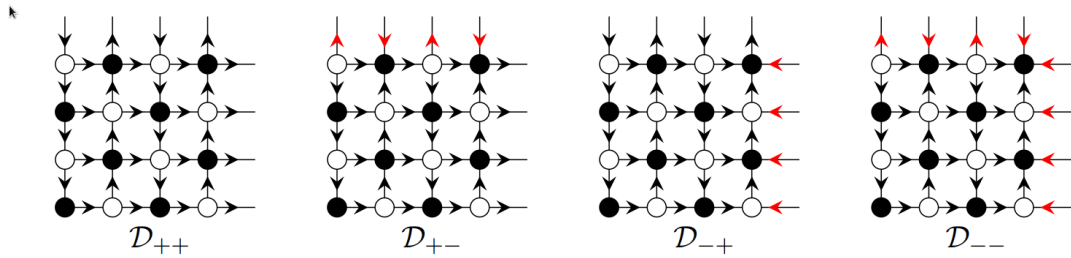

FIGURE 2.10: Orientations of the square lattice with periodic boundary conditions.

Consider an reference configuration Γ_0 and consider it's transition cycles with all other configurations. Let us divide all the configurations in 4 disjoint classes. Class (e, e) comprises dimer configuration for which the set of transition cycles wrap both the horizontal and vertical directions an even number of times. Similarly we define classes $(o, e), (e, o)$ and (o, o), where $e = $ even and $o = $ odd, and the first (resp. second) symbol refers to

the horizontal (resp. vertical) direction. Also, break up the partition function into four components $Z = Z_{ee} + Z_{oe} + Z_{eo} + Z_{oo}$ where $Z_{ee}, Z_{oe}, Z_{eo}, Z_{oo}$ are the contributions from the respective classes.

By taking one example of a configuration in each class and arguing that the 'internal distortions' in Transition cycle do not change the sign much, we can see that $det(D_{++})$ has the correct sign only for the class (e, e). Using the smae method, we arrive at the following relations;

$$|det(D_{++})| = Z_{ee} - Z_{oe} - Z_{eo} - Z_{oo}$$

$$|det(D_{+-})| = Z_{ee} - Z_{oe} + Z_{eo} + Z_{oo}$$

$$|det(D_{-+})| = Z_{ee} + Z_{oe} - Z_{eo} + Z_{oo}$$

$$|det(D_{--})| = Z_{ee} + Z_{oe} + Z_{eo} - Z_{oo}$$

and therefore we have

$$Z = \frac{1}{2}(-|det(D_{++})| + |det(D_{+-})| + |det(D_{-+})| + |det(D_{--})|) \qquad (2.12)$$

Chapter 3

Mean Field Theory

The focus of this chapter will be on "mean-field theory" or "the continuum theory" of the dimer model. In coarse graining, much information about the system is discarded and only their "average" is used for calculation. The calculations become simpler, and fortunately we can gain many useful physical insights by studying the coarse grained model.

For the coarse grained model to be physically relevant, we must restrict ourselves to distances much larger than the lattice constant and also much smaller than the system size so as to ignore the boundary effects. Unlike previous section, we will be dealing mostly with lattices having periodic boundary conditions.

3.1   Coarse Graining

We define a magnetic field $B(\vec{x}, \hat{n})$ on the lattice point $\vec{x}$ in direction $\hat{n}$, pointing from odd vertices to even vertices. If a dimer is present at $\vec{x}$ facing towards $\hat{n}$, then $B(\vec{x}, \hat{n}) = 3$ and if it's absent, $B(\vec{x}, \hat{n}) = -1$.

We define the mean field using "Polarization Vector" $P(\vec{r})$ by taking the average of B on a sphere with radius much larger than the lattice constant. On assuming that $P(\vec{r})$ varies smoothly, We obtain the following constraint on $\vec{P}$-

$$B(\vec{r}, \hat{i}) + B(\vec{r}, -\hat{i}) + B(\vec{r}, \hat{j}) + B(\vec{r}, -\hat{j}) = 0 \implies \nabla \cdot \vec{P} = 0 \tag{3.1}$$

The entropy of the system depends on the number if available microstates, or in our case, the dimer configurations. The ground-state entropy density depends on $\vec{P}$. As

we know, the rearrangements (within the flux constraints) must occur along the closed cycles or strings which cross the system. if $\vec{P}_T = \sum_{\vec{r}} \vec{P}(\vec{r})$ is large, most fluxes have a positive component in that direction. On the one hand, if $\vec{P}_T$ is large, most fluxes have a positive component in that direction and the typical string crosses the systema closed string would require half of its fluxes to have a backward component, but such a local gathering of reversed fluxes is unlikely. On the other hand, when $\vec{P}_T$ is near zero, there are many closed strings in any configuration, and hence many rearrangements that preserve $\vec{P}_T$.

The number of configurations $\mathcal{N}(\vec{P}_T)$ with a given polarization is maximum at $\vec{P}_T = 0$ and goes to zero as $\vec{P}_T$ approaches its saturated value. For large volume, local $\vec{P}(\vec{r})$ fluctuates, and the Central Limit Theorem says that the number of ground states for a given $\vec{P}_T$, in a system of large volume V, approaches a Gaussian form

$$\mathcal{N}(\vec{P}_T) \propto exp(-|\vec{P}_T|^2/(2\sigma_P^2))$$

Having the variance $\sigma_P^2 = 1/KV$ where K is the 'stiffness constant' depending on the system. For small $\vec{P}_T$, the entropy density for this system is

$$s(\vec{P}_T) = \lim_{V \to \infty} \frac{ln\mathcal{N}(\vec{P}_T)}{V} \approx s_0 - \frac{1}{2}K|\vec{P}_T|^2 \tag{3.2}$$

Let us now consider local variations in P. By taking motivation from paramagnetism, we can define the total free energy in units of $k_B T$ as

$$F(\vec{P}) = F_0 + \int d^2\vec{r}\frac{1}{2}K|\vec{P}(\vec{r})|^2 \tag{3.3}$$

The above equation along with the Divergence constraint of $\vec{P}$ looks like those of the magnetic field. As we will see later, the analogy is quite useful.

In a particular configuration, a high value of $P_i(\vec{r})$ signifies the presence of a dimer at position $\vec{r}$ in the direction $\hat{i}$. However, this statement is not quite exact, and is only true in an average sense.

3.2   Dimer Correlation

To find the dimer correlations, it is useful to first go to the Fourier space. The equations 3.1 and 3.3 transforms to

$$\vec{q} \cdot \vec{P}(\vec{q}) = 0 \tag{3.4}$$

$$F = \frac{K}{2} \sum |\vec{P}(\vec{q})|^2 \tag{3.5}$$

To find the correlation in Fourier space, we need to find

$$\langle P_u(-\vec{q})P_v(\vec{q'}) \rangle = \frac{1}{\mathcal{N}} \int d\vec{P} \; P_u(-\vec{q})P_v(\vec{q'})e^{-F} = \frac{1}{\mathcal{N}} \int d\vec{P} \; (P_u(-\vec{q})P_v(\vec{q'}))e^{\frac{-K}{2}\sum_{\vec{q}}|P(\vec{q})|}$$

where $\langle \cdot \rangle$ means taking average over all configurations divided by the normalisation factor(number of configurations) and $d\vec{P}$ means the integration is carried out over all modes. Since $\vec{P}(\vec{r})$ is real, $P(-\vec{q}) = P^*(\vec{q})$. By integration on non-participating modes and observing that only modes $\vec{q}$ and $-\vec{q}$ contributes, the above expression simplifies to

$$\langle P_u(-\vec{q})P_v(\vec{q'}) \rangle = \frac{1}{c} \int d\vec{P} \; (P_u(-\vec{q})P_v(\vec{q'}))e^{\frac{-K}{2}|P(\vec{q})|}$$

where c is the normalization constant given by $\sqrt{\pi/K}$ as because of the constraint $\vec{P}(\vec{q}) \perp \vec{q}$, $\vec{P}$ lies in a single direction. Multiplying the equation by $\frac{1}{c} \int d\vec{Q} \; e^{\frac{-K}{2}\sum_{\vec{q}}|Q(\vec{q})|}$ where $\vec{Q}$ has the same direction as $\vec{q}$, and defining vector $\vec{R} = \vec{P} + \vec{Q}$, such that $\vec{R}$ can vary in any direction and $\vec{P} = \vec{R} - (\vec{R} \cdot \hat{q})\hat{q}$. Then we finally get

$$\langle P_u(-\vec{q})P_v(\vec{q'}) \rangle = \frac{\delta_{qq'}}{c^2} \int d\vec{R} \; (R_u - R_a q_a q_u)(R_v - R_b q_b q_v)e^{\frac{-K}{2}|R(\vec{q})|} = \frac{1}{2K}\delta_{qq'}(\delta_{uv} - \frac{k_u k_v}{k^2}) \tag{3.6}$$

By transforming the above equation in the real space and taking the limit of large r, we get the following correlation in the real space.

$$\langle P_u(\vec{0})P_v(\vec{r}) \rangle \propto \frac{1}{Kr^2}(\delta_{uv} - \frac{2r_u r_v}{r^2}) \tag{3.7}$$

Hence, we observe that the correlation is similar to dipole-dipole interaction. The correlation follows power law decay instead of expected exponential decay suggesting that there are long-range effects arising out of the short range interaction between dimers. It was shown by Youngblood [8] that any field defined by equation 3.1 and 3.3 will have the dipole-dipole correlation.

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