

Numerical Studies of Lattice Systems with Twisted Boundary Conditions

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by

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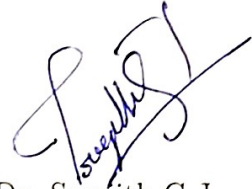
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Certificate

This is to certify that this dissertation entitled Numerical Studies of Lattice Systems with Twisted Boundary Conditions 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 B. Kaarthik Abhinav at Indian Institute of Science Education and Research under the supervision of Dr. Sreejith G.J., Assistant Professor, Department of Physics, during the academic year 2018-2019.

A handwritten signature in blue ink, appearing to read 'Sreejith G.J.', is written over a horizontal line.

Dr. Sreejith G.J.

Committee:

Dr. Sreejith G.J.

Dr. Deepak Dhar

This thesis is dedicated to my family.

Declaration

I hereby declare that the matter embodied in the report entitled Numerical Studies of Lattice Systems with Twisted Boundary Conditions 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 Dr. Sreejith G.J. and the same has not been submitted elsewhere for any other degree.



B. Kaarthik Abhinav

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Abstract

Physical models have been studied with twists being applied to the electric and magnetic fields at the boundary. It is curious to understand what happens if the twist is applied to the lattice, instead of the fields on the lattice[12]. The properties of many models depend on the lattice on which they are studied. We take finite lattices and apply a twist in one direction, and study the behaviour of the models on this lattice. To understand the effect concretely, we perform numerical simulations of two simple systems, the 2D Ising model and 2D dimer model defined on square lattices with twists. We look at the effect of the parity of the twist and the temperature of the model.

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Introduction

Statistical Mechanics studies the emergent properties of the interaction of a large number of entities, typically atoms and molecules. Although we understand the behaviour of isolated atoms to a very good degree and can write down their wavefunctions from the Schrödinger's equation, it is difficult to do so when a large number of particles is involved. The complexity of the problem scales with the number of particles and it is impossible to even write down all the equations for many particles. However, the systems show simpler laws for bulk properties. Statistical mechanics establishes the connection between the microscopic laws and the macroscopic phenomena.

The transport properties of certain topological systems can be related to Chern numbers, which can be implemented by applying a twisted boundary condition on the fields present in the system on a periodic lattice[12]. It is curious to understand what happens when instead of the twisted boundary conditions being present on the fields, they are actually present on the lattice. Of equal interest is to understand the effect of dislocations on the lattice, and the twist on a lattice acts like a column of dislocated atoms. To understand the general effect of twist for various models on the lattice, we can first consider the simplest systems on such twisted lattices.

In equilibrium statistical mechanics, one of the most well studied models is the Ising model, with the exact solution of the 2D Ising Model, provided by Onsager in 1944 and by Kaufman in 1949. In this project, we set out to study some properties of the Ising model when a twist is applied to the boundary condition. For the Ising model, the degrees of freedom live on each site, because of which we expect that the effect of the twist will be minimal. We can look at a slightly more complex model that is closely related to the Ising model, called the dimer model, where the degrees of freedom lie between two adjacent sites, and we expect that the twist must play a more prominent role. The dimer model has

interesting phase transitions and phases depending on the Hamiltonian on the model. This is also a simple model which has been solved exactly for the non-interacting case, and it would be curious to see what happens when a twist is applied.

In Chapter 1, a brief introduction of the two simple models is presented. The work that has been done in these models over the past several decades is also mentioned. The details of the numerical studies for these models using Monte Carlo has been explained in Chapter 2. Once the numerical simulations have been implemented, we can compute various quantities for the models that allows us to study their properties. In Chapter 3, these quantities are described and the implementation of the twist on the lattice has been presented. The results obtained from the numerical simulations is shown in Chapter 4. For the 2D Ising model, an attempt was made to understand the effect of the twist analytically using the solution given by Lieb et.al, which has been presented in Chapter 5. The final chapter contains a brief summary of the work that was done in this project.

Chapter 1

Models in Statistical Physics

In this project, we have worked with the Ising model in 2D and the dimer model in 2D. These models have a long history and have been studied extensively over the past few decades. Our aim is to understand what happens when we apply a *twist* in the lattice. Before we define what we mean by a twist, a brief introduction to the models is helpful. In the next two sections, I give a brief description of the two models and the motivation behind studying them.

1.1 Ising model

This model was proposed by Wilhelm Lenz in 1920 to his student Ernst Ising, who solved the one dimensional version in his PhD thesis. It is a very simple model for ferromagnetism. The one-dimensional Ising model does not show any phase transition, but the 2D Ising model shows a phase transition from ferromagnetic to a paramagnetic phase when the temperature is increased from 0. The zero-field 2D Ising model is one of the very few many-body problems that has been solved exactly till date.

The model consists of a set of points in an n -dimensional lattice, with each lattice site being assigned a spin $\sigma = \pm 1$. If the number of lattice sites is N , the number of different configurations of the system is 2^N . The spins at each site interact with their nearest

neighbours on the lattice, and the Hamiltonian for the system is defined as

$$H = -J \sum_{\langle n.n. \rangle} \sigma_i \sigma_j \quad (1.1)$$

where J is the interaction energy which sets the energy scale. This is the isotropic Ising model where the interaction between spins is the same in all directions. The Ising model has been studied for various kinds of lattices, but for the purpose of this thesis, we will stick to the 2-D square lattice of size $N \times N$, where we can write the Hamiltonian as

$$H = -J \sum_{\substack{i=1,\dots,N \\ j=1,\dots,N}} [\sigma_{i,j} \sigma_{i,j+1} + \sigma_{i,j} \sigma_{i+1,j}]$$

For a given configuration of spins on the lattice, this expression calculates the energy of the system. In order to study the behaviour of this system, we can first write the partition function and then calculate various quantities from there. We know that the partition function can be written as

$$Z(\beta) = \sum_{\{\sigma\}} e^{-\beta H} = \text{Tr}_{\{\sigma\}}(e^{-\beta H}) \quad (1.2)$$

For the two dimensional square lattice with zero external magnetic field, the critical temperature at which the phase transition takes place was found to be $T_c = \frac{2J}{k_B \ln(1+\sqrt{2})}$ by Kramers and Wannier by finding a relation between the low temperature and high temperature expansions. This model has also been solved exactly by Lars Onsager in 1944 using a very sophisticated technique. A lot of work ensued after this to solve the model in a simpler way, with simplifications offered by Kaufman in 1949 and Montroll and Newell in 1953 using spinors and Lie algebras. The history of the model is very nicely summarised by Stephen Brush[3].

1.2 Dimer model

The dimer model has been extensively studied for nearly a century, with the problem being first formulated in the context of adsorption of diatomic molecules on the surface of a metal[7]. The problem of the number of perfect matchings on a planar graph was solved exactly by Kasteleyn in 1961 and Temperley and Fisher in 1961, using Pfaffian techniques.

We study the model of fully-filled dimers on the 2D square lattice with interactions. The square lattice must be of the form $2N \times 2N$ for this model to be fully filled. The dimers lie on the edges between adjacent vertices of the lattice. Each vertex is connected to exactly one other vertex by a dimer. For a $2N \times 2N$ lattice with $4N^2$ sites, the number of dimers would be $2N^2$. For such a system we define the Hamiltonian as:

$$H = v[N^c(\parallel) + N^c(=)] \quad (1.3)$$

Here v sets the interaction energy and we will set it equal to -1. This means that for a given configuration/ matching c , we can calculate the energy of the configuration by counting the number of parallel dimers in the vertical and horizontal directions. Dimers are considered to be parallel to each other if they lie on parallel sides of a plaquette. A typical dimer configuration is shown in Fig 1.1 for a 16×16 lattice.

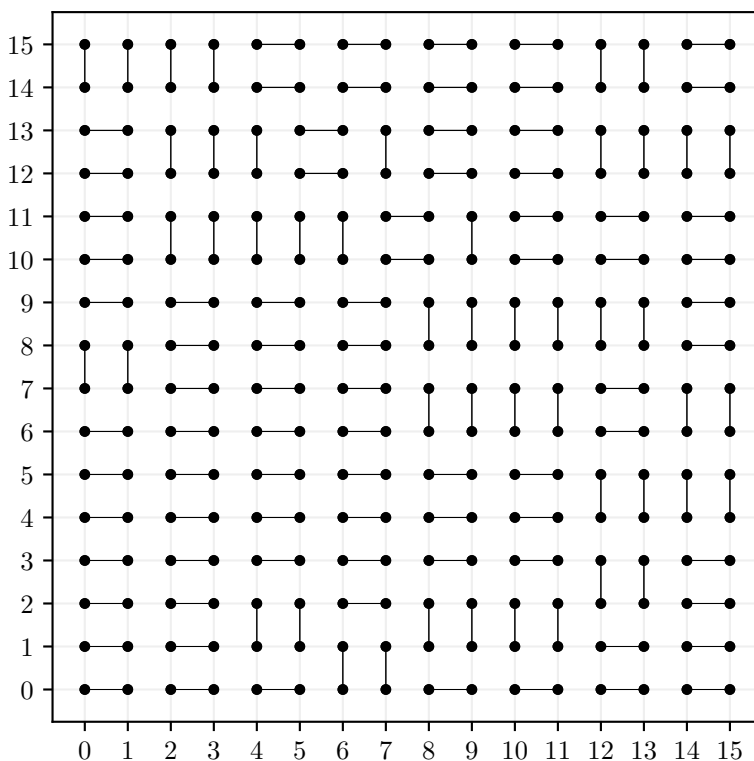


Figure 1.1: A typical configuration of dimers on a square lattice

For every such configuration, the energy can be calculated. We notice immediately that there are four states of the lattice for which the energy is minimum. These correspond to all states pointing along x-direction, or all states pointing along y-direction. The four degenerate ground states are shown in the figure below.

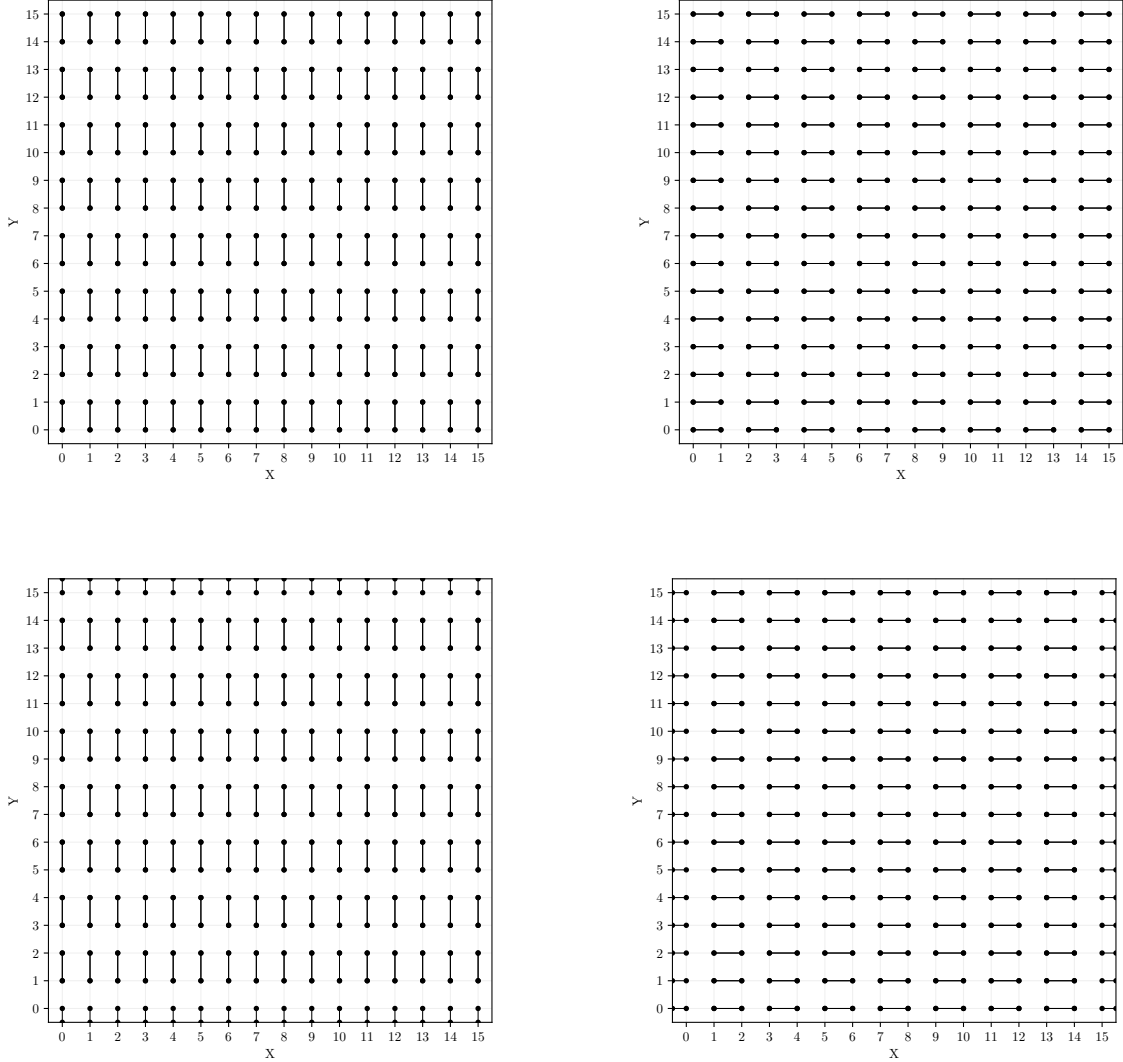


Figure 1.2: The four ground states

This model shows a phase transition from a low-temperature columnar order phase to a high-temperature liquid like phase. The critical temperature of this model has been identified as $T_c = 0.65$ for this model[7]. The four degenerate ground states can only be possible if there

are even number of sites in the x-direction and the y-direction. Square lattices of dimensions $2N \times 2N$ are lattices are bipartite, that is, it is possible to identify two sublattices A and B such that the lattice only contains edges which have one vertex in A and one vertex in B. There are no edges which connect two vertices in the same sublattice. This is only true for the untwisted lattice, and lattices with an even twist, where twist is defined in Chapter 3. For such lattices, it is clearly evident that any dimer must be connecting two sites in opposite sublattices.

The dimer model is one model in which a Coulomb phase is realized. Coulomb phases are those in which the spin-spin correlations, depend on the distance R like dipole-dipole interactions, and proportional to $1/R^2$ for two dimensions. This behaviour is similar to electrostatics. One can also define a mapping for the 2D dimer model from a configuration of dimers to that of a configuration of arrows on the lattice such that there is no net flux at any site in the lattice. These arrows can be thought of as lattice fluxes and they satisfy the same condition of divergence-less flux condition that is satisfied by the electric and magnetic fields in space. For the fully-filled dimer model on a bipartite lattice, we can specify a convention of flux on each dimer as a value $+3$ in the direction from odd to even sublattice, and $+1$ in every other empty bond going from even to odd sublattice. This kind of mapping clearly leads to a divergence-less field at every lattice site. This is a quantity that has generated a lot of interest in recent years[5].

Chapter 2

Numerical Simulations

In order to study these models, we employ numerical simulations which allow us to sample many configurations and perform experiments like in real systems. In principle, if we can write down the partition function of a system exactly we can calculate all the properties of the system. However, in practice this is nearly impossible because of the large number of states for each system. Take the Ising model, for instance, where we study what happens when spins at every site of a lattice takes the values ± 1 , and they consist of nearest neighbour interactions. This simple model is used to understand the ferromagnetic to paramagnetic phase transitions in metals. But when we look at the number of possible configurations of the system, it scales with the number of sites that are present, and so the number of configurations for a system with N sites is 2^N . As an example, if we consider a 2D lattice of dimensions 4×4 , the number of sites is 16 and the number of possible configurations is $2^{16} = 65536$. But if the lattice has dimensions 5×5 , the number of sites is 25 and the number of configurations is $2^{25} = 33554432$, which is 512 times the number of configurations for 4×4 lattice. So it becomes nearly impossible to enumerate all the possible configurations and to calculate the partition function exactly. Numerical simulations are used to study these systems in equilibrium, by evolving the systems to such that they sample most of the configurations that the system can be present in when it is in equilibrium.

Monte Carlo simulations are a set of powerful tools that have been developed to study systems in equilibrium. The basic idea is to take the system at an initial state and evolve it to a new state by making local changes that satisfy the principle of detailed balance, so

that the system tends towards equilibrium. The principle of detailed balance gives a set of equations that any system must satisfy at equilibrium, and it gives us the freedom to choose the probabilities of various transitions.

2.1 Principle of detailed balance

The system at equilibrium is characterized by the fact that the rates of transition from one state to another is balanced by the reverse transition. We know that all systems that are described by a Hamiltonian tend to a Boltzmann distribution of the configurations at equilibrium. So, at equilibrium we have:

$$P_a P(a \rightarrow b) = P_b P(b \rightarrow a) \quad (2.1)$$

where P_a and P_b are the Boltzmann probabilities of the states a and b at equilibrium, and $P(a \rightarrow b)$ and $P(b \rightarrow a)$ are the transition probabilities that need to be chosen for each model. So, if E_a and E_b are the energies of two states of the system, then at equilibrium the contribution to the partition function for each of these states is

$$\begin{aligned} P_a &= e^{-\beta E_a} \\ P_b &= e^{-\beta E_b} \end{aligned}$$

So, the probabilities of transition can be written in terms of these as:

$$\frac{P(a \rightarrow b)}{P(b \rightarrow a)} = e^{-\beta(E_b - E_a)} \quad (2.2)$$

This equation is satisfied for every pair of states a and b . Since the initial state a must transition to one of the states, we also have:

$$\sum_{\{b\}} P(a \rightarrow b) = 1 \quad (2.3)$$

where $\{b\}$ is the set of all states that are accessible from a . These are the fundamental constraints that any system in equilibrium must satisfy. Given these constraints, a suitable set of transition probabilities are chosen, which are time-independent, and the system evolves

through these transitions.

2.2 Ising model

While the principle of detailed balance gives us the general idea of how the system needs to evolve to reach equilibrium, one needs to suitably choose the rates of transition for each model. For the Ising model, we start with an initial configuration of one of the ground states, with all spins either pointing up or down (± 1). For a 2D lattice with $N \times N$ spins, we initialize a variable *states* that contains the values of the spins at each site. We then generate new states from this configuration using the Metropolis Algorithm with single-spin-flip dynamics. The steps that are to be followed can be written as follows[1]:

- Pick a random site and flip the spin on that site.
- Calculate the change in energy of the system ΔE due to the flip.
- If $\Delta E < 0$, then the flip is accepted, otherwise the flip is accepted with a probability $e^{-\beta\Delta E}$ (Metropolis Algorithm). If the initial state is μ with energy given by E_μ , and the new state is ν with energy given by E_ν , then this can be written as

$$P(\mu \rightarrow \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)} & \text{if } (E_\nu - E_\mu) \geq 0 \\ 1 & \text{otherwise} \end{cases} \quad (2.4)$$

- The above steps are repeated N^2 times before the quantities are measured.

Once these steps are complete, a new configuration is obtained which is likely to be different from the initial configuration, but which has been obtained using the probabilities which satisfy detailed balance. The above algorithm is typically repeated around 10^7 times to sample configurations. The system starting at an initial ground state, which corresponds to $T=0$, first needs to be “heated up” to a particular temperature that we are interested in. Once the system reaches equilibrium at our desired temperature, we start sampling configurations at regular intervals by calculating various quantities, which are defined in the next chapter.

2.3 Dimer model

As we saw earlier, the fully filled dimer model in 2D is a model of perfect matchings on a graph. The Hamiltonian for the system gives rise to four ground states which are degenerate and which breaks both the translational and $\pi/2$ rotational symmetry. To simulate this model at a particular temperature, we can use the Monte Carlo methods of picking a random site of the lattice and changing the dimer present on that site. However, in contrast to the Ising model, where it is simple to just flip the spin at a particular site, and accept the flip with some probability, it is not possible to randomly change the dimers at any site. By changing the dimer at one site, the dimer already connected to the site needs to be changed. In effect, the algorithm must keep changing the dimers along a path until many dimers have changed and the path completes a loop by ending at the starting site. An algorithm which achieves this is called the Directed Loop Algorithm and it was first proposed by Sandvik and Syljuåsen [8]. They proposed a method of choosing the transition probabilities for the dimer flips which results in the completion of the loop, while flipping the dimers at different sites and generating a new configuration.

For the dimer model, we implemented the directed loop algorithm as discussed in the appendix of [9], since it is more convenient. The algorithm proceeds as follows:

1. Pick a random site on the lattice, say x . This site would be one end of a dimer connected to y , which is one of the four neighbours of x in the 2D square-lattice.
2. For the site x , calculate the number of dimers that are parallel to it in each direction. This is to calculate the probability of acceptance for the first site.
3. Calculate the probability of accepting the flip along the direction of the current dimer ($x \rightarrow y$) at x as $e^{-\beta N_{\parallel}/2}$, where N_{\parallel} is the number of dimers parallel to xy .
4. If the dimer flip is accepted, two monomers are created at x and y , which is like a worm with the head at y and the tail at x . For convenience, we represent this as though half a dimer is present at the adjacent location (y), with the dimer being destroyed at that site.
5. In the next step, one of the four directions is chosen at y , according to the acceptance probability $e^{-\beta N_{\parallel}/2}$, where N_{\parallel} is calculated for dimers parallel to *each* direction at the head of the worm.

6. After a direction is chosen, if the site that is adjacent to y in that direction is z , then the worm is moved in between y and z with the head pointing towards z and the tail at y . Now a new dimer is being created between y and z .
7. If the site along the chosen direction z is a monomer, then the dimer is completed and the loop update is complete. Otherwise, a dimer is created between y and z , and the dimer between z and its neighbour, say w , is destroyed. The head of the worm moves to the site w and it is present as half a dimer between z and w . The algorithm has reached the same state as it was in the beginning of step 5, and the above steps are repeated until the two monomers are destroyed.

At the end of the loop update, many dimers in the lattice would have been modified. This loop update is performed many times, and once the number of accepted flips is greater than the number of sites present, we consider the current state to be a new configuration and we calculate the various quantities for this state. Once again, the system starts with one of the four ground states, which correspond to $T=0$, and the system is heated to our desired temperature. When the system reaches equilibrium, the various quantities of our interest are measured as detailed in the next chapter.

Chapter 3

Macroscopic observables

For any system that is described by a Hamiltonian, we are interested in understanding the behaviour of some parameters that can be measured experimentally. We know from statistical physics that the partition function Z is related to the free energy of the system by

$$F = -k_B T \ln(Z). \quad (3.1)$$

We also know from thermodynamics that various quantities can be calculated from the free energy, like the specific heat, susceptibility and correlation functions. These quantities can be measured experimentally and used to infer the properties of the system. We define below some of the quantities that are measured in our study of Ising model and dimer model.

3.1 Ising model order parameters

For the Ising model in 2D, we know very well of the existence of a low temperature ferromagnetic phase and a high temperature paramagnetic phase. In order to identify the phase of the system we need to calculate certain order parameters, of which the most commonly calculated ones are as follows (for a 2D square lattice of size $N \times N$)[1]:

- **Energy:** The expectation value of the energy is the simplest quantity to calculate directly from the Hamiltonian. The energy is calculated after every Monte Carlo sweep,

and the average energy can be estimated from these samples. The average energy is calculated as

$$\langle E \rangle = -J \left\langle \sum_{\substack{i=1,\dots,N \\ j=1,\dots,N}} [\sigma_{i,j} \sigma_{i,j+1} + \sigma_{i,j} \sigma_{i+1,j}] \right\rangle \quad (3.2)$$

- **Magnetisation:** This can be calculated as the sum of spins in every site. For a given configuration, $M = \sum_{i,j} \sigma_{i,j}$. The average magnetisation per site is calculated as

$$\langle m \rangle = \frac{1}{N^2} \left\langle \sum_{i,j} \sigma_{i,j} \right\rangle \quad (3.3)$$

- **Specific Heat:** Once the energy is calculated, we can calculate the specific heat capacity per site as

$$c_v = \frac{k_B}{N^2} \beta^2 (\langle E^2 \rangle - \langle E \rangle^2) \quad (3.4)$$

This expression can be derived easily from the relation between the internal energy and the partition function. It is interesting to note that the microscopic fluctuations of the energy is directly related to a macroscopic quantity like specific heat, which is an experimentally measurable quantity.

- **Magnetic Susceptibility:** We can calculate the fluctuations of various quantities from second derivatives of the appropriate fields. The strength of the response of some variable X to changes in the value of a field Y is called the susceptibility of X to Y, and is calculated as

$$\chi = \frac{\partial \langle X \rangle}{\partial Y}$$

For the magnetic susceptibility, which measures the response of the magnetization to changes in the magnetic field, we have the expression per site as

$$\chi = \frac{1}{N^2} \frac{\partial \langle M \rangle}{\partial B} = \frac{\beta}{N^2} (\langle M^2 \rangle - \langle M \rangle^2) \quad (3.5)$$

The second expression is again simple to derive from the relation of the magnetization to the partition function.

- **Binder's Cumulant:** For the Ising model at the critical temperature, the specific heat and magnetic susceptibility must have singularities, which is the indication of the second order phase transition, since they are related to the second derivatives of the

free energy. However, for any finite lattice, we will not observe this singularity, since the partition function is the sum of a finite number of analytic functions. Only in the thermodynamic limit of $N \rightarrow \infty$ do we observe the singularity. However, from finite lattice sizes, we can still identify the critical temperature by varying the lattice sizes and calculating the fourth order cumulant for each size, also called as Binder's cumulant as

$$B = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2} \quad (3.6)$$

This quantity, when plotted as a function of temperature for different lattice sizes shows a crossing point, which is at the critical temperature. This expression is derived using finite size scaling analysis[4].

3.2 Dimer model order parameters

For the dimer model, there is a low temperature ordered phase, also called the Columnar ordered phase, and a high temperature disordered phase, which can be identified using the following quantities[7]:

- **Complex Columnar Order Parameter:** This quantity is defined as:

$$\psi_{col}(\mathbf{r}) = (-1)^{r_x} [\hat{n}(\mathbf{r} + \mathbf{x}/2) - \hat{n}(\mathbf{r} - \mathbf{x}/2)] + i(-1)^{r_y} [\hat{n}(\mathbf{r} + \mathbf{y}/2) - \hat{n}(\mathbf{r} - \mathbf{y}/2)] \quad (3.7)$$

where \mathbf{x} and \mathbf{y} are unit vectors and $\hat{n}(\mathbf{r} - \mathbf{x}/2)$ is the bond occupation number, which takes the value 1 if there is a dimer between the site $\mathbf{r} - \mathbf{x}$ and site \mathbf{r} . This quantity can be calculated for each lattice site and it takes the values $+1, -1, +i$ or $-i$, depending on the direction of the dimer at the lattice site and the parity of that site. In a pure columnar phase, which is one of the four degenerate ground states of the system, all the sites take the same value of this parameter. The average value can be calculated as:

$$\langle |\psi_{col}| \rangle = \frac{2}{N^2} \langle | \sum_{\mathbf{r} \in A} \psi_{col}(\mathbf{r}) | \rangle \quad (3.8)$$

where A is the even sublattice in the 2D bipartite lattice. We can also calculate the

columnar susceptibility as

$$\chi_{col} = \frac{4}{N^2} \left(\left\langle \left| \sum_{\mathbf{r} \in A} \psi_{col}(\mathbf{r}) \right|^2 \right\rangle - \left\langle \left| \sum_{\mathbf{r} \in A} \psi_{col}(\mathbf{r}) \right| \right\rangle^2 \right) \quad (3.9)$$

and the Binder's cumulant as

$$B_{col} = 1 - \frac{\langle |\psi|^4 \rangle}{2 \langle |\psi|^2 \rangle^2} \quad (3.10)$$

This quantity saturates to 1/2 in long range ordered phase and scales to 0 in the thermodynamics limit when there is no long range order. This quantity detects the translational symmetry breaking.

- **Dimer Rotational Symmetry Breaking Parameter:** Another quantity of interest is the order parameter that breaks the $\pi/2$ rotational symmetry, which is present at high temperatures, when there are an equal number of dimers in x and y direction on an average. This can be calculated as

$$D = \frac{2}{N^2} |N^c(|) - N^c(-)| \quad (3.11)$$

which is the difference between the number of vertical and horizontal dimers in the lattice for the configuration c . It has a value of 1 in the columnar state and 0 in the disorder state. We can similarly calculate the susceptibility as

$$\chi_D = N^2 (\langle D^2 \rangle - \langle D \rangle^2)$$

and the Binder's cumulant as

$$B_D = 1 - \frac{\langle D^4 \rangle}{3 \langle D^2 \rangle^2}$$

- **Plaquette Order Parameter:** Along with the columnar ordered phase and the disordered phase, there can exist an intermediate plaquette phase, where there are parallel dimers in plaquettes. To identify if there is a distinct plaquette phase, we can calculate it such that the order parameter vanishes for a columnar phase. So the

plaquette order parameter can be defined as

$$P = \frac{2}{N^2} \left| \sum_{\mathbf{p}} (-1)^{p_x+p_y} v_p \right| \quad (3.12)$$

where $v_p = 1$ if there exists a pair of parallel dimers in the plaquette identified by the site \mathbf{p} . The sum is over all the plaquettes in the lattice, with the plaquette being identified with the top left corner of each square. The factor $(-1)^{p_x+p_y}$ ensures that the expectation value of the plaquettes is zero for the columnar state and non-zero in the plaquette phase. We can also calculate the associated susceptibility as

$$\chi_P = N^2(\langle P^2 \rangle - \langle P \rangle^2)$$

and the Binder's cumulant as

$$B_P = 1 - \frac{\langle P^4 \rangle}{3\langle P^2 \rangle^2}$$

- **Energy:** From the Hamiltonian, we can also calculate the energy of the system for each configuration, and calculate the specific heat at each temperature to see if it indicates a phase transition. The energy is calculated as

$$E_c = v[N^c(\parallel) + N^c(=)]$$

and we can calculate the fluctuation of energy which is related to the specific heat as

$$c_v = \frac{k_B}{N^2} \beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$$

The quantities mentioned above were used to study the model in the paper by F.Alet et.al[7]. They identified the critical temperature for this model to be $T_c = 0.65$ from the Binder's cumulant of the Dimer Rotational Symmetry Breaking parameter. We observe a similar behaviour for the untwisted lattice, and so we can be fairly certain that our implementation of the algorithm is also correct.

In addition to the quantities listed above, we can also study the distribution of the dimers in the x-direction and y-direction, for the twisted and untwisted lattices. We can also define a quantity called the flux for the bipartite lattice, like mentioned in Chapter 1, and calculate its fluctuations.

3.3 Implementing a twist

Now, when we apply a twist to the system, we mean that the usual periodic boundary conditions are applied along one direction and along the other direction, the lattice is slightly shifted by a fixed amount and then connected. As an example, Fig 3.1 shows the lattice when a twist of +1 is implemented along the x-direction, as shown.

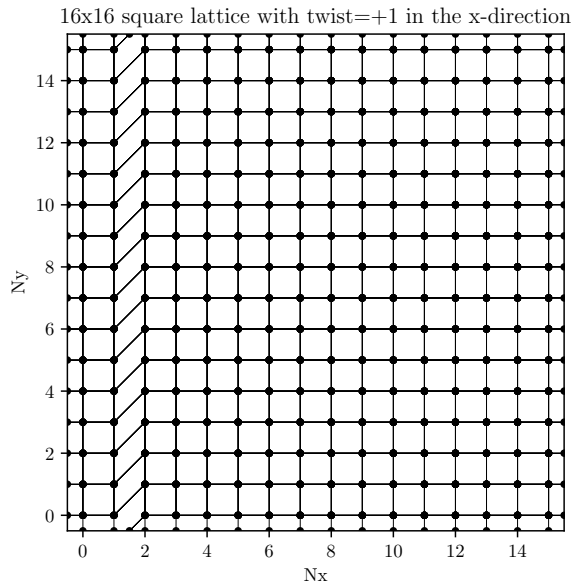


Figure 3.1: Lattice with a twist of +1 in the x-direction

The twist is applied by changing the adjacency matrix of the square lattice. The degree of each vertex, that is, the number of neighbours for each site of the lattice is unchanged when the twist is applied. By applying a twist, the square lattice is no longer bipartite. The twist on the lattice has many interesting properties.

1. The twists are cyclic. So, if the lattice has a twist of k , we can write $k \equiv k \% N_y$.
2. The partition function does not depend on the position of the twist. This can be easily verified using the cyclic property of the trace.
3. It is possible to place various twists at different positions in the lattice. However, the partition function depends only on the total twist of the lattice, which is calculated by

summing over all the individual twists.

4. The partition function of a lattice with twist k and twist $N_y - k$ are identical because of symmetry.

We are interested in understanding the effect of this on different quantities of the system, and consequently on its behaviour in different regimes. The twist can be applied to the lattice, and any model can be implemented on such a lattice to study its behaviour.

Chapter 4

Results of numerical simulations

We have calculated various quantities from the simulation of Ising model and dimer model with twists. The number of Monte Carlo steps was around 10^7 for each such calculation. *For the Ising model, the twist has been applied along the y -direction. The values of twist range from 0 to $N_x - 1$. While for the dimer model the twist has been applied along the x -direction, and the values of the twist range from 0 to $N_y - 1$.*

4.1 Ising model simulations

For the Ising model, we applied a twist to the lattice along the x -direction and simulated such systems. We noticed that the twist has a minimal role to play in the values of statistical quantities in the thermodynamic limit. The effect of twist was only relevant close to the critical temperatures for very slender systems that was elongated in the direction perpendicular to the direction of the twist. We took various approaches to understand whether the twist has any role to play.

4.1.1 Brute Force calculations

The first step to check if the twist has any role to play in the determination of any quantity is to calculate by brute force the various configurations that are present in the system for

various lattice sizes. Since the number of configurations in a system of size $N \times N$ goes as 2^{N^2} , it quickly becomes cumbersome to calculate the number of states in the microcanonical ensemble. It is only possible for very small lattice sizes, like 2×2 , 3×3 and 4×4 . This has been done by numerically exhausting every possible configuration for each of these systems, for the case with the twist and without the twist.

Configurations in 2x2 Lattice		
Energy levels	Twist-0 lattice	Twist-1 lattice
-8J	2	2
0J	12	10
4J	0	4
8J	2	0

Table 4.1: List of all configurations for 2×2 lattice with and without twist

Configurations in 3x3 lattice		
Energy levels	Twist-0 lattice	Twist-1 lattice
-18	2	2
-10	18	18
-6	48	42
-2	198	198
2	144	180
6	102	54
10	0	18

Table 4.2: List of all configurations for 3×3 lattice with and without twist

Configurations in 4x4 Lattice			
Energy levels	Twist-0 lattice	Twist-1 lattice	Twist-2 lattice
-32	2	2	2
-24	32	32	32
-20	64	64	64
-16	424	412	412
-12	1728	1680	1568
-8	6688	6640	6864
-4	13568	14288	14496
0	20524	19298	18660
4	13568	14480	14496
8	6688	6232	6864
12	1728	1904	1568
16	424	400	412
20	64	96	64
24	32	8	32
32	2	0	2

Table 4.3: List of all configurations for 4×4 lattice with and without twist

It is immediately obvious that there are some changes to the energy of various configurations. For the twisted lattice, some new energy levels are present, and some energy levels of the untwisted lattice have fewer number of configurations. We infer that there is no one-to-one mapping between the configurations in the twisted and untwisted lattices. It is to be noted that the lattice with twist τ and $N_x - \tau$ are identical, since it does not matter if the twist is applied in the positive or negative direction. Once it became clear that the twisted and untwisted systems have different energies in the microcanonical ensemble, since we have calculated all the weights of the partition function for these small systems, we can simply plug in those values to calculate

$$Z(\beta, \tau) = \sum_{\{\sigma\}} e^{-\beta E_{\sigma}}$$

From this, we can also calculate the free energy as

$$F(\beta, \tau) = -\frac{1}{\beta} \ln(Z)$$

We can calculate the difference in free energy between the twisted and untwisted lattices as a function of temperature, and is plotted below.

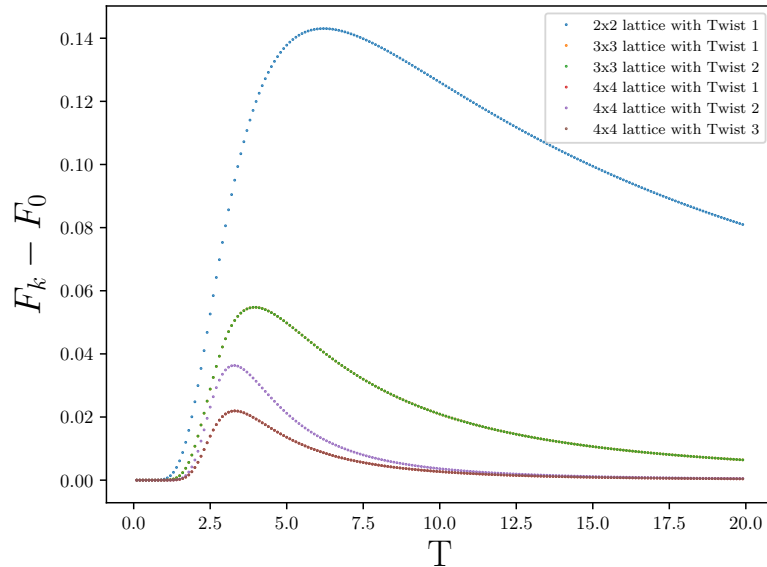


Figure 4.1: Difference in Free Energy between twisted and untwisted lattices vs Temperature

We notice that there is a small difference in the free energy when we twist the lattice. However, that difference rapidly decreases and tends towards 0 for larger lattice sizes. This cannot be calculated by brute force for larger lattices, but one can use Monte Carlo methods to simulate these systems. For slightly larger systems, one can also calculate the partition function using transfer matrices.

4.1.2 Using Transfer Matrices

We know that the partition function can also be written as $Z(\beta) = \text{Tr}(T^{N_y})$, where T is the transfer matrix. From this expression, it is clear that calculating the free energy involves diagonalization of this large matrix of size $2^{N_x} \times 2^{N_x}$, for a lattice of size $N_x \times N_y$. Once again, it is only possible to calculate using this method only for small values of N_x . In the plots below, we see that the difference in free energy is very small for systems that have a larger value of N_y . The following plots are for systems with a twist of +1 along the y-direction.

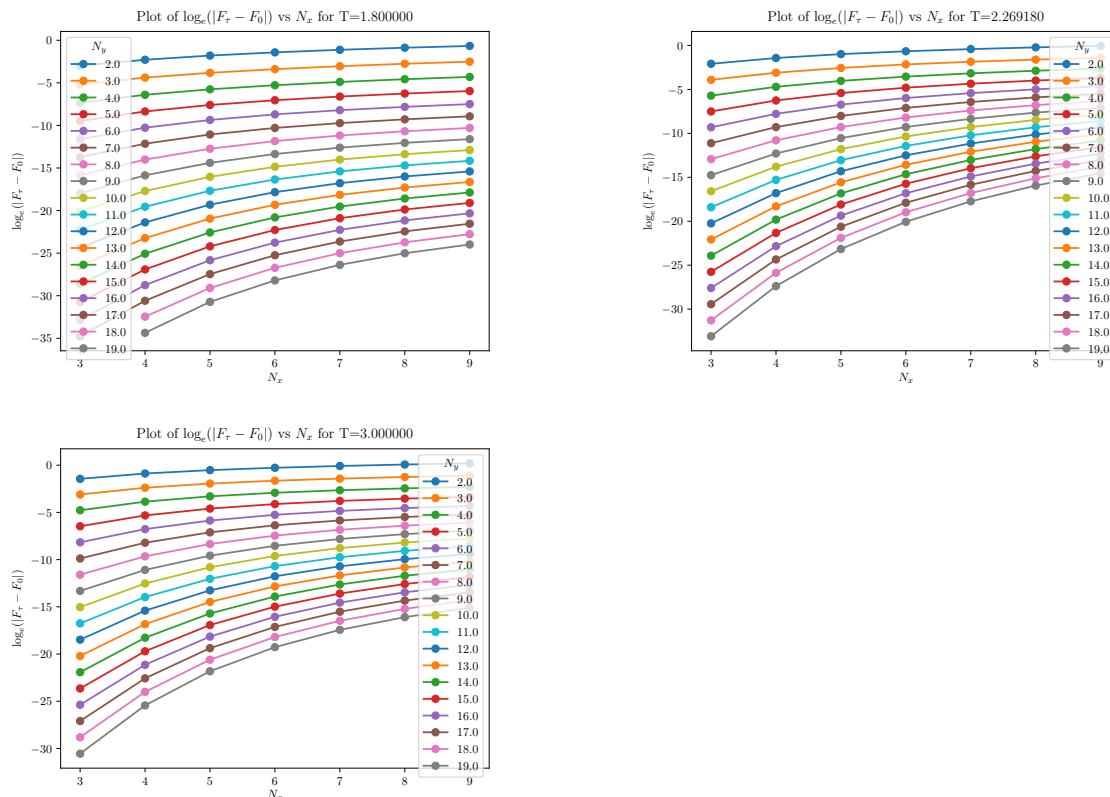


Figure 4.2: Plots of $\ln |F_\tau - F_0|$ versus N_x for different N_y and temperatures.

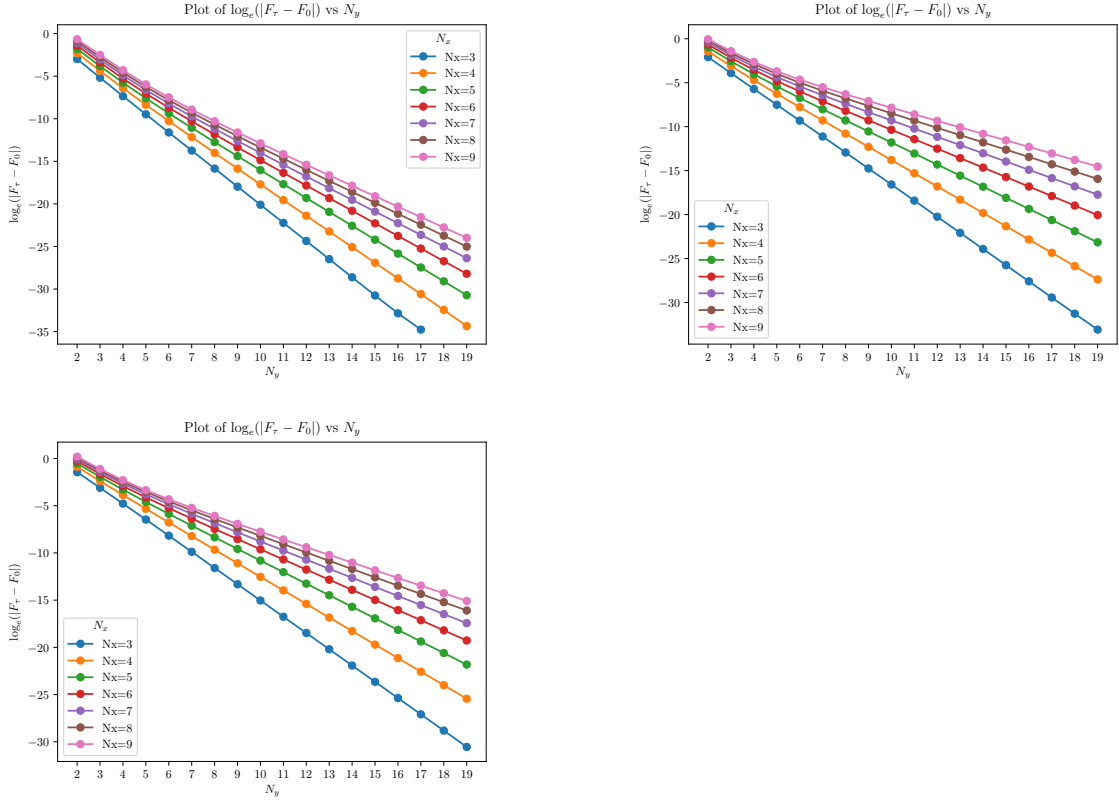


Figure 4.3: Plots of $\ln |F_\tau - F_0|$ versus N_y for different N_x and temperatures.

We see that the difference in free energy is very small for larger lattice sizes and it scales with N_x as shown. For very small values of N_y and very large values of N_x , the effect of twist is observed on the free energy. These are very slender systems. Also, the effect of the twist changes with temperature, as is seen in these plots with the difference in free energy for any given lattice dimension $N_x \times N_y$ being smaller by orders of magnitude away from the critical point $k_B T_c = \frac{2J}{\ln(1+\sqrt{2})} = 2.26918J$ in both directions. This suggests that the effect of twist is more pronounced near the critical temperature. The difference in free energy as the lattice size is increased along N_y decreases rapidly. This suggests that the effect of twist dies out as we increase the lattice size in the direction along which the twist is applied (N_y), and increases as we increase the lattice size in the direction perpendicular to the twist (N_x) increases. From here we can infer that in order to observe any effect of twist in our Monte Carlo systems, we must look at quasi one-dimensional systems, which have a small value of N_y and a large value of N_x . It must be noted that since there is no phase transition exhibited in the Ising model in one-dimension, the quasi one-dimensional version would also

tend towards such a behaviour. Now, since our aim is to understand the effect of these twists on the statistical quantities, we focus on simulating exactly these kinds of systems. From the above plots, we consider looking at systems with $N_y = 4$ and vary N_x to be large, since the decay due to the dependence on N_y is much steeper compared to the increase in N_x . We now look at Monte Carlo simulations to study these systems, since their lattice sizes are larger than what can be used to study using brute force or transfer matrices.

4.1.3 Using Monte Carlo simulations

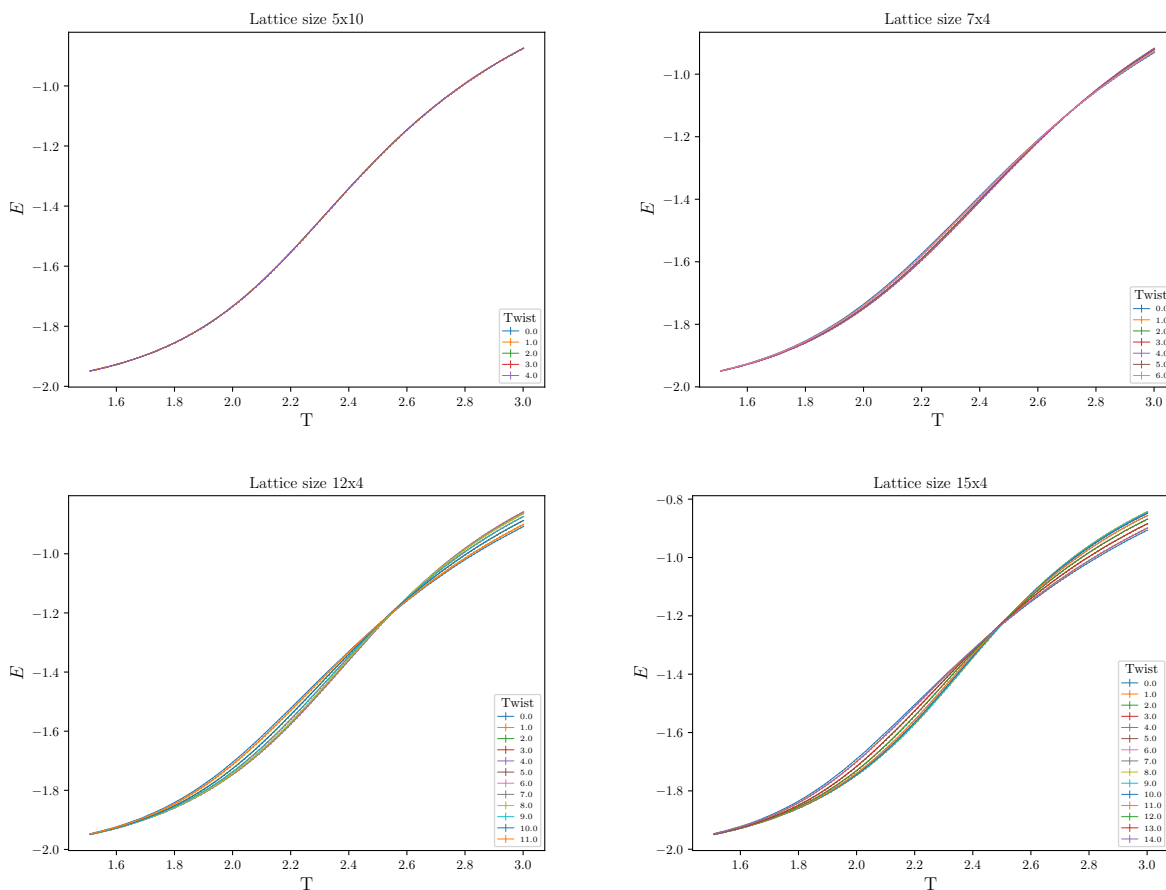


Figure 4.4: Energy vs Temperature for different twists

We have simulated systems with different values of N_x and N_y . When we calculate the average energy of the systems for different twists, we notice that there is a very feeble

dependence on the twist. Such behaviour is only observed for lattices which are elongated in size, and the twist is along this direction. We observe that twists of τ and $-\tau$ have the same value of energy, which is expected. Also, below a temperature $T=2.5$, we observe that the system with larger twist has a lower energy, while for $T > 2.5$, the system with no twist has the lowest energy. Such behaviour is only observed for elongated systems, the dependence on the twist falls rapidly as a function of lattice size. When the system is extended along the direction perpendicular to the twist (y-direction), the differences become negligible. The interesting behaviour is that larger twists have a lower energy for low-temperatures, and smaller twists have a lower energy for high-temperature. This effect is almost absent for systems that have a larger value of N_y and smaller value of N_x .

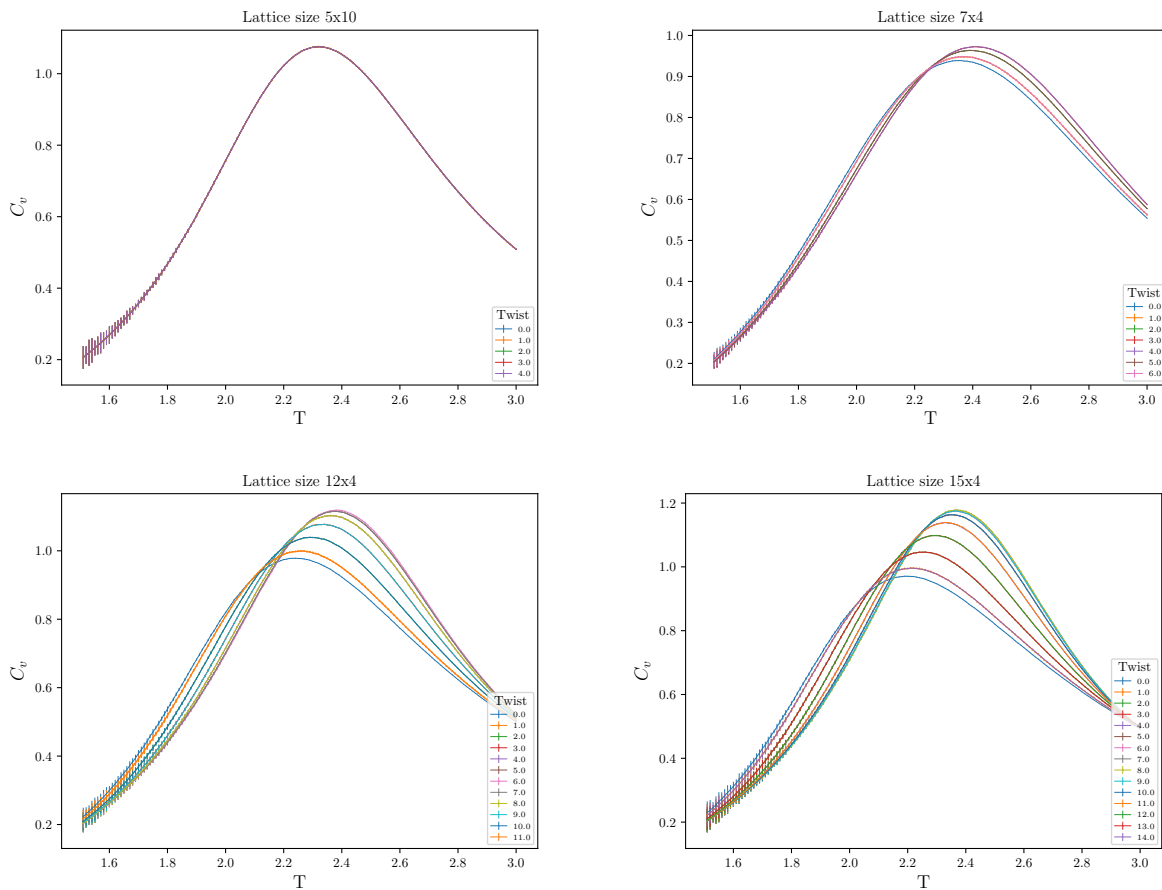


Figure 4.5: C_v vs Temperature for different twists

We notice that the specific heat also has a dependence with twists for different temperatures. At any given temperature the value of specific heat for larger twist is smaller when

$T < T_c$ and is larger for $T > T_c$. This effect is only valid for temperatures that are relatively close to the critical temperature. For temperatures far from the critical temperature, the twist does not play any role. We observe that for the system of size 5×10 , there is no observable effect of the twist anywhere. For the other three systems, where the size in y-direction is smaller, we see the effect of the twist. Below a temperature of around 2.1, the untwisted lattice has the highest value of specific heat while the lattice with the largest twist ($N_x/2$) has the smallest value of specific heat. Beyond $T=2.2$, the lattice with the largest twist has the largest value of specific heat. This suggests some sort of transition taking place around that temperature for the model.

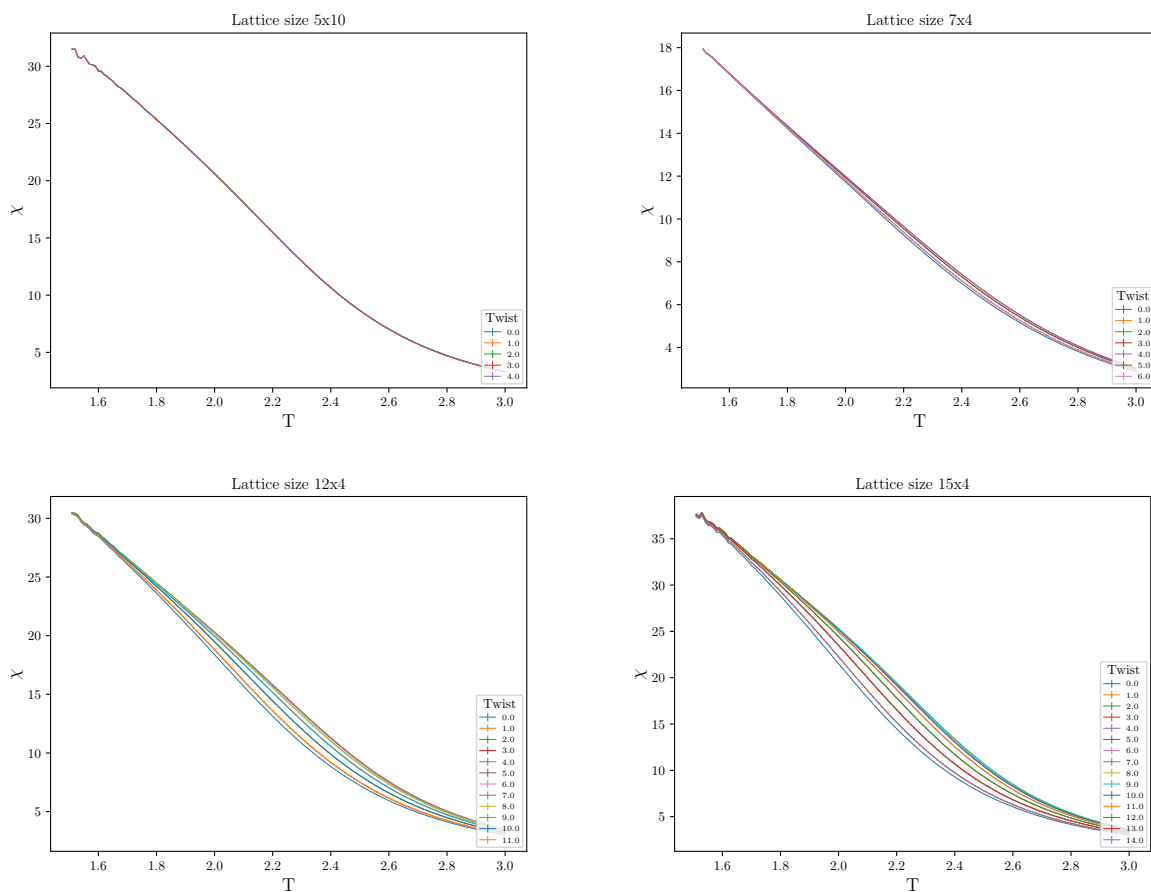


Figure 4.6: χ vs Temperature for different twists

We have not plotted the average magnetisation versus temperature because of the data being very noisy. But the value of susceptibility versus temperature seems to be well behaved and shows some interesting behaviour. Once again, the effect is only around a certain temperature

range around the critical temperature. We don't see a crossing behaviour for this quantity as opposed to the other two quantities previously discussed. Again, the effect of the twists is minimal when the system is larger along the y-direction and smaller along the x-direction. The system with larger twist has a higher magnetic susceptibility compared to that of a system with smaller twist (or no twist) in the region where the twist plays a role.

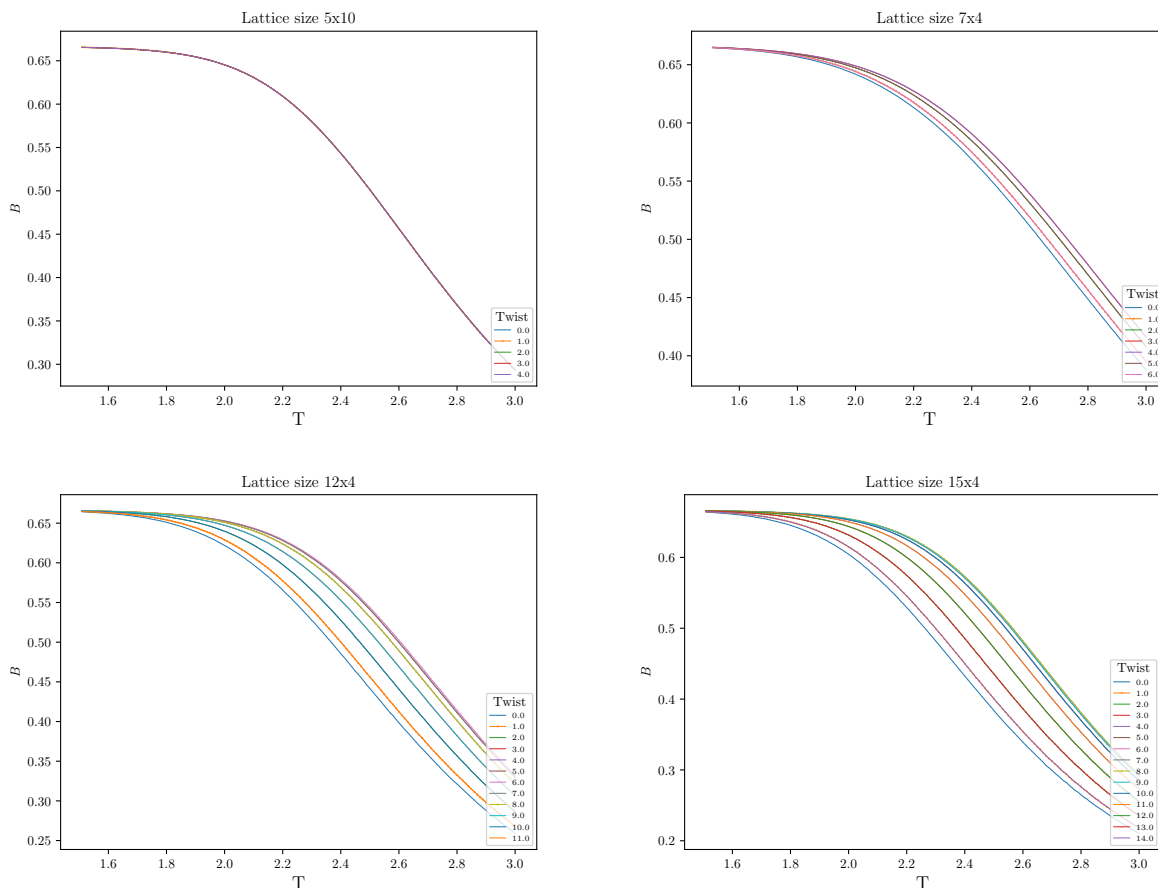


Figure 4.7: Binder's cumulant vs Temperature for different twists

The Binder's cumulant also shows a similar behaviour to that of susceptibility. In the region where the twist plays a role, the system with larger twist has a higher value of Binder's cumulant. For much larger systems, the effect of twist decreases. In the thermodynamic limit of $N_x \rightarrow \infty$ and $N_y \rightarrow \infty$, we do not expect the twist to play any effect. To just confirm if the effect of twist is present for larger systems or not, we performed the same calculations for a 15x15 lattice system.

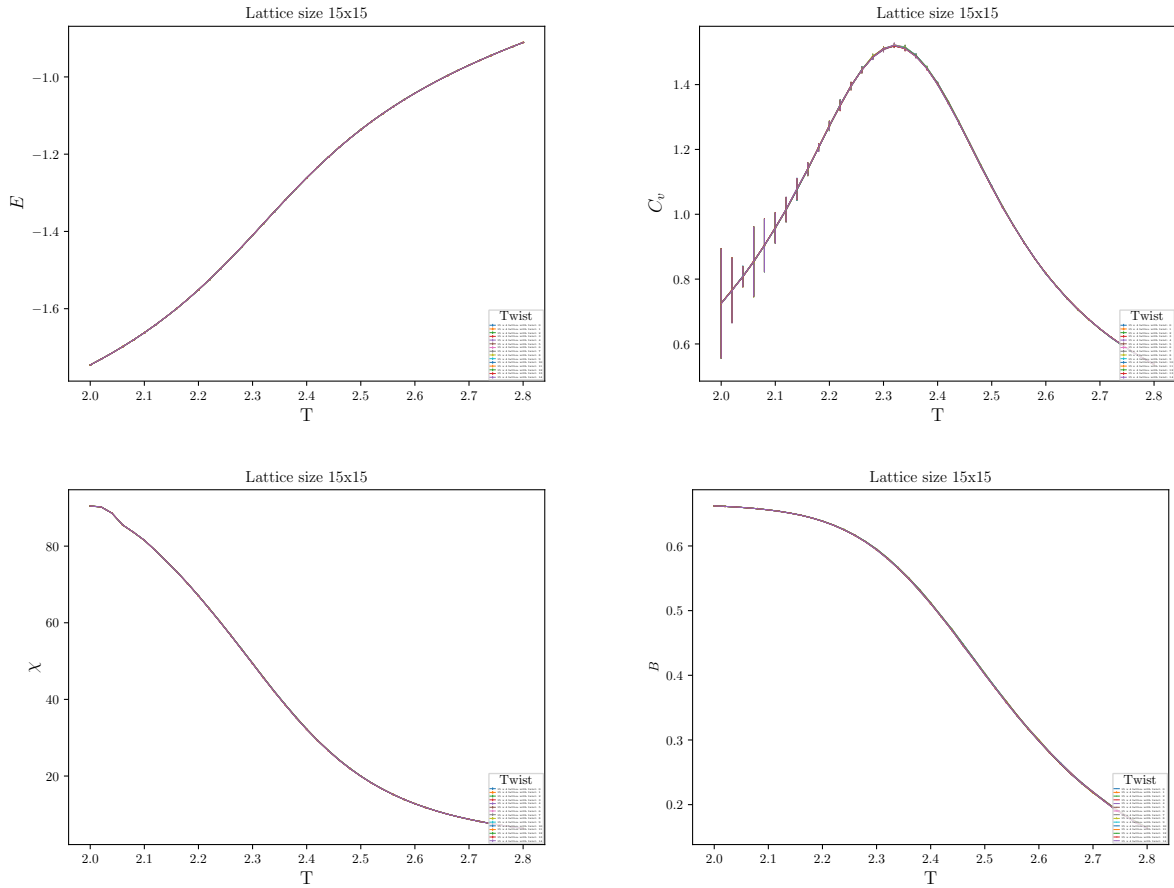


Figure 4.8: All Statistical quantities for a 15x15 lattice

We clearly see that there is no effect of twist on the system. The quantities calculated for a system with $N_x = 15$ and $N_y = 4$ has been plotted earlier, and that system clearly shows the effect of twist. This confirms our belief that if the twist is applied along the y-direction, the effect of twist is observed when the size of N_x is large and the size of N_y is small. The quantities plotted above as a function of temperature for different twists shows this behaviour for elongated systems. The expression for energy was also calculated from the partition function for small lattices by brute force, and the same behaviour was observed. For larger systems also a similar behaviour is observed.

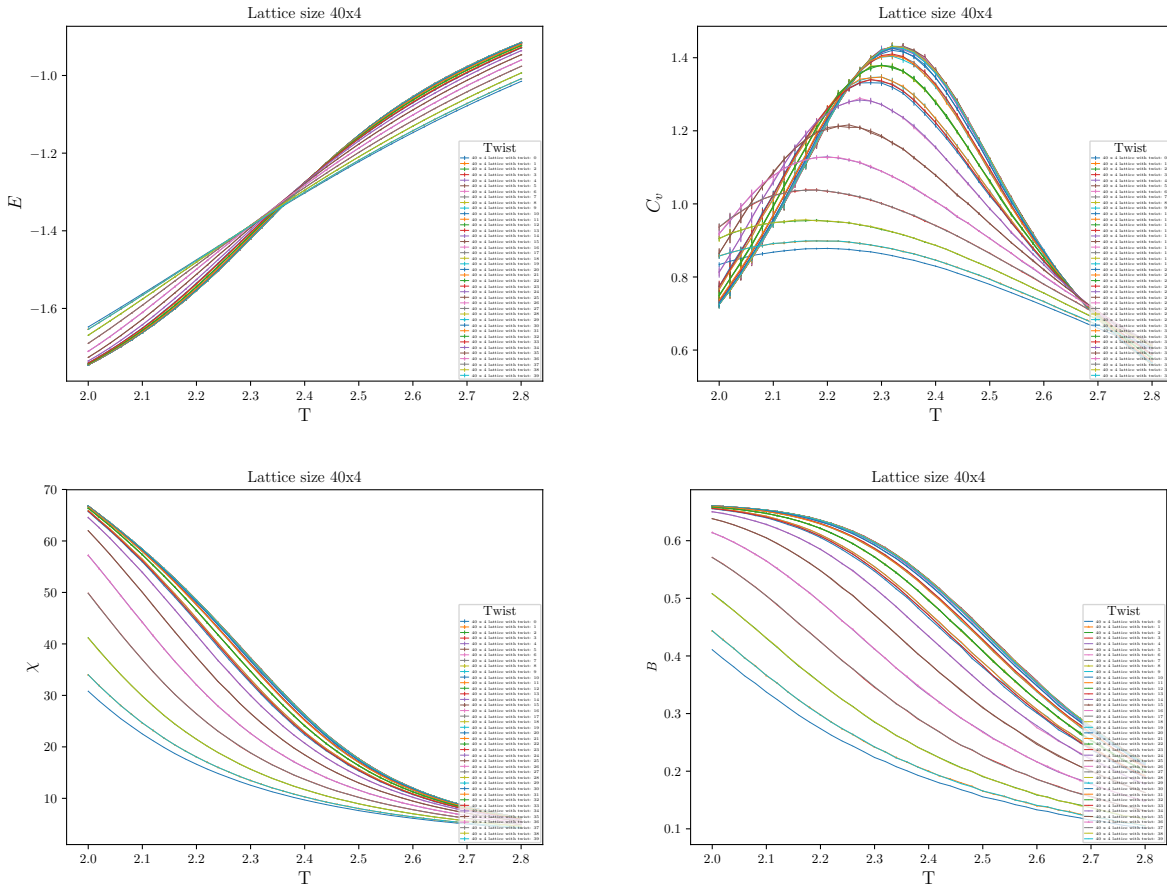


Figure 4.9: All Statistical quantities for a 40x4 lattice

We notice that for lattice of dimensions 40x4 also there is a clear change in the quantities for different twists. The behaviour is same as the cases detailed above.

4.2 Dimer model simulations

After understanding a bit about the effect of twist for the Ising model, we wanted to understand the role of twist in the dimer model. In the dimer model, we have dimers present between adjacent sites on the lattice. For both the Ising model and the dimer model, the implementation of the twist changes the lattice on the level of the system, but locally, the system does not know that a twist has been applied to the lattice. Each lattice site is still connected to four other lattice sites, and locally the interactions remain unchanged. So,

one can define the initial configuration of dimers as one of the four ground states as before. When the algorithm is implemented, only the local interactions are taken into account, and the updates happen without any problem. The system is unaware of a twist being present and all the updates are legal moves. Only when certain global properties are measured do we start noticing the effects of the twist. For all the simulations we considered temperatures that were close to critical temperature. We simulated systems of sizes 16×16 , since larger system sizes was not computationally easy. For instance, even a system of lattice size 32×32 required around 16 times longer runs (since number of samples to be taken is 4 times more and the number of updates to be performed to sample configurations is also 4 times more). Some improvements can be done to the current implementation of the algorithm to make it work for larger system sizes more efficiently, which could not be done within the duration of this project[10]. There are also readily available open-source packages to implement this algorithm efficiently[11], but we wrote it from scratch.

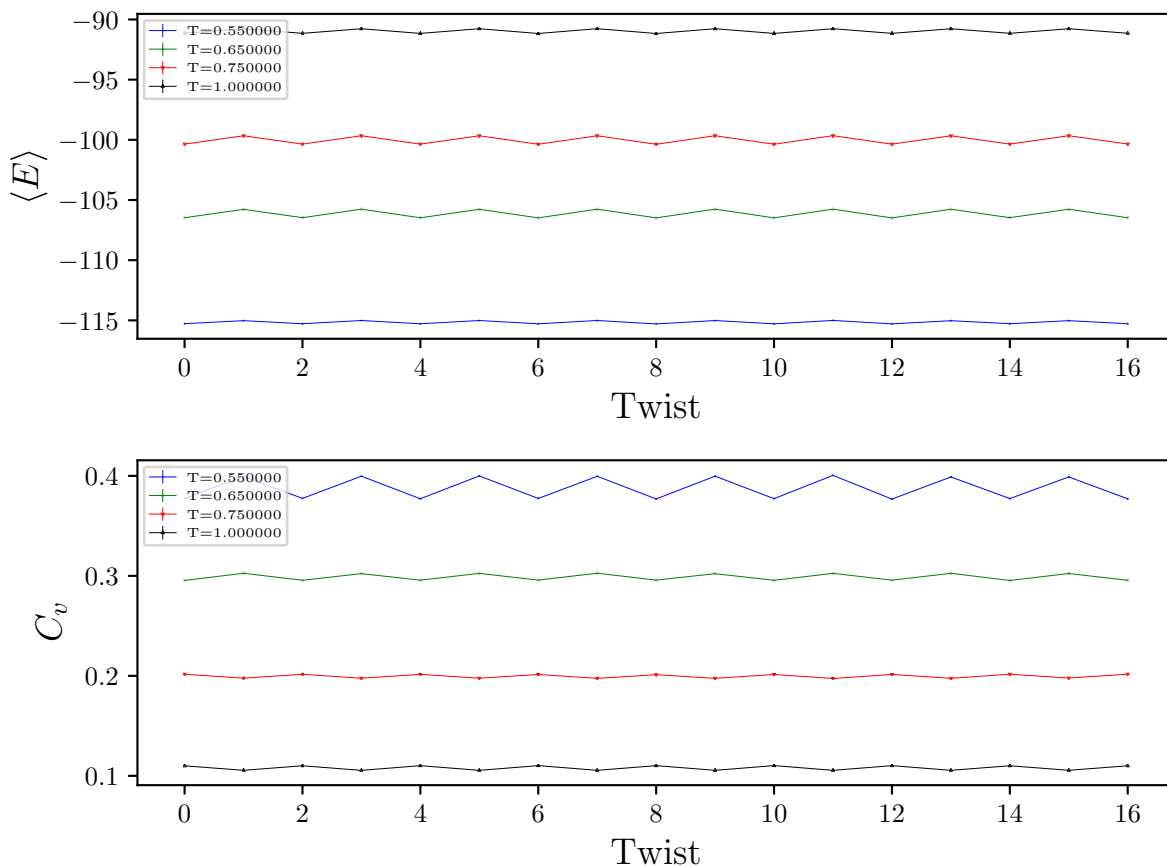


Figure 4.10: Average energy and specific heat as a function of twist for different temperatures

We notice that the energy of the system shows an odd-even effect in the system. All systems with an even twist have identical energy and similarly for odd twists. Apart from that, there does not seem to be any other change. The values of specific heat also show a similar effect. We know that the critical temperature for the dimer model in thermodynamic limit is at $T_c = 0.65$. We observe that the energy shows more difference between odd and even twists close to this temperature. As temperature is increased, the energy of the system is also higher, as expected. The system has a higher energy for lattice with odd twists than for those with even twists.

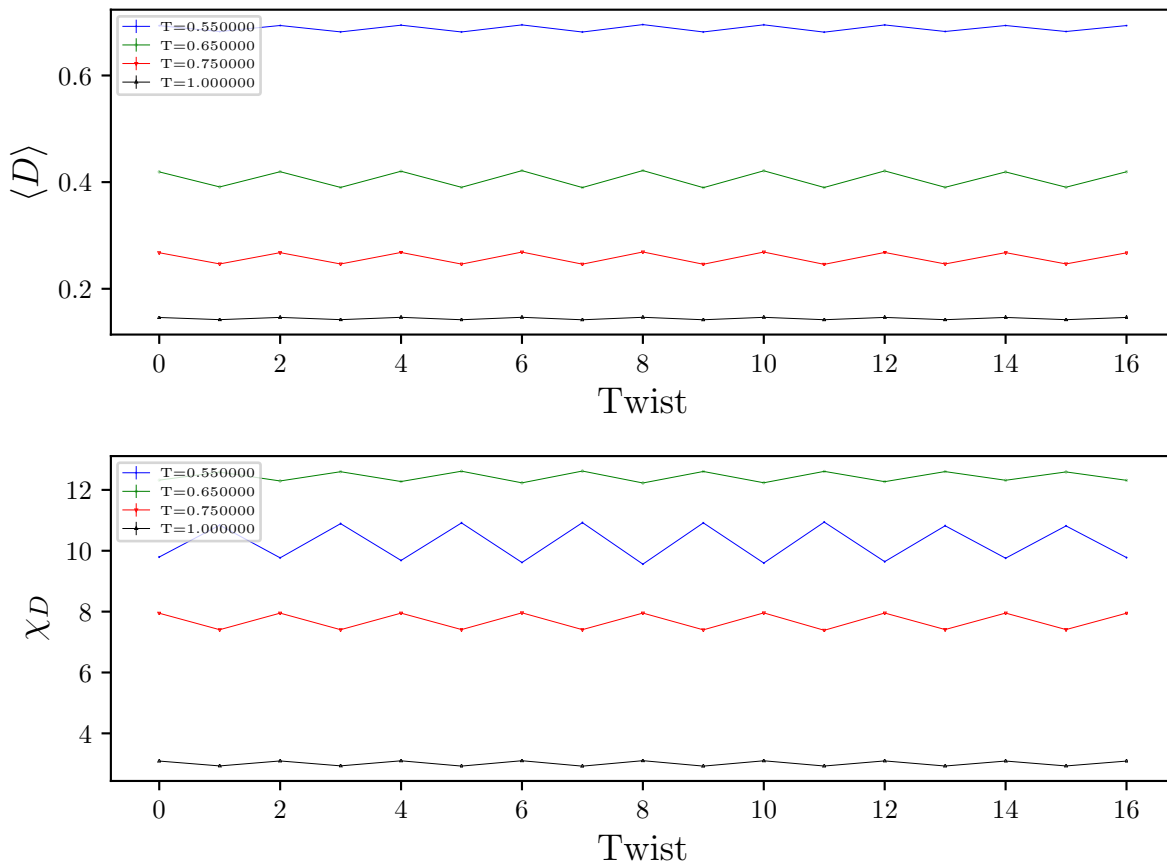


Figure 4.11: Dimer Rotational Symmetry Breaking Order Parameter as a function of twist

Once again we see the effect of odd and even twist on the lattice for this parameter. The average value of the dimer rotational symmetry breaking parameter is supposed to decrease with temperature, as is observed in the plots above. For lattices with odd twists, we see that this value is smaller than for the lattice with even twist. The susceptibility

shows similar odd even effect, but we notice that for $T=0.55$ and $T=0.65$, the lattice with odd twist has higher susceptibility. We also notice that $T=0.65$ has the highest values of susceptibility amongst all the temperatures, indicating a peak in the susceptibility close to this temperature. For temperatures higher than $T=0.65$, we notice that the trend of odd and even values of susceptibility has reversed, with the lattice with odd twist having a lower susceptibility than for the lattice with even twist. For the dimer rotational symmetry breaking parameter, the system with odd twist seems to have a lower expectation value. This means that on an average, the rotational symmetry is unbroken, or rather restored when there is an odd twist. We observe that at low temperatures, the system has a high expectation value, which means the symmetry is broken. This is more clearly illustrated with the next quantity.

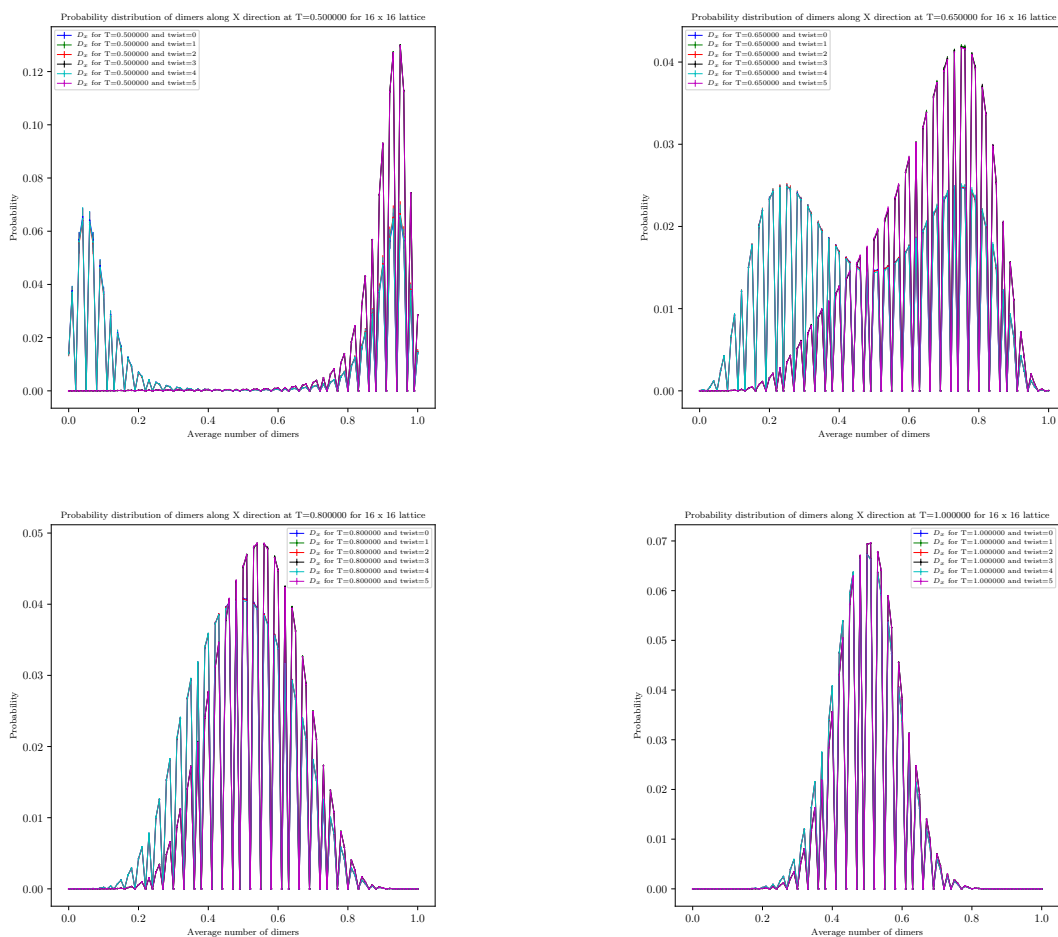


Figure 4.12: Probability distribution of average number of dimers in the x-direction at different temperatures

We observe that there is a higher probability of dimers pointing along the x-direction than in the y-direction in the cases when there is an odd twist in the lattice. For even twists, the system behaves like the case with no twists for this parameter. And as the temperature is increased, the system passes through the critical temperature and the $\pi/2$ rotational symmetry is restored. So, there is an equal probability of dimers to point in either the x-direction or the y-direction. This is the clear evidence of the the effect of twist on the lattice. The dimers align along the direction in which the twist is applied. The twist along a particular direction breaks the symmetry of the lattice and the system accordingly has a larger number of dimers along the x-direction.

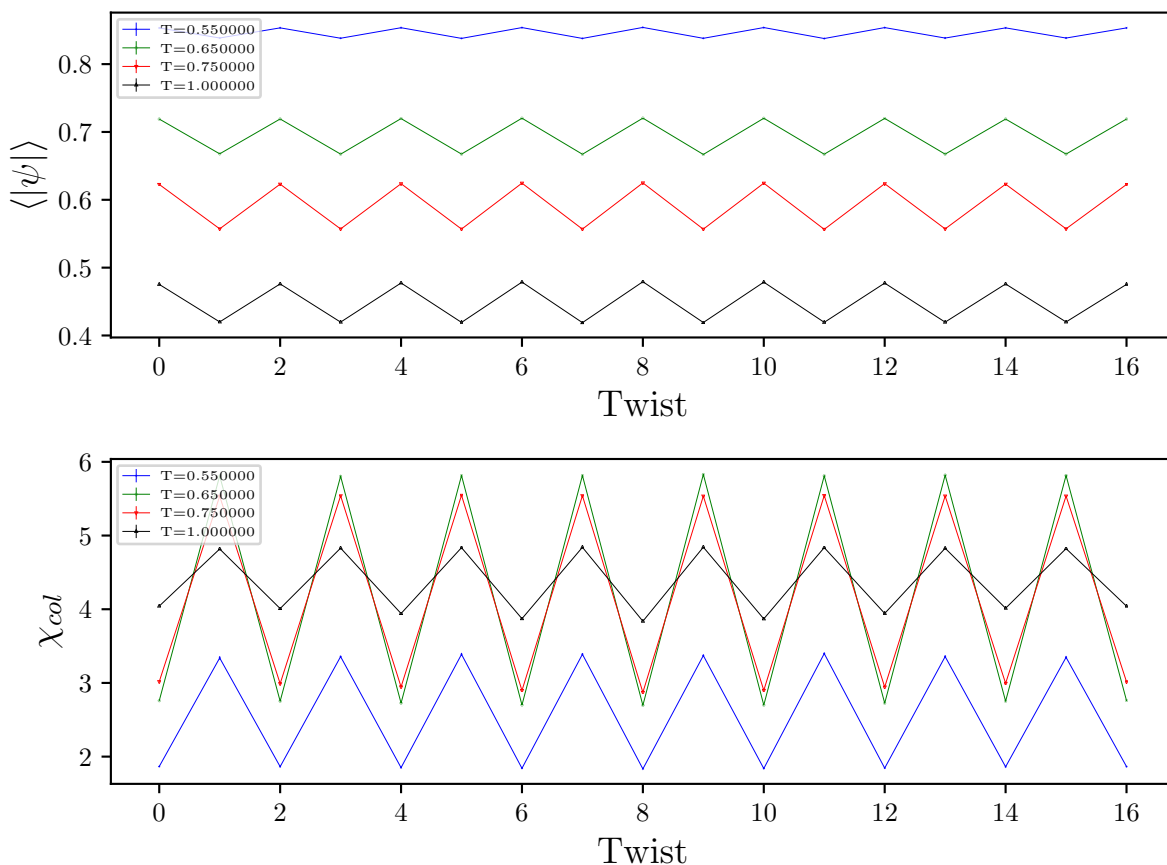


Figure 4.13: Columnar Order Parameter as a function of twist

This quantity also shows different behaviour for odd and even twists. The expectation value of the Columnar order parameter is high for low temperatures and it tends to 0 for high temperatures, indicating the transition to disordered state. For odd twists the

columnar order parameter has a lower value than for even twists. Susceptibility shows some interesting behaviour. For temperatures close to the critical temperature, there is a large difference between the odd and the even twist. For lattices with odd twist, susceptibility has the highest value close to the critical temperature. But for lattices with even twist, the value of susceptibility does not peak at the critical temperature. Due to the algorithm not being optimised enough and the large times taken for sampling, we could not sample these for more temperatures to identify the behaviour of the susceptibility with temperature and twist.

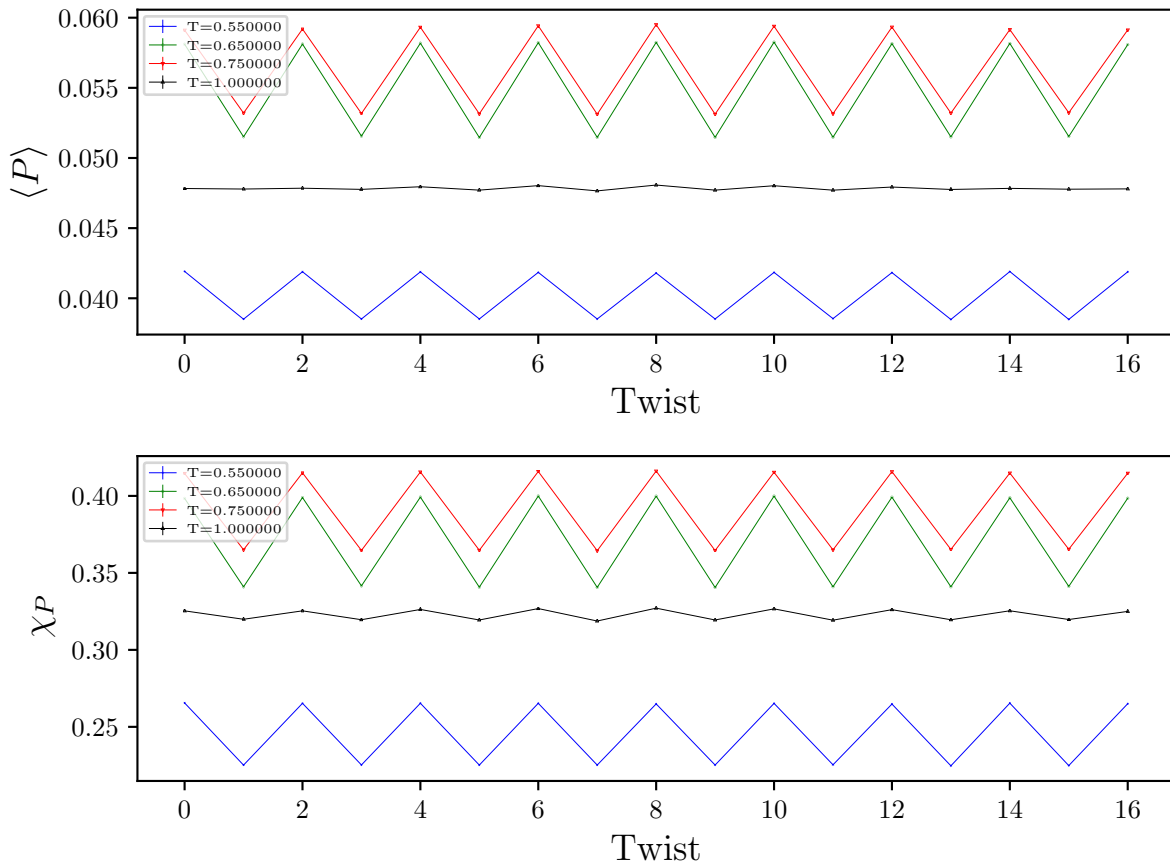


Figure 4.14: Plaquette Order Parameter as a function of twist

We notice that the plaquette order parameter has a very small value (< 0.1) for all these temperatures. This indicates that there isn't a very distinct plaquette phase. Close to the critical temperature we observe the highest value of this plaquette order parameter. Odd twists clearly have a lower expectation value of this quantity, although the difference

is very small, and the behaviour of the susceptibility is similar. For $T=1$, the effect of odd and even twists is even more negligible. We have plotted all the quantities that we have described in the previous chapter. Now, we can also see what happens when we plot the flux across a particular column as a function of twist and temperature. We have already defined fluxes by noting that for any dimer, there is a flux of +3 in the direction from odd to even sublattice, and +1 for all unoccupied bonds from the even to odd sublattice. This quantity is divergenceless, that is, the net flux at each site of the lattice is 0. However, we can compute the net flux through a surface (a line in 2D) that cuts through all the rows at a particular column. This can be done for the x and y direction. The expectation value of the flux $\langle F_x \rangle$ and $\langle F_y \rangle$ must be zero, since there is no charge present in the lattice and the net flux along one direction must on an average be equal to the net flux in the opposite direction. But we can calculate the fluctuations of the flux by simply computing $\langle F_x^2 \rangle$ and $\langle F_y^2 \rangle$.

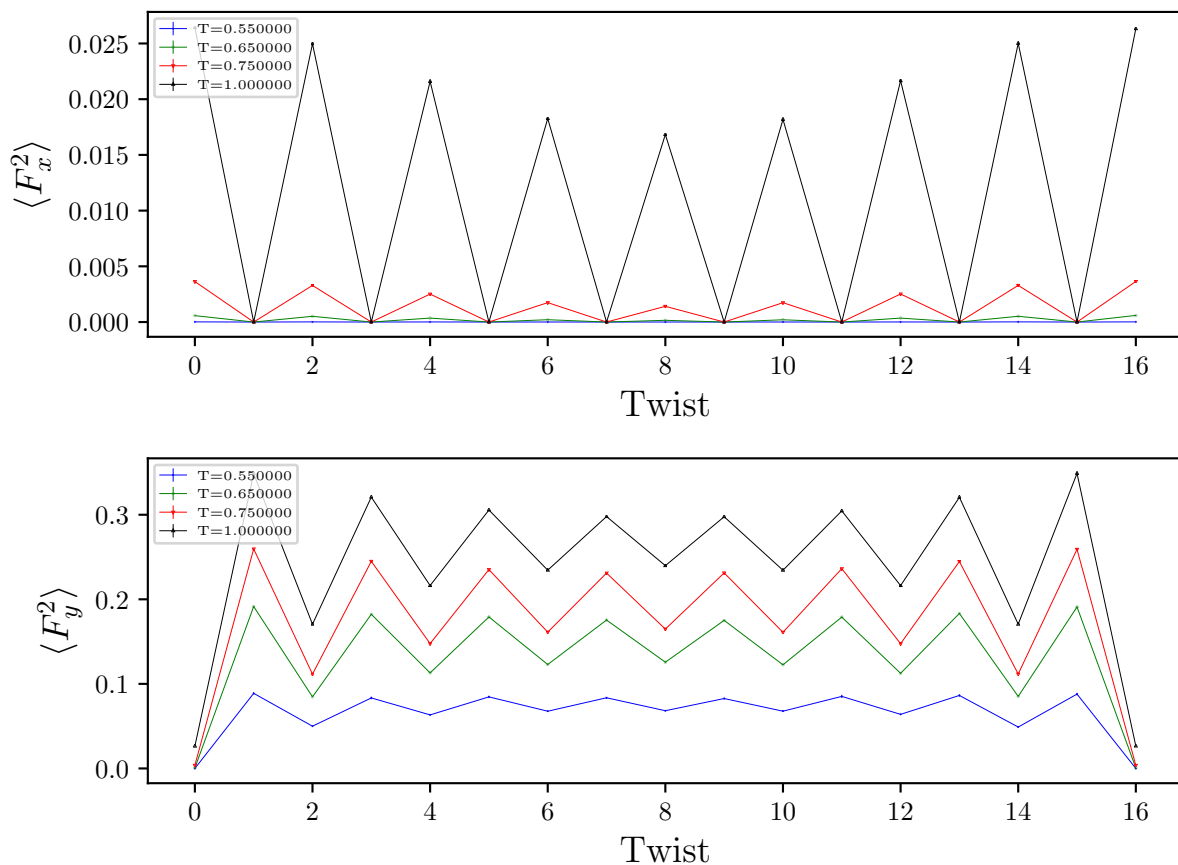


Figure 4.15: Flux fluctuations as a function of twist

This quantity shows some interesting behaviour that is different for the case with the twisted and untwisted lattice. For low temperatures the fluctuations are very small along the x-direction and the y-direction. However, as we increase the temperature, the fluctuations take a higher value. We note that $\langle F_y^2 \rangle$ has a much higher value than $\langle F_x^2 \rangle$ for all temperatures. In the Columnar phase, the value of flux along any column will be small, since the dimers are aligned parallel to each other and every pair of parallel dimers will cancel the fluxes of each other. We note that the values of $\langle F_x^2 \rangle$ is small compared to $\langle F_y^2 \rangle$. For even twists, the value of $\langle F_x^2 \rangle$ is higher for higher temperatures, which indicates that there are fewer dimers which are aligned along the x-direction alone, but since the quantity itself is small, it indicates that overall the system still has an alignment along the x-direction. For odd twists, we see that even $\langle F_x^2 \rangle$ is nearly 0, which indicates that most dimers are aligned along x-direction. This is not a consequence of starting the simulations with an initial alignment along the x-direction, since the simulations were performed starting from each of the four degenerate ground states and equilibrating it well beyond the critical temperature in order to lose the memory of the initial state.

The quantity $\langle F_y^2 \rangle$ has a larger value for lattices with odd twist, which indicates that fewer dimers are aligned along the y-direction. For lattices with even twists, it is smaller. But, we notice for both $\langle F_x^2 \rangle$ and $\langle F_y^2 \rangle$, the value of flux for the system with different twists is clearly different from the untwisted lattice. Strictly speaking, the definition of flux is not possible for a lattice with odd twists, since it is not bipartite. But we can still compute the quantity of flux by enforcing that each site remains as a part of the same sublattice as it was in the untwisted lattice. If we think of sites in the odd sublattice as negative charges, and the sites in the even sublattice as positive charges, then we maintain the charge of each lattice site even in the twisted lattice. In the untwisted lattice (and lattice with even twists), each positive charge is adjacent to only negative charges, and vice versa. But in lattices with odd twist, there are two columns of the lattice along the direction of the twist such that they are connected to the same charge along one direction. In the rest of the lattice, the adjacency remains unchanged.

Now, when we perform the loop update, a dimer is broken and two monomers (opposite charges) are created. One charge is kept fixed and the other moves through the lattice by flipping dimers. In this process, the moving monomer only moves on the sublattice that it is part of. When it completes the loop, a positive and negative charged monomer are adjacent to each other and a dimer is formed between them. This is true for lattices with no

twist or even twists. For odd twists, whenever the monomer destroys a bond that lies along the column at which the twist is implemented, it moves from one sublattice to the other sublattice. So, the charge of the moving monomer changes. When this comes close to the fixed monomer, it would face a “repulsion”, since they have the same charge and a dimer cannot be formed there. We can also explain from the implementation of the algorithm that since they belong to the same sublattice after passing through this column once in lattices with odd twists, they cannot come close enough to form a dimer. This is true only along the direction in which the twist is implemented. So, for lattices with odd twists such that one loop around the system is performed, another loop also needs to be completed in order to complete the loop. If we plot the distribution of the distance along y with the distance along the x -direction (winding number), we see that for odd twists, there are two spots at the positions $-N_x$ and $+N_x$ for which the distance along y cannot be 0.

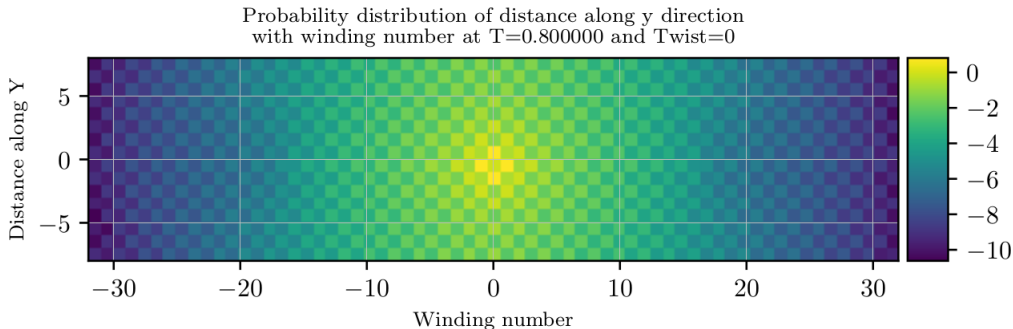


Figure 4.16: Probability distribution of distance along y with the winding along x -direction with 0 twist

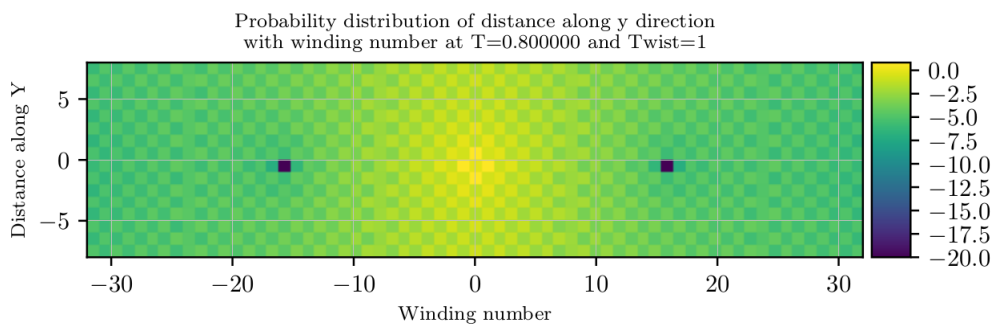


Figure 4.17: Probability distribution of distance along y with the winding along x -direction with 1 twist

The above two plots are the probability distribution of the distance in y -direction with

the the winding number, or more simply the number of steps in the x-direction. This is calculated when the loop is being constructed. For each loop update, we check where the moving monomer is, compared to the stationary monomer, and a distribution is obtained. The colour coding is in the log scale. We notice that for no twist, or even twists, the monomers tend to visit every site on the sublattice, but the probability of winding more than once along x-direction is very small. However, for the odd twists, we notice that the dimers always avoid completing the loop after just one winding of the system.

We can also calculate the monomer monomer correlation function, by looking at the distribution of distances of monomers when the loop is being constructed as discussed in [6] [13]. We expect the pair of monomers to have an attractive entropic potential that increases logarithmically with separation in the disordered regime. This corresponds to their distribution having the behaviour such that $P(r) \sim e^{-\frac{\ln(r)}{2}} \sim r^{-\frac{1}{2}}$. We plot this for a relatively larger lattice system 64x64 at a high temperature of $T=10.0$, on the log-log scale along the directions $(x,0)$ and $(0,y)$. We observe that for even twists, there is no change in the monomer-monomer correlation function, and it is identical to the case with no twists. For the lattice with odd twists (bottom plots in Fig 4.18), we see that the monomer also moves on the opposite sublattice, as seen in the lower values in the plot. We note that for monomers moving on the same sublattice as the original sublattice, the behaviour is identical to that of the behaviour of monomers in the lattice with even twists. For the monomers that move in the opposite sublattice from the original, the two monomers would reside on the same sublattice and hence have the same charge. So, they have a repulsive entropic potential that goes as $V \sim -\frac{\ln(r)}{2}$, which corresponds to the probability distribution having $P(r) \sim e^{\frac{\ln(r)}{2}} \sim r^{\frac{1}{2}}$, which is what we observe.

After plotting the various quantities of interest, we note that the behaviour of the dimer model on the twisted lattice is different from the behaviour of the Ising model on the twisted lattice. While the dimer model only shows a response to whether an odd twist or even twist is present on the lattice, the Ising model in 2D seems to show a response to the amount of twist present, without any differentiation between odd and even twists in particular.

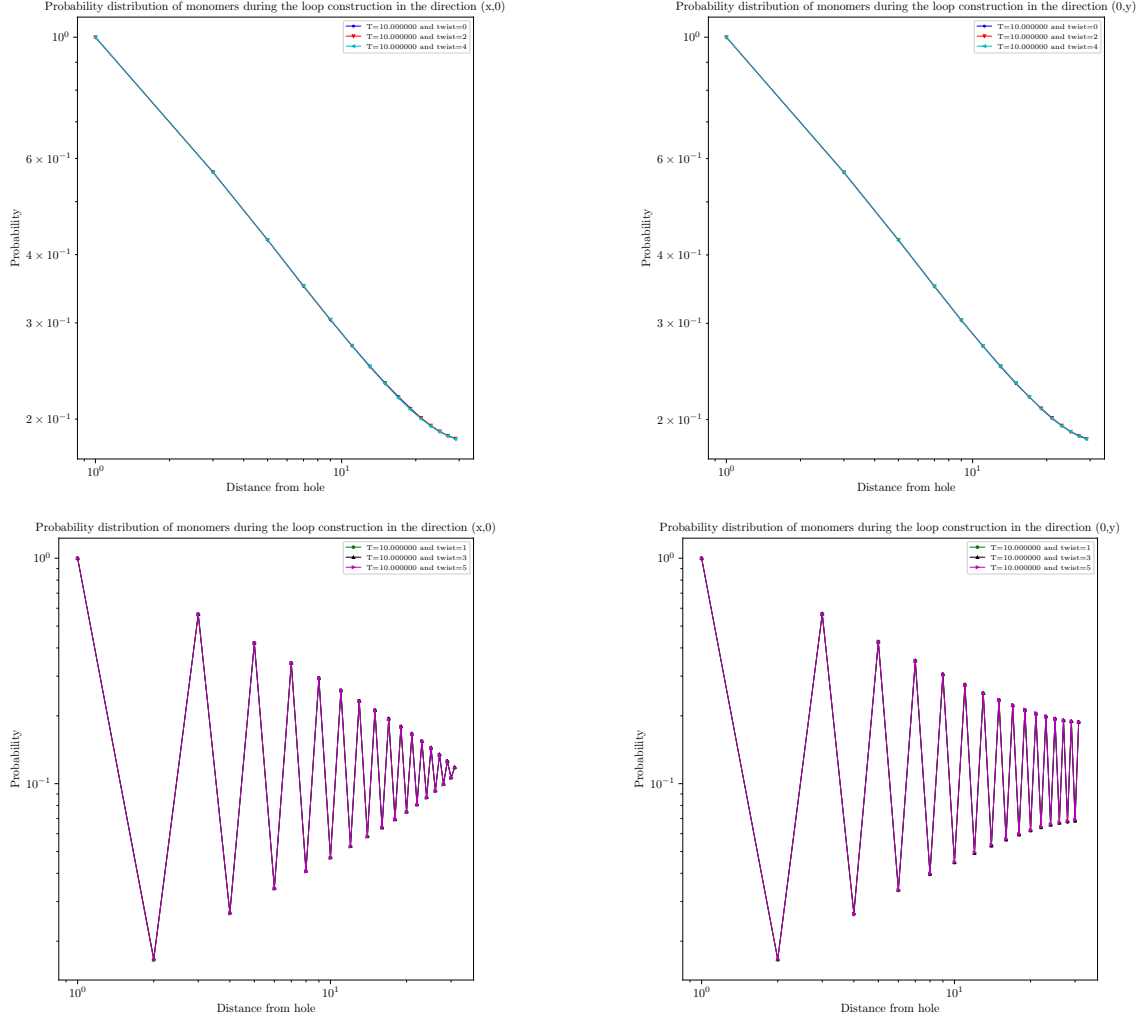


Figure 4.18: Probability distribution of monomer monomer distance at high temperatures

We notice that for odd twists, the scaling is different along the $(x,0)$ direction and along the $(0,y)$ direction. Along the x -direction, in which the twist is applied, the scaling behaviour is different from the monomer-monomer correlation function, since $P(r) \approx r^{-0.64}$ for monomers on opposite sublattices and $P(r) \approx r^{0.64}$ for monomers on the same sublattice (as shown in Fig.4.19). Along the y -direction, we observe a scaling behaviour similar to that of the untwisted lattice with $P(r) \approx r^{-0.52}$ for monomers on opposite sublattices and $P(r) \approx r^{0.51}$ for monomers on the same sublattice (as shown in Fig.4.19). There is clearly an anisotropy due to the presence of odd twists. This needs to be analysed more carefully to understand the behaviour.

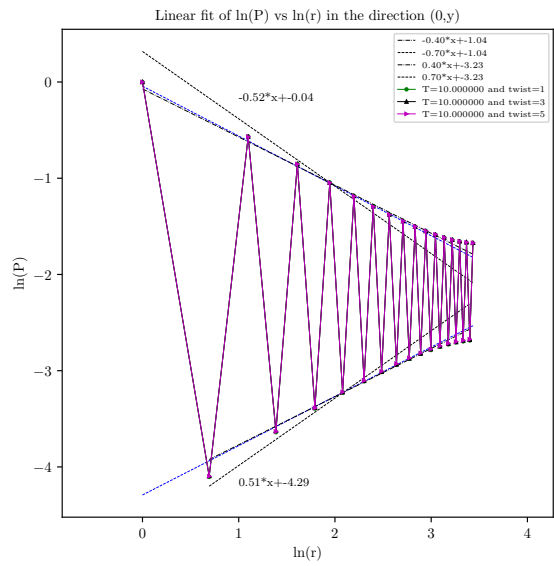
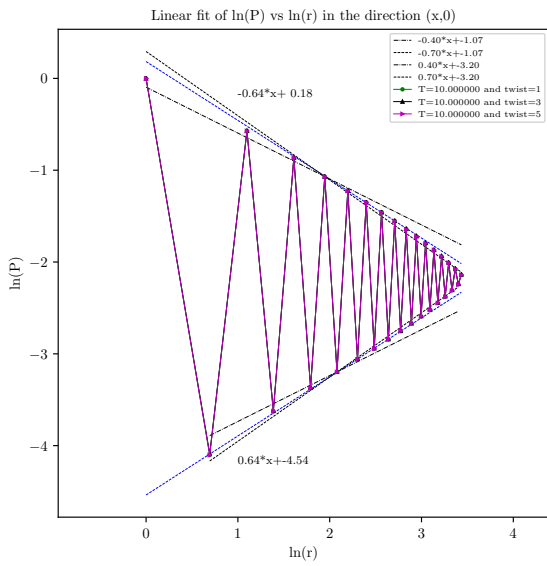
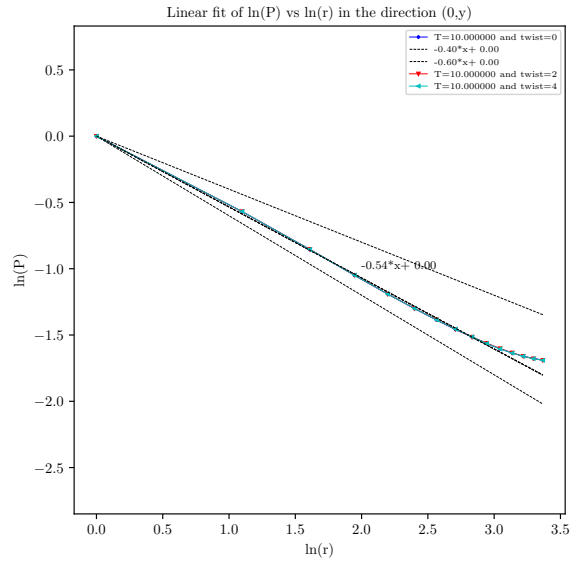
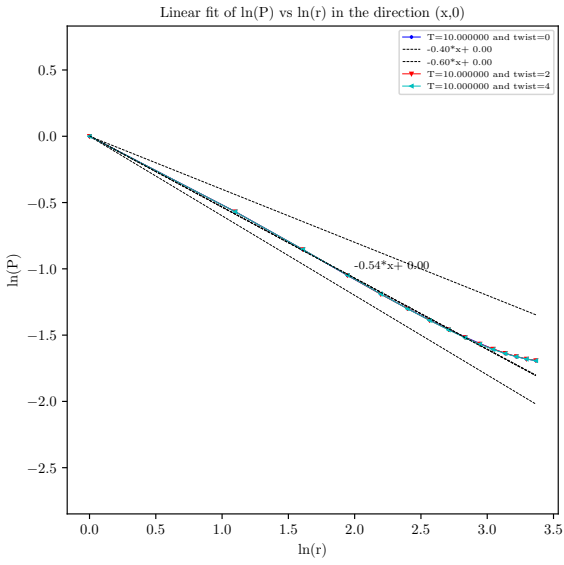


Figure 4.19: Linear fit of $\ln(P)$ vs $\ln(r)$

Chapter 5

Analytical discussion of the Ising model

For the 2D Ising model, we can try to find analytically the effect of the twist on the free energy. This can be done by following Lieb et.al.[2]. First, we map the 2D Ising model to a one-dimensional Transverse Field Ising model.

Let us consider the two-dimensional Ising model on a lattice of size $N_x \times N_y$, which is described by the Hamiltonian:

$$H = - \sum_{\substack{i=1,2,\dots,N_x \\ j=1,2,\dots,N_y}} [J_1 \sigma_{i,j} \sigma_{i+1,j} + J_2 \sigma_{i,j} \sigma_{i,j+1}]$$

where $\sigma_{i,j} = \pm 1$ and we impose periodic boundary conditions, which means $\sigma_{i,N_y+1} = \sigma_{i,1}$ and $\sigma_{N_x+1,j} = \sigma_{1,j}$. This allows us to calculate the energy of the system given a particular configuration of spins. Here the couplings are assumed to be different in the horizontal and vertical directions (Anisotropic Ising Model), since it is more general. We can later set $J_1 = J_2 = J$ to get the usual expression for isotropic Ising model.

Now we can calculate the partition function for this system as

$$Z = \text{Tr}_{\{\sigma\}} e^{-\beta H}$$

where $\beta = \frac{1}{k_B T}$ is the inverse temperature and $k_B = 1.381 \times 10^{-23} JK^{-1}$ is the Boltzmann constant. Here the trace is the sum over all the possible spin configurations.

One way to obtain the solution for this system is by using the Transfer Matrix method, which involves building the partition function step by step in a systematic manner so that it connects the configurations of spins in one row with that in the adjacent row. This allows us to write the exact form of the partition function. Since the matrix contains the interaction of all the possible configurations of one row with the configurations of the adjacent row, in a 2D lattice, we get a $2^{N_x} \times 2^{N_x}$ matrix.

The partition function can be written as

$$Z = \sum_{\{\sigma\}} e^{(K_1 \sum \sigma_{i,j} \sigma_{i+1,j})} e^{(K_2 \sum \sigma_{i,j} \sigma_{i,j+1})} \quad (5.1)$$

where $K_1 = \beta J_1$ and $K_2 = \beta J_2$.

This can be suitably written as a product of matrices using standard algebra to get an expression in terms of transfer matrices T_1 and T_2 , such that

$$Z = \text{Tr}((T_1 T_2)^{N_y}) \quad (5.2)$$

where

$$T_1 = (2 \sinh(2K_1))^{N_x/2} e^{(K_1^* \sum \tau_i^x)} \quad (5.3)$$

and

$$T_2 = e^{K_2 \sum \tau_i^z \tau_{i+1}^z} \quad (5.4)$$

In the process we also use the Kramers-Wannier duality relation $e^{-2K_1} = \tanh(K_1^*)$. Here τ^x and τ^z are the familiar Pauli matrices. This expression appears like a Hamiltonian of the form,

$$H = -K_1^* \sum \tau_i^x - K_2 \sum \tau_i^z \tau_{i+1}^z \quad (5.5)$$

This Hamiltonian is called the 1D Transverse Field Ising model. It contains Pauli operators that act on the spins in the i^{th} site. This is a 1D quantum spin chain with a magnetic field in the transverse direction. This can now be solved using the Jordan-Wigner transformation, which maps this system to a system of non-interacting fermions.

But first we shall do a suitable rotation of the coordinates around the y-axis by $\pi/2$ to simplify our calculations later: $\tau^x \rightarrow -\tau^z$ and $\tau^z \rightarrow \tau^x$

$$T_1 = (2 \sinh(2K_1))^{N_x/2} e^{-(K_1^* \sum \tau_i^z)} \quad (5.6)$$

and

$$T_2 = e^{K_2 \sum \tau_i^x \tau_{i+1}^x} \quad (5.7)$$

The creation and annihilation operators defined by $\tau^+ = \tau^x + i\tau^y$ and $\tau^- = \tau^x - i\tau^y$ can be used to express T_1 as

$$T_1 = (2 \sinh(2K_1))^{N_x/2} e^{-2K_1^* \sum (\tau_i^+ \tau_i^- - \frac{1}{2})} \quad (5.8)$$

If these creation and annihilation operators must act like fermions, then the fermion anti-commutation relations must be satisfied, but instead these operators anti-commute on the same site while commuting on different sites. To ensure that we can solve this equation, we need them to satisfy the fermion anti-commutation relations, which can be done using the Jordan Wigner transformation of the operators:

$$C_m = e^{(i\pi \sum_{j < m} \tau_j^+ \tau_j^-)} \tau_m^- \quad (5.9)$$

$$C_m^\dagger = e^{(i\pi \sum_{j < m} \tau_j^+ \tau_j^-)} \tau_m^+ \quad (5.10)$$

This transformation preserves the quadratic forms of the products of operators in the transfer matrices. Further simplifications using standard algebra allows us to write the expressions as:

$$T = (2 \sinh(2K_1))^{N_x/2} e^{K_2 \sum_m (C_m^\dagger - C_m)(C_{m+1}^\dagger + C_{m+1})} e^{-2K_1^* \sum_m (C_m^\dagger C_m - \frac{1}{2})} \quad (5.11)$$

Once we obtain this expression, we need to diagonalize it to get the eigenvalues. Our motive has been to understand what happens when a twist is applied to the lattice. We can write down a twist operator T_τ which performs the twist on the lattice. We can then

calculate the partition function for the system with the twist as

$$Z = \text{Tr}(T_\tau T^{N_y}) \quad (5.12)$$

Now, if we have a configuration of spins $(\sigma_1, \sigma_2, \dots, \sigma_{N_x})$, the twist matrix acts on it such that we get the new state as $(\sigma_{N_x}, \sigma_1, \sigma_2, \dots, \sigma_{N_x-1})$. So the matrix elements of T_τ are such that

$$\langle (\sigma_{N_x}, \sigma_1, \sigma_2, \dots, \sigma_{N_x-1}) | T_\tau | (\sigma_1, \sigma_2, \dots, \sigma_{N_x}) \rangle = 1, \quad (5.13)$$

and 0 for all other elements. This matrix is also of dimension $2^{N_x} \times 2^{N_x}$, and it acts on the transfer matrix. We can see from the definition of the twist matrix that the states $(1, 1, \dots, 1)$ and $(-1, -1, \dots, -1)$ do not get affected by the twist. So the ground states of the system do not get affected by the twist. Further calculation has not been done exactly, but we can say how this affects the system in a general way. The expression inside the trace can be written in a more symmetric way as

$$Z = \text{Tr}((T_2^{\frac{1}{2}} T_\tau T_2^{-\frac{1}{2}})(T_2^{\frac{1}{2}} T_1 T_2^{\frac{1}{2}}) \dots (T_2^{\frac{1}{2}} T_1 T_2^{\frac{1}{2}})) \quad (5.14)$$

using the cyclic property of trace. If we now define $\tilde{T}_\tau = (T_2^{\frac{1}{2}} T_\tau T_2^{-\frac{1}{2}})$ and $T = (T_2^{\frac{1}{2}} T_1 T_2^{\frac{1}{2}})$, then the expression becomes

$$Z = \text{Tr}(\tilde{T}_\tau T^{N_y}) \quad (5.15)$$

We can now calculate the spectral decomposition of the transfer matrix T_y^N as

$$T^{N_y} = \sum_i \lambda_i^{N_y} |\lambda_i\rangle \langle \lambda_i| \quad (5.16)$$

The partition function can be calculated as

$$\begin{aligned} Z &= \text{Tr}(\tilde{T}_\tau \sum_i \lambda_i^{N_y} |\lambda_i\rangle \langle \lambda_i|) \\ &= \sum_i \lambda_i^{N_y} \text{Tr}(\tilde{T}_\tau |\lambda_i\rangle \langle \lambda_i|) \\ &= \lambda_0^{N_y} \text{Tr}(\tilde{T}_\tau |\lambda_0\rangle \langle \lambda_0|) + \lambda_1^N \text{Tr}(\tilde{T}_\tau |\lambda_1\rangle \langle \lambda_1|) + \dots \end{aligned}$$

where λ_0 is the largest eigenvalue of the matrix. If N is large enough, the other eigenvalues do not contribute to the partition function.

$$Z = \lambda_0^N \left(\text{Tr}(\tilde{T}_\tau |\lambda_0\rangle\langle\lambda_0|) + \left(\frac{\lambda_1}{\lambda_0}\right)^N \text{Tr}(\tilde{T}_\tau |\lambda_1\rangle\langle\lambda_1|) + \dots \right)$$

Now the eigenvalues of the transfer matrix can be calculated by writing it in the momentum space. In the momentum space, the transfer matrix takes the form

$$T = (2 \sinh(2K_1))^{N/2} \prod_{0 \leq q \leq \pi} T_q \quad (5.17)$$

where we have

$$T_q = e^{(2K_2 \cos(q))} \begin{pmatrix} A_q & C_q \\ C_q & B_q \end{pmatrix}$$

and the values A_q , B_q and C_q are

$$\begin{aligned} A_q &= e^{-2K_1^*} (\cosh(K_2) + \sinh(K_2) \cos(q))^2 + e^{2K_1^*} (\sinh(K_2) \sin(q))^2 \\ B_q &= e^{-2K_1^*} (\sinh(K_2) \sin(q))^2 + e^{2K_1^*} (\cosh(K_2) - \sinh(K_2) \cos(q))^2 \\ C_q &= (2 \sinh(K_2) \sin(q)) (\cos(2K_1^*) \cosh(K_2) - \sinh(2K_1^*) \sinh(K_2) \cos(q)) \end{aligned}$$

When we calculate the eigenvalues from here, we get a relation between the eigenvalues and the momentum, and we can plot the dispersion relation. The eigenvalue corresponding that is observed in the partition function is a product of the eigenvalues of the individual transfer matrices in the momentum space. So, the leading eigenvalue is calculated from this as the product of all the largest eigenvalues for each q , which is written as λ_0 .

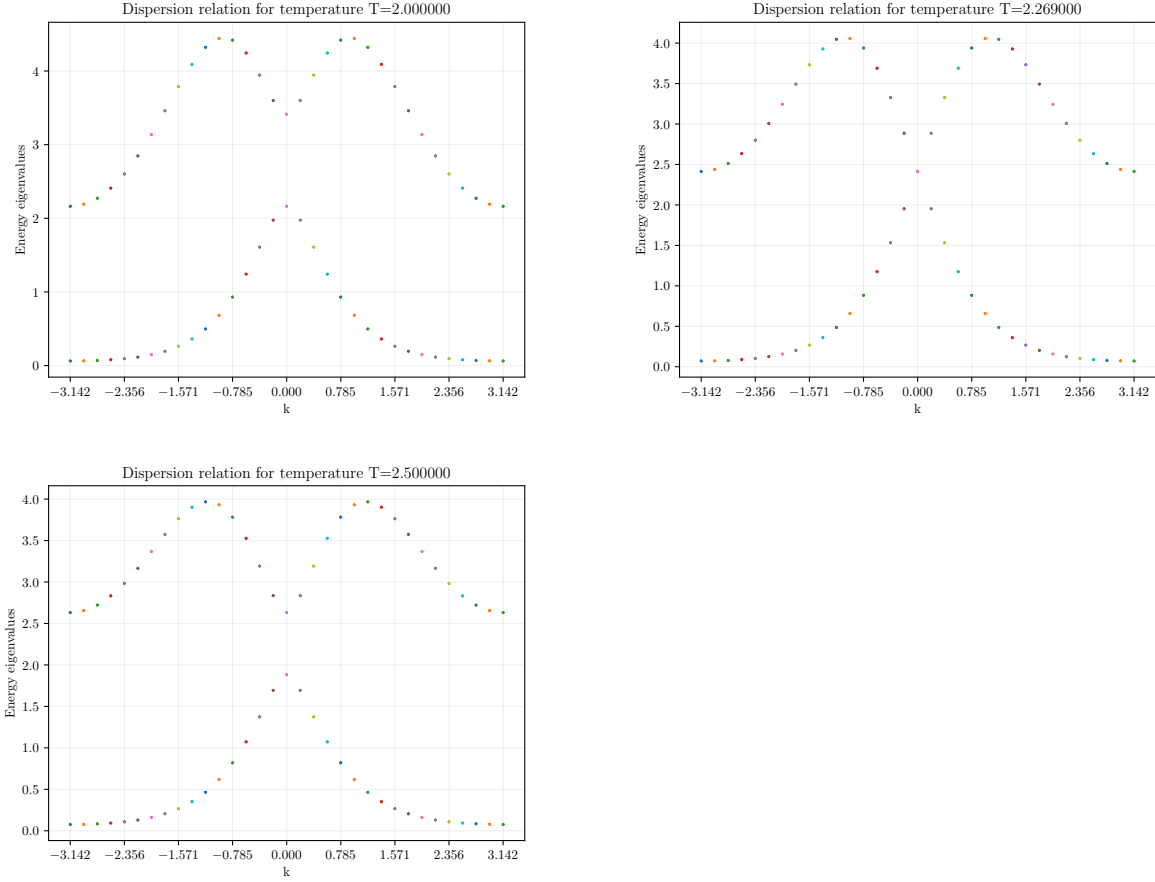


Figure 5.1: Dispersion relation for different temperatures

We see that the product of the largest eigenvalues of T_q is λ_0 . The next highest eigenvalue, λ_1 must be the highest value of the lower band. For temperatures other than the critical temperature, we see that $\frac{\lambda_1}{\lambda_0} < 1$. So the corrections to the partition function will not be present when $N \rightarrow \infty$ since the ratio will go to 0, and the partition function is unaffected by the twist. For temperatures close to the critical temperature, $\lambda_1 \approx \lambda_0$. Then the corrections to the partition function cannot be ignored and the effect of the twist becomes more relevant. It is also relevant when we don't take the thermodynamic limit along the y -direction, since the partition function is calculated as $Z = \text{Tr}(T_y^N)$. If N_y is not very large, it is not accurate to assume $(\frac{\lambda_1}{\lambda_0})^{N_y} \rightarrow 0$. This corresponds to our observations from the simulations where systems with small values of N_y and large value of N_x seem to be most affected by the twist.

Chapter 6

Conclusions

The project was motivated to understand what happens when a twist is applied to a lattice. In order to do this, we took two simple systems, the Ising model and the dimer model, in which it is relatively simple to simulate the effect of twist and to calculate it analytically. After defining what the twist operator is, and its action on the lattice, we performed some numerical simulations of the systems to see how the system is affected by the twist.

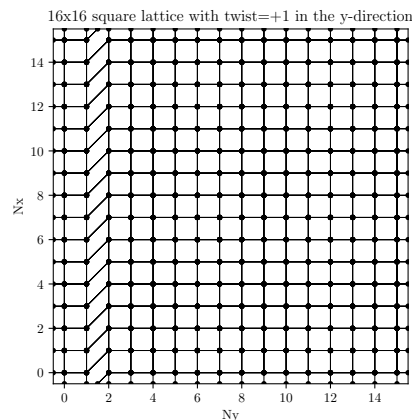


Figure 6.1: Lattice with a twist of +1 in the y-direction; Twist values range from 0 to $N_x - 1$

For the Ising model, the twist was applied along the y-direction, so that the values of twist range from 0 to $N_x - 1$. We observed from the Monte Carlo simulations that:

- The free energy and other statistical quantities show some change with twists for systems with small values of N_y and large value of N_x , but in the thermodynamic limit, the effect of the twist vanishes.
- The expectation value of the energy of the system shows some kind of crossing behaviour around $T=2.5$, below which system prefers larger twists and above which the system prefers smaller twists.
- Through the semi-analytical arguments, we could explain why the twist plays a role close to the critical temperature. More careful calculation could enable us to calculate the exact dependence of the free energy on the twist, and also the dependence of twist for all the other quantities.

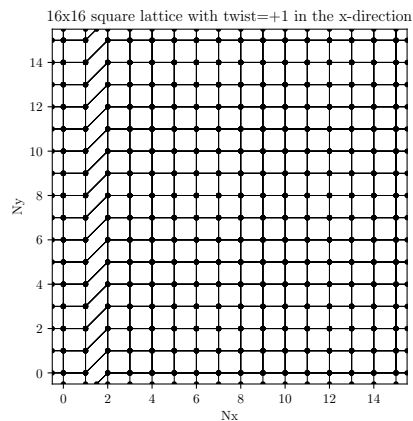


Figure 6.2: Lattice with a twist of +1 in the x-direction; Twist values range from 0 to $N_y - 1$

From the Monte Carlo simulations of the dimer model on the square lattice of size $N_x N_y$, we applied the twist along the x-direction and the values of the twist range from 0 to $N_y - 1$. We observed from simulations that:

- We looked at various quantities that were described in Chapter 3, and they did not show any strong effect of twist. However, we did see a difference between the lattices with odd twists and even twists, which is likely due to the system being non-bipartite for odd twists and bipartite for even twists.

- For low temperatures, the difference between odd and even twists is more pronounced, even away from the critical temperature. But for high temperatures, the effect of the twist vanishes, which is different from the behaviour of the Ising model.

Some interesting questions that one could ask in the case of the Ising model is about the effect of twist on the transport properties of the system. It will be curious to study if twists can transport energy from one region to another. It is also interesting to understand if twists play a role in the 3D Ising model. These lattice twists can be made mobile, and they can keep fluctuating in the system. It would be interesting to understand if the model on the lattice provides a glue-like effect for these lattice twists and freeze the twists in the lattice. We have studied the effect of twist on the classical Ising model and classical dimer model, and it would be interesting to see what happens when the model is a quantum Ising model or quantum dimer model.

For the dimer model, one could ask if the effect of twists persists even for larger systems. While it is not simple to introduce mobile twists (twists on the lattice that are not fixed, and can fluctuate with time) on the dimer model, the implementation of these twists would give rise to monomers at different sites of the lattice, and one can study the behaviour of the system with these monomers present. However, it can be quite challenging to introduce such mobile twists for the dimer model, because in doing so one would introduce many monomers in the lattice and will result in the model not being fully filled. It is trivial to implement such mobile twists for the Ising model, and it would be interesting to develop an algorithm that performs a similar role for the dimer model.

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