# A Study of a Lattice based Symmetry broken Dimer Evaporation - Deposition process 



A thesis submitted towards partial fulfilment of BS-MS Dual Degree Programme
by

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under the guidance of

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## Certificate

This is to certify that this thesis entitled "A STUDY OF A LATTICE BASED SYMMETRY BROKEN DIMER EVAPORATION - DEPOSITION PROCES" submitted towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research Pune represents original research carried out by "VISHNU V. KRISHNAN" at "IISER - PUNE", under the supervision of "ARIJIT BHATTACHARYAY" during the academic year 2014-2015.


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## Declaration

I hereby declare that the matter embodied in the report entitled "A STUDY OF A LATTICE BASED SYMMETRY BROKEN DIMER EVAPORATION - DEPOSITON PROCESS" are the results of the investigations carried out by me at the Department of PHYSICS, IISER-PUNE, under the supervision of ARIJIT BHATTACHARYAY and the same has not been submitted elsewhere for any other degree.


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## Abstract

The analytic and computational study of the probabilistic mechanics of particles is simplified by latticizing space. In this project, we consider a two dimensional, square lattice, with particles interacting via nearest neighbour dimer evaporation-deposition processes. We then use the quantum spin analogy developed by Stinchcombe et al. to analyse the system. Here, we study the analogous Hamiltonians of two systems, one with evaporation and deposition allowed in both spatial directions, and the other with this symmetry, broken. We note that despite differences in the Hamiltonian, both systems have the same ground state, and differ in dynamics of the excitations.

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## Chapter 1

## The Introduction

In this chapter we will establish formalisms and discuss the precedent to this work.

### 1.1 The raison d'être

An exact understanding of non-equilibrium statistical mechanics has long eluded us, and this project was taken up to get closer to such an understanding. Lots of 'many-body' problems ranging from molecular crowding to traffic issues, can be simplified and studied under the ambit of non-equilibrium statistical mechanics. A Lot of emergent behaviour like jamming, shock waves etc., are preserved, and therefore can be analysed.

### 1.2 Structure

As part of this chapter, in the next section, we will discuss some basic stochastic mechanics, as well as the quantum spin analogy introduced by Stinchcombe et al.. In Chapter 2, we will look at the evaporation - deposition Hamiltonian as described by Stinchcombe et al. [5, 1, 2] and the symmetry broken Hamiltonian and attempt to compare the two. Through Chapter 3 , we look at what properties emerge out of a mean field analysis of the two systems, and compare them. The results of numerical simulations comparing various properties of the two systems are included in Chapter 4 .

### 1.3 Humble beginnings

Consider a two dimensional lattice as shown. Let $s$ denote a particular state, or configuration of the system.


Figure 1.1: An arbitrary state s . This is a simple square lattice. The filled sites indicate the presence of a particle, while empty ones indicate absence.

From a description by Schutz [3, 4], a probabilistic evolution of the state may be written as follows, where $P(s, t)$ is the probability that the system is in a state $s$, at time $t$.

$$
\begin{equation*}
P(s, t+\Delta t)=\underset{s^{\prime} \in \chi}{\sum} p_{s^{\prime} \rightarrow s} P\left(s^{\prime}, t\right) \tag{1.1}
\end{equation*}
$$

where $\chi$ is the set of all states, and $p_{s \rightarrow s^{\prime}}$ is the probability of a jump between two states, from $s$ to $s^{\prime}$. Given this microscopic step, the Master equation is derived as follows

$$
\begin{equation*}
P(s, t+\Delta t)-P(s, t)=\sum_{s^{\prime} \neq s} p_{s^{\prime} \rightarrow s} P(s, t)-P(s, t) \tag{1.2}
\end{equation*}
$$

but, note that amongst the jump probabilities is one term that is responsible for a state to remain as it is. And, $p_{s \rightarrow s}=1-\sum_{s^{\prime} \neq s} p_{s \rightarrow s^{\prime}}$. This is used in the equation above to get

$$
\begin{equation*}
P(s, t+\Delta t)-P(s, t)=\sum_{s^{\prime} \neq s}\left[p_{s^{\prime} \rightarrow s} P\left(s^{\prime}, t\right)-p_{s \rightarrow s^{\prime}} P(s, t)\right] \tag{1.3}
\end{equation*}
$$

This equation is now divided by $\Delta t$, and the limit $\Delta t \rightarrow 0$ is taken. Then, the Master equation is

$$
\begin{equation*}
\partial_{t} P(s, t)=\sum_{s^{\prime} \neq s}\left[\omega_{s^{\prime} \rightarrow s} P\left(s^{\prime}, t\right)-\omega_{s \rightarrow s^{\prime}} P(s, t)\right] \tag{1.4}
\end{equation*}
$$

where $\omega$ is a jump rate. Now, as described in [5], we move to a Hamiltonian formalism by taking states $s$ to state vectors $|s\rangle$, and probabilities to probability vectors like

$$
\begin{equation*}
|P(t)\rangle=\sum_{s}[P(s, t)|s\rangle] \tag{1.5}
\end{equation*}
$$

So, given the master equation, a stochastic time dependent Schrödinger equation is written as follows

$$
\begin{equation*}
\partial_{t}|P(t)\rangle=-\mathcal{H}|P(t)\rangle \tag{1.6}
\end{equation*}
$$

Also, the evolution operator at very small time steps is

$$
\begin{equation*}
e^{-\mathcal{H} \Delta t}=1-\mathcal{H} \Delta t \tag{1.7}
\end{equation*}
$$

### 1.4 The Heisenberg model analogy

An occupied site is mapped to an up spin and a vacancy to a down spin [1]. This analogy allows us to write the Hamiltonian in terms of that of the familiar quantum many-body problem, and thereby use all the techniques available to us there.

Before we delve into the evaporation-deposition problem, we look at an instructive one dimensional diffusion model [2]. Two adjacent lattice sites, say $(i \& i+1)$ are considered. The probability that the particle makes the jump, in time $\Delta t$ is $\omega_{i i+1} \Delta t$. So now, a spin Hamiltonian for the system is written by comparing the evolution operator for microscopic steps with equation 1.7 [5]

$$
\begin{equation*}
\mathcal{H}=\sum_{i}\left[-\omega_{i i+1} \sigma_{i}^{-} \sigma_{i+1}^{+}+\frac{1}{4} \omega_{i i+1}\left(1+\sigma_{i}^{z}\right)\left(1-\sigma_{i+1}^{z}\right)\right] \tag{1.8}
\end{equation*}
$$

The first term makes the jump with probability $\omega_{i+1} \Delta t$, while the second term allows it to remain, with a probability $1-\omega_{i i+1} \Delta t$. Accounting for the symmetrically opposite process, the following is obtained

$$
\begin{array}{r}
\mathcal{H}=\frac{1}{4} \Sigma_{i}\left[\frac{1}{2}\left(\omega_{i i+1}+\omega_{i+1 i}\right)\left(\bar{\sigma}_{\mathbf{i}} \cdot \bar{\sigma}_{\mathbf{i}+\mathbf{1}}-1\right)\right]+  \tag{1.9}\\
\frac{1}{4} \sum_{i}\left[\frac{1}{2}\left(\omega_{i i+1}-\omega_{i+1}\right)\left\{i\left(\sigma_{i}^{x} \sigma_{i+1}^{y}-\sigma_{i}^{y} \sigma_{i+1}^{x}\right)+\sigma_{i}^{z} \sigma_{i+1}^{z}\right\}\right]
\end{array}
$$

This is the Hamiltonian for a lattice with asymmetric, hard-core (single occupancy of a lattice site) diffusion, and in case of equal rates ( $\omega_{i i+1}=$ $\left.\omega_{i+1 i}\right)$, it maps to a simple Heisenberg Hamiltonian ( $\bar{\sigma}_{\mathbf{i}} \cdot \bar{\sigma}_{\mathbf{i}+\mathbf{1}}-1$ ).

It is interesting to note that the ground state of this Hamiltonian is a state with all spins pointing in one direction. In a two dimensional lattice the analogy is as follows


Figure 1.2: The jammed and analogous ground states.
With respect to diffusion, this state is 'jammed'; i.e., given diffusion as the only process, the system will remain stuck in this state. So, the analogous ground state seems to correspond to a jammed state in our system.

## Chapter 2

## The Alter(c)ation

We will now look at the interaction that is the main focus of this project: evaporation and deposition. In this chapter we will only describe the two cases. For a discussion on the dynamics of the new Hamiltonian, look at Chapter 5

### 2.1 Unbroken symmetry

Dimer deposition and evaporation occur on adjacent lattice sites that are empty and full, respectively. Similar to a jump rate, evaporation ( $\epsilon^{\prime}$ ) and deposition $(\epsilon)$ rates are defined such that a dimer will evaporate with a probability $\epsilon^{\prime} \Delta t$, and correspondingly deposit.[2]

In the same way as in section 1.4, the Hamiltonian is deduced from the microscopic evolution operator. As in the earlier chapter, we can look at just the one dimensional Hamiltonian, and easily extrapolate to two. The relevant Hamiltonian is

$$
\begin{align*}
\mathcal{H}=-\sum_{i} & {\left[\epsilon_{i i+1}^{\prime}\left\{\sigma_{i}^{-} \sigma_{i+1}^{-}-\frac{1}{4}\left(1+\sigma_{i}^{z}\right)\left(1+\sigma_{i+1}^{z}\right)\right\}\right]+} \\
& -\sum_{i}\left[\epsilon_{i i+1}\left\{\sigma_{i}^{+} \sigma_{i+1}^{+}-\frac{1}{4}\left(1-\sigma_{i}^{z}\right)\left(1-\sigma_{i+1}^{z}\right)\right\}\right] \tag{2.1}
\end{align*}
$$

The first term annihilates while the second creates. When the two rates are equal, this reduces to

$$
\begin{equation*}
\mathcal{H}=-\epsilon_{i i+1} \sum_{i}\left[\sigma_{i}^{-} \sigma_{i+1}^{-}+\sigma_{i}^{+} \sigma_{i+1}^{+}-\frac{1}{2}\left(1+\sigma_{i}^{z} \sigma_{i+1}^{z}\right)\right] \tag{2.2}
\end{equation*}
$$

At this point, a little trick is employed to better utilise this Hamiltonian. Let our current square lattice be made up of two interlaced simple square lattices of $\sqrt{2}$ times the original lattice site separation.


Figure 2.1:

Given any two adjacent points, each will be in a different sub-lattice. Now, given two points, let us perform the following 'flip' in the Hamiltonian, to one of the points. [2]

$$
\begin{equation*}
\sigma_{i+1}^{ \pm} \rightarrow \sigma_{i+1}^{\mp} \sigma_{i}^{z} \rightarrow-\sigma_{i}^{z} \tag{2.3}
\end{equation*}
$$

This then takes the Hamiltonian to the Heisenberg form. The state corresponding to the ground state is represented by figure 2.2 . You can easily see that with respect to dimer evaporation and deposition processes, this is a jammed state. It is so because for either of those processes to occur, there needs to exist a dimer occupancy/vacancy.


Figure 2.2:
Thus, from the two examples of the Heisenberg analogy provided by Stinchcombe et al., we see that the ground state in the spin system corresponds to a jammed state in the lattice. We now would like to look at this with a minor modification.

### 2.2 Broken symmetry

We now break the spatial symmetry of the evaporation-deposition processes. Let us say, we allow evaporation in the x -direction and deposition in y . Then, we now have the Hamiltonian

$$
\begin{align*}
\mathcal{H}=- & -\sum_{i}
\end{align*} \quad\left[\epsilon_{i i+1}^{\prime x}\left\{\sigma_{i, j}^{-} \sigma_{i+1, j}^{-}-\frac{1}{4}\left(1+\sigma_{i, j}^{z}\right)\left(1+\sigma_{i+1, j}^{z}\right)\right\}\right]+,
$$

You can immediately see that a simplification like in the previous case is no longer possible, due to the two terms now acting on different dimensions. But let us proceed in a similar manner anyway.

$$
\begin{align*}
\mathcal{H}=- & \sum_{i}\left[\epsilon_{i i+1}^{\prime x}\left\{\sigma_{i, j}^{-} \sigma_{i+1, j}^{-}-\frac{1}{4}\left(1+\sigma_{i, j}^{z}+\sigma_{i+1, j}^{z}+\sigma_{i, j}^{z} \sigma_{i+1, j}^{z}\right)\right\}\right]+ \\
& -\sum_{j}\left[\epsilon_{j j+1}^{y}\left\{\sigma_{i, j}^{+} \sigma_{i, j+1}^{+}-\frac{1}{4}\left(1-\sigma_{i, j}^{z}-\sigma_{i, j+1}^{z}+\sigma_{i, j}^{z} \sigma_{i, j+1}^{z}\right)\right\}\right] \tag{2.5}
\end{align*}
$$

Now, we perform the same sub-lattice flip, as before. That gives us

$$
\begin{align*}
\mathcal{H}=- & \sum_{i}\left[\frac{\epsilon_{i i+1}^{\prime x}}{4}\left\{\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}+\mathbf{1}, \mathbf{j}}-1-\sigma_{i, j}^{z}-\sigma_{i+1, j}^{z}+i\left(\sigma_{i, j}^{x} \sigma_{i+1, j}^{y}-\sigma_{i, j}^{y} \sigma_{i+1, j}^{x}\right)\right\}\right]+ \\
& -\sum_{j}\left[\frac{\epsilon_{j j+1}^{y}}{4}\left\{\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i} \mathbf{j} \mathbf{j} \mathbf{1}}-1-\sigma_{i, j}^{z}-\sigma_{i, j+1}^{z}+i\left(\sigma_{i, j}^{x} \sigma_{i, j+1}^{y}-\sigma_{i, j}^{y} \sigma_{i, j+1}^{x}\right)\right\}\right] \tag{2.6}
\end{align*}
$$

this reduces to

$$
\begin{align*}
\mathcal{H}=-\sum_{i} & {\left[\frac{\epsilon_{i i+1}^{\prime x}}{4}\left\{\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}+\mathbf{1}, \mathbf{j}}-1-\sigma_{i, j}^{z}-\sigma_{i+1, j}^{z}+4 \sigma_{i, j}^{-} \sigma_{i+1, j}^{-}\right\}\right]+} \\
& -\sum_{j}\left[\frac{\epsilon_{j j+1}^{y}}{4}\left\{\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}, \mathbf{j}+\mathbf{1}}-1-\sigma_{i, j}^{z}-\sigma_{i, j+1}^{z}-4 \sigma_{i, j}^{-} \sigma_{i+1, j}^{-}\right\}\right] \tag{2.7}
\end{align*}
$$

This does not seem tractable due to the pair annihilation terms. So, we may pursue another line of simplification, where we attempt to write the Hamiltonian in terms of the three pauli matrices, without any annihilation or creation matrices.

We begin from equation 2.4 once again, but this time look at both directions together, and introduce the flip at this point. Also, we assume the two rates to be equal.

$$
\begin{equation*}
\frac{1}{-\epsilon} \mathcal{H}=\sigma_{i, j}^{-} \sigma_{i+1, j}^{+}+\sigma_{i, j}^{+} \sigma_{i, j+1}^{-}-\frac{1}{4}\left\{\left(1+\sigma_{i, j}^{z}\right)\left(1-\sigma_{i+1, j}^{z}\right)+\left(1-\sigma_{i, j}^{z}\right)\left(1+\sigma_{i, j+1}^{z}\right)\right\} \tag{2.8}
\end{equation*}
$$

We know the commutation relation $i \sigma^{z}=\left[\sigma^{x}, \sigma^{y}\right]$ as well as the relation $\sigma^{ \pm}=1 / 2\left(\sigma^{x} \pm i \sigma^{y}\right)$. We use these to write the Hamiltonian in terms of the first two pauli matrices

$$
\begin{gather*}
\frac{4}{-\epsilon} \mathcal{H}=\left(\sigma_{i, j}^{x}+i \sigma_{i, j}^{y}\right)\left(\sigma_{i+1, j}^{x}-i \sigma_{i+1, j}^{y}\right)+\left(\sigma_{i, j}^{x}-i \sigma_{i, j}^{y}\right)\left(\sigma_{i, j+1}^{x}+i \sigma_{i, j+1}^{y}\right)  \tag{2.9}\\
\frac{4}{-\epsilon} \mathcal{H}=\sigma_{i, j}^{x} \sigma_{i+1, j}^{x}+\sigma_{i, j}^{y} \sigma_{i+1, j}^{y}+\sigma_{i, j}^{x} \sigma_{i, j+1}^{x}+\sigma_{i, j}^{y} \sigma_{i, j+1}^{y}  \tag{2.10}\\
-i\left(\sigma_{i, j}^{x} \sigma_{i+1, j}^{y}-\sigma_{i, j}^{y} \sigma_{i+1, j}^{x}\right)-i\left(\sigma_{i, j}^{y} \sigma_{i, j+1}^{x}-\sigma_{i, j}^{x} \sigma_{i, j+1}^{y}\right)
\end{gather*}
$$

We re-convert the upper row back into a form involving the Heisenberg Hamiltonian

$$
\begin{array}{r}
\frac{4}{-\epsilon} \mathcal{H}=\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}+\mathbf{1}, \mathbf{j}}-1-\sigma_{i+1, j}^{z}+\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}, \mathbf{j}+\mathbf{1}}-1+\sigma_{i, j+1}^{z}  \tag{2.11}\\
-i\left(\sigma_{i, j}^{x} \sigma_{i+1, j}^{y}-\sigma_{i, j}^{y} \sigma_{i+1, j}^{x}\right)-i\left(\sigma_{i, j}^{y} \sigma_{i, j+1}^{x}-\sigma_{i, j}^{x} \sigma_{i, j+1}^{y}\right)
\end{array}
$$

Comparing this with the Hamiltonian of the system with an un-broken symmetry, we see that apart from the Heisenberg term, there are two field terms, and an angular momentum - like term (it is not, because there are two different spins involved).

A cursory look at a lattice with such a symmetry broken evaporation deposition process tells us, interestingly, that its jammed state is the same as for the original system. We will discuss more about this in Chapter 5

## Chapter 3

## The Mean Field

In this chapter, we are going to discuss the mean field approach, and look at the features it presents.[2] Let us look at the density variation at a site. It would be the average of the particle currents going in and out of that site.

$$
\begin{equation*}
\frac{d \rho_{i}}{d t}=\left\langle J_{i-}+J_{i+}\right\rangle \tag{3.1}
\end{equation*}
$$

### 3.1 Unbroken Symmetry

It is instructive to perform a mean field study of a one dimensional system of the original kind with both evaporation and deposition allowed. Let $n_{i}$ denote the occupancy of a site, with possible values being 0 and 1 .

$$
\begin{align*}
& J_{i+}=\epsilon\left(1-n_{i}\right)\left(1-n_{i+1}\right)-\epsilon^{\prime} n_{i} n_{i+1} \\
& J_{i-}=\epsilon\left(1-n_{i-1}\right)\left(1-n_{i}\right)-\epsilon^{\prime} n_{i-1} n_{i} \tag{3.2}
\end{align*}
$$

Now, we look at the average of these currents. Here is where lies the crux of the mean field simplification: in ignoring higher order correlations. i.e., $\left\langle n_{i} n_{i+1}\right\rangle=\left\langle n_{i}\right\rangle\left\langle n_{i+1}\right\rangle=\rho_{i} \rho_{i+1}$. So now, we have

$$
\begin{equation*}
\frac{d \rho_{i}}{d t}=2-2 \rho_{i}-\rho_{i+1}-\rho_{i-1} \tag{3.3}
\end{equation*}
$$

Since we only consider equal rates, we will set $\epsilon=\epsilon^{\prime}=1$.

### 3.1.1 Uniform average density in 1 dimension

Upon summing over all lattice sites (assume periodic boundaries throughout) and dividing by the number of sites, we obtain the density profile of the whole lattice.

$$
\begin{equation*}
\frac{d \bar{\rho}(t)}{d t}=2-4 \rho(t) \tag{3.4}
\end{equation*}
$$

This is a first order linear ODE. Solving it yields

$$
\begin{equation*}
\bar{\rho}(t)=c e^{-4 t}+\frac{1}{2} \tag{3.5}
\end{equation*}
$$

Plotting for various initial conditions, we see that the average density goes to half.


Figure 3.1: The variation of the average density, with time, for a 1Dimensional system

### 3.1.2 The continuum approximation

Instead of performing the above simplification of equation 3.3, we may rewrite it as follows

$$
\begin{equation*}
\frac{d \rho_{i}}{d t}=2-4 \rho_{i}-\left(\rho_{i+1}-2 \rho_{i}+\rho_{i-1}\right) \tag{3.6}
\end{equation*}
$$

At system sizes much larger than the distance between two adjacent lattice points, we may use the first principles definition of a double derivative to write

$$
\begin{equation*}
\frac{\partial \rho_{i}}{\partial t}=2-4 \rho_{i}-\frac{\partial^{2} \rho_{i}}{\partial^{2} x} \tag{3.7}
\end{equation*}
$$

Under steady state conditions, we get a form for $\rho_{i}$

$$
\begin{equation*}
\rho_{i}=\frac{1}{2}+C_{1} \cos (2 x)+C_{2} \sin (2 x) \tag{3.8}
\end{equation*}
$$



Figure 3.2: The density profile for a 1-Dimensional system, under initial conditions of half, zero and full occupancies.

This density profile, in accordance with the average density of the system, has a mean value of half.

### 3.1.3 Uniform average density in 2 dimensions

Moving to two dimensions with the symmetry retained is trivial. One needs to consider two more currents, resulting in

$$
\begin{align*}
\frac{d \bar{\rho}(t)}{d t} & =4-8 \rho(t) \\
\Rightarrow \bar{\rho}(t) & =c e^{-8 t}+\frac{1}{2} \tag{3.9}
\end{align*}
$$

This signifies a faster (to first order) approach to a constant density of $\frac{1}{2}$. This is also visible upon comparison with its plot for various initial conditions. Note that both figures have the same scale.


Figure 3.3: The variation of the average density, with time, for a 2Dimensional system

### 3.2 Broken Symmetry

We now look at what the mean field approach tells us about our altered system. Let us write down the currents for this.

$$
\begin{gather*}
J_{x}=-\epsilon^{\prime} n_{i, j} n_{i+1, j}-\epsilon^{\prime} n_{i-1, j} n_{i, j}  \tag{3.10a}\\
J_{y}=\epsilon\left(1-n_{i, j-1}\right)\left(1-n_{i, j}\right)+\epsilon\left(1-n_{i, j}\right)\left(1-n_{i, j+1}\right) \tag{3.10b}
\end{gather*}
$$

That gives us a density differential equation of the form

$$
\begin{equation*}
\frac{d \rho_{i, j}}{d t}=2-2 \rho_{i, j}+\rho_{i, j-1} \rho_{i, j}+\rho_{i, j} \rho_{i, j+1}-\rho_{i-1, j} \rho_{i, j}-\rho_{i, j} \rho_{i+1, j} \tag{3.11}
\end{equation*}
$$

### 3.2.1 Uniform average density in 2 dimensions

We may follow the same procedure as before to discern the density profile of our system, but this system introduces non-linear terms. At this point I make the assumption, that at long times, $\rho_{i, j}=\rho_{i, j-1}=\rho_{i, j+1}=\rho_{i-1, j}=\rho_{i+1, j}$. Then, the two non-linear terms cancel out to give

$$
\begin{equation*}
\frac{d \bar{\rho}(t)}{d t}=2-2 \bar{\rho}(t) \tag{3.12}
\end{equation*}
$$

This has a profile as is seen in the following figure. Note that this is slower (to first order) than even the one dimensional symmetric system.

Here, the oversimplification leads to incorrect results.


Figure 3.4: The variation of the average density, with time, for a 2Dimensional system

### 3.2.2 The continuum approximation

From equation 3.11, we have

$$
\begin{gather*}
\frac{d \rho_{i, j}}{d t}=2-2 \rho_{i, j}+\rho_{i, j}\left(\rho_{i, j-1}-2 \rho_{i, j}+\rho_{i, j+1}\right)-\rho_{i, j}\left(\rho_{i-1, j}-2 \rho_{i, j}+\rho_{i+1, j}\right)  \tag{3.13}\\
\frac{\partial \rho_{i, j}}{\partial t}=2-2 \rho_{i, j}+2 \rho_{i, j}\left[\frac{\partial^{2} \rho_{i, j}}{\partial y^{2}}-\frac{\partial^{2} \rho_{i, j}}{\partial x^{2}}\right] \tag{3.14}
\end{gather*}
$$

Even the steady state solution of this diffusion-like equation is not simple.

## Chapter 4

## The Simulation

We will now see the numerical manifestations of the two non-equilibrium systems, and compare \& contrast them. The works of W. Feller [8] and J. Spencer [9] were referred to during this study.

### 4.1 The Anomaly

We have seen that the original and the symmetry broken systems share the ground state. So now, we look at some properties of their first 'excited state'. This is just a jammed state with a one site change, an anomaly.


Figure 4.1: The anomaly in the jammed (or ground) state.

Under evaporation-deposition dynamics, such an anomaly behaves like a random-walker. In the symmetric case, it is a simple, discreet, 2-D random walker, while in the symmetry broken system, its motion is more restricted.

### 4.1.1 Mean Squared Displacement

The first property we will look at is the mean squared displacement of the anomaly. The averaging is performed over an ensemble of a thousand systems.


Figure 4.2: The x -axis represents the number of steps after which the mean square displacement (y-axis) is calculated.

One can see that they are linear to sufficient accuracy, and show the diffusive properties of a simple random walk. It is interesting that the two systems have the same diffusive characteristics when it comes to an anomaly.

### 4.1.2 Probabilities of Return

In the second property we look at, we consider, in a space of all crossings of the x-axis (say) by the anomaly, the probabilities associated with each return length.

At low numbers of steps needed for a return, this quantity exhibits stark differences.


Figure 4.3: The x -axis represents the number of steps for which the probability (y-axis) is calculated.

An anomaly in a symmetry-broken setting has a relatively high probability of return due to the dimensional restriction of its dynamics, that results in there necessarily being a 1 step return every time it hits the x -axis. For the same event in the symmetric setting, there is only a chance of $1 / 2$.

A two step return is impossible in a symmetry-broken system because every two consecutive steps are at right angles to each other.

Large step return frequencies of both the kinds of systems convergent decrease.

## Chapter 5

## The Conclusion

In this chapter, we make the concluding discussion.
Let us begin by taking another look at the final Hamiltonian of the symmetry broken system, equation 2.11

$$
\begin{array}{r}
\frac{4}{-\epsilon} \mathcal{H}=\bar{\sigma}_{\mathbf{i}, \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}+\mathbf{1}, \mathbf{j}}-1-\sigma_{i+1, j}^{z}+\bar{\sigma}_{\mathbf{i} \mathbf{j}} \cdot \bar{\sigma}_{\mathbf{i}, \mathbf{j}+\mathbf{1}}-1+\sigma_{i, j+1}^{z}  \tag{5.1}\\
-i\left(\sigma_{i, j}^{x} \sigma_{i+1, j}^{y}-\sigma_{i, j}^{y} \sigma_{i+1, j}^{x}\right)-i\left(\sigma_{i, j}^{y} \sigma_{i, j+1}^{x}-\sigma_{i, j}^{x} \sigma_{i, j+1}^{y}\right)
\end{array}
$$

We had noted how both systems have the same jammed state. Post the 'flip', this means that the analogous ground states are the same too.

Let us examine each kind of term independently.

1. The Heisenberg terms,
2. The field terms,
3. The 'angular momentum' terms

The first seeks to align all the spins in a particular direction. This is the term responsible for the ground state ( $g s$ ).

The two field terms prefer to align rows \& columns in the up \& down directions respectively. These terms do not make any difference, as, given a spin direction, it is preferred by one field term and not by the other.

The third term is slightly more interesting. It acts to flip the spins of two adjacent points, if they already have opposite spins; otherwise, it has no effect on the dynamics. So, in the $g s$, this term will have no effect. But in the presence of anomalies, this term is responsible for their propagation. When the evaporation and deposition rates are equal, there is no preferred
direction. This explains the random walk like diffusive behaviour seen in figure 4.2.

Figure 4.3, on the other hand is an example of the differences in their dynamics. For small return lengths, their probabilities vary greatly. The symmetry broken system has a high number of length 1 returns due to the fact that every time the anomaly comes to the x -axis, it makes a length 1 movement and remains on it. Also, it has no returns of length 2.

We see from the figure that the probabilities of large return lengths equalise.

The modified Hamiltonian was not analytically tractable, but we could see the implications of the differences.

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