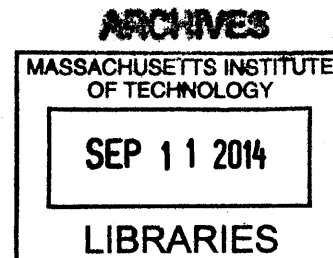Free Approximation of Transport Properties in Organic System

Using Stochastic Random Matrix Theory

By

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Free Approximation of Transport Properties in Organic System Using Stochastic Random Matrix Theory

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Abstract

The proposed research is a study and application of Stochastic analysis- Random Matrix Theory(RMT) to fast calculate the transport properties of large static systems with relatively large disorder in mesoscopic size. As a major topic of Random Matrix Theory(RMT), free convolution managed to approximate the distribution of eigenvalues in an Anderson Model.So the next step is trying to expand RMT to approximate other quantities, such as transmission probability, conductivity and etc. Due to the eigenvectors' shifts, RMT works well only for small disorder. System with larger disorder requires to take in account of the changes in eigenvectors directly or through other approximations of the eigenvectors.

Advisor: Troy Van Voohris
Title: Professor of Chemistry

Preface

I would like to thank my advisor, Troy Van Voorhis for his great help and support in the past years.

I would also like to thank Mike, Matt, Dave, Shuhao, Jiahao and many others in my lab.

Last but not the least, I really appreciate the great amount of knowledge taught by Jeremy and Jian in Cao's Group.

Contents

1 Introduction

People have shown great interest in organic semiconductor in the recent years. Organic semiconductor distinguish itself from the traditional inorganic one, as this new type of material is cheap and efficiency enough to be widely used in ordinary life. Organic materials have been applied to many devices, like solar cells, light emitting diodes(OLED)s and so on.[1, 2, 5-8] However, unlike inorganic material, organic's usually contains more defects. Those defects turn out to be huge influences for the system, by decreasing the transportation ability of the particles.[8] In other words, semiconductors can become insulators if there are too many impurities in the system, e.g disorder is large. Therefore, it is crucial to find the transport properties for systems with disorder, such as transmission probability, conductivity and etc..[2]

Disorder always exists in varies of systems. People can use perturbation theory for small disorder and calculate the exact properties of a small system. However, it is hard to accurately and quickly calculate a large system with relatively large disorder.[9] Random Matrix provides people with a fast and good approximation of such systems. Free probability, as a key part of random matrix, is able to obtain the distribution of eigenvalues for large disorder systems, as it avoids the diagnolization processes which consume the most efforts and appear in most of the traditional spectrum decompositions[11]. Meanwhile, the simulation of eigenvectors is on its way of study, which are crucial properties to be discovered.

Organic materials share many similarities with inorganic's and Anderson impurities model is chosen to simulate them. Usually two other models can be used as an analogy for transport in organic system: band theory and hopping theory. Basically HOMO and LUMO replace the conduction band and the valence band in pure inorganic objects (band theory).[18]

However, due to the molecular structure, static disorder contributes to ruin the band theory in organic system. Meanwhile as organic materials contain way more impurities, particle hopping seems to be untrue at low

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temperature (50K or lower)[3]. Therefore, Anderson model, one of the most fundamental physical models to describe a static system with site coupling, is selected. It has also been called nearest neighbor coupling model.[7] Localization occurs on every sites expect for the coupling between neighbors. Disorder appears at each site, whereas coupling between sites is set to be pure at this moment.[8] In such system, disorder includes but not limited to physical defects, structure disorder, impurities and etc.. [13] However, at high temperature, hopping theory would play a major role in organic transport. Phonon will be enormously generated and becomes a wide source to support the particles to hop through energy barriers and invalidate the localization status.[3] Thus, at high temperature, Anderson model, which behaves as a stochastic model for static time-invariant system, might no longer be a good fit and modifications are required to include the time-dependent variables.

Last but not the least, a great amount of organic semiconductor materials are neither perfectly disordered (polymers) or ordered (molecular crystals) to fit the conventional theory well.[11] Hence, it is expensive and inaccurate to test all these non-perfect materials. As a result, computational chemistry played an important role to approximate those intermediates. [13]

This thesis will be presented in the order of Introduction, Anderson Model, Random Matrix Theory, application of Random Matrix onto Anderson and Conclusion.
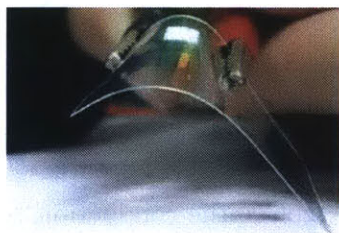

Figure 1. Organic semiconductor

2 Anderson Model

2.1 Background

Anderson model is the most frequently used Hamiltonian model to illustrate a system with impurities at zero degree (low temperature) Kelvin[11] and was first used to study the transition from metal to insulator when impurities were added into the model.[4, 15, 16]
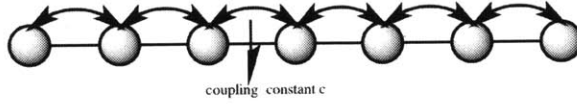

Figure 2. Nearest Neighbor Coupling Model.

In general, Anderson Model has the following formula[4]:

$$H = \sum g_i \, |a\rangle \, \langle a| + c \, |a\rangle \, \langle b|$$

where g_i is a Gaussian Distributed random impurity and c is a constant coupling between site a and b. In the regular nearest neighbor case, $|a-b| = 1$. Considering the nearest neighbor model, its matrix representation is:

$$H_c = \begin{pmatrix} g_1 & c & 0 & \cdots & 0 \\ c & g_2 & c & \ddots & \vdots \\ 0 & c & \ddots & c & 0 \\ \vdots & \ddots & c & g_{n-1} & c \\ 0 & \cdots & 0 & c & g_n \end{pmatrix}$$

Spectrum decomposing the Hamiltonian, people will obtain the eigenvalues and the eigenvectors. Density of states (DOS, ρ) is the histogramming of the eigenvalues and the wave functions at each energy levels are those

eigenvectors[18].

$$\rho(E) = \frac{1}{a} \sum_v (E - E_v)$$

for E_v being the energy spectrum and a is the normalization number. It can also be written in the form of Green function[20],

$$\rho(E) = \frac{1}{\pi a} Tr(ImG(E))$$

with the one particle green function $G(r, r') = \langle r | \frac{1}{E \pm i\epsilon - H} | r' \rangle$. DOS of an Anderson model consists of two parts, a semi-circle and two tails. The states in the semi-circle (Wegner circle) are extended, while these in the tails are localized that wavefuntions of neighbor sites are not overlapping enough with each other.[22] 'Localized' here means that wave functions in neighbor sites can no longer overlap with each other significantly, e.g a single peak appears at one site with probability 1. A special concept is the weak localization in strong disorder system at low temperature. This weak localization idea was first introduced by P.W. Anderson to show that with strong disorder, the regular Boltzmann theory no longer works and the Boltzmann 'conductor' could be an insulator even if the Fermi level contains charge carriers.[4, 23] Instead of the probability, what really needs to be summed up is the quantum mechanical coefficient for all possible approaches from one site to the other. In all, particles can run extra circles during transmission, which increases the resistivity and therefore decreases the conductivity. In another word, at 0 degree Kelvin (or other low temperature), if the Fermi level is located in the tail of DOS, then the system is an insulator, otherwise, it acts as a metal. It is DOS tail that merges into to the semi-circle band, forming the mobility edges.[23, 24] Larger disorder causes the mobility edge extended more into middle of the band and leads into an insulator. How far this phoneme appears, the exponential decay of these asymptotic waves, is defined

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as the localization length.

$$\Phi(r) = f(r)exp(-\frac{r}{\lambda})$$

where λ is the localization length, f is varying function. For infinitely large λ, Φ becomes extended.[23]

As the result of the further study on Anderson model, the Anderson Conjecture implies that for 1-D and 2-D systems, energy states are always localized with even just small amount of disorder, whereas 3-D system has more space for particle to scatter around and therefore has a critical transition point. [23] For convenience, the coupling constant c always has value of 1 unit.
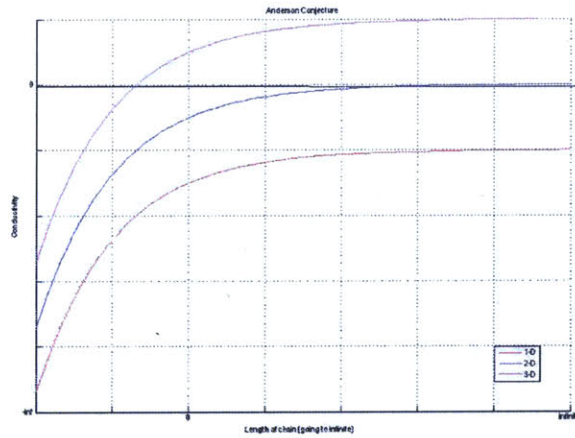

Figure 3. Anderson Conjecture. In 1-D and 2-D systems, states are localized and conductor turns into insulator with the existence of very little impurities. 3-D provides more room for particle to jump though and therefore has some conductivity.

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2.2 Transmission probability

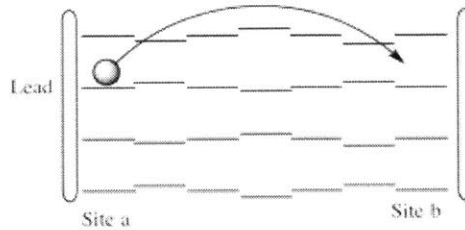The graph below describes the transmission process [20, 21]:

Figure 4. Particle transmitting (elastic) from one site to another in a disordered system.

In general, when people are looking for the transport properties of a system, the first term needed is the transmission coefficient. Transmission coefficient (scattering matrix, S-matrix) describes the rate of a particle appearing at a different location from its origin.[25, 26]

$$|Outgoing\rangle = S * |Injected\rangle$$

Starting with transmission coefficient, people can then easily tell the conductivity, delocalization length and so on.

The transmission probability T for a particle transmitting from site a to b is[25, 35]:

$$T = \left|S_{a,b}^2\right| = |\langle a|G|b\rangle|^2$$

where G is the one-particle green function. In mathematica, Green function always appears in the problems of inhomogeneous differential equations. Physically speaking, the Green function here acts as a filter that distinguishes the values that causes singularities. Moreover, the Green function can be considered as a generalized transmission S-matrix, regardless in or outside of the

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conductor.

$$O * R = S$$

$$R = O^{-1}S = G * S$$

where O is a differential operator, R is the response and S is the excitation (S-matrix).

Then we simply the problem to

$$(E - H_o)\Phi = S$$

which results in

$$G = (E - H_{op})^{-1}$$

for H_{op} being the system Hamiltonian of operator O.[26]

Hence for Anderson Model, we will have

$$G = (H - E + i\epsilon)^{-1}$$

where E is the energy variable, H is the Anderson system and ϵ is an imaginary number to avoid crashing at those singular values and leads the curve to decay. The term of $i\epsilon$ turns to be $exp(i\epsilon * m)$ in further calculation. In addition, ϵ could be viewed as a consequence of 'self-energy', which will be discussed later in this chapter.[25]

The system with impurities are sandwiched between two leads, from which particles with different energy E will be injected into the system. Leads itself can be viewed as a type of impurities in this larger tight binding system. Therefore, leads will impose effects onto the system, which is called the 'self energy' Σ.[25] This self-energy ultimately becomes the imaginary part of the

Green function.

$$G = (H - E + i\epsilon)^{-1} = (H - E + i\Sigma)^{-1}$$
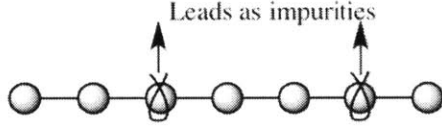

Figure 5. Self Energy implied from leads as impurities.

2.3 Green function and Self Energy

Self Energy[25,26,35] represents the influence of the two leads to the system and will effect the behaviors of the sites close to the leads. If the self energy is large, leads tends to be two huge defects and the system to be studied will be show little active signs. [3, 20]

For Anderson Model, its Hamiltonian has been written above and the corresponding Green function is:

$$G_c = (EI - H_c - \Sigma_l)^{-1}$$

$$\begin{pmatrix} E - \Sigma + g_1 & 1 & & & & \\ 1 & E + g_2 & 1 & & & \\ & 1 & \ddots & \ddots & & \\ & & \ddots & E + g_{n-1} & 1 & \\ & & & 1 & E - \Sigma + g_n \end{pmatrix}$$

where E screens through the continuous energy levels (variable) and Σ_l is the effect imposed from leads to the conductor.

Σ_l can be calculated from:

$$\Sigma_l = \Sigma_L + \Sigma_R$$

$$\Sigma_x = G_{xC}^{\dagger} G_x G_{xC}$$

for x being either the right or the left leads.[25, 26]

Then for either side, the self energy is,

$$\Sigma = \begin{pmatrix} 0 & \cdots & 0 & 0 \\ \vdots & \cdots & 0 & 0 \\ 0 & 0 & \vdots & 0 \\ t & 0 & \cdots & 0 \end{pmatrix} \left(\frac{1}{H_l - EI + i\epsilon} \right) \begin{pmatrix} 0 & \cdots & 0 & t \\ \vdots & \cdots & 0 & 0 \\ 0 & 0 & \vdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

with H_l being the Hamiltonian of a tight binding chain with nearest neighbor coupling of unit 1 and 0 unit for on site energy.

The only existing element in Σ would be the $\Sigma(1,1)$ and $\Sigma(n,n)$ for a lead containing n sites.

Symmetry tridiagonal matrix can be solved analytically.

$$\Sigma(1,1) = \Sigma(n,n) = \frac{cos[(n+1)\lambda] - cos[(n-1)\lambda]}{2sin(\lambda) * sin[(n+1)\lambda]}$$

with $E + i\epsilon = -2cos(\lambda)$.[37]
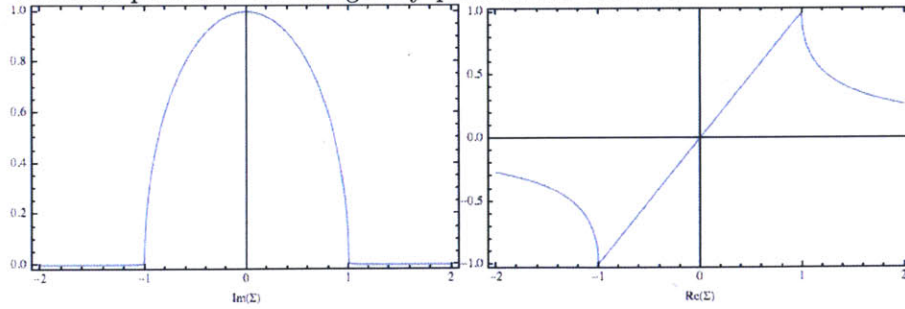
The real part and the imaginary part of the above is:

Figure 6. Real and Imaginary part of self energy.

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Explicit representation of the real and the imaginary parts can also be derived[24, 25],

$$Re\Sigma = \frac{V^2}{t}(\kappa - \sqrt{\kappa^2 - 1}[\theta(\kappa - 1) - \theta(-\kappa - 1)])$$

$$Im\Sigma = -\frac{V^2}{t}\sqrt{1 - \kappa^2}\theta(1 - |\kappa|),$$

$$\kappa = \frac{E}{2t}$$

where V is the coupling constant between lead the conductor, t is the site coupling in between lead (what we used to call J in any tight binding chain). The explicit representations have the same graph as Figure 6.

If $t \gg E$,but t does not have to be infinite large, then the imaginary part can be treated as a constant[26],

$$Im\Sigma = -V^2\frac{\sqrt{4t^2 - 1}}{2t^2}$$

Then for a particle transmit from site a to b, its transmission probability can be calculated as:

$$T = |\langle a|G|b\rangle|^2$$

$$T = |\langle a|G_c|b\rangle|^2$$

$$= |\langle a|(EI - H_c - \Sigma_l)^{-1}|b\rangle|^2$$

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where $|a\rangle$ and $|b\rangle$ are the vectors in position space, e.g the first site

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

and the last site

$$|n\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

[37]

2.4 Conductivity

Conductivity (g) is positively proportional to transmission probability at 0 degree Kelvin and can be directly calculated from the following equations[20, 26]. In a 1-D Anderson Model, infinite long nearest neighbor coupling with impurities, conductivity are supposed to be zero, as all the states are localized. A general Landauer Formula reveals a new page in conductivity. Computational calcualtion of Landauer Fomula uses the form of Kubo equation [32, 33].

$$g \propto |T|$$

$$g = \frac{e^2}{\pi \hbar}(|T|) = Tr(\Sigma G' \Sigma G)$$

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where G is the Green function containing the lead effects and Σ is the self energy.

To derive the Landauer Formulara bove, Fisher-Lee formula in GF representation is required[27, 31, 32].

Fisher-Lee formula in GF representation

To obatin the conductivity in this 1-D model, I need to calculate the current (j) of this system first. Drived by Landauer and Buttker [29, 30,59-61], current in a finite system with possible disorders can be writen as

$$j_l = \frac{ie}{\hbar}(\phi_l H_{lc}\phi_c - \phi_c H'_{lc}\phi_l)$$

where ϕ_l, ϕ_c, ϕ_r are the wave functions of the left lead, conductor and the right lead. It is then necessary to study more in the system, as well the effects brought from both leads.

$$\begin{pmatrix} H_l & H_{lc} & 0 \\ H'_{lc} & H_c & H'_{rc} \\ 0 & H_{rc} & H_r \end{pmatrix} \begin{pmatrix} \phi_l \\ \phi_c \\ \phi_r \end{pmatrix} = E \begin{pmatrix} \phi_l \\ \phi_c \\ \phi_r \end{pmatrix}$$

Solve the equations above, the following is obtained:

$$\phi_l = (\phi_{in} + \phi_l^r) = (1 + G_l H_{lc} G^{self} H'_{ls})\phi_{in}$$

$$\phi_r = G_r H_{tc} G^{self} H'_{ls}\phi_{in}$$

$$\phi_c = G^{self} H'_{lc}\phi_{in}$$

with G^{self} being a full green function with self energy and ϕ_{in} is the incoming wave and ϕ_l^r is reflected wave from left. [33, 34]

Then to calculate the current from lead to conductor, we will have [29,

28, 30]:

$$j_l = \frac{ie}{\hbar}(\phi_l H_{lc}\phi_c - \phi_c H'_{lc}\phi_l)$$

$$= \frac{ie}{\hbar}(\phi'_r H_{rc} G'^{self} \phi'_{lc}(G'_l - G_r) H_{lc} G^{self} H'_{rc}\phi_{in})$$

$$= \frac{-e}{\hbar}(\phi'_{in} H_{lc} G'^{self} \Sigma G^{self} H'_{rs}\phi_{in})$$

Hence, we will have

$$|T| = 2\pi \sum_{\lambda} \delta(E - E_\lambda)(\phi'_{in} H_{lc} G'^{self} \Sigma G^{self} H'_{rs}\phi_{in})$$

$$= 2\pi \sum_{\lambda} \sum_{\delta} \delta(E - E_\lambda)(\phi'_{in} H_{lc}\phi_\delta)(\phi'_\delta G^{self} \Sigma G^{self} H'_{rs}\phi_{in})$$

$$= \sum_{\delta}(\phi'_\delta G^{self} \Sigma G^{self} H'_{rs}(2\pi \sum_{\delta} \delta(E - E_\lambda)\phi_{in}\phi'_{in})H_{rs}\phi_\delta)$$

$$= Tr(\Sigma_r G'^{self} \Sigma_l G^{self})$$

As a result,

$$g(E) = Tr(\Sigma G' \Sigma G)$$

where Σ is the self energy and G is the Green function. This general equation sums up the probability of transmission for particles injected at different E. But since at 0 degree Kelvin, the only active energy level is the Fermi Level, the faster way can be used.[37]

3 Random Matrix Theory

3.1 Background

Random matrices are those matrices who entries are independently identically distribution, the most common of which are Gaussian Distributed entries. Random Matrix Theory (RMT) plays many roles in science for numerical analysis, mostly for stochastic problems[38, 63, 62].

Random matrix theory was first mentioned by Wigner in 1951 to statistically understand the resonances phenomena of neutron scattering in nuclei.[39-43] Because there were no good approaches to calculate the energy levels other than the lower ones, Wigner thought it could be possible to statistically understand the energy level. Application of random matrix theory turns to be a huge success when measuring mean eigenvalue spectrum and its properties for prediction.

Following Wigner, several other scientists kept working on random matrices, such as Dyson, Metha, Porter, Thomas and the others.[44-47, 49, 50, 52] The most famous one is Dyson. Dyson considered random matrix is a new type of statistics as it is over the ensemble of different systems, rather than collections from identical systems or averaging through number theory. Therefore, random matrix theory minimizes the special characteristics of each individual system, which is also named as universal properties.[44, 45] Later on, Dyson explored further in random matrices and defined 1. time reversal invariant with rotational symmetry, Dyson index $\beta = 1$; 2. NOT invariant at time reversal symmetry (i.e charge carriers in external magnetic field), Dyson index $\beta = 2$; 3. time reversal invariant plus half integer spin, $\beta = 4$. These three types of system has been fully studied. So what are the Hamiltonians corresponding to the three systems above? This will be discussed right below.[53]

If the random numbers in the hamiltonians follows Gaussian distribution, then they are Gaussian Ensemble, one of the most well studied matrix

ensembles. The others are

1. Wishart

2. Manoca and

3. Circular.

Gaussian Ensemble consists of the Gaussian unitary ensemble (GUE), Gaussian orthogonal ensemble (GOE) and Gaussian symplectic ensemble (GSE). GUE are $n * n$ unitary matrices with Gaussian distributed entries; GOE are $n * n$ orthogonal matrices and GSE are symplectic matrices.

Given $N = randn(n, n)$ with every numbers in the $n * n$ matrix N being Gaussian randomly selected,

GUE matrices can be generated by $(N + N^H)/2$;

GOE matrices can be generated by $(N + N^T)/2$;

and GSE matrices can be generated by $(N + N^D)/2$, where N^D is the dual transpose of the N. [38] The three types of Gaussian ensembles correspond to the three systems defined by Dyson. GOE is for the system with time invariance and rotational symmetry; GUE is for the system with complex numbers and not invariant under time reversal symmetry; GOE is for the last one. In-between the three ensembles, GUE/GUE are the most frequently used two. One interesting and crucial property of these two ensembles are in their eigenvalue spectrums.[39] Wigner discovered that the distribution of eigenvalues of GUE/GOE presents a semi-circle as the size of the matrix tends to be infinite.[40] The eigenvalues of GUE/GOE can be exactly calculated through a standard procedures. Starting with an arbitrary the probability distribution function (p.d.f) for matrix entries, we need to pick up a good matrix factorization that the derivative of the matrix can be then used to generate the joint density of the ensembles. For example, spectrum decomposition will be a good matrix factorization for GUE/GOE, applying the derivative of the matrix[38]

$$dGOE \ or \ GUE = \prod_{i<j}(\lambda_i - \lambda_j)^\beta (d\Lambda)(Q'dQ)$$
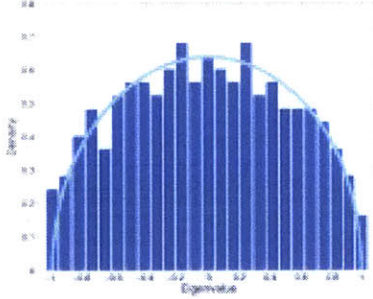
for matrix GOE *or* $GUE = Q\Lambda Q'$. We than can obtain the density by summing over the eigenvectors. Therefore, the following is received:

$$\lim_{N\to\infty} \rho(dx) = \rho(dx) = \frac{1}{2\pi}\sqrt{4-x^2}dx$$

whose moments are

$$\langle \sigma, x^k \rangle = \begin{cases} C_{k/2} & k=odd \\ 0 & k=even \end{cases}$$

where C_n is the nth Catalan number, $C_n = \frac{1}{n+1}\binom{2n}{n}$. [54, 55]

In 1960, Dyson again named a new set of ensemble, the circular ensemble. Circular ensemble can be formed by exponentiating any one of these three ensembles with unitary matrices and then applying the Haar measurement (rotation invariance). [45] This new ensemble works no longer with Hamiltonian of a system, but indeed the unitary scattering matrix for a scattering process. [56]

In mid-1990, as reviewed by C.W. Beenakker, Random Matrix theory has been applied into physics to solve many different questions, including S-Matrix modelling and so on.[57-72] However, those problems usually require diagnoalization of tons of huge matrices and therefore expensive. So is there any better and fast tool that people can use? One newly rise topic in Random Matrix Theory is free probability.65-70 This is a very convenient tool to approximate the eigenvalue density from that of two different matrices.

3.2 Free probability

Free probability is a popular topic in Random Matrix Theory due to its function of an algebraic structure for non-commute matrices[38, 54]. It provides a fast way to approximate the distribution of eigenvalues for random matrices. Free probability view differently from the classical probability, as it takes the eigenvalues of the sum of random matrices.[38, 72, 73] As the eigenvalues λs of the sum of a series of Gaussian random matrices, it is not normal any more. And free probability shows that as the size of the matrix tends to be infinite, as well the number of sample, λ will being a semi-circle distribution. In free probability, Wigner's semi-circle distribution law is similar to the normal distribution in the non-free theory. In addition, free cumulants taken the place of regular cumulant, as free cumulant is simply non-crossing partitions finite set, rather than all partitions for regular cumulant.[74, 68, 69]

Within free probability, one key term is free convolution. People can split a single matrix into two easier matrices and find the distribution of eigenvalues through free convolution. It is always a pity that, regularly, the eigenvalues of the sum of two matrices are not the sum of the eigenvalues of each matrix

$$\text{Eig}(A+B) \neq \text{Eig}(A) + \text{Eig}(B)$$

for non-commuting A and B), as the contribution from eigenvectors are neglected.[38, 75] While in some cases, the distribution of the eigenvalues of Haar measured matrix tends to be additive free convolution for that of two random matrices separated from the origin one.[75] (Haar measured matrix - invariant of base, freely independent matrices.)[41]

3.2.1 Free convolution and Free Rotation

Convolution can tell the p.d.f (probability distribution function) of the third function that is composed of two known functions. Free convolution

involves randomness within probability measures. [40]

Let us denote ρ_A to be the distribution of matrix A and ρ_B to be that of matrix B. Free convolution $A \boxplus B$ is defined as

$$R_{A \boxplus B}(\omega) = R_A(\omega) + R_B(\omega) - \frac{1}{\omega}$$

where R is the R - Transformation of ρ_X[76, 77].

$$\omega = \lim_{\epsilon \to 0} \int_R \frac{\rho_x(z)}{R_X^{-1}(\omega) - (z + i\epsilon)} dz$$

with some R-transform can be obtained through expansion of power series:

$$G_A(\omega) = \lim_{\epsilon \to 0} \int_R \frac{\rho_A(z)}{\omega - z - i\epsilon} dz = \sum_{k=0}^{\infty} \frac{\mu_k(X)}{\omega^{k+1}}$$

where μ_k is the kth moment of ρ_X.

$$R_A(\omega) = \sum_{k=0}^{\infty} \frac{v_k}{\omega^{k+1}}$$

and v_k are the free cumulants, which is the combination of moments and $v_k(A \boxplus B) = v_k(A) + v_k(B)$.[75, 76, 78]

If both Hermitian A and B are Haar based, then after the free rotation Q on B, $A + QBQ'$, has the same p.d.f of the $A \boxplus B$ as the size of the matrix becomes infinite. Here Q is a unitary random matrix generated by QR decomposition of a fully random matrix N.[76]

$$\rho(Eig(A + B)) \approx \rho(Eig(A + QBQ'))$$

3.2.2 Free convolution applied to approximate of density of state

Previously, research has been done to approximate the density of state (equivalent to the p.d.f of eigenvalues) in Anderson Model, mimicking the

non-crystal organic materials. It proves that free convolution did a great job that the error for the approximation can be as small as the 8th moment.[76, ??]

Figure 7 shows how free convolution works as nearly a perfect approximation to the traditional calculation.
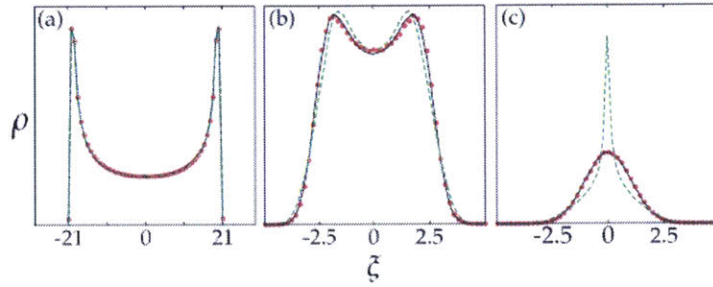

Figure 7. Cropped from [??], Density of States, obtained from 5000 samples pool of 2000 by 2000 matrices with small (a), medium (b), large disorder (c) (disorder $\frac{\sigma}{J}$=0.1, 1 and 1); Red: exact diagonalization, Black: Free convolution with partition of diagonal+tridiagonal, Green: Free convolution with partition of upper left tridiagonal and bottom right tridiagonal.

Errors for the approximation can be calculated from:

$$\omega(\eta) = \omega'(\eta) + \frac{\mu_k - \mu'_k}{k!}(-1)^k \omega'^{(k)} + O(\omega'^{(k+1)})$$

where ω is the p.d.f of eigenvalues from regular calculation

$$\omega(\eta) = exp(\sum_{n=1}^{inf} \frac{\kappa_n - \kappa_{n'}}{n!}(-\frac{d}{d\eta})^n)\omega'(\eta)$$

ω' is the p.d.f of eigenvalues form free approximation, μ_k is the kth moment, and κ_n is the finite cumulants.

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The kth moment

$$\mu_k = \langle (A+B)^n \rangle = \sum (A^{m_1} B^{n_1}....A^{m_k} B^{n_k}),$$

in which $\sum_{j=1}^{k} m_j + n_j = n$ and

$$\langle (AB)^4 \rangle = \frac{1}{n} \langle g_1 g_2 g_3 g_4 c^4 e_{12} e_{23} e_{34} e_{41} \rangle$$

with g_i being the diagonal random entries.

With the partition of

$$\begin{pmatrix} g_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & g_3 \end{pmatrix} + \begin{pmatrix} 0 & c & 0 \\ c & \ddots & c \\ 0 & c & 0 \end{pmatrix},$$

error can be minimized to the 8th moment, $\epsilon = 2\sigma^4 J^4/8!$.

In general, 1-D nearest neighbor model has an error of $(AB)^4 = \frac{J^4 \sigma^4}{2n*8!}$;

2-D square has an error of $(AB)^4 = \frac{J^4 \sigma^4}{4*8!}$;

and 3-D cube has an error of $(AB)^4 = \frac{J^4 \sigma^4}{6*8!}$.

Other way of partition is also tested:

$$A_2 + B_2 = \begin{pmatrix} g_1 & c & 0 \\ c & 0 & 0 \\ 0 & 0 & \ddots \end{pmatrix} + \begin{pmatrix} \ddots & 0 & 0 \\ 0 & g_j & c \\ 0 & c & 0 \end{pmatrix}$$

However, the approximation does not behave as perfect as the previous partition method, due to a difference of $\frac{-\sigma^4}{4}$ for its fourth moment which does not appear until the eighth in the previous partition method.

$$\kappa_4^{(A_2+B_2)} \neq \kappa_4^{(A_2 \boxplus B_2)}$$

and

$$\langle A_2 B_2 \rangle = (J_2 + \sigma^2)J^2$$

instead of $(J_2 + \frac{\sigma^2}{2})^2$.[79]

4   Methods

Taking advantage of free probability, I separated the Hamiltonian of Anderson Model, H_c, into two parts, one matrix with only the site coupling and one with disorder that was free-rotated later on.

$$H_c = H_0 + H_{impurity}$$

4.1   Transmission probability calculation during the earlier period

At the very beginning of the research, more focus is put on the transmission probability and I did not take into the account of the effect of varying eigenvectors from free rotations. Also the model is based on particle in a ring and no influence from the leads is considered.

Transmission probability is set up in ring, analogy to an infinitely long chain, and is obtained by

$$T = |\langle +k |G| + k\rangle|^2$$

for a particle from site 0 $|+k\rangle$ with starting energy E_k and moving towards right. Eventually this particle goes out at site n.

The wave functions and energy for each level k can be written as

$$|+k\rangle = \begin{bmatrix} exp(\frac{2\pi ki}{n}) \\ exp(2\frac{2\pi ki}{n}) \\ exp(3\frac{2\pi ki}{n}) \\ \vdots \\ exp(n\frac{2\pi ki}{n}) \end{bmatrix}$$

and $E(k) = Jcos(\frac{2\pi k}{n})$, respectively. [18]

For larger n, we will be able to get more accurate simulation due to

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smaller errors in Gaussian Distribution. The green function here is a filter that only leaks out the wave at a certain energy level k, $G=\frac{1}{H-IE(k)}$. Hence, the transmission coefficient is now just $\langle +k \,|G| + k\rangle$ and the transmission probability is then $|\langle +k \,|G| + k\rangle|^2$.The result can be random and full of noise due to two problems: 1. errors occur during random selection of the Gaussian numbers; 2. these random numbers changes the states of 'free' particles. Therefore, external energies are added/subtracted from each site. Our matrix turned out to be: $H_0 + H_{imp} - \frac{tr(V)}{n} + xJ$. Since free probability will lead the eigenvalues of $H \approx H_0 + QH_{imp}Q\dagger$, then what would happen if we turn the basis of impurity H_{imp} freely, would that change the transmission coefficient? For simulation with free rotation, a unitary matrix Q is introduced from the QR decomposition of an n by n matrix. As a trial, H_{imp} is rotated first by calculating $QH_{imp}Q\dagger$.[80]

Calculations of the transmission probability are run many times, setting 1000 run as a standard. All data from the 1000 samples are collected, histogram and plotted.

4.2   Conductivity

Later on, more effects, such as self energy and etc, are added into the equations to receive the conductivity of the Anderson Model. The following will show free approximation are applied into conductivity session.

Similar to what I did above, convert the corresponding Green function according to the partition to the Hamiltonian

$$G'^{-1} = H - \Sigma - EI$$

$$= (H_0 - \Sigma - EI) + Q' * H_{imp} * Q$$

$$= \begin{pmatrix} E-\Sigma+g_1 & 1 & 0 & 0 & 0 \\ 1 & E+g_2 & 1 & \ddots & 0 \\ 0 & 1 & \ddots & 1 & 0 \\ 0 & \ddots & 1 & E+g_{n-1} & 1 \\ 0 & 0 & 0 & 1 & E-\Sigma+g_n \end{pmatrix}$$

$$= \begin{pmatrix} E-\Sigma & 1 & & & \\ 1 & E & 1 & & \\ & 1 & \ddots & 1 & \\ & & 1 & E & 1 \\ & & & 1 & E-\Sigma \end{pmatrix} + Q' * \begin{pmatrix} g_1 & & & & \\ & \ddots & & & \\ & & g_i & & \\ & & & \ddots & \\ & & & & g_n \end{pmatrix} * Q$$

where E is the energy of particles injected into the system, Σ is the self energy and Q is a unitary random matrix (note: since I generated Q from matrices with only real numbers, Q is indeed orthogonal).

Here again, for convenience, site coupling constant is set to be 1 unit.

From here, I replaced the G in $T = \frac{e^2}{\pi\hbar}Tr(\Sigma G'\Sigma G)$ by G' as an free approximation.

10000 samples are generated to receive the assemble estimation for the conductance of 1-D Anderson model. For every run, Q (s) are generated from a freshly made Gaussian random matrix. Results were collected and then histogram. Variables are controlled, screening through different sizes of disorder, different length of the chain, different positions of impurities, different injected energy E and etc.

The size of disorder is determined by $\frac{\sigma}{c}$, where σ is the standard deviation of Gaussian distribution and c is the coupling constant. The size of the matrix,

the length of the chain, could be easily set up. Instead of the matrix of impurities, that of site coupling was free rotated. Despite that, impurities were also added onto off-site partition (tridiagonal lanes) for a modified model. E were screened from 0 unit to 5 unit with increment of 0.1 unit, as E ranges from 0 to $2c$ in a pure system. Σ were set to be $1 * i$.

Recall that

$$\Sigma = -\frac{V^2}{t}(\frac{E}{2t} + i\sqrt{1 - (\frac{E}{2t})^2})$$

in which t is the coupling between lead and the system, V is the density of state at energy E. When t is large enough, the imaginary part becomes $-i\frac{V^2}{t}$. If V is not large enough, then the imaginary part will disappear and physically there won't be enough number of particles to go through this test. Hence, V also needs to be large enough to propagate more particles to be injected into the system. After a couple tests, $1i$ turns to be the best value for Σ. One other effect of Σ is that larger self energy will influence almost every sites and curve the conductivity too much, while smaller self energy leads to peaks that are too sharp.

Once all the fixed values are settled, programs are run to reach the 10000 sample pool.

Program Algorithm to calculate conductivity

1. Produce an n by n matrix with every diagonal terms to be Gaussian distributed $N - (0, \sigma)$ and tridiagonal terms to be 1;

2. Partition the matrix in desired structures;

3. Generate a random real matrix N whose entries follows Gaussian again;

4.QR decompose matrix N and receive the orthogonal matrix Q;

5. Apply Q to the part that you want to free rotate by having $Q'XQ$ as

X is the part selected;

6. Calculate the Green function approximate $G' = (H' - EI + i\epsilon)^{-1}$ for each E ranges from from $-2c$ to $2c$;

7. Obtain the Transmission Coefficient by the formula $T = |\langle a | G' | b \rangle|^2$;

8. Finally approach the conductivity by having $g \propto |T|$;

9. Repeat steps 1-8 10000 times;

10. Collect data for conductivity;

11. Histogram the data and plot.

5 Result and Conclusion

5.1 Transmission probability during earlier period

The transmission probability is based on the ideal model of particle in a ring. I consider neither effects from free rotation to the eigenvectors nor the self-energy from the leads (there is no leads).

The graph below shows the transmission probability (x axis) versus the energy E_k (y axis)ranging from -1 to 1 unit, at different disorder size J.
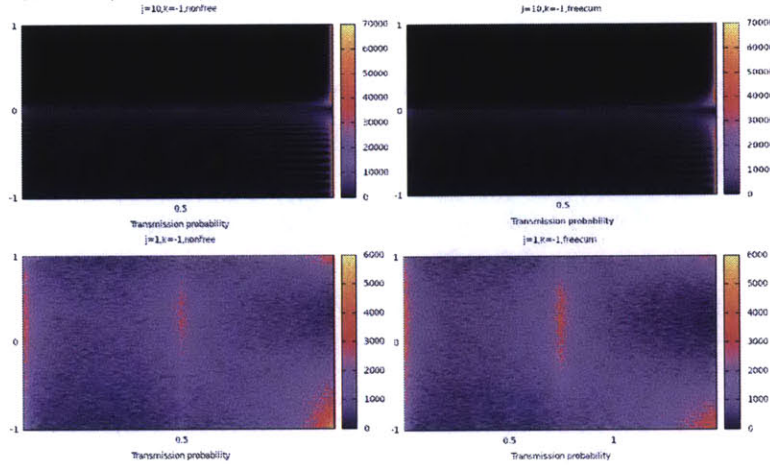
Figure 8. Transmission probability V.S energy shift on sites. J=10, original calculation (Top left); J=10, free rotation included (Top right);J=1, original calculation (Bottom left); J=1, free rotation included (Bottom right).

From the figures above, transmission probability tends to be 1 for large coupling J (J=10) at all other energy levels except for at the resonance state ($x = 0$). As charge can easily transmit in between the 'band' formed by the coupling, transmission is more likely to happen than reflection. On the other hand, for small J (J=1), transmission coefficients tend to be 0 with some to be 0.5, as charges are scattered and localized by relatively large impurities. As in a 1D real system with frozen disorders, transmission coefficient could tell us the trends for waves to be reflected by disorders.

Besides, free rotation plays as good role as the original calculation. Calculations with free rotation show similar patterns to those of the original calculation. As to how accurate the approximation is, we will run a further error analysis.

5.2 Transmission probability and Conductivity (including eigenvector changes due to free rotation)

Following the instruction in the method chapter, I received the data below :

To validate the initial conductivity formula, I tested the transmission coefficient (squared) along the length of the chain with disorder $\sigma = 5$, Self energy $\sum = 1 * i$ and fixed the energy level at 0.1 unit. According to the conjecture, the transmission coefficient should exponentially decay as the length increase. Therefore, I took the logarithm values and a line came up. Due to the capacity of the computation, deviation increased as the value of transmission coefficient got close to zero at long chain.
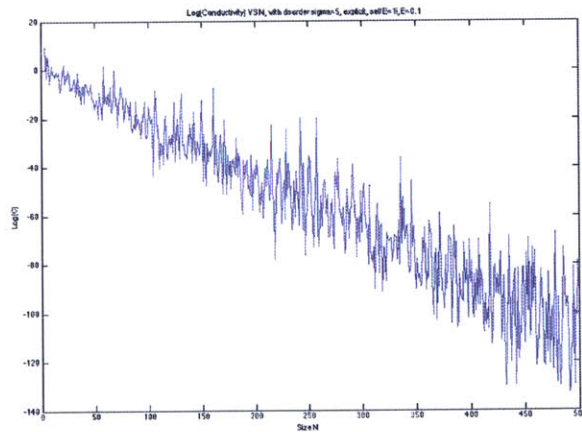

Figure 9. Log(Conductivity) Versus Size N of Matrix. The line proves the exponential decay of conductivity as the size of the matrix is increasing.

Now it is interesting to explore some properties along different energy E . The figure below shows the performance of the logarithm values of conductivity versus the energy E at different disorder sizes σ, the coupling constant was set to be 1, the size of the matrix is 100, the self energy is $1 * i$.
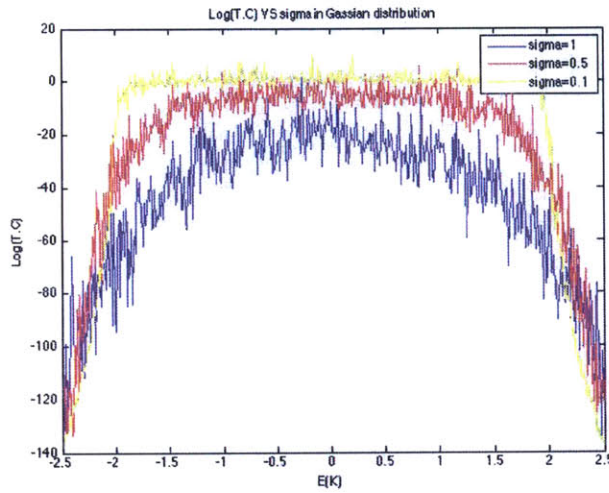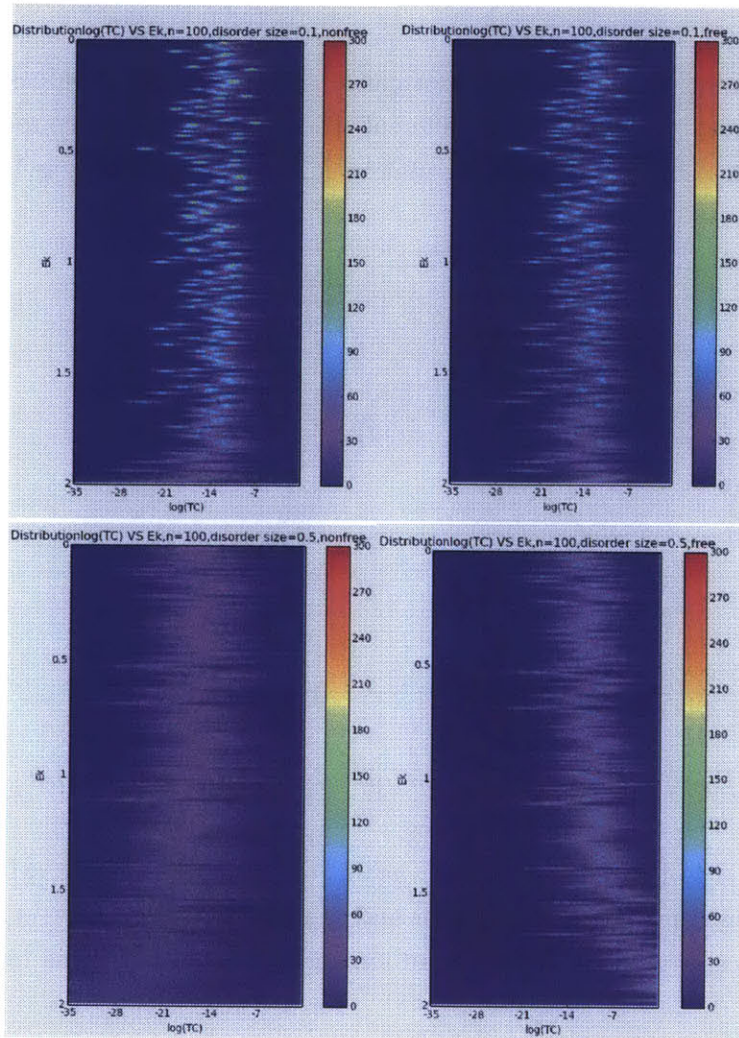

Figure 10. Log(Transmission probability) Versus particles injected with energy E.

As mentioned in the method chapter again, the range of E is $2c$, where c is *the* coupling constant in the system and is fixed to be 1 unit. As the disorder becomes larger, the energy band expanded to 2.5 and turns to be more localized.

Due to the disorder, Figure 10 just shows one shot result for each E_k. What if multiple shots are taken for every E_k? The graph below tells the distribution of log (transmission probability) is at different E_k and disorder sizes.
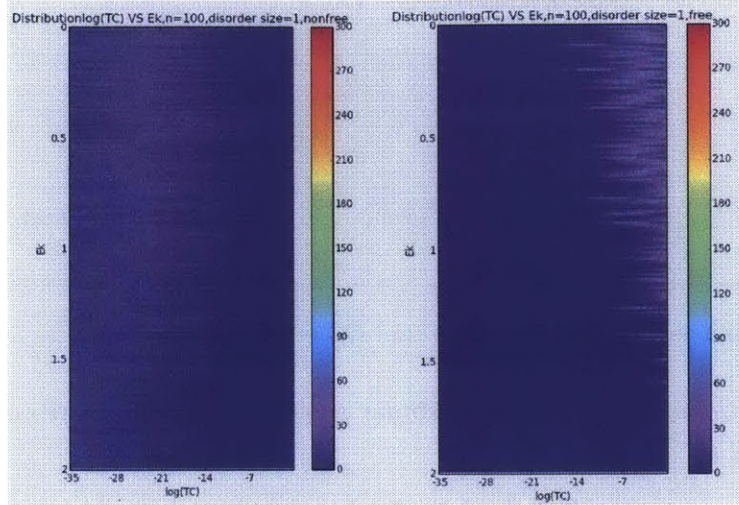
Distributionlog(TC) VS Ek,n=100,disorder size=0.1,nonfree
Distributionlog(TC) VS Ek,n=100,disorder size=0.1,free
Distributionlog(TC) VS Ek,n=100,disorder size=0.5,nonfree
Distributionlog(TC) VS Ek,n=100,disorder size=0.5,free

Figure 11.Distribution of (Log(Transmission Probability)) V.S. E(k) in system with disorder size=0.1,0.5 and 1.

It shows approximation calculation for a system with smaller disorder are much more accurate than for that with larger disorder.

So now I would like to test whether the free probability would work to approximate the conductivity or not. Figure 11 shows the comparison between conductivity (averaged from 10000 runs for each E_k) from regular calculation and free approximation, in which energy E is fixed at 0.1 unit without loss of generality, matrix size n equals to100, self energy is $1i$. Different positions of the disorder were added onto the pure Hamiltonian, either on-site (on the diagonal) or additional off-site (first off-diagonal lanes) disorder.
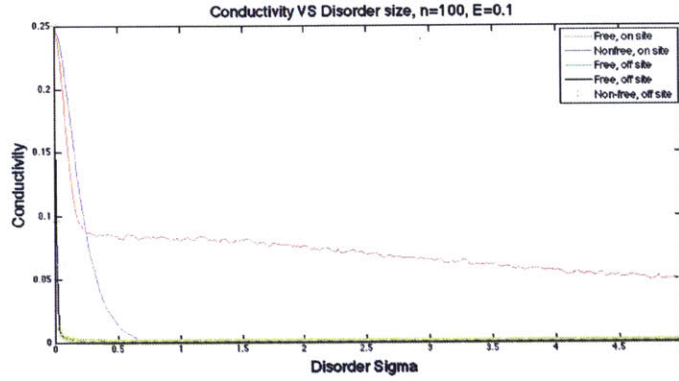
Figure 12. *Conductivity Versus Disorder size σ under only on-site and both on-site and off site impurities.*

It is clear that there is a transition point around $\sigma \approx 0.3$ where free approximation no longer works well for the on-site disorder. While for off-site disorder, curves overlap with each other. In the cases with on-site disorder only, free rotation delocalized the states in additional to shifts caused by the large disorder. Therefore conductivity tends to decay at a slow rate. Figure 12 proves that at small disorder, free approximation works fine. Whereas for off-site disorder, bands for particle to transmit is blocked by the impurities and, consequently, conductivity quickly decays to zero.
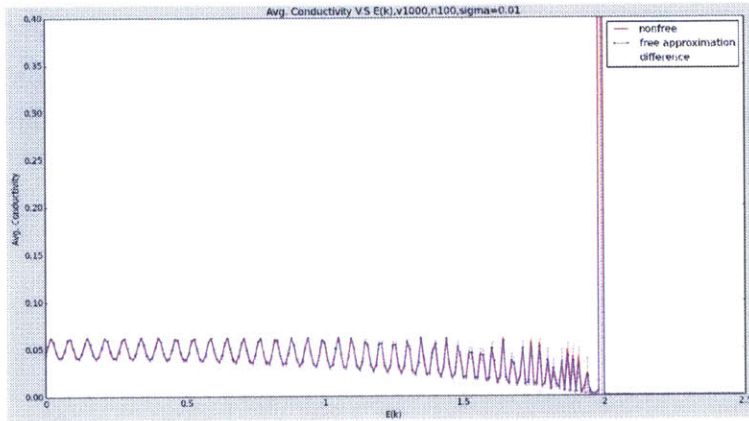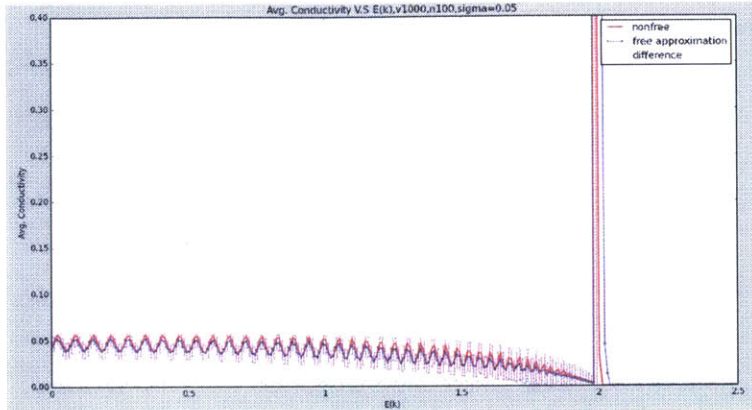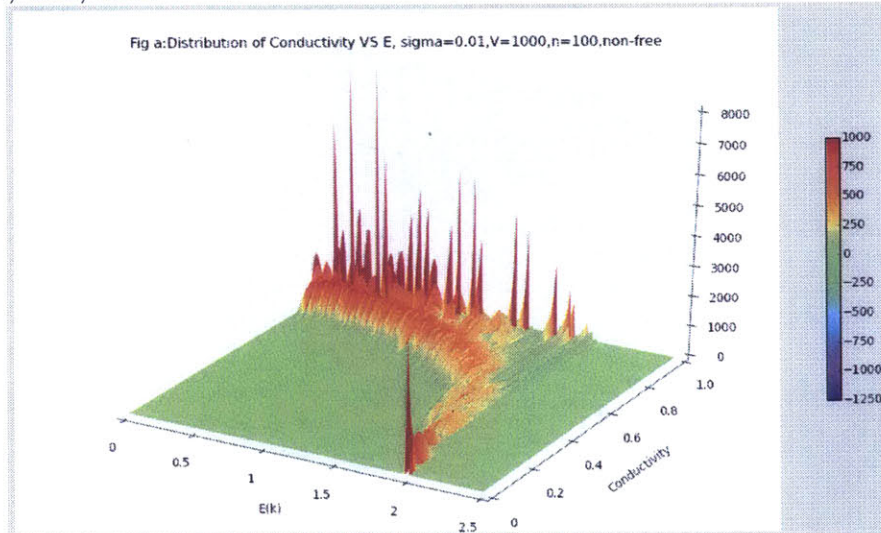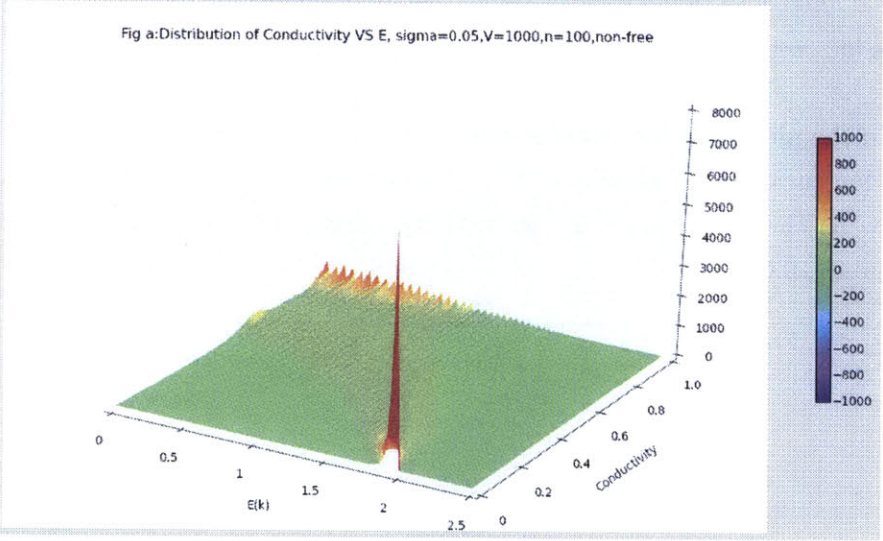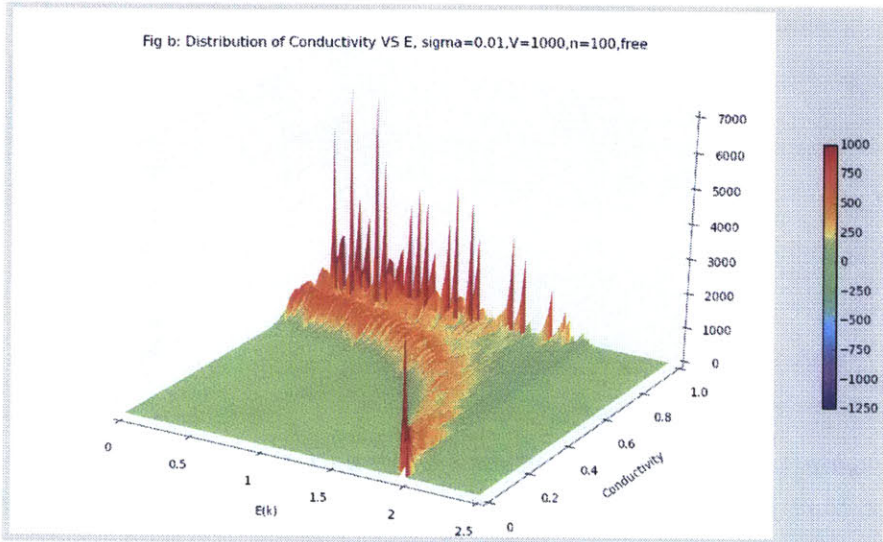
Figure 13. Approximation at disorder of 0.01 and 0.05. When $\sigma = 0.01$, curve from free approximation matches with that from regular calculations; once σ increases to 0.05, curves from free approximation starts shifting lower than the regular calculation.

In the picture above, conductivity is averaged from 10000 samples. Then just for curiosity, I histogram the curves at every $E(k)$ and plot the graph below as the distribution of conductivity versus $E(k)$ at different disorder size, 0.01, 0.05.
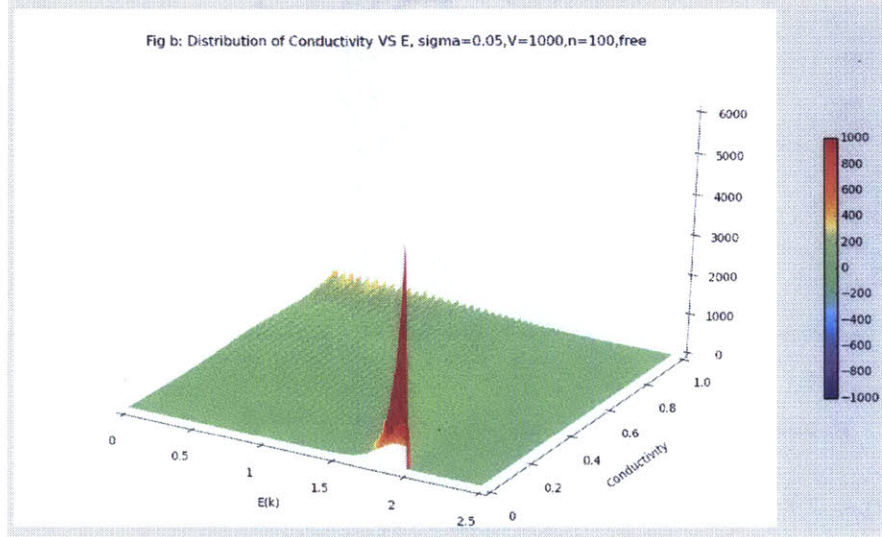
Fig b: Distribution of Conductivity VS E, sigma=0.01,V=1000,n=100,free

Fig a:Distribution of Conductivity VS E, sigma=0.05,V=1000,n=100,non-free

Fig b: Distribution of Conductivity VS E, sigma=0.05,V=1000,n=100,free

Figure 14. *Distribution of conductivity versus E_k at disorder size 0.01 and 0.05.*

Starting with small disorder $\sigma = 0.05$, values of conductivity turns to be have differences. Later on, first order correction from the fourth term in the 8th moment is calculated: $\Delta = \sigma^4 \frac{d^8(\varrho^{(A \oplus B)}(g))}{8! dg^8}$, where g is the value of conductivity. However, this terms is too large to be a possible correction, ranging up to 10^6, which is way higher than the maximum value shown on the color bar, 7000.

Thus it is important to figure out what is happening to the system with only on-site disorder. Figure 14 shows the comparison between of distributions of eigenvalues for of non-free and free -rotated Green function.
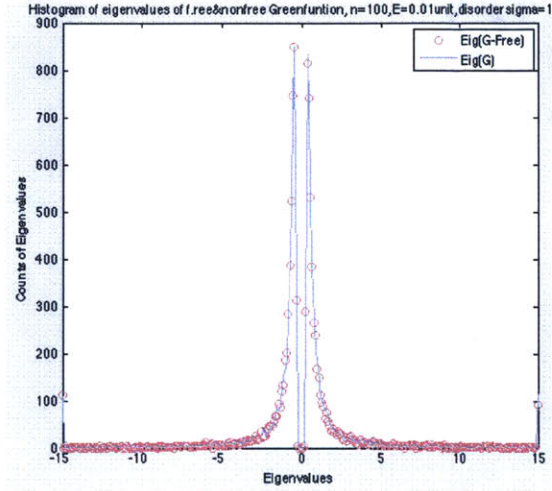
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Figure 15. Comparison between the p.d.f of eigenvalues from regular calculation and free approximation.

It is not surprising to see approximation of the eigenvalue spectrum functioning well, given the eigenvectors are not involved. Hence, it is certain that eigenvector shift causes the approximation of conductivity to fail at large disorder. Then it will great to find a method to estimate the assemble of eigenvectors correctly.

To discover more about the properties of eigenvectors, random states are chosen. Vectors from regular calculation contain only one non-zero number and it is always 1. Vectors from free approximation contains non-zeros everywhere. That means free approximation releases the states from localized status and there are more chances for particle to transport through any sites.

In sum, free approximation of conductivity works effectively around small disorder. However, since the eigenvectors will be shifted and eventually delocalized by the free rotation, this approximation needs to be modified for large on-site disorder system.

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6 Future

Continued from the last chapter, this one will show two possible approaches to estimate the behaviors of eigenvectors. The most direct solution is to find out how eigenvectors are distributed as the disorder is getting larger. The second one will apply quantum algorithms[80-83] to first find the eigenvalues, the ground state and then the rest states through a series of self-similarity quantum gates[83].

As the first approach, distribution of the ground state eigenvectors in a 2-site chain and disorder $\sigma = 1$ were collected and posted in Figure 16:
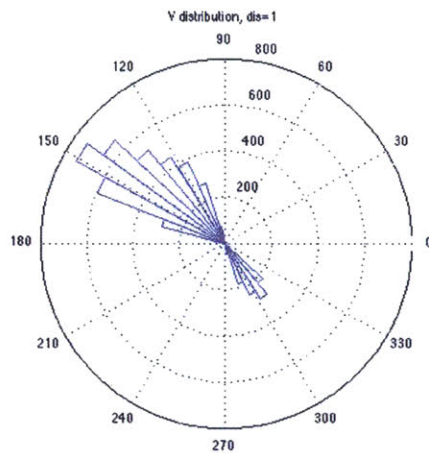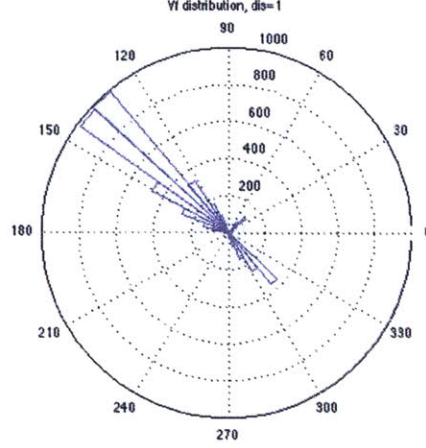
Figure 16. Distribution of non-free and free approximated eigenvectors, with disorder $\sigma = 1$ and site $n=2$.

Converting the the polar coordinate to Cartesian and increasing the disorder gradually, I formed a short video clip which tells the trends of the distribution of eigenvectors with increasing disorder. Then curve fittings were run to find the analytical expression for their variation. Curve fitting uses exponential modified Gaussian distribution. A third modification of x^n was added to follow up with the fast changing rate in long chains. The proposed curve should be in the form of

$$f(x,\mu,\sigma',\lambda) = x^n \frac{\lambda}{2} exp(\frac{\lambda}{2}(2\mu + \lambda\mu^2 - 2x)) erfc(\frac{\mu + \lambda\sigma^2 - x}{\sqrt{2}\sigma})$$

The second approach is a lot more complicated. Basically, it will apply the tradition quantum algorithms to find eigenvalues of random matrices[84, 85]. Repeating quantum gates will be used for a long time scale.[86] Each repeat will help stabilize and clarify the energy levels and the corresponding eigenvectors. Eventually an approximation on eigenvalues, after tons of repeats, can be found. [86, 87]

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