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HOPPING CONDUCTIVITY OF ELECTRON GLASS

A Thesis Presented

by

MINGZHU CUI

Submitted to the Office of Graduate Studies,
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Applied Physics Program

HOPPING CONDUCTIVITY OF ELECTRON GLASS

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ABSTRACT

HOPPING CONDUCTIVITY OF ELECTRON GLASS

August 2017

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Directed by Associate Professor Stephen Arnason

Hopping conductance between the sites in disordered systems is mapped to a random resistor network named Miller-Abrahams network. The conductance between two sites is in an exponential form depending on two parameters, the space separation and energy separation between sites. Our effort is focused on the visualization of the random resistor network. We find all the realizations for one electron hop and plot out the according random resistor networks. By comparing the random resistor network structures, we find that Coulomb interaction plays an important role in calculating the hopping conductance between sites. Furthermore, we rank the realizations by total energy and plot out its distribution. We find out that the total energy of all these realizations for one electron hop may follow a Gaussian distribution.

ACKNOWLEDGMENTS

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I would like to thank Prof. Bala Sundaram for being my committee member and he gives me some great advices about how to improve the results and what to try in the future. And his careful corrections make the thesis more rigorous.

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CHAPTER 1

INTRODUCTION

The interest in the properties of disordered systems revolutionized research in solid state physics, which traditionally dealt with materials whose properties were mostly determined by crystalline symmetry. The conventional methods for treating such systems are based on equilibrium statistical mechanics because the ground state of a solid is assumed to have translational symmetry, which do not apply to disordered systems. Hence, a disordered system is always out of thermodynamic equilibrium. Nevertheless, most materials in nature are disordered; therefore, the understanding of disordered systems is relevant for a wide class of materials [1]. This thesis focuses specifically on the conductivity of disordered solids.

At sufficiently low temperatures, transport effects in lightly doped semiconductors are not due to free carriers but occur as a result of hopping charge transport between localized impurity states. The term impurity conduction denotes this type of transport. When the impurity concentration is high, the impurity states overlap strongly and lose their localized character. It is often said that an impurity band is formed and that conduction takes place in this "band. " At low concentrations banding does not occur and conduction takes place by hopping of electrons from occupied to unoccupied localized donor states [2]. In this thesis, the impurity transport is restricted to hopping processes and impurity bands are not considered.

The process of “hopping” was first studied by Conwell [3] and Mott [4]. They individually attributed the lower activation energy to transitions between impurity states [1]. The same mechanism was independently proposed by Pines, Abrahams, and Anderson in connection with the study of electron relaxation processes in Si [2].

The electron hop is the fundamental transport process in the Anderson insulator. Anderson insulator is an insulator that can undergo Anderson transition, which is a metal-insulator transition as a function of concentration or disorder for disordered electronic system. The conductivity in such an insulator is often found to be non-Arrhenius [1]. N. F. Mott published a paper named “On the Transition to Metallic Conduction in Semiconductors” [4]. He conceived of the reason for this effect and called it variable range hopping. The basic mechanism is phonon-assisted tunneling between localized states. Such a process is governed by a competition between tunneling and activation. The greater the distance between the sites, the more difficult the tunneling – the larger the energy separation, the more difficult the activation. Thus the optimal hopping distance is temperature dependent, which explains the non-Arrhenius behavior. This non-Arrhenius dependence of the conductivity, which is characteristic of the hopping was observed in a variety of noncrystalline materials such as amorphous chalcogenides, amorphous silicon, amorphous germanium and other materials [1]. Fig.1.1 is a schematic description of variable range hopping process. Here E_f is the energy of Fermi level, E_c is the mobility edge of conductance band, and ξ is the localization length.

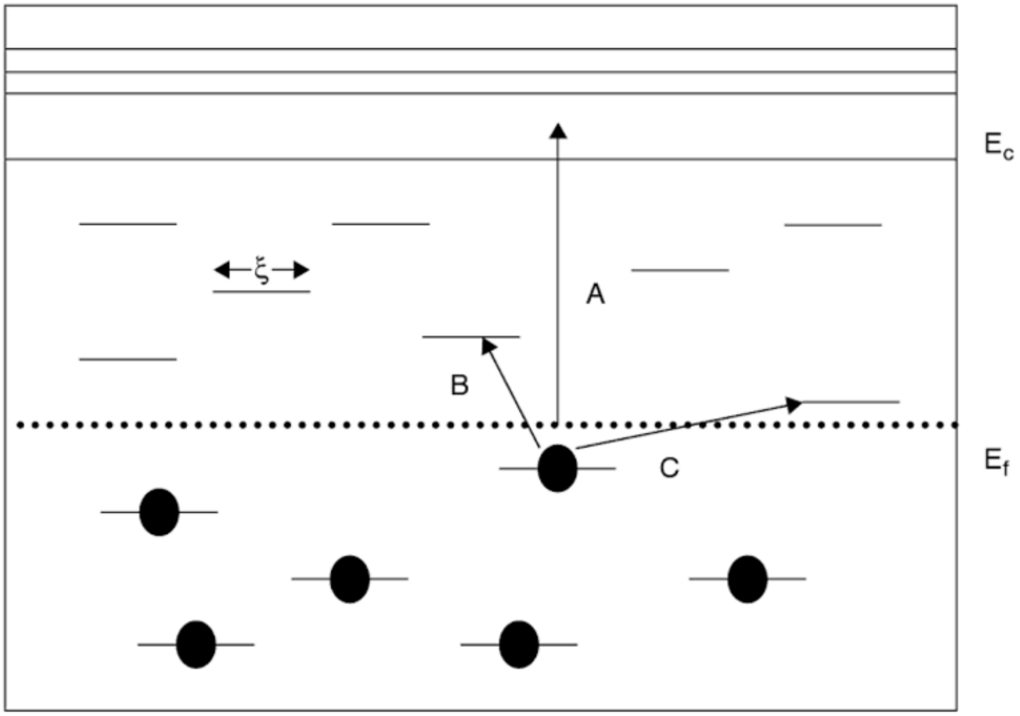


Fig. 1.1 Schematic description of the localized states as a function of space and energy. Three hopping processes are possible. At high energies the dominant process is excitation above the mobility edge (A). At lower temperatures an electron hops to a n nearest neighbor available site (B). At yet lower temperatures the preferred hop is to a distant site which is closer in energy (C) [1].

Based on the explanation for hopping process, Miller and Abrahams [2] showed that the problem of hopping conduction can be mapped on a random network of resistors, each resistor connecting a pair of impurities with a resistance in accordance with the hopping rate between them [1], which is true according to Landauer formula [5]: the conductance of a nanoscale conductor is given by the sum of all the transmission possibilities (hopping rate) an electron has when propagating with an energy equals to the chemical potential. Besides, Miller and Abrahams were the first to calculate the hopping conductivity of semiconductors using reduced networks. They assumed that the statistical distribution of the resistances depends only on the distances between sites and not the site energies. This was justified because the experimental data for some semiconductors indicated that impurity conduction exhibits a well-defined activation energy. But Mott [6] [7] pointed out that the exponential dependence of the resistances on the site energies cannot be ignored in most cases; if the activation energy of a nearest-neighbor site is large, a hop to a distant site whose energy is lower may be easier than one to a nearest-neighbor site. This mechanism of hopping conduction is usually called variable range hopping. It contrasts with the original work of Miller and Abrahams, which was restricted to nearest-neighbor hopping and may be appropriate at high temperatures [8].

However, Mott's optimization process of variable range hopping was not verified in detail. Ambegaokar et.al [9], Shklovskii and Efros [10], Pollak [11] reexamined the transport paths independently and started to form the percolation theory of hopping to deal with hopping conduction. The theories are based on the fact that there is an enormously broad distribution of resistances in the Miller and Abrahams network, which implies that the resistivity is determined by the largest resistances in an optimal current carrying path. Thus there exists an optimal percolation network that maximizes the conductivity; hence, much of the material does not participate in carrying the current [1]. If we always proceed through nearest-neighbors as in the Miller-Abrahams theory, we are certain to arrive at a site where our nearest-neighbor is a large distance away, so it may be more efficient to go through non-nearest-neighbors. That is why the Miller-Abrahams paths do not usually carry current [8].

Later people realize that Coulomb interaction energies are often at least as large as the energy band of the random potential due to disorder [1]. Efros and Shklovskii [12] showed that the Coulomb interaction between localized electrons is shown to create a ‘soft’ gap in the density of states near the Fermi level--a depletion of the single-particle density of states(DOS). The effect of Coulomb interaction can modify the conductance from Mott’s variable range hopping dramatically.

In the early 1980s, a number of groups realized that the combination of disorder and interactions may lead to glassy behavior that would show up as very slow relaxation to equilibrium and memory effects. Davies et al. [13] were the first to name this phenomenon the “electron glass” [1]. Glass behaviors were also observed in later experiments. Electron glass is an appropriate system to study glassy effects because it is easy to prepare, easy to excite in many ways, such as temperature, gate voltage, electric field and electromagnetic radiation, and easy to measure accurately. Also, due to the light mass of the electrons, the electron glass is a prototypical example for quantum glass in which the relaxation toward equilibrium involves quantum transitions such as tunneling [1].

Electron glass is a lightly doped semiconductor, and the electrons in materials are strongly localized. So the transport effects for electrons are mainly variable range hopping. Coulomb interaction between sites can play an important role in calculating conductance for a disordered system, so it should be taken into account as well. Besides, it will be helpful if we can visualize the structure for the conductance between sites. So we are going to adopt Miller-Abrahams network and map the conductance onto a network formed by random resistors. By doing electron hops on the random resistor network, we can see how the conductance between sites changes. And by calculating the average conductance of different network generated by electron hops, we can check if there is a Coulomb gap formed.

CHAPTER 2

THEORETICAL BACKGROUND

2.1 Laudauer formula:

Laudauer formula provides theoretical support for Miller and Abrahams when they are trying to map the hopping conduction on a random network of resistors which connects a pair of impurities with a resistance in accordance with the hopping rate between them. Laudauer's assumption, that the system is connected to reservoirs by ideal quantum wires which behave as waveguides for the electron waves [14], is the prototype for calculating hopping conductance between a pair of sites.

The ideal quantum wire is a pure narrow channel that separates 2 large electron gas reservoirs having the difference δn in electron density. If δn is small, one can assume that there is a difference in a chemical potential, $\delta\mu = \delta n / g(\epsilon F)$. Suppose the Fermi level of non-biased system is the origin for the chemical potentials. Thus the chemical potential for the α-th reservoir will be μ_α. If the channel is long and uniform, then the total current carried by the state is characterized by a transverse mode n and a given direction of spin which propagates without scattering. The transverse mode n current is

$$J_{n=}e \int \frac{dk_z}{2\pi\hbar} \frac{\partial \mathcal{E}_n(k_z)}{\partial k_z} = \frac{2}{2\pi\hbar} \int_{\epsilon F+\mu_\alpha}^{\epsilon F+\mu_\beta} d\varepsilon \, \frac{\partial \mathcal{E}_n(k_z)/\partial k_z}{|\partial \mathcal{E}_n(k_z)/\partial k_z|} = \frac{2}{h} \delta\mu \qquad (2\text{-}1)$$

If electron spin is taken into account and N transverse modes are open, then the conductance is given by the expression $G = \frac{2e^2}{h}$ [14]. This means an ideal quantum wire has finite conductance, which is independent of the length of the wire. Fig.2.1 describes a system including a barrier connected to reservoirs by ideal quantum wires. Only a part of the current is transmitted if there is some reflection.

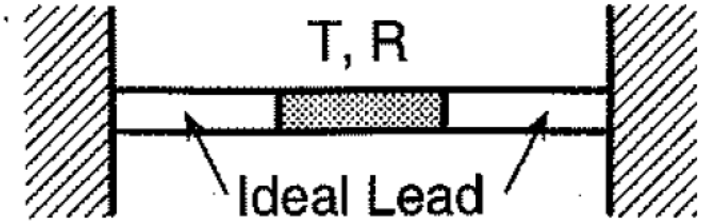


Fig.2.1 Schematic diagram of configuration for Landauer formula [14]. The shadows on both sides stand for two large electron gas reservoirs. The ideal lead in between stands for an ideal quantum wire. T stands for transmission and R stands for reflection.

In this case one can introduce the transmission probability of the mode n, T_n, to obtain (including spin degeneracy)

$$J = \frac{2}{h}\,\delta\mu \sum_{n=1}^{N} T_n \tag{2-1}$$

And the conductance between the two reservoirs is

$$G = \frac{2e^2}{h} \sum_{n=1}^{N} T_n \tag{2-3}$$

The expression above is called two terminal Landauer formula.

From Landauer formula we can know that the conductance of a nanoscale conductor is given by the sum of all the transmission possibilities (hopping rate) an electron has when propagating with an energy equal to the chemical potential [15].

2.2 The Miller-Abrahams network:

Miller-Abrahams extend the idea of a quantum conductance channel to a network of resistors model and is a foundation for the thesis, providing us a very convenient way to calculate the conductance between two sites.

Miller and Abrahams developed a model consisting of two parts, the quantum mechanical theory of the wave functions and of the transition rates W_{ij} from a localized state i to a localized state j, and a statistical mechanical theory of transport that employs such transition rates. They also showed how their model can be reduced to a random resistor network and be used for computing the hopping conductivity of disordered solids [8].

The derivation of the Miller-Abrahams equation starts from Boltzmann equation

$$\frac{\partial P_i}{\partial t} = \sum_j [W_{ji} P_j (1 - P_i) - W_{ij} P_i (1 - P_j)] \tag{2-4}$$

P_i is the probability that site i is occupied. As mentioned before, W_{ij} is the transition rates from a localized state i to a localized state j.

$$P_i = P_i^0 + \Delta P_i \tag{2-5}$$

$$W_{ij} = W_{ij}^0 + \Delta W_{ij} \tag{2-6}$$

Superscript 0 denotes the equilibrium value. Δ is an increment proportional to an applied electric field. Here $\Delta W_{ij} = -\Delta W_{ji}$.

Then the linearized version obtained is as following

$$\frac{\partial \Delta P_i}{\partial t} + \sum_j A_{ij}\,\Delta P_i - \sum_j A_{ji}\,\Delta P_j = \sum_j B_{ji}\Delta W_{ji} \tag{2-7}$$

Where

$$A_{ij} = W_{ij}^{0}\left(1 - P_j^{0}\right) + W_{ji}P_j^{0} \tag{2-8}$$

$$B_{ij} = P_i^{0}\left(1 - P_j^{0}\right) + P_j^{0}\left(1 - P_i^{0}\right) \tag{2-9}$$

(2-7) is a set of linear equations for the unknown ΔP_i . The equilibrium values P_i^0 are given by the Fermi distribution

$$P_i^0 = \frac{1}{\exp(E_i/k_bT)+1} \tag{2-10}$$

E_i is he energy of a carrier on site i measured from the Fermi level, k_b is the Boltzmann constant, and T is temperature of the system. The equilibrium value W_{ij}^0 are given by

$$W_{ij}^0 = \frac{u_{ij}}{\left|\exp\left[(E_j - E_i)/k_bT\right] - 1\right|} \tag{2-11}$$

with

$$u_{ij} = u_{ji} = \frac{1}{\tau_0}\exp\left(-\frac{2r_{ij}}{a}\right) \tag{2-12}$$

In (2-12) $\frac{1}{\tau_0}$ is of the order of a phonon frequency, r_{ij} is the distance between i and j, and a is Bohr radius. It is assumed that τ_0 depends only weakly on r_{ij} and T.

Suppose that F is the intensity of the applied electric field, and r_i is the radius vector of site i, the applied field changes the energy differences Δ_{ij} between the energies of sites i and j [8]. Then for a linearized theory we should have

$$\Delta W_{ij} = \frac{dW_{ij}}{d\Delta_{ij}}e\boldsymbol{F}\cdot\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right) = \frac{e\boldsymbol{F}\cdot\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)}{sinh^2\left(\frac{\Delta_{ij}}{k_bT}\right)}u_{ij} \tag{2-13}$$

where e is the charge of an electron. Miller and Abrahams defined the electrical potential for site i as V_i, which means the potential at each site is unique and varies through the sample. Then

$$P_i = P_i^0 + \Delta P_i \equiv \frac{1}{\left|\exp\left[\frac{E_i - eV_i}{k_b T}\right] + 1\right|} \tag{2-14}$$

so that to first order

$$\Delta P_i = \frac{dP_i^0}{dE_i} eV_i = \frac{eV_i}{4k_b T cosh^2\left(\frac{E_i}{2k_b T}\right)} \tag{2-15}$$

In the linear regime the variable V_i is proportional to F. We can transform the set of linear equations for P_i to another set for V_i. The resulting set of linear equation is then given by

$$D_i \frac{\partial V_i}{\partial t} = \sum_j D_{ji} V_j - \sum_j D_{ij} V_i + \sum_j G_{ij} \boldsymbol{F} \cdot \boldsymbol{r}_{ij} \tag{2-16}$$

where $D_i = P_i^0(1 - P_i^0)$, $D_{ij} = D_i A_{ij}$, and $G_{ij} = B_{ij} W_{ij}^0 W_{ji}^0 / u_{ij}$.

We can now discuss the construction of a network model for calculating the hopping conductivity. First consider the steady state. A temperature dependent conductance G_{ij} is defined by

$$\frac{k_b T G_{ij}}{e^2} = P_i^0\left(1 - P_j^0\right) W_{ij}^0 = P_j^0(1 - P_i^0) W_{ji}^0 \tag{2-17}$$

If one substitute (2-17) into (2-16), then

$$\sum_j \left\{\left[V_i - \frac{\boldsymbol{F} \cdot \boldsymbol{r}_i\left(W_{ij}^0 + W_{ji}^0\right)}{u_{ij}}\right] - \left[V_j - \frac{\boldsymbol{F} \cdot \boldsymbol{r}_j\left(W_{ij}^0 + W_{ji}^0\right)}{u_{ij}}\right]\right\} G_{ij} = 0 \tag{2-18}$$

where $\left(W_{ij}^0 + W_{ji}^0\right)/u_{ij}$=coth $(|\Delta_{ij}|/2k_b T)$. We mainly consider the regime for which coth $(|\Delta_{ij}|/2k_b T) \sim 1$, in which case (2-18) becomes

$$\sum_j \left[(V_i - \boldsymbol{F} \cdot \boldsymbol{r}_i) - \left(V_j - \boldsymbol{F} \cdot \boldsymbol{r}_j\right)\right] G_{ij} = 0 \tag{2-19}$$

Equation (2-19) represents a network of resistors. We think of $(V_i - \boldsymbol{F} \cdot \boldsymbol{r}_i)$ as the potential at site i. Then, $Z_{ij} = 1/G_{ij}$ is the resistance between sites i and j, and (2-19) is simply Kirchhoff's equation for site j. Miller and Abrahams treated Z_{ij} more generally and considered it as an impedance [8].

For the unsteady state, the time-dependent term of (2-16) does not vanish, and (2-19) must be rewritten as

$$\frac{P_i^0 e^2 (1-P_i^0)}{k_b T} \frac{\partial V_i}{\partial t} = \sum_j [(V_i - \boldsymbol{F} \cdot \boldsymbol{r}_i) - (V_j - \boldsymbol{F} \cdot \boldsymbol{r}_j)] G_{ij} \qquad (2\text{-}20)$$

To make a more general network for this case, we define a capacitance $C = P_i^0 e^2 (1 - P_i^0)/k_b T$ with a potential V_i across it. We now refer all the potentials to the "ground" potential, which is zero. Because $\boldsymbol{F} \cdot \boldsymbol{r}_i$ is the applied potential at i, it is represented as an output from a generator connected in series with C between the ground and site i. There is an impedance Z_{ij} connected between any two junctions i and j. There is also a capacitor C_i in series with a generator connected to the ground [8]. Using the expression for P_i^0 and W_{ij}^0, and restricting our attention to the case where various site energies are of the order or larger than $k_b T$, we obtain

$$Z_{ij} = k_b T \frac{\exp\left[(|E_i| + |E_j| + |E_i - E_j|)/2k_b T\right]}{e^2 u_{ij}} \qquad (2\text{-}21)$$

$$C_i = \frac{e^2}{k_b T} \exp\left(-\frac{E_i}{k_b T}\right) \qquad (2\text{-}22)$$

using (2-12) and (2-22), we can rewrite (2-21) as

$$Z_{ij} = \frac{k_b T}{e^2} \exp\left(\frac{E_{ij}}{k_b T} + \frac{2 r_{ij}}{a}\right) \tau_0 \qquad (2\text{-}23)$$

E_{ij} is either the energy difference between site i and j or E_{ij}= $(|E_i| + |E_j| + |E_i - E_j|)/2$. The conductance G_{ij} is

$$G_{ij} = \frac{1}{Z_{ij}} = \frac{e^2}{k_b T} \exp\left(-\frac{E_{ij}}{k_b T} - \frac{2r_{ij}}{a}\right)\frac{1}{\tau_0} \tag{2-24}$$

In this thesis, there is no electric field applied to the system. However, there is a random site dependent energy drawn from a Gaussian distribution. And there will be an energy difference between site i and site j, which is analogous to the energy difference changed between two sites by the applied electric field in Miller-Abraham networks. And there is also an interaction energy between sites to mimic the Coulomb correlations amongst electrons. Recall that the original work of Miller and Abrahams was restricted to nearest neighbor hopping. However, according to Mott's work both hopping distance and energy difference should be taken into account. So we will see there is a trade-off between space separation and energy difference in our case. Also, the conductance in the network can vary by orders of magnitude because of the exponential dependence on both the spatial separation and energy difference, so I choose to use a logarithmic scale when trying to visualize the conductance between sites.

CHAPTER 3

CONDUCTANCE FOR ELECTRON GLASS

3.1 Introduction for electron glass

In 1982, J. H. Davies, P. A. Lee, and T. M. Rice published a paper named "Electron Glass" [13], and they were the first to name a phenomenon "Electron Glass". The phenomenon is that the combination of disorder and interactions may lead to a glassy behavior that would show up as very slow relaxation to equilibrium and memory effects [1]. Electron glass is a lightly doped semiconductor, in which the impurity states are strongly localized. Transport effects are not due to free carriers in conductance band but occur as a result of electron hopping between localized impurity states. The disorder in electron glass has two aspects: one is the disorder for the position of sites, which means that the sites in electron glass are randomly displaced; the other one is that the energy on each site is unique and site dependent, which follows a Gaussian distribution in our case. Usually electron glasses are noncrystalline materials, such as amorphous silicon, amorphous chalcogenides, amorphous germanium and some other materials like amorphous Indium Oxide which is the material that motivated this project. This thesis focuses on the conductivity of electron glasses, which is mainly caused by electron hops inside the materials.

3.2 Variable range hopping

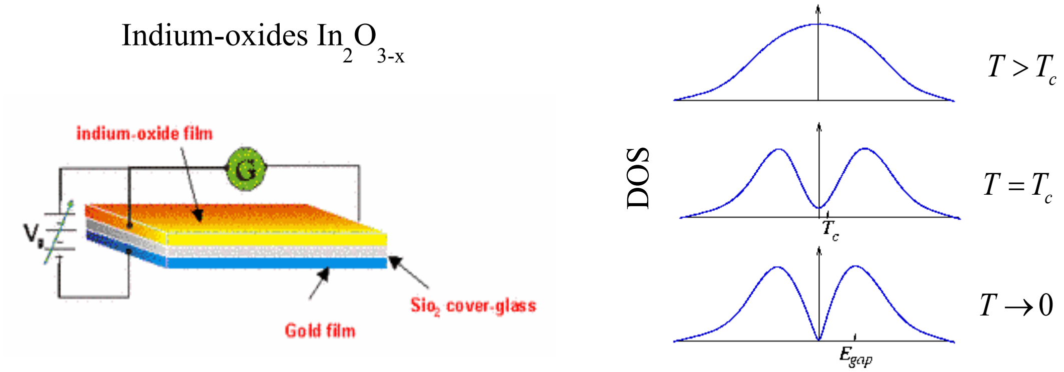
Mott [4] realized that if the electrons are localized at the Fermi level, the material becomes insulating at low temperatures; if they are extended, the system is metallic. Hence, a disordered electronic system can undergo a metal-insulator transition as a function of concentration or disorder. This transition is called the Anderson transition and the insulator is called and Anderson insulator. The conductivity in such an insulator is often found to be non-Arrhenius. Mott conceived of the reason for this effect and called it variable range hopping [1]. Fig. 1.1 shows that hopping processes depend both on energy separation and space separation. Then he gives out that the hopping probability at a given temperature depends on two parameters: R, the space separation of the sites, and ΔE, their energy separation. The relationship between hopping probability and the two parameters is as following

$$P \sim \exp\left[-2\alpha R - \frac{\Delta E}{kT}\right] \tag{3-1}$$

Here α^{-1} is the attenuation length for a hydrogen-like localized wave function.

Later people realized that Coulomb interaction can play a very important role in electron glass because Coulomb interaction energies are often at least as large as the energy band of the random potential due to disorder [1]. Efros and Shklovskii [12] showed that the Coulomb interaction between localized electrons creates a ‘soft’ gap in the density of states near the Fermi level. In fact, this ‘soft’ gap is a depletion of the single-particle density of states(DOS), which is the distribution of the energy E_i required to add or remove an electron to the system in site i holding the rest of the electrons fixed. Fig.3.1 describes the configuration for MOSFET used in experiment and the distribution of DOS under different temperatures. From Fig.3.1 (B) we can see there is a gap formed as the temperature goes down because of the Coulomb interaction between localized impurity states. Also because of Coulomb interaction, the energy in site i, E_i, not only includes the random energy due to the disorder of system, also includes the Coulomb interaction energy with all other sites. Thus, if an electron is transferred from site i to site j, the energy of this one electron hop is

$$\Delta E_{j,i} = E_j - E_i - \frac{e^2}{\kappa r_{i,j}} \tag{3-2}$$



(A) (B)

Fig.3.1 (A) Schematic graph for the equipment used to do experiment about electron glass. The main part is a field effect transistor with a conduction channel made of amorphous indium oxide. V_g is the gate voltage. (B) shows the 2D density of states for the weak disordered system in part (A). T_c is a finite temperature at which one can find a replica symmetry breaking glass transition and E_{gap} is the mobility edge for conduction band [16] [17].

Recall that electron glass has memory effects. A phenomenon called conductance memory, which is caused by Coulomb interaction, is going to be introduced. Fig.3.2 illustrates the two dips experiment. A. Vaknin and his collaborators [18] cool down the MOSFET structure to liquid He temperature. By scanning the gate voltage, they find there is a dip in conductance at around 5V. This dip is caused by the suppression of density of states and it is a Coulomb gap. At time t=0, they fix the gate voltage at a new voltage around -6V, which is equivalent to changing the chemical potential for the system. After 0.15h, they scan the gate voltage again. They find there is a memory of the old dip at 5V and a new correlation gap appears at the new gate voltage. The memory of the old dip slowly goes away and the magnitude of the new correlation gap slowly increases. In fact, the slow changes are the glassiness. Also from the top line on the graph, we can see if we change the system energy either a little bit larger or a little bit smaller by increasing or decreasing the gate voltage around 5V, the conductance of the system will go up in both cases.

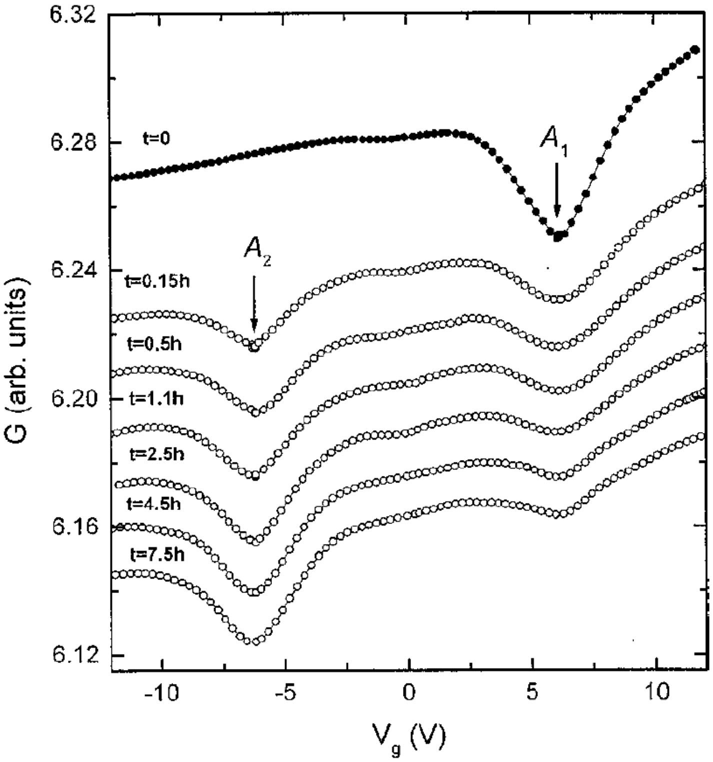


Fig.3.2 An illustration of the TDE (two dips experiment). G is the conductance for the MOSFET structure. V_g is the gate voltage. $A_1$and $A_2$are the magnitudes of the two dips. The right dip (A1) occurs at the cool-down value of V_{g1} and decays in time. The left dip (A2) occurs at the value to which V_{g2} is switched at time t=0 and grows with t. R_s=3.8MΩ and T=4.2 K [18].

3.3 Motivation for computer simulation

Our aim is to visualize the conductance of the disordered system. Furthermore, we want to check if we can see the emergence of the Coulomb gap while we are able to visualize the percolating network. In the next chapter, we are going to generate a random network with all the bonds standing for the conductance between sites. By doing one electron hops, we are going to check if there are some changes for the bonds because of

Coulomb interaction. By comparing the average conductance for all one electron hop realizations, we can know if a Coulomb gap forms or not.

CHAPTER 4

RESULTS

In our simulations of the model, we use 100 sites with random positions and random site energies following a Gaussian distribution. The gray scale and linewidth of bonds stand for the magnitude of the conductance between sites. Black bonds, with color character [0,0,0] and linewidth 2.5, denote relatively large conductance. Grey bonds, with color character [0.5,0.5,0.5] and linewidth 2, stand for smaller conductance. The lighter grey bonds, with color character [0.8, 0.8, 0.8] and linewidth 1.5, denote yet smaller conductance. In all the graphs showing network structures, the solid blue dots are the sites occupied by electrons and the open blue circles are the unoccupied sites. Fig.4.1 is a random network we generate.

To study the range of changes in energies associated with changes in the configuration, we considered single electron excitations, moving an electron from an occupied site to an unoccupied site. We can then see how the energy fluctuations are correlated with the structure of the resulting percolating networks. We find all realizations for one electron hop, then calculate the total energy for all those realizations. By ranking all the total energies we get, we find the realization with the lowest energy for one electron hop, which is shown in Fig.4.2.

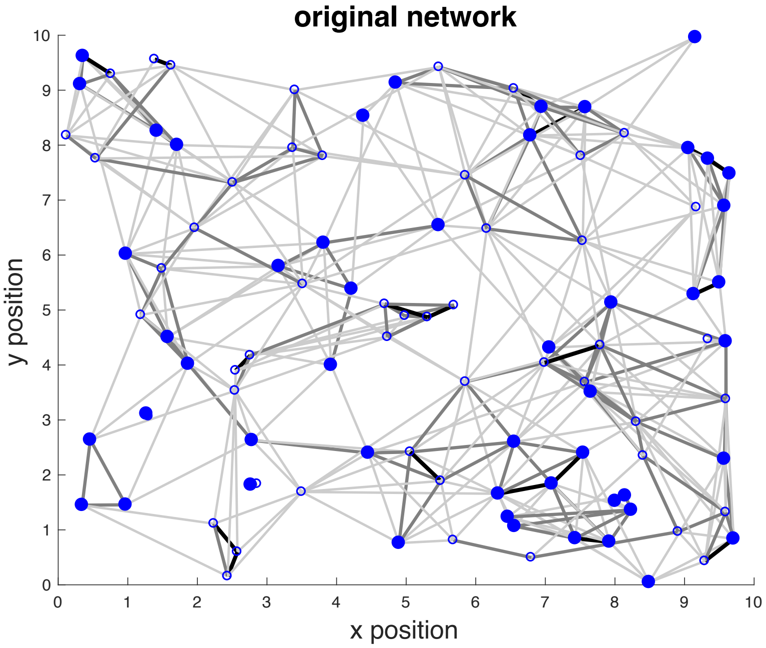


Fig.4.1 A random network generated (Original Realization).

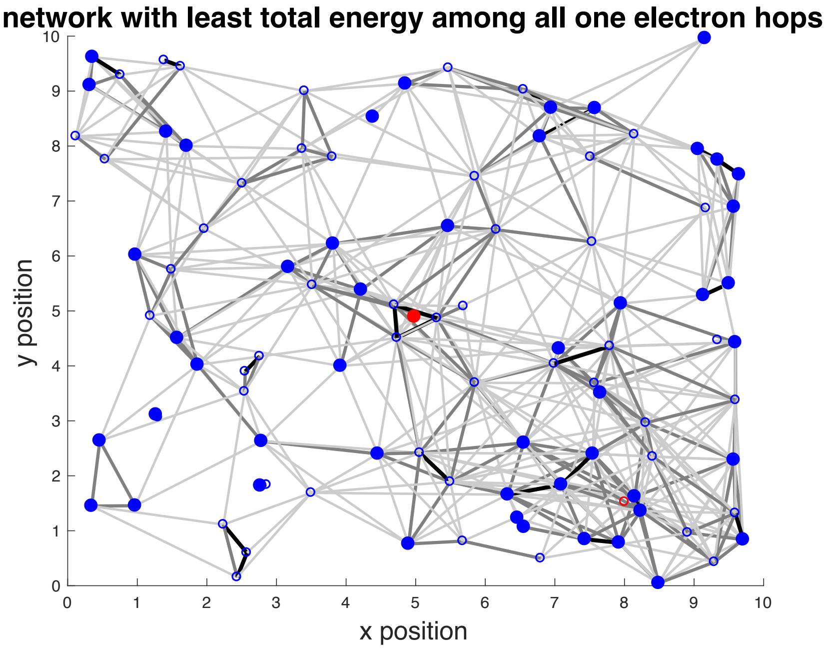
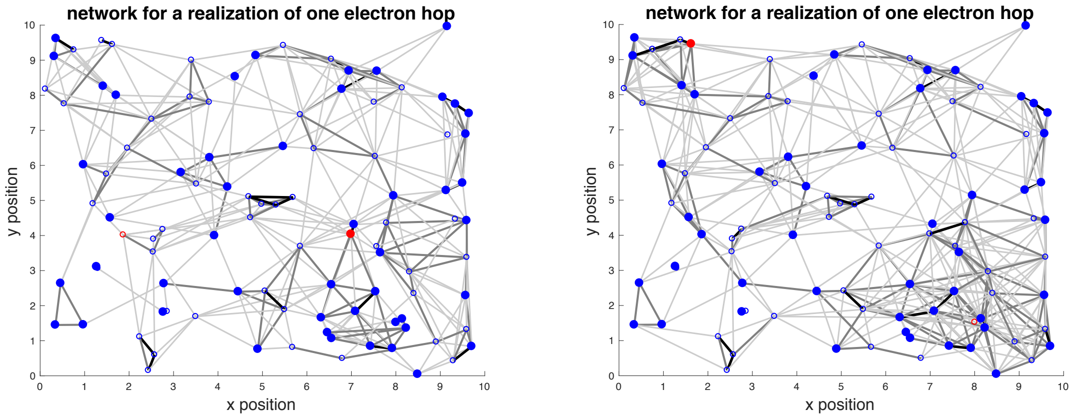


Fig.4.2 Network for the realization with lowest total energy after one electron hops from original configuration. The red open circle denotes the site that the electron leaves and red solid dot denotes the sites that the electron hops to.

By comparing Fig.4.1 and Fig.4.2, we can see at least for this set of configurations the electrons tend to be more uniformly distributed at lower total energy, which is what one would expect. Besides comparing the original network and the network with lowest energy for one electron hops, we still need to see what happens to more general networks. Fig.4.3 shows the networks for two different realizations of one electron hop. By comparing Fig.4.3(A) and Fig.4.3(B) we can see there are some obvious changes to the conductance around the sites which the electrons leave and hop to. When an electron hops from site i to an unoccupied site j, the charge on site i changes from e to –e and the charge on site j changes from –e to e. Thus, the sign for Coulomb interaction energy between site i (j) and the other sites is inverted. As the coulomb interaction energy is usually as large as the energies in this problem, this change for Coulomb interaction energy can significantly influence the conductance between sites. We can also see there are some changes for the conductance on the bottom left corner and bottom right corner, which are the conductance between sites that are relatively far from the according site i and site j.



(A)

(B)

Fig.4.3 Two different realizations for one electron hop.

Since we have already calculated the energy for all realizations of one electron hop, we can order them from low to high to see the distribution of the energy changes for one electron hops. It is shown in Fig.4.4 (A). Fig.4.4 (B) is the distribution of total energy shown in Fig.4.4 (A). We can see the distribution is close to a Gaussian distribution but there is a noticeable fat tail showing up at high energies.

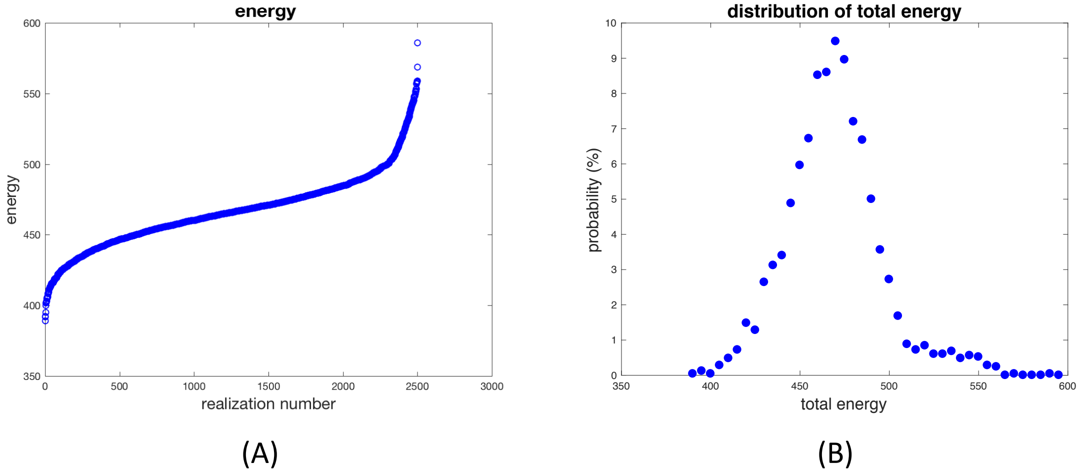


Fig.4.4 Statistical calculation for the energy of all realizations for one electron hop.

To check whether the fat tail is an artifact of a small sample size, we calculate the distribution of total energy for random networks with site number N=50, 100,150 ,200. Half of the sites are occupied by electrons in all of the networks. The result is shown in Fig.4.5. From Fig.4.5 we can see the distribution of total energy for one electron hops is getting more and more close to a Gaussian distribution and the fat tail disappears as the number of sites in the networks increases.

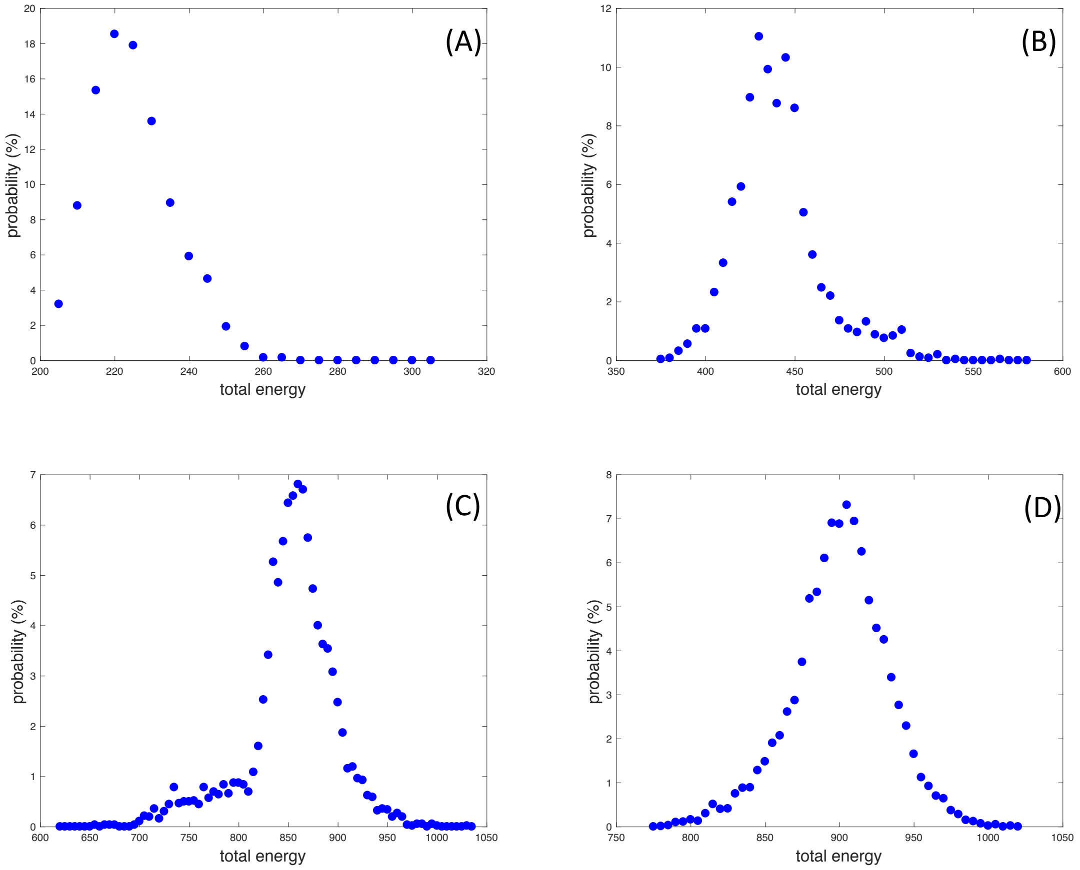


Fig.4.5 Distribution of energy for one electron hops. (A) N=50 (B) N=100 (C) N=150 (D) N=200.

To check whether there is a Coulomb gap emerging when we excite the random network showing in Fig.4.2, we calculate the average conductance for all the realizations of one electron hop. The result is shown in Fig.4.6. We can see that in some excited networks the average conductance becomes smaller than the network with lowest energy, which is the data with the realization number equals one in Fig.4.6. The result does not match the tendency of conductance showing in Fig.3.2. This means that the network with lowest energy from one electron hops is not the network with the global minimum energy.

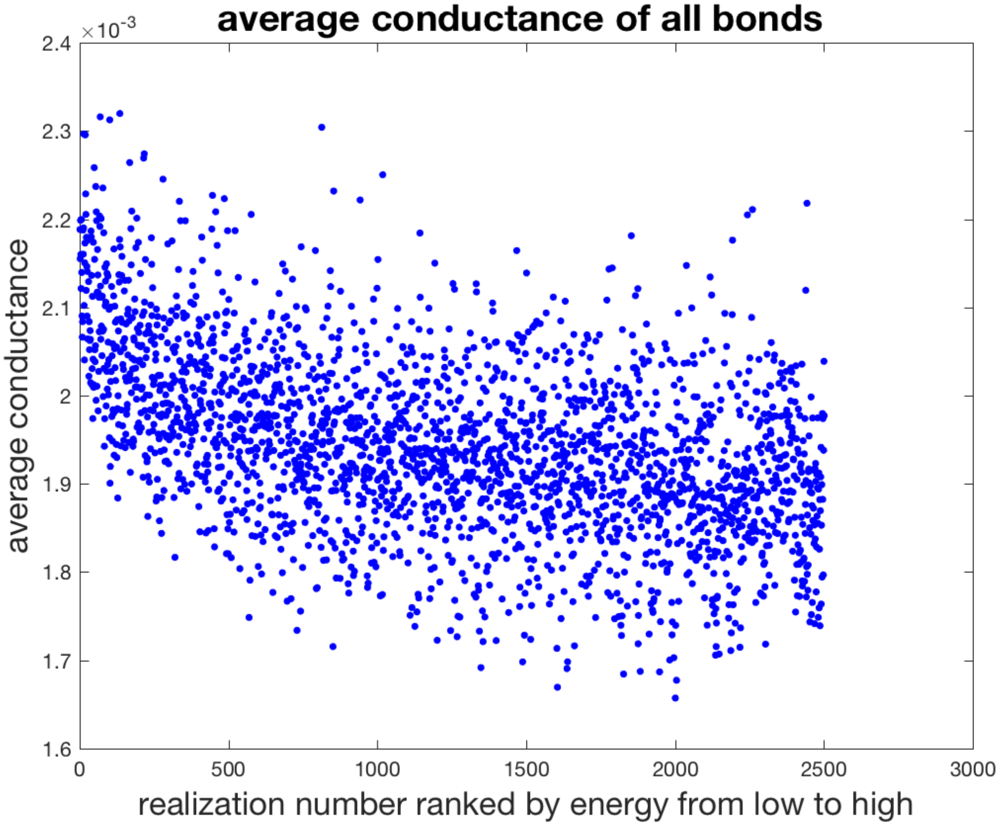


Fig 4.6 Average conductance for all realizations of one electron hop based on the network showing in Fig.4.1.

CHAPTER 5

CONCLUSIONS

By visualizing the conductance network of the disordered system, we can see how the individual conductances change between sites when we consider single electron changes of the network. Through statistical calculation of total energy and average conductance for all realizations of one electron hop, we can know the distribution for total energy and whether the system can form a Coulomb gap via one electron hops. The conclusions we can obtain are listed as following:

- Nearly all the sites are coupled together by the bonds. If we do one electron hops, the conductance between two remote sites may change because of coupling effect. The network shows strong correlations between occupational configurations and conductance.
- By finding the network with the least total energy among all possible cases for one electron hops, we can see the electrons are more uniformly distributed than the original network.
- The distribution of total energy for all one electron hops may follow Gaussian distribution, within the uncertainty that is inherent in our small network size.
- Considering the excitations of the one electron hops relative to lowest energy configuration we observed, sometimes the average conductance of the new

system does not increase, which may show that the one electron hop lowest energy system found is not the global lowest energy system.

There is still a long way to go for this research. To test whether there is a Coulomb gap formed during an excitation process, we need to find the global lowest energy network. And to have better knowledge about the disordered system, we may need to do more statistical calculations such as calculating the inverse participation ratio for the system.

APPENDIX

MATLAB

For generating the random network and find all realizations for one electron hop

Main program:

```
M=100;              % number of dots
kb=1;               % Boltzman constant
T=1;                % temperature
xi=1;               % localization length
e=1;                % charge for electron
kappa=1;            % dielectric permittivity of the lattice

A=zeros((M*M/4+1),8);% save results
R=zeros(M,M);       % matrix of distance
R1=zeros(M,M);      % matrix of distance after changing position
E=zeros(1,M);       % matrix of energy without coulomb interaction
deltE=zeros(M,M);   % matrix of energy difference
x=rand(1,M)*10;     % define original position for dots
y=rand(1,M)*10;
E=5+sqrt(1.25)*randn(1,M); % for each sites energy distribution is fixed
% load x
% load y
% load E
energy=zeros(1,M);        % energy for sites including Coulomb interaction

num=1;                  % generate results saving matrix
for i=1:(M/2)
   for j=(M/2+1):M
      num=num+1;
      A(num,1)=i;
      A(num,2)=j;
   end
end

for i=1:M               % calculate r(i,j)
   for j=1:M
```

```
        if i==j
            R(i,j)=0;
        else
            R(i,j)=sqrt((x(i)-x(j))^2+(y(i)-y(j))^2);
        end
    end
end
%************Calculate total energy ******
charge_sign=zeros(1,M);
for i=1:(M/2)              % electrons
    charge_sign(i)=(-1);
end
for i=(M/2+1):M            % holes
    charge_sign(i)=1;
end
energy=E;
for i=1:M
    for j=1:M
        if (i~=j)
            energy(i)=energy(i)+charge_sign(i)*charge_sign(j)*(e^2)/kappa/R(i,j);
        end
    end
end
energy_total_before=0;     % Calculate total energy
for i=1:M
    energy_total_before=energy_total_before+energy(i);
end
A(1,3)=energy_total_before;

for j=1:M                  % Conductance
    for k=1:M
      deltE(j,k)=abs(energy(j)-energy(k));
    end
end
    gamma_total=0;
    gamma_average=0;
    numb=0;
%     numb1=0;
    for j=1:M
        for k=1:M
            if j==k
                gamma(j,k)=0;
            else
                gamma(j,k)=exp(-(deltE(j,k)/kb/T)-(2*R(j,k)/xi));
            end
```

```
%           if gamma(j,k)>(10^(-3))
         gamma_total=gamma_total+gamma(j,k);
         numb=numb+1;
%           end
      end
   end
   gamma_average=gamma_total/(numb);
   A(1,4)=gamma_average;
% A(1,4)=numb;
%******************* draw the graph for resistance ************
figure
% subplot(2,2,1)
Con_line(M,x,y,energy,R)
for i=1:(M/2)
   plot(x(i),y(i),'b.','MarkerSize',25)
   hold on
end
for i=(M/2+1):M
   plot(x(i),y(i),'bo','MarkerSize',5)
   hold on
end
title(['\fontsize{18}original network'])
xlabel('x position','FontSize',16)
ylabel('y position','FontSize',16)
%******************* change an electron with a hole ***********
for i=2:(M*M/4+1)
   x1=x;
   y1=y;
   n=A(i,1);
   N=A(i,2);
   tempx=x1(n); % just change the storage of positions
   tempy=y1(n);
   x1(n)=x1(N);
   y1(n)=y1(N);
   x1(N)=tempx;
   y1(N)=tempy;

   R1=zeros(M,M); % calculate rij
   for j=1:M
      for k=1:M
         if j==k
            R1(j,k)=0;
         else
            R1(j,k)=sqrt((x1(j)-x1(k))^2+(y1(j)-y1(k))^2);
         end
```

```
    end
  end

  charge_sign=zeros(1,M);    %Calculate total energy for each dot
  for j=1:(M/2)              % electrons
    charge_sign(j)=(-1);
  end
  for j=(M/2+1):M            % holes
    charge_sign(j)=1;
  end
  energy=E;
  for j=1:M
    for k=1:M
      if (j~=k)
        energy(j)=energy(j)+charge_sign(j)*charge_sign(k)*(e^2)/kappa/R1(j,k);
      end
    end
  end

  changed_total_energy=0;    % Calculate total energy
  for j=1:M
    changed_total_energy=changed_total_energy+energy(j);
  end
  A(i,3)=changed_total_energy;

  for j=1:M                  % Conductance
    for k=1:M
      deltE(j,k)=abs(energy(j)-energy(k));
    end
  end
  gamma_total=0;
  gamma_average=0;
  numb=0;
%   numb1=0;
  for j=1:M
    for k=1:M
      if j==k
        gamma(j,k)=0;
      else
        gamma(j,k)=exp(-(deltE(j,k)/kb/T)-(2*R1(j,k)/xi));
      end
%       if gamma(j,k)>(10^(-3))
      gamma_total=gamma_total+gamma(j,k);
      numb=numb+1;
%       end
```

```
        end
    end
    gamma_average=gamma_total/(numb);
    A(i,4)=gamma_average;
%   A(i,4)=numb;
end
%******************* reorder A ***************************
for i=1:(M*M/4+1)
    A(i,5)=A(i,1);
    A(i,6)=A(i,2);
    A(i,7)=A(i,3);
    A(i,8)=A(i,4);
end
for i=1:(M*M/4)
    for j=(i+1):(M*M/4+1)
        AA1=0;
        AA2=0;
        AA3=0;
        AA4=0;
        if A(i,7)>A(j,7)
            AA1=A(j,5);
            A(j,5)=A(i,5);
            A(i,5)=AA1;

            AA2=A(j,6);
            A(j,6)=A(i,6);
            A(i,6)=AA2;

            AA3=A(j,7);
            A(j,7)=A(i,7);
            A(i,7)=AA3;

            AA4=A(j,8);
            A(j,8)=A(i,8);
            A(i,8)=AA4;
        end
    end
end
%********************************draw the graph after changing *************
if (A(1,3)~=A(1,7))
    x1=x;
    y1=y;
    n=A(1,5);
    N=A(1,6);
    tempx=x1(n); % just change the storage of positions
```

```
   tempy=y1(n);
   x1(n)=x1(N);
   y1(n)=y1(N);
   x1(N)=tempx;
   y1(N)=tempy;

   R1=zeros(M,M); % calculate rij
   for j=1:M
      for k=1:M
         if j==k
            R1(j,k)=0;
         else
            R1(j,k)=sqrt((x1(j)-x1(k))^2+(y1(j)-y1(k))^2);
         end
      end
   end

   charge_sign=zeros(1,M);
   for j=1:(M/2)              % electrons
      charge_sign(j)=(-1);
   end
   for j=(M/2+1):M            % holes
      charge_sign(j)=1;
   end
   energy=E;
   for j=1:M
      for k=1:M
         if (j~=k)
            energy(j)=energy(j)+charge_sign(j)*charge_sign(k)*(e^2)/kappa/R1(j,k);
         end
      end
   end
%     subplot(2,2,2)
  figure
   Con_line(M,x1,y1,energy,R1)
   for i=1:(M/2)
      if (i==n)
         plot(x(i),y(i),'ro','MarkerSize',5)
         hold on
      else
         plot(x(i),y(i),'b.','MarkerSize',25)
         hold on
      end
   end
   for i=(M/2+1):M
```

```
        if (i==N)
            plot(x(i),y(i),'r.','MarkerSize',25)
            hold on
        else
            plot(x(i),y(i),'bo','MarkerSize',5)
            hold on
        end
    end
  %title(' network with least total energy among all one electron hops', 'Size',16)
  title(['\fontsize{18}network for a realization of one electron hop'])
  xlabel('x position','FontSize',16)
  ylabel('y position','FontSize',16)
end

figure
% subplot(2,2,3)
for i=1:(M*M/4+1)
    plot(i,A(i,7),'bo')
    hold on
end
title(['\fontsize{18}energy '])
xlabel('realization number','FontSize',16)
ylabel('energy','FontSize',16)
figure
% subplot(2,2,4)
for i=1:(M*M/4+1)
    plot(i,A(i,8),'b.','MarkerSize',10)
    hold on
end
title(['\fontsize{18}average conductance of all bonds '])
xlabel('realization number ranked by energy from low to high','FontSize',16)
ylabel('average conductance','FontSize',16)
figure
for i=1:50
    plot(i,A(i,8),'b.','MarkerSize',10)
    hold on
end
ylim([1.6*10^(-3) 2.4*10^(-3)])
title(['\fontsize{18}average conductance of all bonds '])
xlabel('realization number ranked by energy from low to high','FontSize',16)
ylabel('average conductance','FontSize',16)
```

The function for drawing the bonds which denote conductance between sites

```
function Con_line(M,x,y,E,R)
kb=1;
T=1;
xi=1;
gamma=zeros(M,M);   % conductance
sign=zeros(M,M);
% ******************************calculate deltE
for i=1:M
   for j=1:M
      deltE(i,j)=abs(E(i)-E(j));
   end
end
%************************************conductance
for i=1:M
   for j=1:M
      if i==j
         gamma(i,j)=0;
      else
         gamma(i,j)=exp(-(deltE(i,j)/kb/T)-(2*R(i,j)/xi));
      end
   end
end
%*********************************************gamma
for i=1:M
   for j=1:M
      if gamma(i,j)==0
         sign(i,j)=0;
      elseif gamma(i,j)>(10^(-1))
         sign(i,j)=1;
      elseif ((10^(-1))>=gamma(i,j))&&(gamma(i,j)>(10^(-2)))
         sign(i,j)=2;
      elseif ((10^(-2))>=gamma(i,j))&&(gamma(i,j)>(10^(-3)))
         sign(i,j)=3;
      elseif ((10^(-3))>=gamma(i,j))&&(gamma(i,j)>(10^(-4)))
         sign(i,j)=4;
      elseif ((10^(-4))>=gamma(i,j))&&(gamma(i,j)>(10^(-5)))
         sign(i,j)=5;
      elseif ((10^(-5))>=gamma(i,j))&&(gamma(i,j)>(10^(-6)))
         sign(i,j)=6;
      elseif ((10^(-6))>=gamma(i,j))&&(gamma(i,j)>(10^(-7)))
         sign(i,j)=7;
      elseif ((10^(-7))>=gamma(i,j))&&(gamma(i,j)>(10^(-8)))
         sign(i,j)=8;
      elseif ((10^(-8))>=gamma(i,j))
         sign(i,j)=9;
```

```
        end
    end
end
for i=1:M
    for j=i:M
        if sign(i,j)==1
            line([x(i),x(j)],[y(i),y(j)],'linewidth',2.5,'color',[0,0,0]); % dark black
            hold on
        elseif sign(i,j)==2
            line([x(i),x(j)],[y(i),y(j)],'linewidth',2,'color',[0.5,0.5,0.5]);% lighter black
            hold on
        elseif sign(i,j)==3
            line([x(i),x(j)],[y(i),y(j)],'linewidth',1.5,'color',[0.8,0.8,0.8]); % light black
            hold on
%         elseif sign(i,j)==4
%             line([x(i),x(j)],[y(i),y(j)],'linewidth',4.5,'color','k');%black
%             hold on
%         elseif sign(i,j)==5
%             line([x(i),x(j)],[y(i),y(j)],'linewidth',4,'color','r');%red
%             hold on
%         elseif sign(i,j)==6
%             line([x(i),x(j)],[y(i),y(j)],'linewidth',3.5,'color','y');% yellow
%             hold on
%         elseif sign(i,j)==7
%             line([x(i),x(j)],[y(i),y(j)],'linewidth',3,'color',[0.5 0.5 0.5]);
%             hold on
%         elseif sign(i,j)==8
%             line([x(i),x(j)],[y(i),y(j)],'linewidth',2.5,'color',[0.1 0.1 0.1]);
%             hold on
%         elseif sign(i,j)==9
%             line([x(i),x(j)],[y(i),y(j)],'linewidth',2,'color',[0.7 0.7 0.7]);
%             hold on
        end
    end
end
end
```

Code for finding the distribution of total energy of all realization for one electron hops

```
load A_1.mat
num=zeros(42,1);
for i=1:2501
    for j=1:42
        if ((370+5+j*5)>A(i,7))&(A(i,7)>(370+j*5))
```

```
            num(j)=num(j)+1;
        end
    end
end
for k=1:42
    plot((370+k*5),num(k)/2501*100,'b.','MarkerSize',25)
    hold on
end
% title(['\fontsize{18}distribution of total energy'])
xlabel('total energy','FontSize',16)
ylabel('probability (%)','FontSize',16)
```

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