QUANTUM DYNAMICS OF NOISE ASSISTED EXCITATION TRANSPORT

A Thesis Submitted to
the Graduate School of Engineering and Sciences of
İzmir Institute of Technology
in Partial Fulfillment of the Requirements for the Degree of

MASTER OF SCIENCE

in Physics

by
Hazan ÖZKAN

March 2018

We approve the thesis of **Hazan ÖZKAN**

_____

Assoc.Prof.Dr Özgür Çakır
Supervisor

_____

Assoc.Prof. Dr. Sevilay Sevinçli
Committee Member

_____

Assist.Prof. Dr. Aziz Kolkıran
Committee Member

02 March 2018

_____   _____

Prof. Dr. R. Tuğrul SENGER   **Prof. Dr. Aysun SOFUOĞLU**
Head of the Department of   Dean of the Graduate School of
Physics   Engineering and Sciences

ACKNOWLEDGMENTS

ABSTRACT

QUANTUM DYNAMICS OF NOISE ASSISTED EXCITATION TRANSPORT

In this thesis, different types of systems are studied to investigate the effects of the environmental factors on diffusion and transfer time. Each system consists of different energy levels and excitation transfers between them. The mismatch between the energy levels leads to the Anderson localization. Localization has a negative effect on transport. It is shown that Anderson localization is suppressed due to interaction with the environment. To describe the dynamical evolution of the open quantum system Lindblad master equation is used. The transition times of the system from the pure state to the completely mixed state are examined with the help of the density matrix. In consequence of our study, because of the interaction between the system and environment the change in the wavefunction, the loss in the interference terms and an irreversible information flow in the total system are observed. Destructive effects of the environmental noise on localization are observed for different scenarios and diffusion enhanced. However, when the interaction with the environment becomes larger than a critical value, the system exhibits Zeno effect. In the Zeno regime, the time evolution of the quantum state of the system as well as the diffusion is suppressed.

ÖZET

GÜRÜLTÜ ETKİSİNDE UYARIMLARIN TAŞINIMININ KUANTUM DİNAMİĞİ

Bu tezde, açık kuantum sistemlerinde çevresel etkilerin sistemin difüzyon ve taşınım süreleri üzerindeki etkileri çalışılmıştır. Her bir sistem farklı enerji seviyelerinden oluşur ve egziton bu seviyeler arasında transfer olur. Enerji seviyeleri arasındaki bu fark Anderson lokalizasyonuna neden olur. Lokalizasyonun transfer üzerinde negatif bir etkisi vardır. Çevre ile etkileşimler sayesinde Anderson lokalizasyonun azaldığı gösterilmiştir. Açık kuantum sisteminin zaman içerisindeki değişimini matematiksel olarak ifade edebilmek için Lindblad master denklemi kullanılmıştır. Yoğunluk matrisinin yardımıyla sistemin saf durumdan karmaşık duruma geçiş süreleri incelenmiştir. Çalışmalarımız sonucunda, çevre ve sistem arasındaki etkileşim nedeniyle dalga denkleminde değişim, girişim terimlerinde kayıp ve sistemde tek yönlü bilgi kaybı gözlemlendi. Çevresel gürültünün bazı bölgelerde lokalizasyon üzerindeki yok edici etkisi farklı durumlar için gözlemlendi ve taşınım hızlandı. Ancak çevre ile etkileşim kritik değerden büyük olduğ unda, sistem Zeno alanının özelliklerini gösterdi. Zeno alanında sistemin kuantum durumlarının zaman içerisindeki değişimi ve difüzyon baskılandı.

TABLE OF CONTENTS

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

Excitation transport in open quantum systems is a highly crucial topic nowadays and concepts of the mechanism of several physical systems. Energy transfer in photosynthetic system(Lee, Cheng, and Fleming 2007; Ishizaki and Fleming 2012; Rebentrost et al. 2009; Engel et al. 2007) and Rydberg gases(Schönleber et al. 2015) are generally preferred as a model to study these mechanisms.

The Fenna-Matthews-Olson protein complex which is present in the green sulphur bacteria used as a prototype to explain the effects of the quantum coherence on energy transfer in photosynthetic systems. Green sulphur bacteria consists of chlorosome antenna and the Fenna-Matthews-Olson protein (Blankenship 2014). When light harvesting antenna interacts with light, the Fenna-Matthews-Olson protein achieves energy transfer between the chlorosome antenna complex and reaction center. On the other hand Rydberg atoms generally used to observe coherent excitation transfer experimentally because of their controllability(Singer et al. 2004; Saffman, Walker, and Mølmer 2010). They can be used as background atoms around aggregate atoms and act like environment (Schönleber et al. 2015). When laser is applied to the system, the background atoms get transparent. However, the strong interaction between Rydberg atoms disturbed transparency. When transparency lost, atoms become detectable and excitation transport can be observed. In the classical limit excitation transfer is described by Brownian motion which is result in very long transfer times with low transfer efficiency. On the other hand according to quantum mechanical description, the system should exhibit Anderson localization which again leads to low transfer efficiency. Therefore, it is important to model these systems as an open quantum system taking into account the quantum mechanical effects as well as noise due to environment

An open quantum system interacts another quantum system with a high number of degrees of freedom which is called the environment (Breuer and Petruccione 2002). Both open system and environment compose to total system together. The total system generally is a closed system and evolves under unitary dynamics. Unlike closed quantum systems, the interaction between the system and the environment leads to a different dynamical evolution in the open quantum system. Since there is a noise on the environment, the dynamics of the open system should also contain a non-unitary part as well. This part

includes a dephasing term which is responsible for the decay of the coherences.

In this thesis, the effects of the noisy environment on the quantum transfer efficiency for different systems was investigated. As a basic toy model, first two-level system was studied. Then a ring, a ribbon and a two-dimensional lattice was used as an higher dimensional cases. For each system, it was assumed that there is an energy difference between sites which is called disorder. The disorder has a negative effect on quantum transport and lead to localization (Anderson 1958). To break this localization, dephasing and artificial magnetic was introduced into systems.

In open quantum systems, the interaction between the system and the environment leads to uncertainty in the knowledge of the system state. In this case, the state of the quantum system was described by using ensemble of the known states by using the density operator (Joos et al. 2013). To describe the evolution of the density matrix the Lindblad master equation was used. For each type of system, first the system Hamiltonian and Lindblad operators were defined. Then, boundary conditions were determined. Finally, the Lindblad master equation was converted to the first order linear differential form and this linear equation was solved with MATLAB numerically.

The first chapter includes a review of some basic concepts of open quantum systems. In Chapter 2, the effects of dephasing on localization are investigated for two-level system both analytically and numerically. The changes in the population dynamics of the density matrix with respect to disorder and dephasing are investigated. Energy difference between sites(disorder) caused Anderson localization. However, localization is broken by dephasing in some regions. In Chapter 3, the system is generalized to N sites with closed boundary conditions. The relation between participation number and entropy is obtained. Numerical solutions are given for ring of 20 sites in the presence of dephasing. It is observed that, in the weak dephasing regime quantum transport increases. In Chapter 4, the effects of the artificial magnetic field on localization is investigated for a ring and ribbon type configurations with closed boundary conditions and a 2D lattice with open boundary conditions. For ring and 2D lattice, under weak magnetic field quantum transfer increases.

1.1. Dynamics of the Open Quantum Systems

An open system is a quantum system which is coupled to another quantum system called environment. Since there is an information flow between system and environment, the state of the open system depends on both its own dynamics and also on surroundings(Breuer and Petruccione 2002).

Depending on this information flow open systems can be Markovian or non-Markovion. If there is an information flow from the system to the environment, these systems are Markovian systems. If there is also backflow information from the environment to the system, then these systems called non-Markovian open systems.

The total Hamiltonian can be written as

$$H(t) = H_S \otimes \hat{1} + \hat{1} \otimes H_E + H_{SE}(t) \tag{1.1}$$

where H_S is system Hamiltonian, H_E is environment Hamiltonian and H_{SE} is the interaction Hamiltonian.

1.2. Density Matrix

When there is an incomplete information about a system, we can specify probability distribution over possible states. The system can be represented as a large collection of systems in different states with different probabilities. This collection called ensemble. The same approach can also be used in quantum mechanics too. Instead of specifying a unique state vector $|\Psi\rangle$, a collection of state vectors in different states with different probabilities can be listed by using density operator (Joos et al. 2013). The density operator can be written in terms of an ensemble of normalized states as

$$\rho = \sum_n p_n |\phi_n\rangle \langle\phi_n| \tag{1.2}$$

where p_n refers the probability of being in the state $|\phi_n\rangle$. Total probability must be equals to 1 and $0 \le p_n \le 1$.

$$\sum_n p_n = 1 \tag{1.3}$$

Any density matrix satisfy the following properties: (Schaller 2014)

- Normalization: $\operatorname{tr}(\rho) = 1$

- Positivity: $\langle \Psi_n | \rho | \Psi_n \rangle \geq 0$

- Hermiticity : $\rho^\dagger = \rho$

In the matrix formalization

$$
\rho = \begin{pmatrix}
p_{11} \langle \psi_1 | \rho | \psi_1 \rangle & \dots & p_{1N} \langle \psi_1 | \rho | \psi_N \rangle \\
\vdots & & \vdots \\
p_{N1} \langle \psi_N | \rho | \psi_1 \rangle & \cdots & p_{NN} \langle \psi_N | \rho | \psi_N \rangle
\end{pmatrix} \tag{1.4}
$$

The diagonal elements of the density matrix represent the population terms while the off-diagonal elements represent the interference terms. The interference terms determine the correlation between states which is called coherence. Eventually because of the interactions between system and environment these terms decay. This is called dephasing. For pure states (Ableitinger et al. 2008)

$$
\operatorname{tr}\rho^2 = 1, \tag{1.5}
$$

For mixed states

$$
\operatorname{tr}\rho^2 < 1. \tag{1.6}
$$

The evolution of the density operator is different for pure states and mixed states. A system called as in a pure state if we know where the system exactly is. For pure states density operator can be written as

$$
\rho(t) = | \Psi(t) \rangle \langle \Psi(t) | \tag{1.7}
$$

and evolves according to Liouville-von Neumann equation.

$$
\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)] \tag{1.8}
$$

However, in open quantum systems because of the interaction between the system and

environment, there is a partial knowledge or no knowledge of the system and these system states called mixed states. For mixed states it is not relevant to use unitary evolution and the Liouville-von Neumann equation needs to be modified.

$$\frac{d}{dt}\rho_S(t) = -itr_E[H(t), \rho(t)]$$ (1.9)

To do that reduced system dynamics can be used and to obtain the reduced system dynamics environment degrees of freedom can be traced out.

$$\rho_S = tr_E\rho$$ (1.10)

1.3. The Lindblad Master Equation

The Lindblad master equation (Lindblad 1976) is a first order differential equation and describes the equation of motion of the density matrix. It can be derived from the Liouville-von Neumann equation by using two approximations (Breuer and Petruccione 2002). These are Markov approximation and Born approximation.
The combined Hamiltonian consists of three parts and can be written as

$$\hat{H}(t) = \hat{H}_S + \hat{H}_E + \hat{H}_{SE},$$ (1.11)

where $\hat{H}_S$, $\hat{H}_E$ and $\hat{H}_{SE}$ describe system Hamiltonian, environment Hamiltonian and interaction Hamiltonian respectively. By the Liouville-Von Neumann equation

$$\frac{d}{dt}\hat{\rho}_{SE} = -\frac{i}{\hbar}\left[\hat{H}_S + \hat{H}_E + \hat{H}_{SE}, \hat{\rho}_{SE}\right]$$ (1.12)

Equation (1.12) can be written in the interaction picture as

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar}\left[\hat{V}(t), \hat{\rho}(t)\right]$$ (1.13)

where

$$\hat{\rho}(t) = e^{\frac{i}{\hbar}(\hat{H}_S + \hat{H}_E)t} \hat{\rho}_{SE}(t) e^{-\frac{i}{\hbar}(\hat{H}_S + \hat{H}_E)t} \qquad (1.14)$$

and

$$\hat{V}(t) = e^{\frac{i}{\hbar}(\hat{H}_S + \hat{H}_E)t} \hat{H}_{SE} e^{-\frac{i}{\hbar}(\hat{H}_S + \hat{H}_E)t}. \qquad (1.15)$$

Here, $\hat{V}$ indicates the total Hamiltonian in the interaction picture.

The integration of Equation (1.12) yields

$$\hat{\rho}(t) = \hat{\rho}(0) - \frac{i}{\hbar} \int_0^t \left[\hat{V}(t'), \hat{\rho}(t') \right] dt'. \qquad (1.16)$$

Substituting Equation(1.15) into Equation (1.12), Equation (1.12) becomes

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar} \left[\hat{V}(t), \hat{\rho}(0) \right] - \frac{1}{\hbar^2} \left[\hat{V}(t), \int_0^t \left[\hat{V}(t'), \hat{\rho}(t') \right] dt' \right]. \qquad (1.17)$$

where

$$\rho(t) = \rho_E(0) \otimes \rho_S(t). \qquad (1.18)$$

According to the Born approximation, the environment has a large number of degrees of freedom and not affected by coupling much. Therefore, it is possible to trace out environment degrees of freedom.

Equation(1.17) will be

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{i}{\hbar} tr_E \left\{ \left[\hat{V}(t), \hat{\rho}(0) \right] \right\} - \frac{1}{\hbar^2} tr_E \left\{ \left[\hat{V}(t), \int_0^t \left[\hat{V}(t'), \hat{\rho}(t') \right] dt' \right] \right\}. \qquad (1.19)$$

Assume that

$$tr_E[V(t), \rho(0)] = 0 \qquad (1.20)$$

Therefore,

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{1}{\hbar^2} tr_E \left\{ \left[\hat{V}(t), \int_0^t \left[\hat{V}(t'), \hat{\rho}(t') \right] dt' \right] \right\}. \qquad (1.21)$$

After inserting the Equation (1.18) inside the integral in the Equation (1.20), Equation (1.20) becomes

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{1}{\hbar^2} \int_0^\infty dt' tr_E \left\{ \left[\hat{V}(t), \left[\hat{V}(t'), \hat{\rho}_E(0)\hat{\rho}_S(t) \right] \right] \right\}. \qquad (1.22)$$

Equation (1.22) is called Born-Markov master equation. The interaction Hamiltonian is defined as (Brasil, Fanchini, and Napolitano 2013)

$$\hat{H}_{SE} = \hbar(\hat{S}\hat{E}^\dagger + \hat{S}^\dagger \hat{E}) \tag{1.23}$$

where $\hat{S}$ indicates the part of the Hamiltonian that acts only on the system and $\hat{E}$ indicates the part of the Hamiltonian that acts only on the environment.

If $\hat{S}$ and $\hat{H}_S$ commute,

$$[\hat{S}, \hat{H}_S] = 0, \tag{1.24}$$

Then the system $\hat{S}$ does not depend on time. In the case of a Bosonic environment, the environmental part of the Hamiltonian can be written as

$$\hat{H}_E = \hbar \sum_k w_k \hat{a}_k^\dagger \hat{a}_k. \tag{1.25}$$

$\hat{a}_k$ and $\hat{a}_k^\dagger$ indicate the annihilation and creation operators for environment respectively and w_k are the characteristic frequencies of each mode.

The environment operator is defined in the interaction picture as

$$\hat{E} = \sum_k g_k^\star \hat{a}_k e^{-iw_k t} \tag{1.26}$$

where $g_k^\star$ are coupling constants. Inserting these assumptions into the Equation (1.20)

$$\frac{d}{dt}\hat{\rho}_S(t) = \int_0^t \mathrm{tr}_E\left\{ \left(\hat{S}^\dagger \hat{E}(t) - \hat{E}^\dagger(t)\hat{S}\right), \left[(\hat{S}^\dagger \hat{E}(t') - \hat{E}^\dagger(t')^\dagger \hat{S}), \hat{\rho}_E(0)\hat{\rho}_S(t')\right] \right\} dt'. \tag{1.27}$$

Define

$$\mathrm{tr}_E\left\{ \hat{E}(t)\hat{\rho}_E(0)\hat{E}^\dagger(t') \right\} = \mathrm{tr}_E\left\{ \hat{E}^\dagger(t')\hat{E}(t)\hat{\rho}_E(0) \right\} = \left\langle \hat{E}^\dagger(t')\hat{E}(t) \right\rangle \tag{1.28}$$

and

$$\mathrm{tr}_E\left\{ \hat{E}^\dagger(t')\hat{E}(t)\hat{\rho}_E(0) \right\} = \mathrm{tr}_E\left\{ \hat{E}^\dagger(t')\hat{E}(t)\hat{\rho}_E(0) \right\} = 0. \tag{1.29}$$

The equation can be written in the form

$$
\begin{aligned}
\frac{d}{dt}\hat{\rho}_S(t) = \int_0^t dt' \Big(&[\hat{S}\rho_S(t')\hat{S}^\dagger - \hat{S}^\dagger\hat{S}\rho_S(t')]\langle\hat{E}(t)\hat{E}^\dagger(t')\rangle \\
&+ [\hat{S}\rho_S(t')\hat{S}^\dagger - \rho_S(t')\hat{S}^\dagger\hat{S}]\langle\hat{E}(t')\hat{E}^\dagger(t)\rangle \\
&+ [\hat{S}^\dagger\rho_S(t')\hat{S} - \hat{S}\hat{S}^\dagger\rho_S(t')]\langle\hat{E}^\dagger(t)\hat{E}(t')\rangle \\
&+ [\hat{S}^\dagger\rho_S(t')\hat{S} - \rho_S(t')\hat{S}\hat{S}^\dagger]\langle\hat{E}(t')^\dagger\hat{E}(t)\rangle \\
&- [\hat{S}^\dagger\rho_S(t')\hat{S}^\dagger - (\hat{S}^\dagger)^2\rho_S(t')]\langle\hat{E}(t)\hat{E}(t')\rangle \\
&- [\hat{S}^\dagger\rho_S(t')\hat{S}^\dagger - \rho_S(t')(\hat{S}^\dagger)^2]\langle\hat{E}(t')\hat{E}(t)\rangle \\
&- [\hat{S}\rho_S(t')\hat{S} - \hat{S}^2\rho_S(t')]\langle\hat{E}^\dagger(t)\hat{E}^\dagger(t')\rangle \\
&- [\hat{S}\rho_S(t')\hat{S} - \rho_S(t')\hat{S}^2]\langle\hat{E}^\dagger(t')\hat{E}^\dagger(t)\rangle \Big)
\end{aligned}
\tag{1.30}
$$

$$
\begin{aligned}
\frac{d}{dt}\hat{\rho_S}(t) = &-[\hat{S}\hat{S}^\dagger\hat{\rho_S}(t) - \hat{S}^\dagger\hat{\rho_S}(t)\hat{S}]\langle\hat{E}^\dagger(t)\hat{E}(t')\rangle - [\hat{\rho_S}(t)\hat{S}^\dagger\hat{S}]\langle\hat{E}(t')\hat{E}^\dagger(t)\rangle \\
&-[\hat{S}^\dagger\hat{S}\hat{\rho_S}(t) - \hat{S}\hat{\rho_S}(t)\hat{S}^\dagger]\langle\hat{E}(t)\hat{E}^\dagger(t')\rangle - [\hat{\rho_S}(t)\hat{S}\hat{S}^\dagger - \hat{S}^\dagger\hat{\rho_S}(t)\hat{S}]\langle\hat{E}^\dagger(t')\hat{E}(t)\rangle
\end{aligned}
\tag{1.31}
$$

If the environment is initially in the vacuum state

$$
\hat{\rho_E} = (|0\rangle|0\rangle...) \otimes (\langle0|\langle0|...)
\tag{1.32}
$$

Then

$$
\langle\hat{E}^\dagger(t')\hat{E}(t)\rangle = \text{tr}_E\Big\{\hat{E}^\dagger(t')\hat{E}(t))\hat{\rho}_E(0)\Big\} = 0
\tag{1.33}
$$

and

$$
\langle\hat{E}(t)\hat{E}^\dagger(t')\rangle = \langle\hat{E}(t')\hat{E}^\dagger(t)\rangle
\tag{1.34}
$$

where

$$
\langle\hat{E}(t)\hat{E}^\dagger(t')\rangle = \sum_{k,k'} g_k^\star g_{k'} \int_0^t dt' e^{-i(w_k t - w_k' t')}
\tag{1.35}
$$

Consider the environment as a harmonic oscillators. To understand the characterization of the frequencies of the bath modes and the coupling between the environment and system, spectral density can be defined as

$$J(w) = \sum_n |g_n|^2 \delta(w - w_n). \tag{1.36}$$

The Equation (1.35) can be expressed in terms of the spectral density as

$$\left\langle \hat{E}(t) \hat{E}^\dagger(t') \right\rangle = \int_0^\infty dw J(w) \int_0^t dt' e^{-iw(t-t')}. \tag{1.37}$$

The integral can be simplified by using change of variable

$$\tau = t - t',$$

$$d\tau = -dt'.$$

Therefore,

$$\left\langle \hat{E}(t) \hat{E}^\dagger(t') \right\rangle = \int_0^\infty dw J(w) \int_0^t d\tau e^{-iw\tau}. \tag{1.38}$$

According to the Markov approximation, the memory time of the environment is shorter than the time scale of the system. In other words, system has no memory effects. When limit as t goes to infinity, by the Cauchy principle value integral

$$\int_0^\infty dr e^{-i\epsilon r} = \pi \delta(\epsilon) - i\mathcal{P}\frac{1}{\epsilon} \tag{1.39}$$

Therefore,

$$\left\langle \hat{E}(t) \hat{E}^\dagger(t') \right\rangle = \pi \delta(w) - i\mathcal{P}\frac{1}{w} \tag{1.40}$$

where $\mathcal{P}$ refers to Cauchy principle part and contains imaginary part. This part is responsible for the frequency shift.

Equation 1.39 becomes

$$\pi \int_0^\infty dw J(w)\delta(w) - i\mathcal{P}\int_0^\infty dw \frac{J(w)}{w} \tag{1.41}$$

To simplify the equation, define

$$\gamma \equiv 2\pi \int_0^\infty dw J(w)\delta(w) \tag{1.42}$$

and

$$\epsilon \equiv -2\mathcal{P} \int_0^\infty dw \frac{J(w)}{w} \tag{1.43}$$

Then Equation 1.41 becomes

$$\frac{\gamma + i\epsilon}{2} \tag{1.44}$$

and Equation 1.31 will be

$$\frac{d}{dt}\hat{\rho}_S(t) = \left[\hat{\rho}_S(t)\hat{S}^\dagger\hat{S} - \hat{S}\hat{\rho}_S(t)\hat{S}^\dagger\right]\frac{\gamma - i\epsilon}{2} - \left[\hat{S}^\dagger\hat{S}\hat{\rho}_S(t) - \hat{S}\hat{\rho}_S(t)\hat{S}\right]\frac{\gamma + i\epsilon}{2}. \tag{1.45}$$

For the case $\epsilon = 0$

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{\gamma}{2}\left[\hat{\rho}_S(t)\hat{S}^\dagger\hat{S} - \hat{S}\rho_S(t)\hat{S}^\dagger + \hat{S}^\dagger\hat{S}\hat{\rho}_S(t) - \hat{S}\hat{\rho}_S(t)\hat{S}^\dagger\right]. \tag{1.46}$$

$$\hat{\rho}_S(t) = e^{\frac{i}{\hbar}\hat{H}_S(t)}\hat{\rho}_S e^{-\frac{i}{\hbar}\hat{H}_S(t)} \tag{1.47}$$

Using Equation (1.46), transform Equation (1.45) to the initial picture form

$$\frac{d\hat{\rho}_S}{dt} = -\frac{i}{\hbar}\left[\hat{H}_S, \hat{\rho}_S\right] + \gamma\left[\hat{S}\hat{\rho}_S\hat{S}^\dagger - \frac{1}{2}\{\hat{S}^\dagger\hat{S}, \hat{\rho}_S\}\right]. \tag{1.48}$$

General form of the Lindblad equation is

$$\frac{d}{dt}\hat{\rho}_S = -\frac{i}{\hbar}[H_S, \hat{\rho}_S] + \sum_n \gamma_n\left[\hat{L}_n\hat{\rho}_S\hat{L}_n^\dagger - \frac{1}{2}\hat{L}_n^\dagger\hat{L}_n\hat{\rho}_S - \frac{1}{2}\hat{\rho}_S\hat{L}_n^\dagger\hat{L}_n\right] \tag{1.49}$$

where γ indicates dephasing term and $\hat{L}$ operators are Lindblad operators.

Lindblad master equation can be examined in two parts. The first term on the right hand side of the equation describes the unitary evolution of the density operator.

The second term describes possible transitions and non-unitary evolution of the density matrix. This term includes dephasing term and Lindblad operators and describes possible transitions.

1.4. Anderson Localization

According to Einstein, at too short scales process is not Markovian. There is a memory effect and there is no diffusion. On the other hand, at large scales if the system has no memory there will be always diffusion. (Einstein 1905)

$$\langle r^2 \rangle = Dt \tag{1.50}$$

where D is the diffusion constant.

According to Anderson, it is not always true for quantum particles. The wave is coherently scattered by impurities. Interferences of multiple scatterings with higher return probability leads to quantum correction to diffusion. If disorder is strong enough, for infinitely long time disorder may leads to localization (Anderson 1958)

$$\langle r^2 \rangle \xrightarrow[t \to \infty]{} constant \tag{1.51}$$

and

$$D = 0$$

(a)   (b)

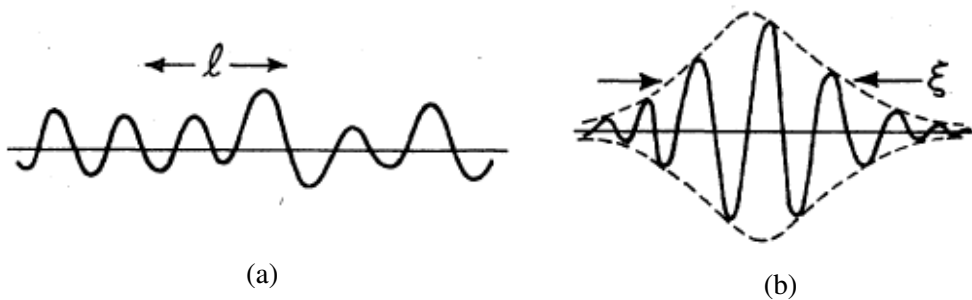Figure 1.1. The wave function of (a)extended state, (b)localized state
Source: (Lee and Ramakrishnan 1985)

The wave function decays

$$| \Psi(\vec{r}) | \sim exp(-\frac{| \vec{r} - \vec{r_0} |}{\xi})$$

(1.52)

where ξ is localization length and l is the mean free path.

Since dephasing leads to loss of the interference terms, in this study we used dephasing to break Anderson localization.

CHAPTER 2

DELOCALIZATION IN A TWO LEVEL SYSTEM WITH DISORDER

As a basic toy model first a two level system was studied. Energy difference between sites which is called disorder was introduced to the system and effects of disorder on localization was observed. To break the localization dephasing was introduced to the system. The Hamiltonian of two level system for a spin $\frac{1}{2}$ particle in the presence of the
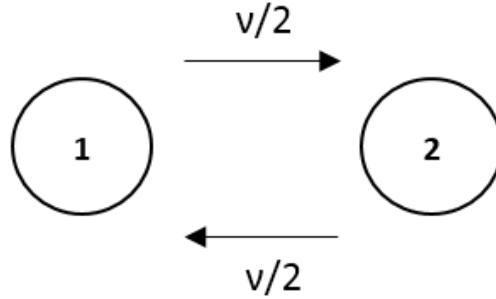
Figure 2.1. A two-level system with a hopping strength $v/2$

single excitation is

$$H_S = \frac{\epsilon}{2}(|1\rangle\langle 1| - |2\rangle\langle 2|) + \frac{v}{2}(|1\rangle\langle 2| + |2\rangle\langle 1|) \tag{2.1}$$

where ϵ indicates site energies and v is the hopping strength between two sites. $|1\rangle$ and $|2\rangle$ refer to the localization site of the particle.

The system Hamiltonian can be written in terms of Pauli spin matrices as

$$H_S = \frac{\epsilon}{2}\hat{\sigma}_z + \frac{v}{2}\hat{\sigma}_x. \tag{2.2}$$

The Hamiltonian of a charged particle under the magnetic field is

$$H = -\vec{\mu}\vec{B}, \tag{2.3}$$

The magnetic dipole moment of a spinning charge particle which is proportional to spin angular momentum (S) is

$$\vec{\mu} = \gamma \vec{S} \tag{2.4}$$

where γ is the gyromagnetic ratio.

In terms of the gyromagnetic ratio, the Hamiltonian can be written as

$$H = -\gamma \vec{S} \vec{B}. \tag{2.5}$$

$$H = (-\gamma \frac{\hbar}{2}) \vec{\sigma} \vec{B} = \frac{\Omega}{2} \vec{n'} \vec{\sigma} \tag{2.6}$$

where $\hat{n'} = cos\theta \hat{z} + sin\theta \hat{x}$ is the unit vector in the xz plane.

The Larmor frequency Ω is defined as

$$\Omega = \sqrt{\frac{\epsilon^2}{4} + \frac{v^2}{4}}. \tag{2.7}$$

Initially particle localized at site 1 and system rotates in the x-z plane. Eventually, displays from z axis by Ω.

Density matrix can be written in terms of Pauli spin matrices as

$$\rho = \frac{1}{2}(\mathbb{1} + \vec{n}\vec{\sigma}) \tag{2.8}$$

which can be represented in the matrix formalism as

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + n_z & n_x - in_y \\ n_x + in_y & 1 - n_z \end{pmatrix} \tag{2.9}$$

where $n = (n_x, n_y, n_z)$ is an arbitrary real vector.

Bloch sphere is a graphical representation of two level systems. (Nielsen and Chuang 2010) The points on the top of the sphere $|0\rangle$ and the bottom of the sphere $|1\rangle$ represent excited and ground states or spin up and spin down states. These points refer to pure states. The radius of the Bloch sphere can be used to determine whether the system mixed or pure. If radius is one, the point is on the surface of the sphere and indicates pure state. If radius is less than one the point is inside the sphere and corresponds to the mixed
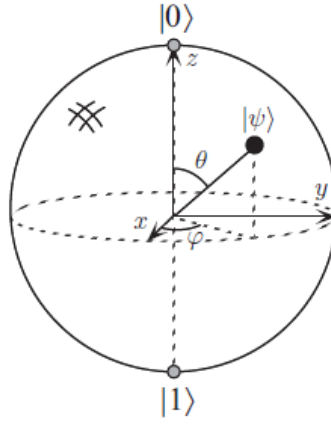
Figure 2.2. Bloch sphere for spin $1/2$ particle. $|\Psi\rangle$ is any qubit represented by angles θ and ϕ where $0 \le \theta \le \pi$ and $0 \le \phi \le 2\pi$ and r is the radius of the Bloch sphere Source: (Nielsen and Chuang 2010)

state.

The qubit $|\Psi\rangle$ can be represented as a linear combination $|e\rangle$ and $|g\rangle$

$$|\Psi\rangle = cos\frac{\theta}{2}\,|e\rangle + e^{i\phi}sin\frac{\theta}{2}\,|g\rangle\,. \tag{2.10}$$

Here, θ and ϕ are the arbitrary real numbers. $|e\rangle$ and $|g\rangle$ are the excited state and the ground state respectively.

The Lindblad master equation for two level system is given by

$$\dot{\rho} = -i[H_S, \rho] + \sum_{n=1}^{2} \gamma_n [A_n \rho(t) A_n^\dagger - \frac{1}{2} A_n A_n^\dagger \rho(t) - \frac{1}{2}\rho(t) A_n^\dagger A_n] \tag{2.11}$$

where A_n are projection operators. For a two level system, there are two different projection operators $A_1 = |1\rangle\,\langle 1|$ and $A_2 = |2\rangle\,\langle 2|$ respectively.

The Lindblad master equation in terms of the Bloch vectors is

$$\dot{\rho} = -i[\frac{\Omega}{2}\vec{n'}\vec{\sigma}, \frac{1+\vec{n}\vec{\sigma}}{2}] - \frac{\gamma_1 + \gamma_2}{2}(n_x\sigma_x + n_y\sigma_y) \tag{2.12}$$

15

$$\frac{\dot{\vec{n}}\vec{\sigma}}{2} = \frac{\Omega}{2}\vec{\sigma}(\vec{n'} \times \vec{n}) - \frac{\gamma}{2}(\vec{n} - n_z)\vec{\sigma} \tag{2.13}$$

The final form of the equation is

$$\frac{\dot{\vec{n}}}{2} = \frac{\Omega}{2} \times \vec{n} - \frac{\gamma}{2}(\vec{n} - n_z). \tag{2.14}$$

Equation (2.13) can be written in the matrix form to simply the calculations

$$\begin{bmatrix} \dot{n_x} \\ \dot{n_y} \\ \dot{n_z} \end{bmatrix} = \begin{bmatrix} -\gamma & -\delta & 0 \\ \delta & -\gamma & -v \\ 0 & v & 0 \end{bmatrix} \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} \tag{2.15}$$

where δ is disorder, γ is dephasing and v is a hopping strength between two sites.
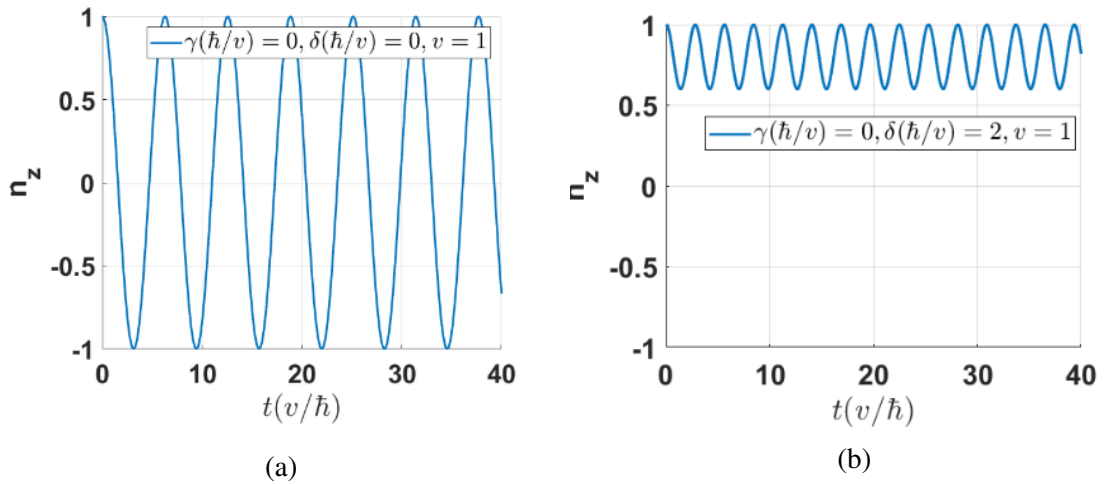

Figure 2.3. The time evolution of the diagonal elements of the density matrix.(a) in the absance of disorder (b) in the presence of disorder

Initially, particle is localized at site 1. In Figure 2.3.a, there is no energy difference between sites. Since there is no disorder, particle can easily hops between the site one and site two with a hopping strength v. In the Figure 2.3.b, there is an energy difference(disorder) between sites.n_z changes between 1 and 0.5 but cannot reach -1 (site 2). In this case disorder leads to localization.

To break this localization, different values of dephasing introduced to the system. According to Figure 2.4, when dephasing increases fluctuations decreases and system
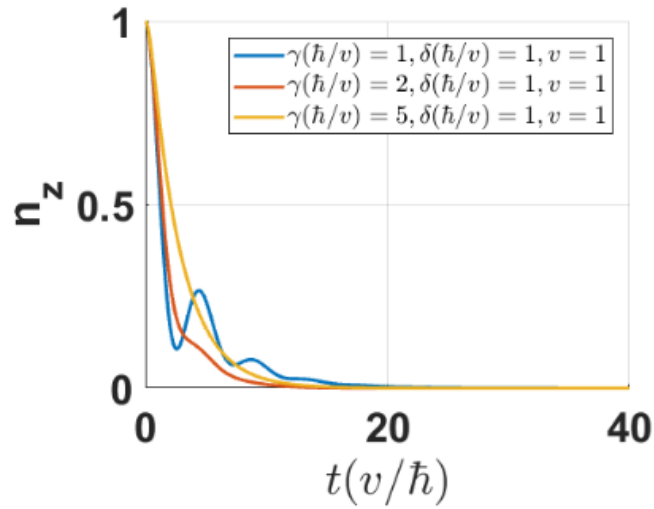

Figure 2.4. Time evolution of the diagonal elements of the density matrix for three different dephasing values in the presence of disorder

becomes mixed faster. Therefore, introducing dephasing can break the localization. For the case $\delta = 0$ the solution of the linear system in Equation (2.13) is

$$
\begin{aligned}
\dot{n_x} &= -\gamma n_x \\
\dot{n_y} &= -v n_z - \gamma n_y \\
\dot{n_z} &= v n_y
\end{aligned}
\tag{2.16}
$$

$$
\ddot{n_z} + \gamma \dot{n_z} + v^2 n_z = 0
\tag{2.17}
$$

System behaves like a damped harmonic oscillator $\left(m\ddot{x} + \gamma \dot{x} + \omega^2 x = 0 \right)$ with the roots:

$$
r = -\frac{\gamma}{2} \pm \sqrt{\frac{\gamma^2}{4} - v^2}
\tag{2.18}
$$

There are three different cases for a damped harmonic oscillator

- $\frac{\gamma^2}{4} - v^2 > 0$ over damped

- $\frac{\gamma^2}{4} - v^2 = 0$ critically damped

17

- $\frac{\gamma^2}{4} - v^2 < 0$ under damped

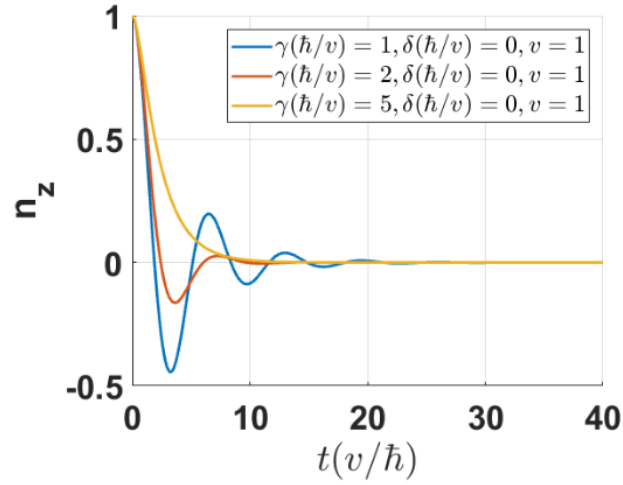where $\gamma/v = 2$ is critical point

Figure 2.5. The evolution of the diagonal elements of the density matrix for three different dephasing values in the absance of disorder

When the Lindblad master equation is solved for different dephasing rates, three different case are obtained. Figure 2.5 shows the time evolution of the diagonal elements of the density matrix for three characteristic values of γ. According to Figure 2.5, $\gamma/v = 2$ is the critical point for this system. For $\gamma/v > 2$ overdamped oscillation is observed while for $\gamma/v < 2$, underdamped oscillation is observed.

CHAPTER 3

TRANSPORT ON A DISORDERED RING

In this chapter as a higher dimensional model a ring was studied. Random energy differences between sites which is called disorder was introduced into the system. Then dephasing was addded to remove the effect of disorder and to break the Anderson localization. To solve the dynamical evolution of the system Lindblad master equation was used in the more general form with closed boundary conditions.
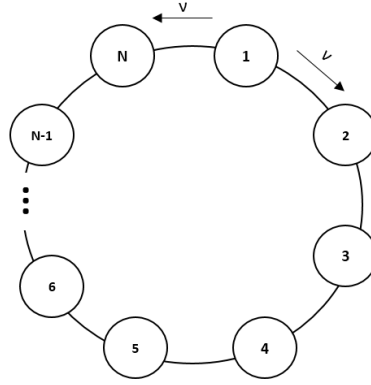

Figure 3.1. N-site ring with a nearest neighbors hopping v

The Hamiltonian of N level system in the presence of single excitation is (May et al. 2008)

$$H_S = \sum_{m=1}^{N} \epsilon_m(|m\rangle\langle m|) + \sum_{n<m}^{N} v_{mn}(|m\rangle\langle n| + |n\rangle\langle m|) \tag{3.1}$$

where ϵ_m indicates site energies and v_{mn} is the hopping strengths only between the nearest neighbour interactions. $|n\rangle$ and $|m\rangle$ is the localization site of the particle at site n and m respectively. The equation of motion for the density operator is given by

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H_S(t), \rho(t)] + L(\rho(t)). \tag{3.2}$$

where

$$L(\rho(t)) = \gamma \sum_n [A_n\rho(t)A_n^\dagger - \frac{1}{2}A_n A_n^\dagger \rho(t) - \frac{1}{2}\rho(t)A_n^\dagger A_n] \tag{3.3}$$

Here Lindblad operators are projection operators. $A_n = |n\rangle \langle n|$ and γ is pure dephasing rate.

Lindblad master equation is impractical for calculations especially for higher level systems. To simplify the calculations we converted Lindblad master equation into the first order linear differential form. To do that we mapped density matrix to the density vector form by using f function

$$f(i, j) = (i - 1)N + j. \tag{3.4}$$

In our systems the Hilbert space is a N dimensional space. When converting density matrix to density vector form, we are mapping $N \times N$ matrix to N^2 dimensional vector. (Schaller 2014)

After using this mapping density matrix becomes

$$\rho = \begin{pmatrix} \rho_{11} & \cdots & \rho_{1N} \\ \vdots & & \vdots \\ \rho_{N1} & \cdots & \rho_{NN} \end{pmatrix} \Leftrightarrow ||\rho\rangle\rangle = \begin{pmatrix} \rho_{11} \\ \vdots \\ \rho_{1N} \\ \rho_{21} \\ \vdots \\ \rho_{NN} \end{pmatrix} \tag{3.5}$$

This process decreases our dimension of work space and makes easier our calculations. Eventually Lindblad master equation gains linear form

$$\dot{\rho} = \mathbf{L}\rho \tag{3.6}$$

Here ρ is a N^2 dimensional vector and L is $N^2 \times N^2$ matrix. In our systems complexity scales with O(6) for $N^2 \times N^2$ L matrix.

The equilibration time was defined by taking weighted average over diagonal elements of the density matrix. Equilibration time describes diffusion dynamics of the diagonal elements of the density matrix.

$$t_{eq} = \frac{\sum_n |c_{1n}| \frac{1}{Re(\lambda_n)} + \sum_n |c_{2n}| \frac{1}{Re(\lambda_n)} + \ldots + \sum_n |c_{nn}| \frac{1}{Re(\lambda_n)}}{\sum_{i,n} |c_{in}|} \tag{3.7}$$

where

$$\rho_{ii} = \sum_n c_{in} e^{-\lambda_n t} \tag{3.8}$$

Here, λ is eigenvalues of $\mathbf{L}$ matrix.

The random disorder was introduced into the system as $-0.5 \leq \eta \leq 0.5$ where $\eta = \epsilon/v$.
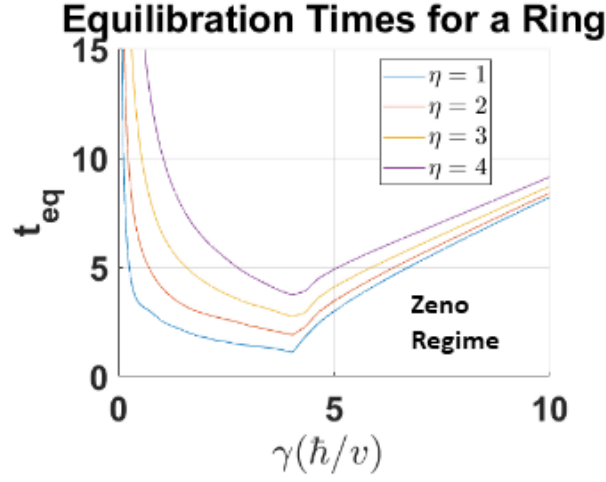

Figure 3.2. The relation between the equilibration time and dephasing rate for ring of 20 sites

According to Figure 3.2, when disorder increases entropic time increases. Disorder leads to localization. To break the localization we introduce dephasing into the system. If dephasing is weak ($\eta < 4$), equilibration time decreases with γ and quantum transfer increases. However at the strong dephasing regime, particle enters Zeno regime and time increases again.

In the Zeno regime because of the frequent measurements system cannot evolve and quantum transfer always suppressed. Here, dephasing acts like measurement on the system and suppressed quantum trasnport (Misra and Sudarshan 1977).

To understand whether system mixed or pure we used entropy and participation number definition.Von Neuman entropy can be calculated from (Neumann 2013)

$$S(\rho) = -\mathrm{tr}\rho log_2\rho. \tag{3.9}$$

If entropy is zero that indicates system is in a pure state and pure quantum states corresponds to maximum information. When system becomes mixed entropy increases and in that case there is a missing information.

For completely mixed state entropy reaches maximum value and can be calculated from

$$S(\frac{1}{N}\mathbb{1}) = -\frac{1}{N}\text{tr}(log_2\frac{1}{N}\mathbb{1}) = log_2 N. \tag{3.10}$$

We defined participation number as

$$PN = \sum_n \rho_{nn}^2 \tag{3.11}$$

Participation number describes the diffusion dynamics of the system and can be expressed in terms of the diagonal elements of the density matrix.
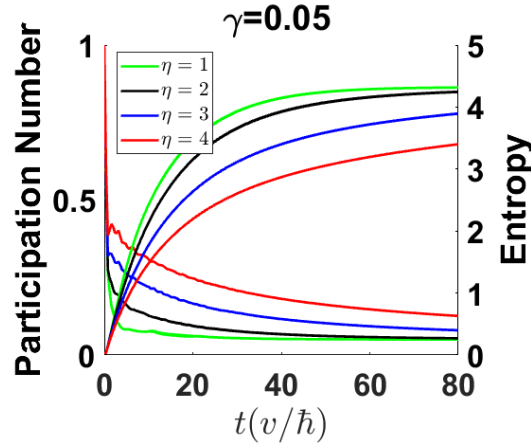
Initially particle is localized at the middle site.

Figure 3.3. The relation between participation number and entropy with respect to time for ring of 20 sites

Since there is a localization, participation number is 1. According to Figure 3.3, eventually participation number increases and converges to its minimum value. On the other hand,initially entropy is 0 because system is in a pure state.

When system becomes mixed, entropy increases and attains its asymptotic value which can be calculated as

$$S(\frac{1}{20}\mathbb{1}) = log_2 20 = 4.32 \tag{3.12}$$

for ring of 20 sites.

3.1. Rate Equations for a Ring (Zeno Regime)

In this part the Lindblad master equation was solved analytically. The quantum transport in the strong dephasing regime0 (Zeno regime) was investigated. The Lindblad master equation is

$$\dot{\rho} = -i[H, \rho] + \frac{\gamma}{2}L[\rho]. \tag{3.13}$$

By the Einstein summation convention

$$\dot{\rho}_{nm} = -(H_{nk}\rho_{km} - \rho_{nk}H_{km}) - \gamma\rho_{nm}(1 - \delta_{nm}) \tag{3.14}$$

$$= -(\epsilon_n\rho_{nm} - \epsilon_m\rho_{nm}) - iv\sum_{\sigma=\pm1}(\rho_{n+\sigma,m} - \rho_{n,m+\sigma}) - \gamma\rho_{nm}(1 - \delta_{nm}) \tag{3.15}$$

where ϵ_m and ϵ_n refers to site energies.

If n=m, the first terms of the equation gives zero. Then equation becomes

$$\dot{\rho}_{nn} = -iv\sum_{\sigma=\pm1}(\rho_{n+\sigma,n} - \rho_{n,n+\sigma}). \tag{3.16}$$

If $n \neq m$, there is a mismatch between site energies.

$$\dot{\rho}_{nm} = -\gamma\rho_{nm} - i\epsilon_{nm}\rho_{nm} - iv\sum_{\sigma=\pm1}(\rho_{n+\sigma,m} - \rho_{n,m+\sigma}) \tag{3.17}$$

where $\epsilon_{nm} = (\epsilon_n - \epsilon_m)$. Integrate both sides of the Equation (3.17)

$$\rho_{nm} = e^{-(i\epsilon_{nm}+\gamma)t}\rho_{nm}(0) - i\int_0^t e^{-(i\epsilon_{nm}+\gamma)(t-t')}[-iv\sum_{\sigma=\pm1}(\rho_{n+\sigma,m} - \rho_{n,m+\sigma})]dt. \tag{3.18}$$

In case of a strong dephasing ($\gamma \gg v$), first term yields zero. Hence

$$\rho_{nm} = -iv\frac{1}{\gamma + i\epsilon_{nm}}\sum_{\sigma=\pm1}(\rho_{n+\sigma,m} - \rho_{n,m+\sigma}) \tag{3.19}$$

case 1: If $\epsilon = 0$, there is no disorder

Letting $n = m$ in Equation (3.16) yields

$$\dot{\rho}_{nn} = -iv(\rho_{n+1,n} + \rho_{n-1,n} - \rho_{n,n+1} - \rho_{n,n-1}). \tag{3.20}$$

If $n \neq m$ from the Equation (3.19), we get

$$\rho_{nm} = -iv(\rho_{n+1,n} + \rho_{n-1,n} - \rho_{n,n+1} - \rho_{n,n-1})\frac{1}{\gamma}. \tag{3.21}$$

Insert Equation (3.21) into Equation (3.20) and assume that there is only nearest neighbour interactions

$$\dot{\rho}_{nn} = \frac{(-iv)(-iv)}{\gamma}[(\rho_{n,n} + \rho_{n+1,n+1} + \rho_{n,n} - \rho_{n-1,n-1} - \rho_{n+1,n+1} + \rho_{n,n} - \rho_{n-1,n-1} + \rho_{n,n}] \tag{3.22}$$

Equation (3.22) can be reduced to the form

$$\dot{\rho}_{nn} = -\frac{v^2}{\gamma}[4\rho_{nn} - 2(\rho_{n+1,n+1} + \rho_{n-1,n-1})]. \tag{3.23}$$

For a two level system

$$\dot{\rho}_{11} = \frac{v^2}{\gamma}[-4\rho_{11} + 4\rho_{22}] \tag{3.24}$$

$$\dot{\rho}_{22} = \frac{v^2}{\gamma}[-4\rho_{22} + 4\rho_{11}] \tag{3.25}$$

where $\sum_n \dot{\rho}_{nn} = 0$

case 2: Disorder different than zero

By the Equation (3.20)

$$\dot{\rho_{nn}} = -iv(\rho_{n+1,n} + \rho_{n-1,n} - \rho_{n,n+1} - \rho_{n,n-1}) \tag{3.26}$$

and the Equation (3.19)

$$\rho_{nm} = -iv(\rho_{n+1,n} + \rho_{n-1,n} - \rho_{n,n+1} - \rho_{n,n-1})\frac{1}{\gamma + i\epsilon_{nm}} \tag{3.27}$$

Insert the Equation (3.27) into Equation (3.26)

$$\dot{\rho_{nn}} = (-iv)(-iv)[(\frac{1}{\gamma + i\epsilon_{n+1,n}}(\rho_{n,n} - \rho_{n+1,n+1}) + \frac{1}{\gamma + i\epsilon_{n-1,n}}(\rho_{n,n} - \rho_{n-1,n-1}))$$

$$+ \frac{1}{\gamma + i\epsilon_{n,n+1}}(-\rho_{n+1,n} - \rho_{n,n}) + \frac{1}{\gamma + i\epsilon_{n-1,n-1}}(-\rho_{n-1,n-1} + \rho_{n,n})]$$

$$\dot{\rho_{nn}} = v^2[(\frac{1}{\gamma + i\epsilon_{n+1,n}} + \frac{1}{\gamma + i\epsilon_{n-1,n}} + \frac{1}{\gamma + i\epsilon_{n,n+1}} + \frac{1}{\gamma + i\epsilon_{n,n-1}})(-\rho_{nn})]$$

$$+ v^2[(\frac{1}{\gamma + i\epsilon_{n+1,n}} + \frac{1}{\gamma + i\epsilon_{n,n+1}})(\rho_{n+1,n+1})]$$

$$+ v^2[(\frac{1}{\gamma + i\epsilon_{n,n-1}} + \frac{1}{\gamma + i\epsilon_{n-1,n}})(\rho_{n-1,n-1})]$$

The equation becomes

$$\dot{\rho_{nn}} = (\frac{\gamma v^2}{\gamma^2 + \epsilon_{n+1,n}^2}(\rho_{n+1,n+1}) + \frac{\gamma v^2}{\gamma^2 + \epsilon_{n-1,n}^2}(\rho_{n-1,n-1}) - \frac{\gamma v^2}{\gamma^2 + \epsilon_{n+1,n}^2}(\rho_{n,n}) - \frac{\gamma v^2}{\gamma^2 + \epsilon_{n-1,n}^2}(\rho_{nn})$$

Let us assume that

$$A = \frac{\gamma v^2}{\gamma^2 + \epsilon_{n+1,n}^2} \tag{3.28}$$

and

$$B = \frac{\gamma v^2}{\gamma^2 + \epsilon_{n-1,n}^2}. \tag{3.29}$$

Then, the result can be written in the form

$$\dot{\rho}_{nn} = -(A + B)\rho_{nn} + A\rho_{n+1,n+1} + B\rho_{n-1,n-1}. \tag{3.30}$$

In the Zeno regime, there are only population terms. If dephasing is strong enough, coefficient A and B proportional to $\frac{1}{\gamma}$. When γ increases diffusion rate decreases.

CHAPTER 4

THE EFFECTS OF THE MAGNETIC FIELD ON TRANSPORT

In this chapter, the effects of the artificial magnetic field on localization was investigated in addition to dephasing. A ring and a ribbon with closed boundary conditions and a two-dimensional lattice with open boundary conditions was used. The Aharanov-Bohm phase was introduced into these systems to break the Anderson localization.

According to the Aharonov-Bohm effect, when a charged particle moves along a closed path in the presence of a vector potential, it acquires a geometric phase after completes one tour. This phase called Aharonov Bohm phase (Aharonov and Bohm 1959).

$$\Phi_{AB} = -\frac{e}{\hbar} \oint_C A \cdot dr \tag{4.1}$$

4.1. Transport on a Ring
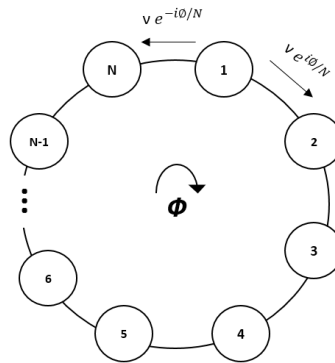

Figure 4.1. N-site ring with nearest neighbor hoppings $ve^{-i\phi/N}$ and $ve^{i\phi/N}$ under artificial magnetic field Φ where $\Phi = N\phi$

The Hamiltonian of N level ring in the presence of single excitation under the magnetic field is

$$H_S = \sum_{n=1}^{N} \epsilon_n (|n\rangle\langle n|) + \sum (ve^{-i\phi} |n\rangle \langle n+1| + ve^{i\phi} |n+1\rangle \langle n|) \qquad (4.2)$$

where ϵ_n are site energies and $ve^{\pm i\phi}$ are hopping strengths only nearest neighbours. where

$$\phi = \Phi/N \qquad (4.3)$$

and Φ is Aharanov- Bohm phase which is called Peierls phase on lattice.

The extra phase terms is introduced to the system as

$$v \to v\, exp(i \int_{r_n}^{r_m} A \cdot dr) \qquad (4.4)$$
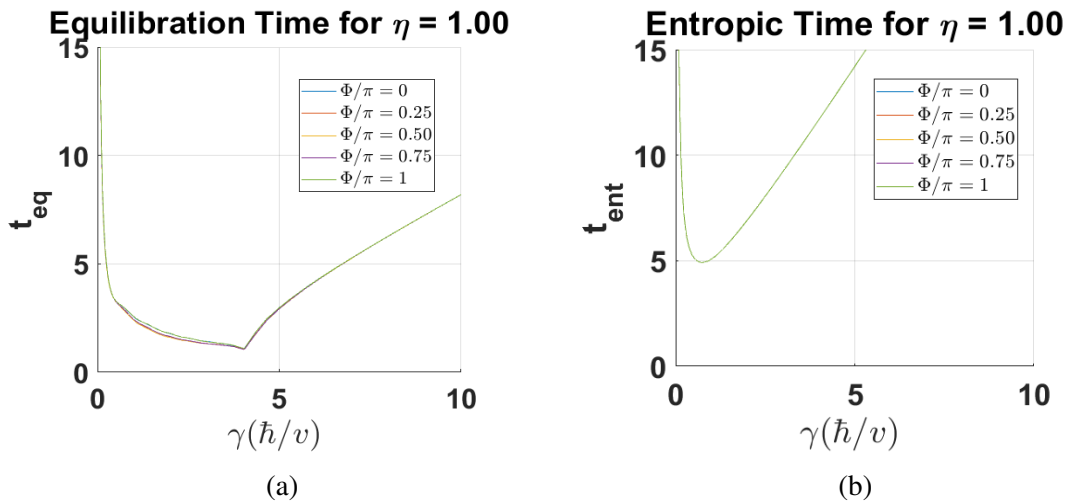

Figure 4.2. The relation between the dephasing and time for a ring of 20 sites under the magnetic field (a) for equilibration time (b) for entropic time

According to Figure 4.2, in the weak dephasing regime time decreases with dephasing while in the strong dephasing regime time increases again. In the Figure 4.2.a, Zeno regime can still be observed.
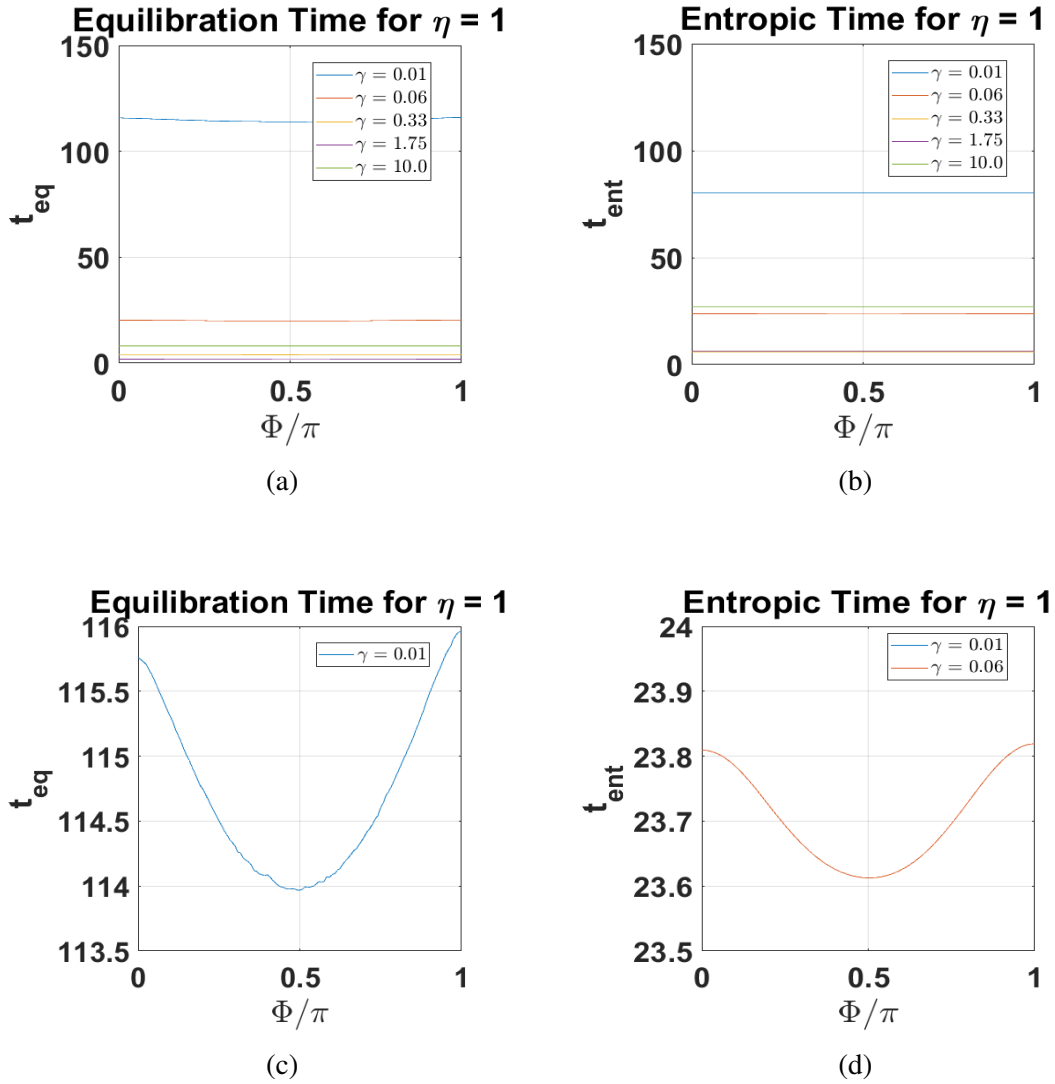
Figure 4.3. The relation between magnetic field and time for a ring of 20 sites (a) for equilibration time (b) for entropic time (c) for equilibration time scaled down to 100-120 (d) for entropic time scaled down to 18-21

Figure 4.3 shows the relation between magnetic field and time for different values of dephasing. According to Figure 4.3.a and 4.3.b, the magnetic field is independent of time. However on a closer inspection it is possible to see the effects of magnetic field on localization clearly. According to Figure 4.3.c and 4.3.d, when $\phi < \pi/2$ time decreases with magnetic field and when $\phi > \pi/2$ time increase again. So for ring, in some regions magnetic field can increase the quantum transport.

In this case in addition to equilibration time dephasing relation the entropic time dephasing relation was also investigated too. t_{ent} was described from the entropy defini-

tion. According to Figure 4.4, τ indicates the time where entropy reaches maximum value and t' is an entropic time for our calculations.
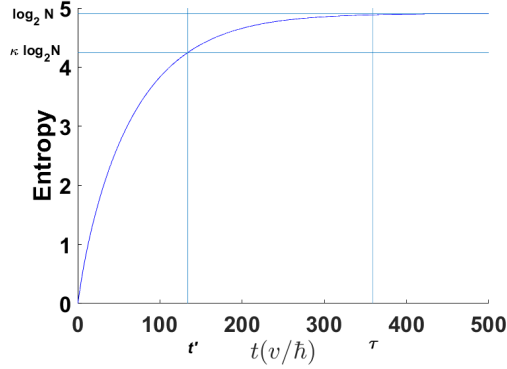

Figure 4.4. The relation between entropy and time where $\kappa = 1 - 1/e^2$

Then the effects of the magnetic field on both participation number and entropy for ring of 20 sites was investigated.
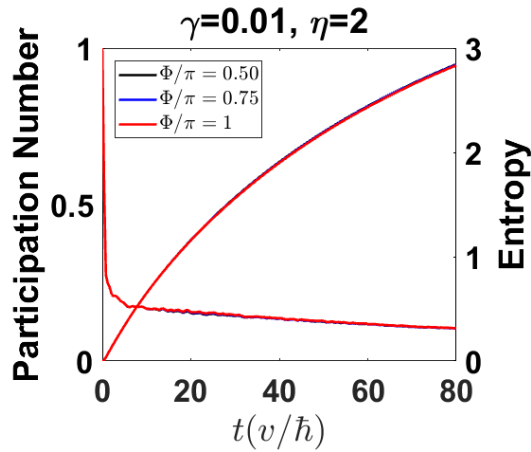

Figure 4.5. The relation between participation number and entropy with respect to time for ring of 20 sites under magnetic field

According to Figure 4.5, entropy and participation number are inversely proportional to each other. For a ring, magnetic field is independent of both participation number

and entropy. Eventually entropy reaches its asymptotic value and participation number converges to it minimum value.
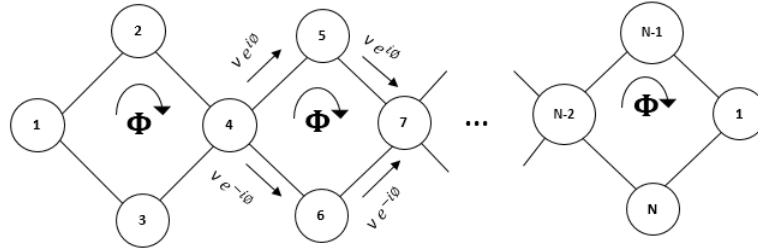
4.2. Transport on a Ribbon

Figure 4.6. N-site ribbon with nearest neighbor hoppings $ve^{-i\phi/4}$ and $ve^{i\phi/4}$ under magnetic field Φ where $\Phi = 4\phi$

The Hamiltonian of N level ribbon in the presence of a single excitation under the magnetic field is

$$H_S = \sum_{n=1,4,7...}^{N} \epsilon_n(|n\rangle\langle n|) + \sum (ve^{-i\phi}|n\rangle\langle n+1| + ve^{i\phi}|n+1\rangle\langle n|) \qquad (4.5)$$

where ϵ_n are site energies at the knots and v is hopping strength for only nearest neighbours.

$$v \rightarrow v\,exp(i\int_{r_n}^{r_m} A \cdot dr) \qquad (4.6)$$

where

$$\phi = \Phi/4 \qquad (4.7)$$

According to Figure 4.7, in the weak dephasing regime time decreases with dephasing while in the strong dephasing regime time increases. In the Figure 4.7.a, for strong dephasing the effects of the magnetic field on time begin to disappear. However, Zeno effect can still be observed.
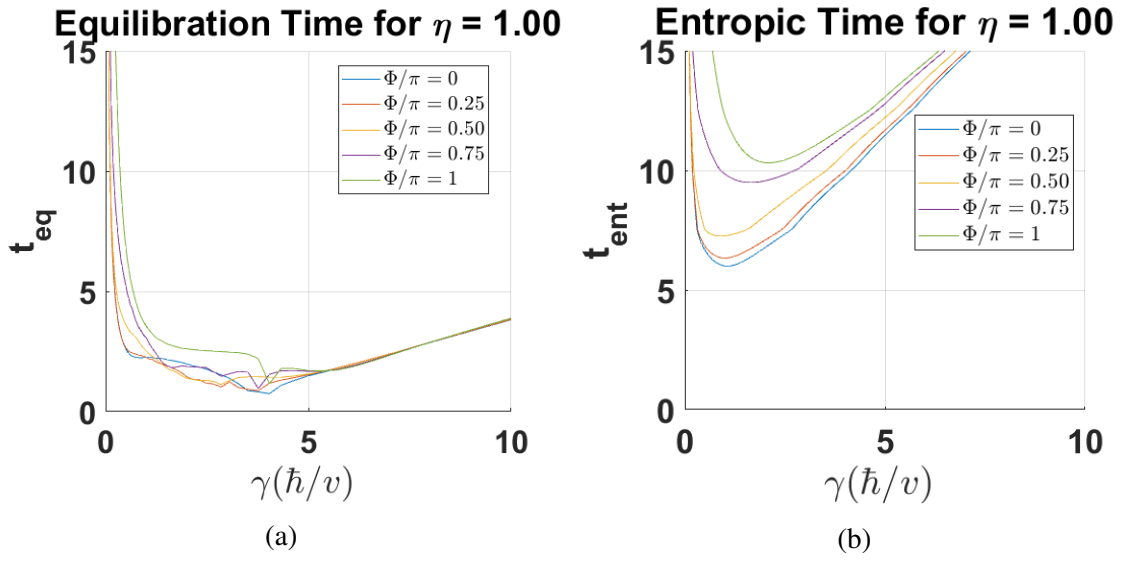
Figure 4.7. The relation between the dephasing and time for a ribbon of 30 sites under the magnetic field (a) for equilibration time (b) for entropic time
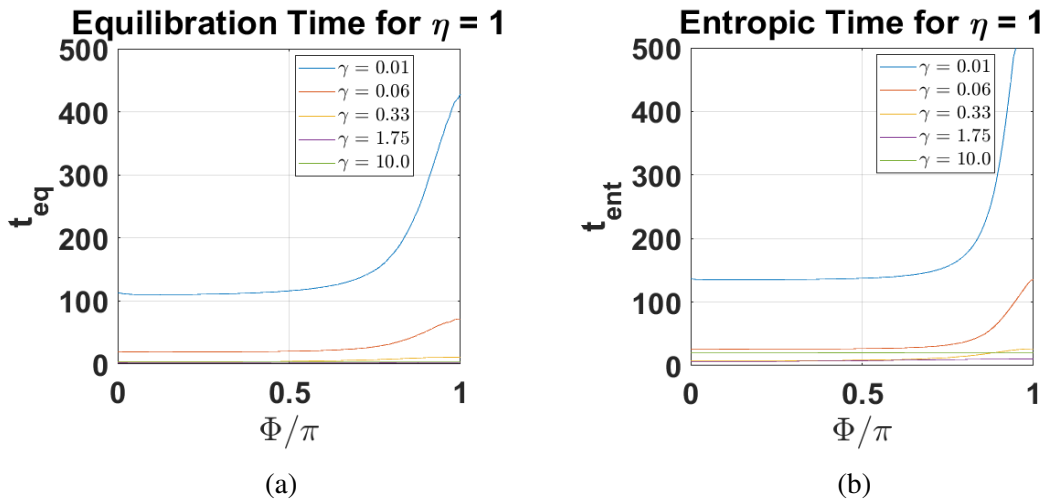

Figure 4.8. The relation between magnetic field and time for a ribbon of 30 sites (a) for equilibration time (b) for entropic time
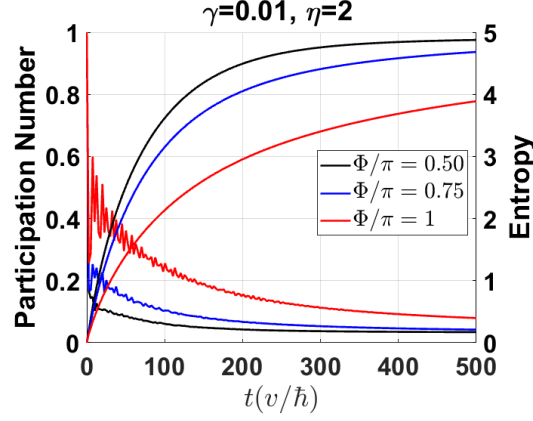
Figure 4.9. The relation between participation number and entropy with respect to time
for ribbon of 30 sites under magnetic field

According to Figure 4.8, time increases with magnetic field. In the strong dephasing regime effects of magnetic field begin to disappear. When $\phi = \pi$ time reaches maximum value. At this point destructive interferences lead to strong localization. According to Figure 4.9, when ϕ increases entropy attains its asymptotic value and participation number converges to minimum value at a later time.

4.3. Transport on a 2D Lattice

The Hamiltonian for $N \times N$ lattice in the presence of single excitation under the magnetic field is

$$H = \sum_{n_x, n_y = 1}^{N=5} \epsilon \left| n_x, n_y \right\rangle \left\langle n_x, n_y \right| + v \sum [e^{i n_x \phi} \left| n_x, n_y + 1 \right\rangle \left\langle n_x, n_y \right|$$
$$+ e^{-i n_y \phi} \left| n_x + 1, n_y \right\rangle \left\langle n_x, n_y \right|) + h.c] \tag{4.8}$$

Here n_x and n_y indicate lattice sites along the x and y direction respectively. ϵ indicates site energies and the hopping strength along both directions is given by v. Extra phase term is introduced into the hopping term and to create the artificial magnetic field symmetric gauge is used.
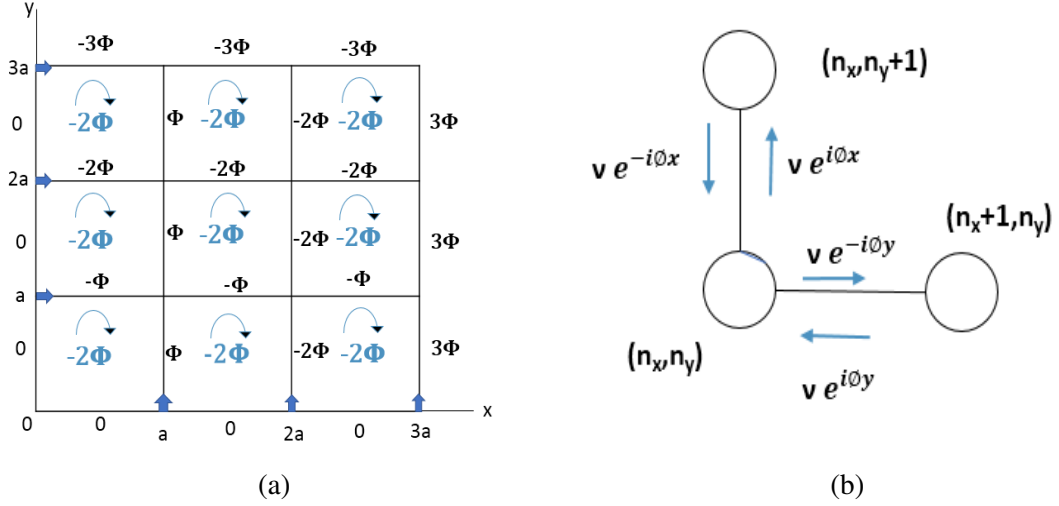
$$\vec{A} = \frac{B_0}{2}(-y, x, 0) \tag{4.9}$$

Figure 4.10. (a) A two dimensional lattice in the x-y plane with an artificial magnetic field 2Φ (b) Schematic representation of lattice sites with hopping strengths $ve^{\pm i\phi_x}$ and $ve^{\pm i\phi_y}$ where $\phi = \Phi/2$.

where

$$\phi = \Phi/2 \tag{4.10}$$

According to symmetric gauge, when particle hops nearest neighbors along the x axis, it gains phase in terms of y while along the y axis it gains phase in terms of x. These interactions cause extra phase contribution for each plaquette as 2ϕ.

According to Figure 4.11, for two-dimensional lattice it is possible to observe Zeno effect for both entropic time and equilibration time figures. In the entropic time figure when phi increases equilibration time decreases.

According to Figure 4.12, there are degenerate states in the system initially. These degeneracies lead to localization. When degeneracies break, ΔE increases and Δt decreases. As a result, quantum transfer increases. Eventually new degeneracies occur at the new points and time increases again.

By the energy-time uncertainty relation

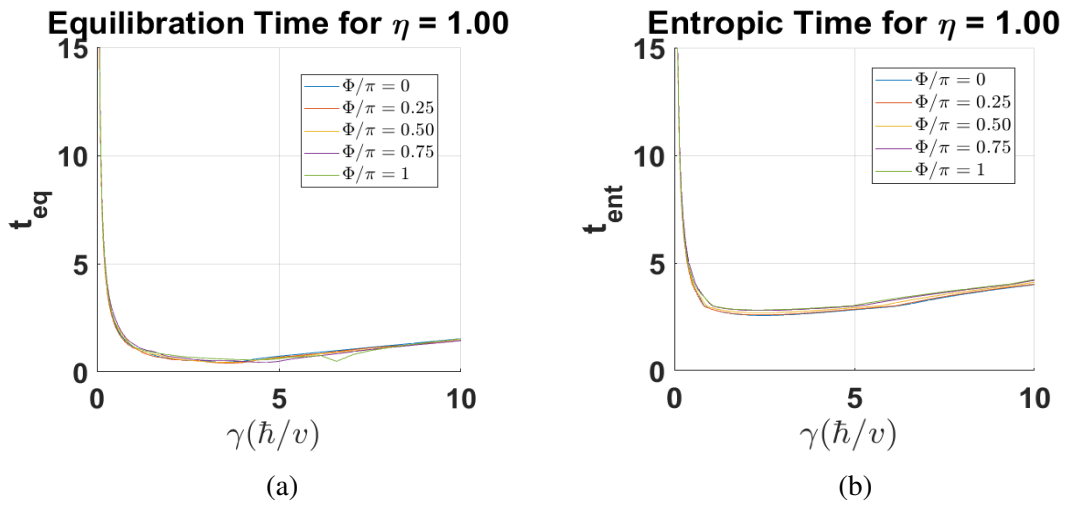$$\Delta E \cdot \Delta t \geq \hbar/2 \tag{4.11}$$

Figure 4.11. The relation between the dephasing and time for 5×5 lattice under the magnetic field (a) for equilibration time (b) for entropic time
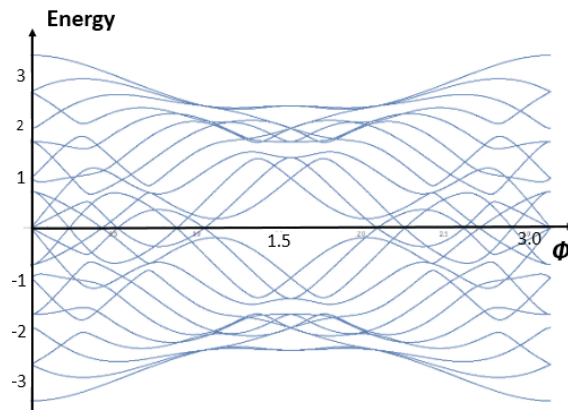

Figure 4.12. Energy-ϕ relation for 5×5 lattice where $\Phi = 2\phi$
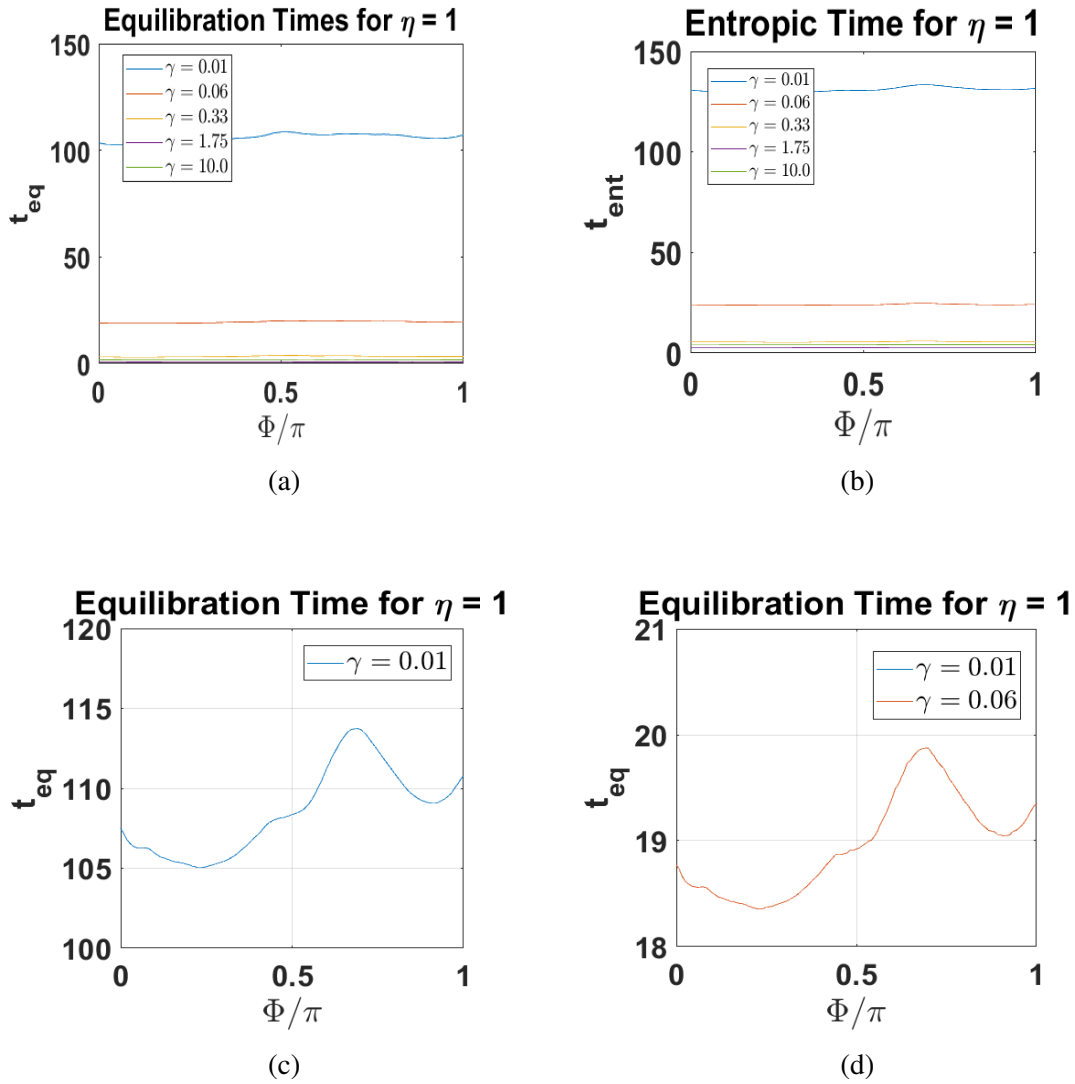
Figure 4.13. The relation between the magnetic field and time for 5×5 lattice (a) for equilibration time (b) for entropic time (c) for equilibration time scaled down to 100 to 120 (d) for equilibration time scaled down to 18 to 21

According to Figure 4.12, when ϕ equals to 0 or π, there are maximum number of degeneracies in the system. Therefore, at these points there is a strong localization.

According to Figure 4.13, the relation between the magnetic field and time for $2D$ lattice is different from ring and ribbon. There are local maximum and minimum points due to lifting of degeneracies. According to Figure 4.14, the participation number and entropy relation for $2D$ lattice is similar as ring. However for lattice entropy and participation number are slightly dependent on ϕ.
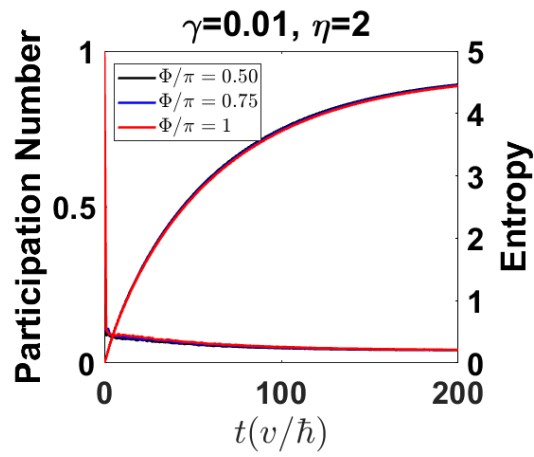
Figure 4.14. The relation between participation number and entropy with respect to time for 5×5 lattice under the magnetic field

CHAPTER 5

CONCLUSIONS

In open quantum systems, there is an interaction between the system and the environment. Therefore, the dynamics of the evolution of the open quantum system is different than closed quantum system. In addition to the unitary part, the open quantum systems contains also non-unitary part. The dynamical evolution of the open system can be described by Lindblad master equation. In this study the Markovian limit of the Lindblad master equation is used. According to Markovian dynamics, the memory effects of the environment can be neglected. Hence, the environment degrees of freedom is traced out and reduced system dynamics is obtained. After the Hamiltonian is constructed for each system the Lindblad master equation is solved numerically.

In this thesis, the effects of the dephasing and the magnetic field on the localization was studied for different type of systems. The energy difference between the sites of these systems leads to localization and make difficult to transition of the exciton. If energy difference (disorder) is high enough, excitation cannot spread to other sites. When dephasing is introduced to these systems, Anderson localization is lifted, both equilibration time and entropic time decrease. However, at the Zeno regime where dephasing is higher than a critical value, transfer is suppressed again.

Then, the relation between the participation number and entropy is observed. Since system is in a pure state initially, participation number equals to one and entropy is zero. When system becomes mixed, participation number converges to its minimum value and entropy increases and attains to its asymptotic value.

Finally, magnetic field is introduced to these systems. In that case, the effects of the magnetic field and dephasing on quantum transport is investigated together. Our results indicate that, the magnetic field also influences quantum transport. At low magnetic field, the localization is weakly suppressed thus the diffusion gets faster. However at strong magnetic field, destructive interference due to magnetic field leads to localization and diffusion is suppressed.

Generally the effects of environment on quantum transport is expected to be negative. However in open quantum system under proper conditions the interaction between the system and environment can increase quantum transport.

REFERENCES

Ableitinger, Alexander, RA Bertlmann, K Durstberger, BC Hiesmayr, and P Krammer. 2008. "Decoherence of open quantum systems."

Aharonov, Yakir, and David Bohm. 1959. "Significance of electromagnetic potentials in the quantum theory." *Physical Review* 115 (3): 485.

Anderson, Philip W. 1958. "Absence of diffusion in certain random lattices." *Physical review* 109 (5): 1492.

Blankenship, Robert E. 2014. *Molecular mechanisms of photosynthesis.* John Wiley & Sons.

Brasil, Carlos Alexandre, Felipe Fernandes Fanchini, and Reginaldo de Jesus Napolitano. 2013. "A simple derivation of the Lindblad equation." *Revista Brasileira de Ensino de Física* 35 (1): 01–09.

Breuer, Heinz-Peter, and Francesco Petruccione. 2002. *The theory of open quantum systems.* Oxford University Press on Demand.

Engel, Gregory S, Tessa R Calhoun, Elizabeth L Read, Tae-Kyu Ahn, Tomáš Mančal, Yuan-Chung Cheng, Robert E Blankenship, and Graham R Fleming. 2007. "Evidence for wavelike energy transfer through quantum coherence in photosynthetic systems." *Nature* 446 (7137): 782.

Griffiths, David J. 2016. *Introduction to quantum mechanics.* Cambridge University Press.

Ishizaki, Akihito, and Graham R Fleming. 2012. "Quantum coherence in photosynthetic light harvesting." *Annu. Rev. Condens. Matter Phys.* 3 (1): 333–361.

Joos, Erich, H Dieter Zeh, Claus Kiefer, Domenico JW Giulini, Joachim Kupsch, and Ion-Olimpiu Stamatescu. 2013. *Decoherence and the appearance of a classical world in quantum theory.* Springer Science & Business Media.

Lee, Hohjai, Yuan-Chung Cheng, and Graham R Fleming. 2007. "Coherence dynamics in photosynthesis: protein protection of excitonic coherence." *Science* 316 (5830): 1462–1465.

Lee, Patrick A, and TV Ramakrishnan. 1985. "Disordered electronic systems." *Reviews of Modern Physics* 57 (2): 287.

Lindblad, Goran. 1976. "On the generators of quantum dynamical semigroups." *Communications in Mathematical Physics* 48 (2): 119–130.

May, Volkhard, et al. 2008. *Charge and energy transfer dynamics in molecular systems.* John Wiley & Sons.

Misra, Baidyanath, and EC George Sudarshan. 1977. "The Zenoâs paradox in quantum theory." *Journal of Mathematical Physics* 18 (4): 756–763.

Neumann, Johann v. 2013. *Mathematische grundlagen der quantenmechanik.* Vol. 38. Springer-Verlag.

Nielsen, Michael A, and Isaac L Chuang. 2010. *Quantum computation and quantum information.* Cambridge university press.

Rebentrost, Patrick, Masoud Mohseni, Ivan Kassal, Seth Lloyd, and Alán Aspuru-Guzik. 2009. "Environment-assisted quantum transport." *New Journal of Physics* 11 (3): 033003.

Saffman, Mark, Thad G Walker, and Klaus Mølmer. 2010. "Quantum information with Rydberg atoms." *Reviews of Modern Physics* 82 (3): 2313.

Schaller, Gernot. 2014. *Open quantum systems far from equilibrium.* Vol. 881. Springer.

Schönleber, DW, Alexander Eisfeld, Michael Genkin, S Whitlock, and Sebastian Wüster. 2015. "Quantum simulation of energy transport with embedded Rydberg aggregates." *Physical review letters* 114 (12): 123005.

Singer, Kilian, Markus Reetz-Lamour, Thomas Amthor, Luis Gustavo Marcassa, and Matthias Weidemüller. 2004. "Suppression of excitation and spectral broadening induced by interactions in a cold gas of Rydberg atoms." *Physical Review Letters* 93 (16): 163001.