Anderson Localization in Low-Dimensional Systems with Long-Range Correlated Disorder

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ABSTRACT

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It has been known for over a half century that when disorder is introduced into a crystalline system through impurities, vacancies, grain boundaries, or other mechanisms that break the translational invariance of the system, the electronic eigenstates will localize in space. This phenomenon is called Anderson localization after Phillip Anderson who first predicted it in 1958. Since then, Anderson localization has remained a vibrant topic of research due to new experimental methods of probing localized states, an increase in computational power, and its accurate phenomenological representation of many physical systems. To date, a large amount of effort has been dedicated to the study of uncorrelated, or short-range correlated, disorder distributions. However, more recent efforts on long-range correlated disorder distributions have yielded richer results, challenging the foundations of Anderson localization theory. In this document, we focus on characterizing the naturally occurring $\sim 1/r$ correlation, and the phenomenologically rich $\sim 1/k$ correlation in one-dimensional systems. We will discuss several important numerical and analytical methods for determining a localization-delocalization transition along with the localized phase itself. Finally, we will discuss on-going work related to novel two-dimensional disordered materials where random spin-orbit interactions are predicted to cause suppressed spin transport.
DEDICATION

To my parents
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# Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>3</td>
</tr>
<tr>
<td>Dedication</td>
<td>4</td>
</tr>
<tr>
<td>Acknowledgments</td>
<td>5</td>
</tr>
<tr>
<td>List of Figures</td>
<td>8</td>
</tr>
<tr>
<td>1  Introduction</td>
<td>13</td>
</tr>
<tr>
<td>2  Basic Concepts in Ordered and Disordered systems</td>
<td>17</td>
</tr>
<tr>
<td>2.1 Ordered systems</td>
<td>17</td>
</tr>
<tr>
<td>2.2 The Tight-Binding Model</td>
<td>18</td>
</tr>
<tr>
<td>2.2.1 Example: Single Chain of Atoms</td>
<td>21</td>
</tr>
<tr>
<td>2.3 Transport in Ordered Systems</td>
<td>23</td>
</tr>
<tr>
<td>2.4 Disordered Systems</td>
<td>24</td>
</tr>
<tr>
<td>2.5 The Anderson Transition</td>
<td>25</td>
</tr>
<tr>
<td>2.6 Single Parameter Scaling Hypothesis</td>
<td>26</td>
</tr>
<tr>
<td>2.7 The Localization Length</td>
<td>27</td>
</tr>
<tr>
<td>2.8 Kotani Theory of Random Ergodic Operators</td>
<td>28</td>
</tr>
<tr>
<td>2.9 Correlated Disorder</td>
<td>29</td>
</tr>
<tr>
<td>3  Numerical Methods</td>
<td>32</td>
</tr>
<tr>
<td>3.1 Disorder Generation</td>
<td>32</td>
</tr>
<tr>
<td>3.2 The Transfer Matrix Method</td>
<td>34</td>
</tr>
<tr>
<td>3.3 Conductance Calculation Method</td>
<td>38</td>
</tr>
<tr>
<td>3.3.1 Calculation of Self-Energies</td>
<td>42</td>
</tr>
<tr>
<td>3.3.2 Recursive Green’s Function Method</td>
<td>45</td>
</tr>
<tr>
<td>3.4 Example: One-Dimensional Single Site Anderson Hamiltonian</td>
<td>47</td>
</tr>
<tr>
<td>4  Power-Law Spectral Correlated Disorder Distributions in One-Dimension</td>
<td>50</td>
</tr>
<tr>
<td>4.1 Long-Range $1/\kappa^\alpha$ Correlations</td>
<td>50</td>
</tr>
<tr>
<td>4.2 The Exact Correlation Function</td>
<td>51</td>
</tr>
<tr>
<td>4.2.1 $\alpha &lt; 1$</td>
<td>54</td>
</tr>
<tr>
<td>4.2.2 $\alpha &gt; 1$</td>
<td>56</td>
</tr>
<tr>
<td>4.3 Comparison to the Random Dimer Model</td>
<td>59</td>
</tr>
<tr>
<td>4.4 On-going Projects Related to Correlation Driven Anderson Transitions</td>
<td>60</td>
</tr>
</tbody>
</table>
5 Scale-Free Correlated Disorder in One-Dimension .................................. 62
  5.1 Experimental Observation of Matter Wave Localization .......................... 62
  5.2 Validity of Single Parameter Scaling Hypothesis ................................ 63
     5.2.1 1st Cumulant ...................................................... 64
     5.2.2 2nd Cumulant ..................................................... 67
  5.3 Previous Scaling Results for the Localization Length ............................ 69
  5.4 Scale-Free Correlation at the Band Edge ......................................... 71
  5.5 Extension of Band Edge Scaling Results ......................................... 73
  5.6 The Crossing Energy ...................................................... 76

6 Disordered Rashba Spin-Orbit Interaction in Graphene .......................... 79
  6.1 Graphene ............................................................... 79
     6.1.1 Graphene Nanoribbons .............................................. 80
  6.2 Spin Coherence in Graphene ................................................. 84
  6.3 Rashba Spin-Orbit Interaction ................................................. 85
  6.4 Zigzag Boundaries and Rashba Interaction ....................................... 87
     6.4.1 Band Structure Calculation ........................................... 87
     6.4.2 Conductance Calculation .............................................. 93
  6.5 Random Rashba Field ...................................................... 96

7 Discussion and Conclusions ............................................................. 99

References ................................................................. 101

Appendix A: Participation Ratio ......................................................... 106

Appendix B: Anomalous Diffusion of a Wavepacket ................................ 109

Appendix C: Derivation of Graphene Band Structure ................................ 113
## List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Band structure of a single chain of atoms with on-site energy $\epsilon = 0$. If $\epsilon \neq 0$, the band is shifted by a factor of $\epsilon/t$.</td>
<td>23</td>
</tr>
<tr>
<td>2.2</td>
<td>Cartoon of a localized wavefunction vs an extended Bloch wavefunction. If we consider that a source is connected to the left hand side of the system with drain to the right, then the electron occupying the extended state has a probability of going from the source to drain while the electron in the localized state cannot leave the conductor.</td>
<td>25</td>
</tr>
<tr>
<td>2.3</td>
<td>A small distribution for the random dimer model with black colored points indicating sites with energy $\epsilon_A$ and red being sites with $\epsilon_B$. The top figure is the uncorrelated binary distribution with the middle figure indicating the non-dimer pairs (note that these include all odd numbered groups of $B$ atoms). The final figure shows the final disorder distribution with the correlation introduced by replacing all non-dimer pairs of $B$ atoms with $A$ atoms.</td>
<td>30</td>
</tr>
<tr>
<td>3.1</td>
<td>The resulting correlation function from the spectral disorder generation method for different system sizes. The solid red and orange lines are the expected values (Eq. (3.9)) of the correlation function for $\alpha = 0.5$ and $\alpha = 0.6$. The purple, blue, and black lines represent systems of size $2^{10}$, $2^{14}$, and $2^{16}$ respectively. For each numerical data set, $\alpha = 0.5$, $w/t = 1$. For the smallest system size, we see that the curve more closely follows a correlation of $\alpha \sim 0.6$ instead of the expected correlation value of $\alpha = 0.5$. As the system size increases, the generated values follow more closely the expected output.</td>
<td>35</td>
</tr>
<tr>
<td>3.2</td>
<td>(Top) Results from Ref. [55], (Bottom) Our results for a cosine incommensurate potential. Both methods discussed were applied producing identical results. Parameters: $N = 5000$, $r = 3$, and $\Delta_\alpha = 1.9$ which correspond to the system size, the variable determining the irrational factor in the incommensurate potential, and the amplitude of the cosine incommensurate potential respectively. The graph is symmetric around $E = 0$ and only the negative portion is shown for clarity.</td>
<td>39</td>
</tr>
<tr>
<td>3.3</td>
<td>(Top) A system with two semi-infinite perfect leads (Black) and a disordered conductor (Green). The squares represent any repeated unit cell with the Hamiltonian for intra-cell interactions given by $h_{n,n}$ and inter-cell interaction given by $h_{n,n+1}$. (Bottom) An example of a specific unit cell, in this case a graphene nanoribbon of width 3 (See Sec. 6.1 for further details on graphene).</td>
<td>40</td>
</tr>
<tr>
<td>3.4</td>
<td>Density of states versus energy for a clean single atomic chain. Here, $\epsilon_n = 0$ which indicates the lack of disorder. The black dots correspond to numerical calculation while the red curve is the theoretical predicted density of states given in Eq. (3.70).</td>
<td>48</td>
</tr>
</tbody>
</table>
3.5 Density of states for a uncorrelated disorder distributions (black dots). The red line is the density of states of the clean system as given in Eq. (3.70).

4.1 Plot of the correlation function as a function of the dimensionless quantity $\gamma$. The red solid line corresponds to the critical value of $\alpha = 2$ which is given by Eq. (4.40). The other curves correspond to various values of $\alpha$ from Eq. (4.37).

4.2 Plot of the correlation for the largest separation distance, $\gamma = 1$, of the function $\Gamma$. The origin corresponds to the critical value of $\alpha = 2$ and yields a correlation of $-1/2$. For larger values of $\alpha$, the correlation becomes more negative and results in a larger region of extended states[19].

4.3 Typical disorder realization of a $1/k^\alpha$ spectral correlation. In this figure, $N = 1000$ and the same set of random numbers $\{\phi_k\}$ for $\alpha = 2$ (solid, blue), $\alpha = 4$ (dotted, red), and $\alpha = 10$ (dashed, black) have been used. Energy is normalized such that $\langle \epsilon^2 \rangle = 1$. Plots show tendency for strong correlations that induce a sinusoidal structure in the disorder distribution.

4.4 A numerical calculation of the random dimer model for $N = 1000$, $\epsilon_A = t$ and $\epsilon_B = -t$. As the system size is increased, the correlation function approaches a constant value of 0.3 for all $\gamma$.

5.1 (Top) Plot of the typical conductance versus system size. Different symbol shapes represent different values of disorder strength with $W/t = 1.0$ (triangles), 0.5 (squares), and 0.2 (circles). Different colors correspond to $\alpha = 0.25$ (Red), 1.00 (Black), and 1.50 (Blue). Finally, different sizes correspond to energies $E = 0$ (Large Filled), 1.0 (Large Hollow), and 1.8 (Small Solid). (Bottom) Same data as top figure except that $L$ is rescaled for each data set by $\xi$ to cause a data collapse which confirms SPS.

5.2 Plot of the ratio of first and second cumulant as a function of $E/t$. Colors correspond to $\alpha = 0.5$ (Red), 1.0 (Black), and 1.5 (Blue) while shapes correspond to $W/t = 1.0$ (Triangles), 0.5 (Squares), and 0.2 (Circles). The dashed black line is the expected ratio of Eq. (5.8). Note that each data set diverges at some energy which we refer to as $E_{sps}$. For $\alpha = 0.5$, $W/t = 1.0$, all energies violate this condition which we represent by $E_{sps} = 0$.

5.3 Plot of the SPS violation energy versus $\alpha$ for multiple disorder strength. The shapes and colors correspond to disorder strengths of $w/t = 1/3$ (red triangles), 1/5 (purple squares), 1/8 (orange circles), 1/10 (blue rectangles), 1/15 (green up-side-down triangles), and 1/20 (black stars). These values were determined from systems of size $2^{17}$ sites and 1000 disorder distributions. The error associated with each points is between 5 – 10% with the error bars omitted for clarity.

5.4 Plots of $E_{sps}$ versus the ratio $\frac{W}{\mu_\alpha}$. Data is extracted from all permutations of $\alpha = 0.50, 0.75, 1.00, 1.25, 1.50$ and $W/t = 1.00, 0.50, 0.33, 0.25, 0.20$. Solid line is a guide to the eye. (Top) Linear scale. (Bottom) Logarithmic scale.
5.5 Plots of the inverse localization length versus energy. The different colored curves correspond to numerical results calculated from transfer matrix methods for $W/t = 1/3$ (blue), $W/t = 1/5$ (red), and $W/t = 1/10$ (yellow) with the vertical dark lines indicating the values of $E_{sp}$ with the leftmost line correspond to the blue curve and the rightmost to the yellow. The dashed black curves are calculated from Eq. (5.10). (Top) $\alpha = 0.5$ (Bottom) $\alpha = 1.0$.

5.6 Raw localization length data plotted versus $x$ and scaled with $\lambda_0$ for systems of size $L = 2^{17}$ (red circles), $2^{18}$ (purple triangles), $2^{19}$ (blue squares), and $2^{20}$ (green diamonds). The black stars represent the extrapolated value of the localization length, $L \to \infty$, with the line being a guide to the eye.

5.7 Plot of the extrapolated localization length versus $x$ for $x > 1$. The slope of the linear region when $x \gg 1$ as exemplified in Fig. 5.7. The different data sets correspond to, from top to bottom, $\alpha = 0.25, 0.50, 0.75, 1.00, 1.25, 1.50$, and $2.00$. The solid line running through each data set is given by the anticipated value of $\gamma = (3 - \alpha)/2$.

5.9 The inverse localization length $\lambda$ for three values of $\alpha$ at disorder strength $w/t = 1$. Data is extrapolated to $L \to \infty$ from systems of size $L = 2^{17} - 2^{20}$ and averaged over 1000 disorder configurations. This figure presents two distinct regions in energy. For states near the band center, the localization length increases as correlations increase while at the edge, the localization length decreases as correlations increase. The energy where the change of behavior occurs is $E_c$. (Inset) The crossing energy $E_c$ for various disorder strengths.

5.10 The scaling for $E_c$ (black) and $E_{sp}$ (blue) as given by Eqs. (5.23) and (5.24) respectively. The different lines correspond to the values of $\alpha = 0.1$ (dashed), $\alpha = 0.5$ (solid), and $\alpha = 1.0$ (dotted) respectively.

6.1 The graphene lattice. This geometry requires the use of a two site basis that we label A and B with the highlighted area being the smallest possible unit cell.

6.2 The $\pi$ band for graphene. The red and green dots correspond to the $K$ and $K'$ points. This is an extended zone scheme to show the hexagonal symmetry (i.e. we are plotting points that are equivalent up to a translation in $\vec{K}$) with the only unique values between $aK, \sqrt{3}/2 \in [0, \pi]$ and $aK, 3/2 \in [0, \pi]$. The $K$ and $K'$ are located at $(\pi/3, 0)$ and $(2\pi/3, 0)$.

6.3 The zigzag and armchair edge geometries and width characterization scheme. The width is determined by the number of dimer pairs that make up the GNR unit cell (shaded regions with alternating blue and green regions highlighting the different dimer pairs). This armchair width is insulating as $M = 3m - 1$ cannot be satisfied for any value of $m$. 
6.4 The band structure for different width armchair GNRs. (Top) \( M = 4 \). (Middle) \( M = 8 \). (Bottom) \( M = 10 \). For the top and bottom plots, a band gap exists between the conductance and valence band. For the middle plot, \( M = 8 \) satisfies the condition \( M = 3m - 1 \) and the bands touch at \( K = 0 \).

6.5 Diagram of a graphene ribbon with the three displacement vectors \( \delta_i \) defined in Eqs (6.8)-(6.10). The solid points represent the A sublattice while the hollow points represent the B sublattice. The Rashba term in Eq. (6.12) is defined as a summation over the A sublattice only.

6.6 A zigzag GNR of width M=4. The green box represented the repeated unit cell used in the band structure calculation. The translational distance between each unit cell is \( a \sqrt{3} \) as indicated.

6.7 Zigzag GNR with added Rashba spin-orbit interaction. The plots show the band structure of ribbons of width \( W = 2, 3, \) and 4 without and with Rashba spin-orbit interaction. This term breaks the degeneracy of the spin-up and spin-down bands as can be seen from the \( \Delta_r/t = 0.4 \) plots. Note: we have only plotted 1/4 of the full band structure as it is mirror symmetric around energy as well as \( K \). Finally, notice a flat band region around \( E = 0 \) with and without Rashba. These are the conducting states of the zigzag GNR.

6.8 Density of states for a (top) \( M = 4 \) and (bottom) \( M = 8 \) zigzag GNR with added Rashba spin-orbit interaction of \( \Delta_r/t = 0.4 \). The red dots correspond to the calculation of the density of states through the Green’s function method while the black line corresponds to the density of states calculated from the band structure in Sec. 6.4.1.

6.9 Conductance for a (top) \( M = 4 \) and (bottom) \( M = 8 \) zigzag GNR with added Rashba spin-orbit interaction of \( \Delta_r/t = 0.4 \) compared to the band structure. The Blue curves correspond to the conductance \( G \) with respect to the energy. We can see clear conductance plateaus that are related to the number of conducting channels available. To emphasize this, we have plotted the band structure (purple curves) from Fig. 6.7 (which has been rotated 90 degrees such that the momentum states are on the y-axis and the energy on the x-axis). For each energy, the conductance is equal to the number of times a band crosses the chosen energy. To illustrate this, in the top figure a dashed line through \( E/t = 1.6 \), with all band crosses circled, illustrates this point.

A.1 The participation ratio exponent \( D \) as a function of energy for systems with scale-free disorder correlations. The colors correspond to \( \alpha = 0.5 \) (blue), \( \alpha = 1.0 \) (red), and \( \alpha = 1.5 \) (yellow). These results are extracted from system sizes of \( N = 200 - 1000 \) and confirm the absence of a critical point.
B.1 Diffusion of a wavepacket in a 1000 site disorder chain with scale-free correlations. (a) Raw diffusion data versus time $\tau$. (b) The value of the exponent theta calculated from Eq. B.17. We can see that as we go to longer ranged correlations, $\alpha = 0.5$ for example, a plateau begins to develop around $\tau \approx 5$. However, this region is still time dependent and does not correspond to an anomalous diffusive regime. (Inset) Logarithmic scale.

C.1 Diagram of a graphene ribbon with the three displacement vectors $\delta_i$. The solid points represent the $A$ sublattice while the hollow points represent the $B$ sublattice.
1 Introduction

Like so many examples in great science, condensed matter theory was originally dismissed by the general scientific community as well as by some of the greatest minds of the early twentieth century. Wolfgang Pauli, in a personal correspondence to Rudolph Peierls, discouraged the study of this field saying, "...one shouldn’t wallow in dirt"[9] while Isidor Rabi flat out rejected condensed matter as a valid scientific discipline calling it, "The physics of dirt."[9]. One is left to wonder if these two Nobel laureates might have changed their minds on the subject if they had foreseen the advent of the first microchip, the discovery of superconductivity, or if they had known that, after more than a century of study, the physics of dirt remains technologically impactful, often surprising, and continues to challenge and fascinate us.

From the layman’s point of view, condensed matter physics would appear to be, more or less, a form of applied elementary particle physics. However, the distinction of condensed matter physics from the study of elementary particle physics is precisely due to the fact that "more is different"[5]. More precisely, the simple reductionist approach to physics (i.e. all physical phenomena can be predicted from the phenomena of its smallest possible constituents) is incomplete as new physical phenomena appear when considering collective effects which are typically driven by breaking a symmetry associated with the single particle picture. This so called constructionist viewpoint, unique but non-contradictory to the reductionist viewpoint, provides a basic distinction between elementary particle physics and condensed matter.

The term condensed matter thus, is a broad classification used to describe the condensed phases of matter. These include, solid state, liquid state, ferromagnetic, paramagnetic phases, amorphous states, superconducting states among others. The quantity that classifies the change between two states is usually referred to as the order-parameter, which varies between different physical systems. As an example, the
order parameter that distinguishes between ferromagnetic and paramagnetic phases is the net magnetization, while the order parameter associated with the freezing transition (liquid to solid state) is the spatial periodic component of the particle density[72].

Typically, the order parameter is 0 for the disordered state (paramagnetic and liquid state) and non-zero for the ordered one (ferromagnetic and solid state). The temperature at which the transition takes place is called the critical temperature $T_c$.

It is well established by now that phase transitions come in two flavors. First-order phase transitions imply a discontinuous change in some parameters of the system, while second-order phase transitions imply a continuous change. As an example, the solid-liquid transition is first order while the ferromagnetic-paramagnetic transition is second order. The former is typically characterized by a latent heat and mixed phase of matter (e.g. ice in water) while the latter is characterized by a set of critical exponents, $\alpha, \gamma, \beta, \nu$, etc., which are defined for the heat capacity, susceptibility, order-parameter and correlation length respectively. To illustrate this point, assume that we are in a non-ordered phase (order-parameter equal to 0) and the temperature of the system is the parameter driving the transition. While on average the system will be unordered, for each fluctuation of a physical property, there may exist a finite range of order where the chosen physical property has an average value greater than its fluctuations. The average value of these ranges of order that characterize the extent of spatial fluctuations is defined as the correlation length $\xi$. Near the critical temperature $T_c$, the fluctuations become so large that the correlation length, or range of order, goes to infinity. This diverging behavior takes the universal form of

$$\xi \sim \frac{1}{|T - T_c|^\nu}$$  \hspace{1cm} (1.1)

with similar critical relationships for $\alpha, \beta, \gamma$ for the other physical quantities.

Inspired by the theory of classical phase transitions, an analogous theory of quantum phase transitions (transitions occurring at $T = 0$) was developed. In this case, the driving
force behind the phase transition must come from quantum fluctuations that arise from the intrinsic fluctuating nature of matter at the quantum level that is enhanced in the presence of external magnetic fields, disorder, or other such non-thermal mechanisms. These transitions are usually second order as they can be described by a set of critical exponents similar to classical phase transitions. We can define an analogous relationship to Eq. (1.1) in terms of some tuning parameter $x$ as

$$\xi \sim \frac{1}{|x - x_c|^\nu}$$

(1.2)

where $\xi$ is the correlation length associated with quantum fluctuations.

One of the seminal examples of a quantum phase transition[27] is the Anderson metal-insulator transition[4] in which disorder induced quantum fluctuations produce a metal-insulator transition depending on the dimensionality and disorder statistics of the system[1, 24, 19]. Typically the two tuning parameters that drive the transition are the disorder strength $W$ and the energy $E$[64]. The driving force behind the phase transition is the spatial extent of the eigenstates. If the states are extended across the entire system, we are in a metallic phase while if the states are localized, we are in the insulating phase. Thus, the Anderson model is often referred to as a localization-delocalization transition model. The correlation length in this case is referred to as the localization length[4, 27] $\lambda$, which characterizes the average extension of an electronic state by an exponentially decaying envelope

$$|\psi_E(\vec{r})|^2 \sim exp(-|\vec{r} - \vec{r}_0|/\lambda),$$

(1.3)

with $\vec{r}$ the position and $\vec{r}_0$ the "center" of the localized state. Also, $\lambda$ follows the relationship

$$\lambda \sim \frac{1}{|E - E_c|^\nu}$$

(1.4)

near the critical energy $E_c$. For the uncorrelated three dimensional Anderson model, numerical results predict[84] that $\nu \approx 1.6$, while scale-free correlated disorder (which will
be discussed in detail later) makes \( \nu \) a function of the correlations strength, analogous to general classical second order phase transitions with scale-free correlations\[92, 64\]. For dimension \( d < 3 \), no phase transition exists for uncorrelated disorder. However, if the disorder correlations are adequately long-ranged, an Anderson transition can appear\[48\].

The goal of this document is to examine the role of various long-ranged disordered correlations on the localized (\( \lambda < \infty \)) and extended (\( \lambda = \infty \)) phases of the Anderson transition as well as the existence of the transition itself in one- and two-dimensional systems. We begin with an overview of the basic concepts in localization theory and the numerical methods used to probe different physical quantities. After having established this basic framework we proceed to analyze the nature of the Anderson transition for one-dimensional systems with different types of correlated potentials.

First, we calculate the exact correlation function that is generated from \( \sim 1/k^\alpha \) spectral correlations to resolve an apparent contradiction between analytic conditions and numeric simulations. We find that there is no contradiction, and the misunderstanding occurs due to a short range cutoff that is used to incorrectly calculate the correlation function.

Second, we test the validity of a key concept in localization physics, the single parameter scaling hypothesis, for \( \sim 1/r^\alpha \) correlations in one-dimensional systems. We compare these results to perturbative weak disorder calculations of the localization length and find the two results coincide. We argue that these results shows that correlations can induce strong localization due to suppressed tunneling.

Finally, we outline on-going work in random spin-orbit interactions in the novel two-dimensional material, graphene.
2 Basic Concepts in Ordered and Disordered Systems

2.1 Ordered systems

In this section, we will briefly review the basic theory of ordered systems.[7] To begin, consider a translationally invariant crystal. The electronic degrees of freedom in this crystal are represented by the Hamiltonian

$$H = \frac{\vec{p}^2}{2m_e} + U(\vec{r})$$

(2.1)

with $\vec{p}$ being the momentum operator for an electronic state, $m_e$ the mass of the electron, and $U(\vec{r})$ being a static potential generated by the atomic lattice. This potential satisfies the conditions

$$U(\vec{r} + m\vec{a}_i) = U(\vec{r})$$

(2.2)

where $m$ is an integer, $\vec{a}_i$ is the displacement along the $i$ direction with $i = [1, d]$, with $d$ being the dimensionality. The vectors $\vec{a}_i$ define the periodicity of the crystal and are used to define every repeated set of points on the lattice through the expression

$$\vec{R} = \sum_{i=1}^{d} m_i \vec{a}_i.$$  

(2.3)

This vector defines an underlying structure called the Bravais lattice with each point on the lattice being a repeated unit cell which can be any combination of atoms. Due to the discrete translational symmetry of the Bravais lattice, the electronic eigenstates $\Psi_{nk}(\vec{r})$ of this system will be extended Bloch states defined by

$$\Psi_{nk}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{n,k}(\vec{r})$$

(2.4)

where $\vec{r}$ is the position, $n$ is the band index, and $\vec{k}$ is a wave vector that defines the quasi-momentum, or crystal momentum, of the electronic states by $\vec{p}_{\text{crystal}} = \hbar \vec{k}$. The function $u_{n,k}(\vec{r})$ must have the periodicity of the lattice as

$$u_{n,k}(\vec{r}) = u_{n,k}(\vec{r} + \vec{R}).$$  

(2.5)
From these previous two expressions, we can derive the Bloch condition

\[ \Psi_{n\kappa}(\vec{r} + \vec{R}) = e^{i\vec{k} \cdot \vec{R}} \Psi_{n\kappa}(\vec{r}) \]  

This expression is remarkably powerful as it essentially demonstrates that the entire set of electronic wavefunctions are determined by the properties of a single unit cell.

In general, two limiting cases are used to take advantage of the Bloch condition. The first approach is known as the nearly free electron approximation. In this case, we would start with the basis states of the free particle Hamiltonian and add a small perturbation that accounts for the crystal structure. This method is most useful in determining the properties of metals typically found in groups I-IV on the periodic table[7].

The second limiting case is known as the tight-binding approximation which assumes that the electrons are so tightly bound that the wavefunctions are best approximated by an expansion in terms of single atomic orbitals (s, p, d, ...). This method is most useful in describing covalent materials, transition metals, insulators, along with semi-conductors and will be the main approximation used in the proceeding work.

2.2 The Tight-Binding Model

As stated previously, in order to take advantage of the Bloch condition, Eq. (2.6), we work in the tight-binding (TB) approximation which assumes that each atomic site gives rise to bound states that are only weakly coupled to one another.

We begin by considering a single atomic site where the eigenstates \( \psi_n(\vec{r}) \) will be the typical s, p, d, states that satisfy

\[ H_{at}\psi_n(\vec{r}) = E_n\psi_n(\vec{r}) \]  

where \( H_{at} \) is the atomic Hamiltonian and \( E_n \) is the atomic eigenenergy. If we have a lattice of these non-interacting atomic sites, the full eigenstate will be given by a sum of single atomic site solutions with an exponential factor that is included to satisfy the Bloch
condition.
\[
\Psi_{nk}(\vec{r}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \psi_n(\vec{r} - \vec{R})
\]  
(2.8)

The summation is over all atomic sites with the position of each site given by \(\vec{R}\). We can show that this expression satisfies Eq. (2.6) by replacing \(\vec{r}\) with \(\vec{r} + \vec{R}'\). This gives
\[
\Psi_{nk}(\vec{r} + \vec{R}') = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \psi_n(\vec{r} - \vec{R} + \vec{R}')
\]  
(2.9)

and defining a new distance \(\Delta\vec{R} = \vec{R} - \vec{R}'\) giving
\[
\Psi_{nk}(\vec{r} + \vec{R}') = e^{i\vec{k}\cdot\vec{R}} \sum_{\vec{R}} e^{i\vec{k}\cdot\Delta\vec{R}} \psi_n(\vec{r} - \Delta\vec{R})
\]  
(2.10)

which by inserting Eq. (2.8) reproduces the Bloch condition
\[
\Psi_{nk}(\vec{r} + \vec{R}') = e^{i\vec{K}\cdot\vec{R}} \Psi_{nk}(\vec{r}).
\]  
(2.11)

Now, if we add a weak interaction potential
\[
H = H_{at} + U(\vec{r}),
\]  
(2.12)

the eigenstates will no longer be atomic orbitals. However, since the potential is weak it would be prudent to work in the atomic orbital basis. Using this, we will recast the problem in Fock space and construct the general tight-binding model.

First, we find the matrix elements of \(H\) through
\[
\int \psi^*_n(\vec{r} + \vec{R}') H \psi_m(\vec{r} + \vec{R}) d\vec{r} = E_m \int \psi^*_n(\vec{r} + \vec{R}') \psi_m(\vec{r} + \vec{R}) d\vec{r}
\]  
(2.13)

\[
+ \int \psi^*_n(\vec{r} + \vec{R}') U(\vec{r}) \psi_m(\vec{r} + \vec{R}) d\vec{r}.
\]

where we have taken advantage of Eq. (2.7). For simplicity and clarity, we will define the matrix elements
\[
H_{n,m}^{\vec{R},\vec{R}'} = \int \psi^*_n(\vec{r} + \vec{R}') H \psi_m(\vec{r} + \vec{R}) d\vec{r},
\]  
(2.14)
\[ U_{n,m}^{R,R'} = \int \psi_n^*(\vec{r} + \vec{R}') U(\vec{r}) \psi_m(\vec{r} + \vec{R}) d\vec{r}, \quad (2.15) \]

and

\[ S_{n,m}^{R,R'} = \int \psi_n^*(\vec{r} + \vec{R}') \psi_m(\vec{r} + \vec{R}) d\vec{r}, \quad (2.16) \]

which can be used to rewrite Eq. (2.13) as

\[ H_{n,m}^{R,R'} = E_m S_{n,m}^{R,R'} + U_{n,m}^{R,R'}. \quad (2.17) \]

The overlap integral \( S_{n,m}^{R,R'} \) is a measure of the amount of non-orthogonality between the electronic eigenstates centered at different atomic positions and its divergence from unity is often taken as a sign that the tight-binding model is invalid. In this work, we will assume that the crystalline objects we study are adequately described by the tight-binding model. Thus, we replace the overlap matrix by a unit matrix. This gives us

\[ H_{n,m}^{R,R'} = E_m \delta_{R,R'} \delta_{n,m} + U_{n,m}^{R,R'}. \quad (2.18) \]

From this point, we are now in a position to reforge the Hamiltonian in terms of a second quantization picture through Fock space operators[23] as

\[ H = \sum_{n,m} \sum_{R,R'} H_{n,m}^{R,R'} c_{n,R'}^\dagger c_{m,R} \quad (2.19) \]

where \( c^\dagger \) and \( c \) are the fermionic creation and annihilation operators which satisfy the anti-commutation relations

\[ \{ c_{n,R'}^\dagger, c_{m,R} \} = \delta_{R',R} \delta_{n,m} \quad (2.20) \]

\[ \{ c_{n,R}, c_{m,R} \} = \{ c_{n,R'}^\dagger, c_{m,R}^\dagger \} = 0 \quad (2.21) \]

where \( \delta \) is the Kronecker delta function.

For the systems addressed in this document, a single orbital description is sufficient. Thus, we will assume no interaction between different orbitals which makes the Hamiltonian diagonal in this subspace and drop the \( n \) and \( m \) subspace labels as a
consequence. Finally, since we have assumed that potential interactions between atomic sites are small, we will assume that interaction energies between neighboring sites are larger in comparison to more widely separated sites. Thus, we will assume that the only significant contributions to the Hamiltonian will come from on-site interactions and nearest-neighbor interactions. This allows us to write our final Hamiltonian as

\[
H = \epsilon \sum_R c_R^\dagger c_R + t \sum_{\langle R, R' \rangle} \left( c_R^\dagger c_{R'} + h.c. \right) \tag{2.22}
\]

where \( \langle ... \rangle \) stands for a sum over nearest-neighbor pairs, \( \epsilon \) is commonly called the on-site energy and is given Eq. (2.18) for \( R = R' \), and \( t \) is referred to as the hopping energy and is given by Eq. (2.18) for \( |R - R'| = a \) where \( a \) is the lattice constant (or in other words, the nearest-neighbors distance). Note that the label \( R \) corresponds to relevant quantum numbers in the system.

This model is mainly phenomenological as we have truncated the details of the crystal structure into the factors \( t \) and \( \epsilon \). Nevertheless, it has been shown to capture many physical phenomena and is an invaluable tool in the study of disordered electronic systems.

### 2.2.1 Example: Single Chain of Atoms

To illustrate the framework we have just presented, consider a one-dimensional chain of \( N \) atoms. The position of each site in the chain will be given by

\[
\vec{R} = a n \hat{x} \tag{2.23}
\]

where \( a \) is the spacing between the sites and \( n \) is an integer. We will assume the system has periodic boundary conditions,

\[
\Psi_K(NA) = \Psi_K(0) \tag{2.24}
\]

which when compared with the Bloch condition, Eq. (2.6), gives us

\[
e^{iKNA} = 1 \tag{2.25}
\]
with $K$ given by

$$K = \frac{2\pi m}{Na}. \quad (2.26)$$

The Hamiltonian for this system is

$$H = \epsilon \sum_{n=0}^{N-1} c_n^\dagger c_n - t \sum_{n=0}^{N-1} \left( c_n^\dagger c_{n+1} + h.c. \right) \quad (2.27)$$

where we have explicitly assumed $t$ is negative which corresponds to a lowering of energy when electrons move from site-to-site. We rewrite Eq. (2.8) in terms of Fock space operators as

$$\tilde{c}_m = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{i2\pi mn/N} c_n \quad (2.28)$$

where $\tilde{c}_m$ is the fermionic annihilation operator on wave vector state $K = 2\pi m/Na$ and the $\sqrt{N}$ comes from the normalization conditions. We can solve for $c_n$ by using properties of the discrete Fourier transform to find

$$c_n = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} e^{-i2\pi mn/N} \tilde{c}_m \quad (2.29)$$

Using this, we can rewrite our Hamiltonian in terms of $K$ as

$$H = \frac{1}{N} \sum_{m,m' = 0}^{N-1} \left( \epsilon \tilde{c}_m^\dagger \tilde{c}_{m'} - te^{iKa} \tilde{c}_m^\dagger \tilde{c}_{m'} + te^{-iKa} \tilde{c}_m \tilde{c}_{m'} \right) \sum_{n=0}^{N-1} e^{i2\pi (m-m')/N} \quad (2.30)$$

with the sum over $n$ being

$$\sum_{n=0}^{N-1} e^{i2\pi (m-m')/N} = N\delta_{m,m'} \quad (2.31)$$

and leading to the purely diagonal Hamiltonian

$$H = \sum_{m=0}^{N-1} (\epsilon - 2t \cos Ka) \tilde{c}_m^\dagger \tilde{c}_m \quad (2.32)$$

with each eigenstate having an energy

$$E(k) = \epsilon - 2t \cos Ka. \quad (2.33)$$

We plot the energy band in Fig. 2.1.
2.3 Transport in Ordered Systems

By using a modified version of the previous method or one of many solution methods that shall be discussed in subsequent sections, it is possible to solve any generic tight-binding model to find the energies of the system $E_n(\vec{k})$ (Note we have returned to a general description where in the previous section we assumed $n = 1$). At zero temperature, the electrons will occupy the lowest possible energy states until reaching the Fermi energy (the highest occupied energy level at zero temperature). For any perfect periodic crystal, the electron with energy $E_n(\vec{k})$ can be shown to travel with a mean velocity given by

$$v_n(\vec{k}) = \frac{1}{\hbar} \nabla E_n(\vec{k})$$  \hspace{1cm} (2.34)

where $n$ labels the energy band and $\vec{k}$ is the crystal momentum. In this case, we have stationary states that move at constant speed without dissipation. If the velocity of the states at the Fermi energy is non-zero, the material will be conducting regardless of the type of periodicity the crystal contains as the eigenstates of any ordered system will be completely extended across the crystal.
However, it is possible to have a system with a forbidden energy region directly above the Fermi level. This forbidden energy region is known as the band gap and its extent determines if a material is classified as a semiconductor or insulator when no disorder is present. We would like to stress that this classification system relies solely on the energy spectra and is irrespective of the details of the eigenstates.

2.4 Disordered Systems

As stated previously, in systems with discrete translational symmetry Bloch states extend across the entire system with a non-dissipative velocity making an analysis of the energy spectra sufficient for determining the metal/insulator classification of the material. However, if the electron were to be excited into a state that does not extend across the lattice and is instead localized in a small region of space, the system would not conduct as the electron could not traverse the lattice (See Fig. 2.2). In order to generate a state with this type of geometry, we would need to break the discrete translational symmetry of the system such that Bloch states no longer were eigenstates of the Hamiltonian. To this end, we will modify our tight-binding Hamiltonian, Eq. (2.22), to include an on-site disorder term

\[ H = \sum_{\vec{R}} \epsilon_{\vec{R}} c_{\vec{R}}^\dagger c_{\vec{R}} + t \sum_{\langle \vec{R}, \vec{R}' \rangle} \left(c_{\vec{R}}^\dagger c_{\vec{R}'} + h.c.\right) \]

(2.35)

where the new term $\epsilon_{\vec{R}}$ is the sum of the constant site energy $\epsilon$ and a disorder term. The new quantity $\epsilon_{\vec{R}}$ is a random variable which effectively breaks the translational invariance of the crystal. Historically, Phillip Anderson [4] first studied this model in 1958 by analyzing the diffusion of an electron. What he found was that even weak potential perturbations caused a suppression of electronic diffusion. He postulated that a disordered potential will cause the plane wave like Bloch states of the non-disordered system to scatter and destructively interfere with one another. This interference causes the new eigenstates of the system to be spatially localized in the material. As a consequence, an
electron that occupies a localized state will not be able to conduct through the system. This phenomena is commonly known as Anderson localization and Eq. (2.35) is referred to as the Anderson Hamiltonian.

![Figure 2.2: Cartoon of a localized wavefunction vs an extended Bloch wavefunction. If we consider that a source is connected to the left hand side of the system with drain to the right, then the electron occupying the extended state has a probability of going from the source to drain while the electron in the localized state cannot leave the conductor.](image)

In practice, many mechanisms can break the discrete translational symmetry and cause Anderson localization. For instance, in graphene (See Sec. 6.1), these mechanisms include magnetic impurities [14], strain[66], adsorbents[33], topological defects[59], corrugations[60], vacancies[36], and substrate interactions[98]. Alloys and amorphous materials naturally lack crystalline order and can also be considered as disordered[15]. A review of disorder effects in graphene can also be found in Ref. [61].

### 2.5 The Anderson Transition

We have argued previously that disorder has the ability to localize electronic states and that this can critically affect the conductivity of a material. However, this does not mean that disorder always localizes every eigenstate[99]. As we will show in Sec. 2.6, the dimensionality of the system and strength of the disorder play a key role in determining which energy states are localized and which remain extended[1]. In three-dimensional
systems, as well as some low-dimensional systems, there appear regions, in energy space, of localized and extended states that are sharply separated at particular values of energy. These energies are referred to as mobility edges. If we are able to pass through one of these energies, whether by changing the disorder statistics or the Fermi energy, the system undergoes an Anderson quantum phase transition[27]. We will now discuss some key concepts in Anderson localization theory.

### 2.6 Single Parameter Scaling Hypothesis

The criteria for inducing an Anderson transition are well understood for the case of uncorrelated disorder distributions. The keystone theory comes from analyzing the scaling function

$$\beta = \frac{d \ln \mathcal{G}}{d \ln L}$$

(2.36)

which was first introduced in Ref. [1].

It is argued that the only independent variable in Eq. (2.36) is the dimensionless conductance $\mathcal{G}$. However, a rigorous proof of this statement does not exist and the use of a single scaling variable is normally taken as an assumption. This is known as the single parameter scaling hypothesis (SPS). If SPS holds, the scaling trajectory is solely dependent on $\mathcal{G}$ and the existence of an Anderson transition depends on the dimensionality of the system: For 1D and 2D systems, all states will localize, while in 3D an Anderson transition occurs for weak disorder[1].

To verify the SPS hypothesis, it is necessary to look at the entire probability distribution $P(\ln \mathcal{G})$ or equivalently the cumulants of the distribution[6]. We define the first two as

$$C_1 = \langle \ln \mathcal{G} \rangle$$

(2.37)

and

$$C_2 = \langle (\ln \mathcal{G} - C_1)^2 \rangle$$

(2.38)
For SPS to hold, each cumulant must only depend on the value of $C_1$, however to find violations we need only show that $C_2$ is a function of more than one variable.

In the case of weakly disordered one-dimensional systems, it has been shown that the first and second cumulant follow the relationship\cite{6, 22}

$$C_2 = -2C_1$$

while similar relations can be obtained for all higher cumulants. This relationship is commonly used to test the validity of SPS against numerical results for the dimensionless conductance\cite{22, 81}. While this cannot be considered a proof of SPS, it is sufficient to show violations of the hypothesis.

In the case of uncorrelated disorder, no violation of SPS are found with the exception of states near the band edge ($E/t=2$) \cite{80} and band center ($E/t=0$)\cite{81}. For $E/t = 0$, it has been argued that this anomaly is due to the intersection of two bands that result from a hidden spatial symmetry in the tight-binding Hamiltonian\cite{21}.

### 2.7 The Localization Length

As we have shown, verifying the SPS hypothesis is difficult due to the statistical variations of the dimensionless conductance. Thus, it is convenient to introduce a new variable

$$\tilde{\lambda}(L) = \frac{1}{2L} \ln \left( 1 + \frac{1}{G} \right) = \frac{1}{2L} \left( \ln(1 + G) - \ln G \right).$$

called the Lyapunov exponent with $L$ the length of the one-dimensional system. The reason we choose to work with $\tilde{\lambda}(L)$ is that in the $L \to \infty$ limit, it converges to a Gaussian distribution with a non-random average\cite{6}. Furthermore, the limit of $\tilde{\lambda}(L)$ is related to the localization length $\lambda$ by

$$\lambda = \lim_{L \to \infty} \frac{1}{\tilde{\lambda}(L)}.$$
where $\lambda$ is a measure of the range of a localized state\[99\]. It should be noted that the localization length gives us much more than just a tool to verify the SPS hypothesis. Rather this quantity gives us a physical length scale that can be used to measure the range of an eigenstate. I.e. if the localization length approaches infinity in the thermodynamic limit, the corresponding state is extended. If the localization length approaches a finite value, it is localized.

An equivalent definition\[99\] of the Lyapunov exponent is

$$\tilde{\lambda} = \lim_{N \to \infty} \frac{1}{N} \ln |T_N \ldots T_1 \Psi|$$

(2.42)

where $T_n$ is called a transfer matrix. This concept will be discussed in greater detail in Sec. 3.2.

### 2.8 Kotani Theory of Random Ergodic Operators

A general advancement in classifying the existence of an Anderson transition was put forward in the early 1980’s by S. Kotani\[49\]. This initial work applied to continuous one-dimensional random Schrödinger operators of the form

$$H\psi(x) = -\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)$$

(2.43)

and proved that the Lyapunov exponent, using the definition provided in Eq. (2.42), could only have zero values when the disorder was deterministic. Deterministic in this sense implies that the disorder potential operator $V(x)$ is a.e. a measurable function\[83\] which in terms of probability theory means $V(x)$ must be predictable based on available information. A possible way to create a deterministic potential is through strong long-range correlations. For rigorous mathematical proofs of determinism see Refs. \[49, 83\].
These results were extended to encompass the set of discrete random Schrödinger operators that satisfy

$$H\psi(n) = \psi(n+1) + \psi(n-1) + V(n)\psi(n)$$

(2.44)
in the following year by B. Simon[83]. This model Hamiltonian is precisely the tight-binding Anderson Hamiltonian for 1D systems.

While the theorems developed by Kotani and Simon apply to many classifications of random potentials, we would like to point out the results of example 2 presented in Ref. [48]. There they show that, regardless of its exact form, a decaying correlation function for a stationary Gaussian process with $\langle V(x) \rangle = 0$ will yield non-zero Lyapunov exponents. In other words, a correlation function that goes to zero in the thermodynamic limit will not produce extended states. This result is a vital and strong necessary condition in the theory of Anderson transitions.

### 2.9 Correlated Disorder

From the arguments of Sec. 2.8, we have seen that an Anderson transition in a one-dimensional system would be possible only through long-range correlations[48] (e.g. correlations that approach finite values in the thermodynamic limit). This is only a necessary condition and does not predict what features the disorder correlations should have to guarantee the appearance of an Anderson transition. To provide some insight, we will review some previous numerical results on correlated one-dimensional systems.

The first numerical observation of extended states comes from the random dimer model[24]. This work provides an algorithm for generating a correlated distribution that causes the existence of extended states. It begins with generating an uncorrelated binary disorder potential that can take values $\epsilon_A$ or $\epsilon_B$. After generating the uncorrelated disorder distribution, correlations are added by replacing all odd clusters of $\epsilon_B$ with $\epsilon_A$. This effectively leaves only even clusters of $\epsilon_B$ or in other words, $\epsilon_B - \epsilon_B$ dimer pairs. The result
is the appearance of extended states when the condition $-2t < \epsilon_A - \epsilon_B < 2t$, where $t$ is the nearest-neighbor hopping energy in the tight-binding model, is satisfied. This demonstrates the existence of extended states and a dependence on the disorder strength and hopping energy $t$ that was seen in three dimensional single parameter scaling theory[1]. A visualization of this disorder generation process is presented in Fig. 2.3.

Figure 2.3: A small distribution for the random dimer model with black colored points indicating sites with energy $\epsilon_A$ and red being sites with $\epsilon_B$. The top figure is the uncorrelated binary distribution with the middle figure indicating the non-dimer pairs (note that these include all odd numbered groups of $B$ atoms). The final figure shows the final disorder distribution with the correlation introduced by replacing all non-dimer pairs of $B$ atoms with $A$ atoms.

The seminal example of a continuous correlated disorder distribution that generates a set of extended states involves a spectral density of the form $S(k) \sim 1/k^{\alpha}[19]$ with the spectral density related to the correlation function of the disorder potential by an inverse Fourier transformation. This correlation gives rise to a band of extended states around $E = 0$ for $\alpha > 2$. However, this correlation has received a good deal of criticism due to the
correlation function’s unphysical dependence on the system size [76, 96]. In Ref. [31], it was suggested that the correlation function associated with this model fails to satisfy the conditions for a metallic state laid down by Kotani theory (Sec. 2.8).

Before addressing this matter, we will first introduce the numerical methods used throughout the rest of this dissertation.
3 **Numerical Methods**

3.1 Disorder Generation

In general, it is difficult to generate a set of correlated random variables for any arbitrary correlation, especially those with long-range order. Some success has been found in generating random variables by adjusting a set of uncorrelated random values by the spectral density[99, 30]. However, this methods tends to fail when correlations become longer ranged. For the specific case of $\sim 1/x^\alpha$ correlations (where $x$ is the real space position), the spectral method has been adjusted[56] such that very small values of $\alpha$ (or very long-ranged correlations) can be generated to great accuracy. A more novel approach to disorder generation borrows concepts from thermal annealing algorithms to create long-range correlations. Proof of concept has been shown for fractional Brownian motion[34] but a general algorithm has not been developed. Since ultimately we would like to test a wide range of correlations, we will focus our efforts on the general spectral method.

Let the element $\epsilon_n \in \mathbb{R}$ and be determined from the probability distribution $P(\epsilon_n)$ with average value $\langle \epsilon_n \rangle = 0$, variance $\langle \epsilon_n^2 \rangle = 1$, and two-point correlation $\Gamma(n, m)$. We define the Fourier transform and inverse Fourier transform of $\epsilon_n$ by

$$\epsilon_n = \sum_{k=0}^{N-1} \tilde{\epsilon}_k e^{-i2\pi nk/N}$$  \hspace{1cm} (3.1)

$$\tilde{\epsilon}_k = \frac{1}{N} \sum_{n=0}^{N-1} \epsilon_n e^{i2\pi nk/N}$$  \hspace{1cm} (3.2)

where $k$ and $n$ are integers, $N$ is the total number of elements in the sample space, and $\tilde{\epsilon}_k$ is the reciprocal value of the sample space. The spectral density is defined as $S(k) = \langle |\tilde{\epsilon}_k|^2 \rangle$. Using this definition and Eq. (3.2), we can relate the spectral density to the two-point correlation function of $P(\epsilon_n)$ by

$$S(k) = \langle |\tilde{\epsilon}_k|^2 \rangle = \frac{1}{N^2} \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} \Gamma(n, m)e^{i2\pi k(n-m)/N}.$$  \hspace{1cm} (3.3)
In many physical systems, the correlation function is isotropic, \( i.e. \) 
\[ \Gamma(n, m) \rightarrow \Gamma(|n - m|), \]
and can be fully described by the relative distance \( \Delta n = n - m \) where 
\( \Delta n \in [-N + 1, N - 1] \). This allows the sums to be expanded as

\[
S(k) = \Gamma(N - 1)e^{-i2\pi k(N - 1)/N} + 2\Gamma(N - 2)e^{-i2\pi k(N - 2)/N} + \\
+3\Gamma(N - 3)e^{-i2\pi k(N - 3)/N} + ... + 3\Gamma(N - 3)e^{i2\pi k(N - 3)/N} + \\
+2\Gamma(N - 2)e^{i2\pi k(N - 2)/N} + \Gamma(N - 1)e^{i2\pi k(N - 1)/N}
\]  
\[ (3.4) \]

where the prefactor in each term is the number of ways \( n \) and \( m \) can be arranged to yield 
\( \Delta n \) (e.g. \( \Delta n = N - 3 \) has 3 possible configurations of \([n, m], [N - 1, 2], [N - 2, 1], \) or 
\([N - 3, 0]\)). The terms can be combined to give the expression

\[
S(k) = \frac{1}{N^2} \left[ N\Gamma(0) + 2 \sum_{n=1}^{N-1} (N - n)\Gamma(n) \cos \frac{2\pi kn}{N} \right].
\]  
\[ (3.5) \]

where we have used \( n \) in place of \( \Delta n \) for notational simplicity. This expression is general 
and can be applied to any isotropic correlation function.

Next, the values of \( S(k) \) are used to generate a set \( \{\tilde{\epsilon}_k\} \) from uncorrelated Gaussian 
probability distributions, \( \Omega_k \), with a variance equal to the spectral density

\[
\Omega_k(\tilde{\epsilon}_k) = \frac{1}{\sqrt{2\pi S(k)}} e^{-|\tilde{\epsilon}_k|^2/2S(k)}. 
\]  
\[ (3.6) \]

We explicitly write the magnitude of \( \tilde{\epsilon}_k \) as this quantity should be complex to generate any 
possible set of random real values. Since the spectral density only depends on the 
magnitude of \( \tilde{\epsilon}_k \), a phase \( \theta \) can be chosen arbitrarily from a uniform distribution between 0 
and \( 2\pi \). Thus, each element in the set \( \{\tilde{\epsilon}_k\} \) is given by

\[
\tilde{\epsilon}_k = |\tilde{\epsilon}_k|e^{i\theta}. 
\]  
\[ (3.7) \]

Since we require \( \epsilon_n \in \mathbb{R} \), the elements of \( \{\tilde{\epsilon}_k\} \) must be related to one another by

\[
\tilde{\epsilon}_k = \tilde{\epsilon}_{N-k}^*.
\]  
\[ (3.8) \]
with the exception of \( k = 0 \) and \( k = N/2 \) which must be real. This condition is explicitly applied after the initial generation of \( \{\tilde{\epsilon}_k\} \).

Finally, the Fourier transform (eq. 3.1), is applied on \( \{\tilde{\epsilon}_k\} \) and a set of real random variables satisfying the mean, variance, and two-point correlation function requirements are generated.

To test our procedure, we will apply this method to the correlation function

\[
\Gamma(n) = \langle \epsilon_i \epsilon_j \rangle = \frac{1}{(1 + |n|)^\alpha}.
\]

which will give a spectral density of

\[
S(k) = \frac{1}{N^2} \left[ N + 2 \sum_{n=1}^{N-1} \frac{(N-n)}{(1+n)^\alpha} \cos \frac{2\pi kn}{N} \right].
\]

(3.10)

We numerically calculate the correlation function from the generated disorder by

\[
\Gamma(n) = \sum_{m=0}^{N-1} \epsilon_m \epsilon_{m+n}
\]

(3.11)

and average over multiple disorder realizations. Some of these results are plotted in Fig. 3.1. From these results, the numerics seem to overshoot the expected correlation strength for smaller system sizes and are more similar, yet not exact, to correlations with larger values of \( \alpha \). When the system size is increased the numerically generated correlation function matches with the expected correlation function. This result emphasizes the difficulty in numerically generating long-range correlations and the need to test if the correlation put in are obtained in the output.

Now that we have addressed the generation of correlated disorder, we shall discuss a few common methods for solving the Anderson Hamiltonian.

### 3.2 The Transfer Matrix Method

Transfer matrix techniques have been shown to be one of the most efficient ways to determine the existence of a localization/delocalization transition [50]. This method can
Figure 3.1: The resulting correlation function from the spectral disorder generation method for different system sizes. The solid red and orange lines are the expected values (Eq. (3.9)) of the correlation function for $\alpha = 0.5$ and $\alpha = 0.6$. The purple, blue, and black lines represent systems of size $2^{10}$, $2^{14}$, and $2^{16}$ respectively. For each numerical data set, $\alpha = 0.5$, $w/t = 1$. For the smallest system size, we see that the curve more closely follows a correlation of $\alpha \sim 0.6$ instead of the expected correlation value of $\alpha = 0.5$. As the system size increases, the generated values follow more closely the expected output.

be used to extract the localization length by a series of matrix multiplications and finite size scaling\[99\]. Let us consider a quasi-one dimensional system that stretches to infinity in the $\hat{x} - axis$ and is finite in the $\hat{y} - axis$ and $\hat{z} - axis$. If this system is periodic in $\hat{x} - axis$, there will exist a unit cell which describes the system at each point along the infinite direction. The Hamiltonian describing this system can be broken into two components, one describing the energy interactions within the unit cell, and one describing the interactions between unit cells. We refer to these as $h_{n,n}$ and $h_{n,n+1}$ respectively, where $n$ labels the position of the unit cell.

The matrix $T_n$, which satisfies the condition

$$
\begin{pmatrix}
\psi_{n+1} \\
\psi_n
\end{pmatrix} = T_n \begin{pmatrix}
\psi_n \\
\psi_{n-1}
\end{pmatrix}
$$

(3.12)
is defined as the transfer matrix where \( \psi_n, \psi_{n+1}, \) and \( \psi_{n-1} \) are the wavefunctions at unit cell positions \( n, n+1, \) and \( n-1 \) respectively. In general, the transfer matrix is given by

\[
T_n = \begin{pmatrix}
    h_{n,n+1}^{-1}(E - h_{n,n}) & -h_{n,n+1}^{-1}h_{n,n-1} \\
    1 & 0
\end{pmatrix}
\]

(3.13)

This matrix is an equivalent representation of the standard Schrödinger equation

\[
E\psi_n = H\psi_n = h_{n,n}\psi_n + h_{n,n+1}\psi_{n+1} + h_{n,n-1}\psi_{n-1}.
\]

(3.14)

which is derived by carrying out the matrix multiplication in Eq. (3.12).

By successive matrix multiplication, we can calculate the total transfer matrix across sites 1 to \( N \) as

\[
\tilde{T}_N = T_1T_2T_3...T_N.
\]

(3.15)

The smallest positive eigenvalue of the matrix

\[
\Omega_N = \ln(\tilde{T}_N\tilde{T}_N^+)\]

(3.16)

will be the Lyapunov exponent \( \tilde{\lambda} \), which is a function of the energy \( E \) and system size. As stated earlier, this can be related to the localization length of the system through the limit relation

\[
\frac{1}{\lambda} = \lim_{N \to \infty} \frac{\tilde{\lambda}}{2N}.
\]

(3.17)

We now turn our attention to a similar approach outlined in Ref. [55] for a single chain with a one-site unit cell. For this system, the transfer matrix is given by

\[
T_n = \begin{pmatrix}
(E - \epsilon_n)/t & -1 \\
1 & 0
\end{pmatrix}
\]

(3.18)

where \( E \) is the energy of the eigenstate under examination, \( t \) is a constant hopping energy between nearest neighbor sites, and \( \epsilon_n \) is the on-site potential at site \( n \). The choice of the initial state in Eq. (3.12) is arbitrary. Thus, we will choose an initial state \( (\psi_1, \psi_0) = (1, 0) \).
Using this initial vector in tandem with the transfer matrices, we can find the final vector \((\psi_N, \psi_{N-1})\). This final vector can then be related to the lowest Lyapunov exponent by

\[
\tilde{\lambda} = \lim_{N \to \infty} \frac{1}{N} \ln(|\psi_N|^2 + |\psi_{N-1}|^2).
\]  

(3.19)

To solve for the final vector \((\psi_N, \psi_{N-1})\), we use a recursive method based on successive multiplications of the initial vector \((1, 0)\). Please note that the variables \(C_i\) do not refer to cumulants in this section. The first multiplication is

\[
T_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{(E - \epsilon_1)}{t} \\ 1 \end{pmatrix} = \begin{pmatrix} C_1 \\ 1 \end{pmatrix}
\]  

(3.20)

where

\[
C_1 = \frac{(E - \epsilon_1)}{t}.
\]  

(3.21)

Now, we take the second matrix multiplication

\[
T_2 \begin{pmatrix} C_1 \\ 1 \end{pmatrix} = C_1 \begin{pmatrix} \frac{(E - \epsilon_2)}{t} - \frac{1}{C_1} \\ 1 \end{pmatrix} = C_1 \begin{pmatrix} C_2 \\ 1 \end{pmatrix}
\]  

(3.22)

where

\[
C_2 = \frac{(E - \epsilon_2)}{t - C_1^{-1}}.
\]  

(3.23)

The new vector, aside from a prefactor of \(C_1\), is identical to the vector after the first multiplication. Thus, another matrix multiplication will give us the same form with an additional prefactor of \(C_2\) as

\[
T_3 \begin{pmatrix} C_2 \\ 1 \end{pmatrix} = C_1C_2 \begin{pmatrix} \frac{(E - \epsilon_3)}{t} - \frac{1}{C_2} \\ 1 \end{pmatrix} = C_1C_2 \begin{pmatrix} C_3 \\ 1 \end{pmatrix}
\]  

(3.24)

where

\[
C_3 = \frac{(E - \epsilon_3)}{t - C_2^{-1}}.
\]  

(3.25)

Thus we arrive at a general recursive form for all \(C_n\)’s

\[
C_n = \frac{(E - \epsilon_n)}{t - C_{n-1}^{-1}}
\]  

(3.26)
and a final state vector of

$$\begin{pmatrix}
\psi_N \\
\psi_{N-1}
\end{pmatrix} = \tilde{T}_N \begin{pmatrix} 1 \\ 0 \end{pmatrix} = C_1 C_2 C_3 \ldots C_{N-1} \begin{pmatrix} C_N \\ 1 \end{pmatrix}.$$  

(3.27)

Placing the final state vector into eq. 3.19, we arrive at

$$\gamma(E) = \frac{1}{N} \ln \left[ |C_N|^2 + 1 \right] + \frac{2}{N} \sum_{n=1}^{N-1} \ln |C_n|$$

(3.28)

after $C_1 C_2 C_3 \ldots C_N$ is separated into a sum of logarithms.

To test our routines, we duplicate the results of incommensurate potentials presented in Ref. [55]. Here, we study a disorder potential that is of the form $\epsilon_n = \Delta_n \cos nQ$ where $\Delta_n$ is the amplitude of the disorder, $n$ is an integer, and $Q$ is an irrational number multiplied by $\pi$. $Q$ is generated by a continued fraction expansion where

$$Q = \frac{2\pi}{r + \frac{1}{r + \frac{1}{r + \ldots}}}$$

(3.29)

and is uniquely determined by a rational value $r$.

Our results are plotted in Fig. 3.2 and some differences between the two results appear, namely, small fluctuations in the data for $\lambda^{-1} \sim 0$. Since the results in Ref. [55] were produced in 1984, we believe that the discrepancy is more than likely due to the limits of precision at that time.

### 3.3 Conductance Calculation Method

Another quantity of interest in disordered systems is the dimensionless conductance $G$ whose importance was discussed previously in Sec. 2.6. Along with its relation to scaling theory, the conductance is one of the typical quantities that can be measured in a laboratory setting, unlike the localization length (However, recent advances in cold atomic gases[8] provided a method for imaging the wavefunction and allowing the extrapolation of the localization length). It was proposed more than half a century ago[53] that the
Figure 3.2: (Top) Results from Ref. [55], (Bottom) Our results for a cosine incommensurate potential. Both methods discussed were applied producing identical results. Parameters: $N = 5000$, $r = 3$, and $\Delta_\alpha = 1.9$ which correspond to the system size, the variable determining the irrational factor in the incommensurate potential, and the amplitude of the cosine incommensurate potential respectively. The graph is symmetric around $E = 0$ and only the negative portion is shown for clarity.

electrical conductance was related to the sum of all electronic transmission channels by the simple formula

\[ G(E) = \frac{2e^2}{h} \sum_n T_n(E) \]  

which is typically referred to as the Landauer formula. In this expression, $T_n$ refers to the transmission through channel $n$ with $2e^2/h$ being the universal electron conductance quantum. In the following, we will consider $G$ to be dimensionless by setting $\frac{2e^2}{h} = 1$. In a clean system, the total transmission at energy $E$ is equal to the number of propagating
modes at $E$. For the case of a clean one-dimensional chain we only have a single conducting channel implying $G = T_1$.

Figure 3.3: (Top) A system with two semi-infinite perfect leads (Black) and a disordered conductor (Green). The squares represent any repeated unit cell with the Hamiltonian for intra-cell interactions given by $h_{n,n}$ and inter-cell interaction given by $h_{n,n+1}$. (Bottom) An example of a specific unit cell, in this case a graphene nanoribbon of width 3 (See Sec. 6.1 for further details on graphene).

Because of the proximity of this theoretical quantity to experimental measurements, it seems natural to consider a system that closely resembles a general transport experiment. Therefore, consider an infinite one-dimensional lattice separated into three regions as shown in Fig. 3.3. When the position $n \in (-\infty, 1)$ and $n \in (N, \infty)$ the lattice will be clean while the middle section, $n \in [1, N]$, will contain disorder. This allows us to write the general tight-binding matrix as

$$H = \begin{pmatrix}
H_L & H_{LC} & 0 \\
H_{LC}^\dagger & H_C & H_{RC} \\
0 & H_{RC}^\dagger & H_R
\end{pmatrix}$$

where $H_L$ and $H_R$ are the Hamiltonian’s for all sites to the left and right of the conductor, $H_C$ is the Hamiltonian of the conductor, and $H_{LC}$ and $H_{LR}$ are the coupling between the leads and conductor. This model was first solved in Ref. [11] with several detailed reviews
of the numeric solution method that we will present in the following chapter given in Refs. [52, 63].

Since the conductance is a response function, it can be represented, within linear response theory, in terms of Green’s functions[3]. The most physically relevant is the retarded Green’s function operator

$$G^r(E) = \frac{1}{E - H - i\eta}$$  \hspace{1cm} (3.32)$$

where $E$ is the energy level, $H$ is Hamiltonian, and $\eta \ll 1$ which is included to remove the pole when $H\psi = E\psi$ and reproduce causality. Once the Green’s function is known, we are able to calculate the density of states as well as the transmission. Mathematically, this boils down to taking the inverse of the infinite matrix $(E - H - i\eta)$. In the same block-matrix form presented previously, the Green’s function can be written as

$$\begin{pmatrix}
G_L^r & G_{LC}^r & G_{LCR}^r \\
G_{CL}^r & G_C^r & G_{CR}^r \\
G_{RCL}^r & G_{RC}^r & G_R^r \eta
\end{pmatrix} = \begin{pmatrix}
E - H_L - i\eta & -H_{LC} & 0 \\
-H^\dagger_{LC} & E - H_C - i\eta & -H_{RC} \\
0 & -H^\dagger_{RC} & E - H_R - i\eta
\end{pmatrix}^{-1}$$  \hspace{1cm} (3.33)$$

where the Green’s functions have been divided into there areas of propagation (e.g. $G_L^r$ is the green’s function across the left lead). Of these matrix elements, we need only concern ourselves with the Green’s function across the conductor of the system: $G_C^r$. Through a matrix inversion, we find that

$$G_C^r = \left[ E - H_c - i\eta - H_{LC}^\dagger \frac{1}{E - H_L - i\eta} H_{LC} - H_{RC}^\dagger \frac{1}{E - H_R - i\eta} H_{RC} \right]^{-1}.$$  \hspace{1cm} (3.34)$$

We define the latter two terms as the self-energies

$$\Sigma_L(E) = H_{LC}^\dagger \frac{1}{E - H_L - i\eta} H_{LC}$$  \hspace{1cm} (3.35)$$

and

$$\Sigma_R(E) = H_{RC}^\dagger \frac{1}{E - H_R - i\eta} H_{RC}.$$  \hspace{1cm} (3.36)$$
The self energies are used to define the hybridization functions

\[ \Gamma^{L,R}(E) = i[\Sigma^r_{L,R}(E) - \Sigma^a_{L,R}(E)] \] (3.37)

that contain all information regarding the connection of the conductor to the leads. Using these definition, we can relate the Green’s function of the conductor, along with any contribution from inter-facial scattering, by the Caroli formula [11]:

\[ G(E) = tr\{\Gamma^L G^r \Gamma^R (G^r)^\dagger\} \] (3.38)

where \( tr \) stands for the trace.

3.3.1 Calculation of Self-Energies

As things stand now, we are not able to numerically solve the Green’s function due to the semi-infinite leads. To progress further, we will make use of a recursive numerical method that can summarize the effects of a lead in a single matrix element. We will follow the procedure outlined in Refs. [78, 63].

Since the leads are made up of repeated non-disordered unit cells, the Hamiltonian of the system contains only two unique matrices \( h_0 = h_{n,n} \) and \( h_1 = h_{n,n+1} \) which contain the intra-cell and inter-cell interactions respectively with all other \( h_{n,m} = 0 \) as we do not consider interactions between non-nearest neighbor cells. We will refer to these matrices as block matrices as they are of dimension \( b \times b \) where \( b \) is the total number of states in a single unit cell. In block matrix form, Hamiltonian of the lead is

\[
H_{L,R} = \begin{pmatrix}
    h_0 & -h_1 & 0 & 0 & \ldots \\
    -h_1^\dagger & h_0 & -h_1 & 0 & \ldots \\
    0 & -h_1^\dagger & h_0 & -h_1 & \ldots \\
    0 & 0 & -h_1^\dagger & h_0 & \ldots \\
    \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\] (3.39)
We can find a set of coupled equations for every Green’s function element through the definition of the retarded Green’s function pertaining to the left lead

$$(\omega - H_L)G'_L = \mathbb{1}$$

(3.40)

where $\omega = E - i\eta$ and $\mathbb{1}$ is the semi-infinite unitary matrix. This equation can be represented in matrix form as

$$\mathbb{1} = \begin{pmatrix}
\omega - h_0 & h_1 & 0 & 0 & \ldots \\
-\bar{h}_1 & \omega - h_0 & h_1 & 0 & \ldots \\
0 & -\bar{h}_1 & \omega - h_0 & h_1 & \ldots \\
0 & 0 & -\bar{h}_1 & \omega - h_0 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix} G'_r. 
$$

(3.41)

Note that though we are using the notation for the left lead, an identical equation exists for the right. Thus, we can see that by performing a matrix multiplication, we can derive a set of coupled equations that lead to the relationships

$$(\omega - h_0)G'_{0,0} = \mathbb{1} - h_1 G'_{1,0}$$

(3.42)

where $\mathbb{1}$ in this expression is of order $b \times b$ and

$$-(\omega - h_0)G'_{n,0} = \bar{h}_1 G'_{n-1,0} + h_1 G'_{n+1,0}$$

(3.43)

for any $n$. Note that the subscripts of the Green’s functions correspond to their matrix element. From the previous set of equations, we can define a new variable $t_n$ as

$$t_0 = (\omega - h_0)^{-1}h_1 \bar{h}_1$$

(3.44)

$$\bar{t}_0 = (\omega - h_0)^{-1}h_1$$

(3.45)

and a recursive relationship for all $n$ given by

$$t_n = (\mathbb{1} - t_{n-1}\bar{t}_{n-1} - \bar{t}_{n-1}t_{n-1})^{-1}t_{n-1}^2.$$ 

(3.46)
\[ \tilde{t}_n = (1 - t_{n-1}\tilde{t}_{n-1} - \tilde{t}_{n-1}t_{n-1})^{-1/2\tilde{t}_{n-1}}. \] (3.47)

The recursion continues until the desired precision is obtained, i.e. \( t_n < \delta \) where \( \delta \) is an arbitrarily small value. Similar to our derivation of the localization length, we can define the transfer matrices \( T \) and \( \tilde{T} \) as

\[ G_{n+1,0}^r = TG_{n,0}^r, \] (3.48)

and

\[ \tilde{T}G_{n+1,0}^r = G_{n,0}^r, \] (3.49)

which are related to the \( t_n \) variables by

\[ T = t_0 + \tilde{t}_0t_1 + \tilde{t}_0\tilde{t}_1t_2 + ... + \tilde{t}_0\tilde{t}_1\tilde{t}_2...t_n \] (3.50)

\[ \tilde{T} = \tilde{t}_0 + t_0\tilde{t}_1 + t_1t_2\tilde{t}_3 + ... + t_0t_1t_2...\tilde{t}_n. \] (3.51)

Finally, we can find the self-energies

\[ \Sigma_L(E) = H_{LC}^\dagger \tilde{T} \] (3.52)

and

\[ \Sigma_R(E) = H_{RC}T. \] (3.53)

Through this recursive method, what we have effectively done is encapsulated the effect of both the left and right semi-infinite leads, along with their connections to the conductor, within two block matrix elements of size \( b \times b \).

The size of \( H_C \) is \( N \times N \) block matrices of size \( b \times b \). Also, the \( \Gamma \) matrices in Eq. (3.37) are the same size as \( H_C \) but are largely zero. The only non-zero values for these matrices are the block matrix elements \( \Gamma_{1,1}^L \) and \( \Gamma_{N,N}^R \) which are determined from the self-energy calculation procedure above.

Substituting Eq. (3.37) and Eq. (3.34) into Eq. (3.38), we find that the only necessary element of the conductor Green’s function is \( G_{1,N}^r \) (note we have dropped the subscript \( c \)
for brevity) and the conductance reduces to

\[ G = tr[\Gamma_{1,1}^L G_{1,N}^r \Gamma_{N,N}^R (G_{1,N}^r)^\dagger] \]  

(3.54)

### 3.3.2 Recursive Green’s Function Method

To find \( G^r \), we need to take the inverse of \( \omega - H_C - \Sigma^L - \Sigma^R \) which can be represented in matrix form as

\[
[G^{-1}] = \begin{pmatrix}
\omega - h_{1,1} - \Sigma^L & h_{1,2} & 0 & \ldots & 0 & 0 \\
h_{2,1} & \omega - h_{2,2} & h_{2,3} & \ldots & 0 & 0 \\
0 & h_{3,2} & \omega - h_{3,3} & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & h_{N-2,N-1} & 0 \\
0 & 0 & 0 & h_{N-1,N-2} & \omega - h_{N-1,N-1} & h_{N-1,N} \\
0 & 0 & 0 & 0 & h_{N,N-1} & \omega - h_{N,N} - \Sigma^R
\end{pmatrix}
\]  

(3.55)

Numerically, a direct inverse of this matrix requires an order \((Nb)^3\) operations and delivers every matrix element of \( G^r \). However, since we only need a single element of the inverse to calculate the conductance, we will employ the recursive Green’s function technique that delivers only the diagonal elements of the green’s function along with \( G_{1,N}^r \). By focusing on these necessary elements, the order of operations is reduced to \( Nb^3 \) which greatly reduces the computation time as long as \( b \) is small[45].

The recursive Green’s function technique relies on taking the partial inverse, \( g_n^r \), of the diagonal elements of \( G^r \), and using this partial inverse to recursively find all of the true diagonal elements \( G_{n,n}^r \) as well as the Green’s function across the conductor \( G_{1,N}^r \). This method is explained in detail in Refs. [52, 45].

First, we find the partial inverse of the top-left block of Eq. (3.63)

\[ g^r = (\omega - h_{1,1} - \Sigma^L)^{-1} \]  

(3.56)
where the effect of the left lead is contained in \( \Sigma^L \). Next, we must connect the partial inverse at site 1 to the partial inverse at site 2. These two elements are connected solely by the hopping elements \( h_{1,2} \) and \( h_{2,1} \) in Eq. (3.63), giving

\[
g'_2 = (\omega - h_{2,2} - h_{1,2}g'_1h_{1,2})^{-1}
\]

(3.57)

which can be generalized to all sites as

\[
g'_n = (\omega - h_{n,n} - h_{n,n-1}g'_{n-1}h_{n-1,n})^{-1}.
\]

(3.58)

For the final case, the partial inverse contains an extra term, \( \Sigma^R \) that contains the effect of the right lead

\[
G'_{N,N} = g'_N = (\omega - h_{N,N} - \Sigma^R - h_{N,N-1}g'_{N-1}h_{N-1,N})^{-1}
\]

(3.59)

and \( G'_{N,N} \) is first true inverse of the Green’s function. To find the remaining diagonal elements of the green’s function, we use the recursion equation

\[
G'_{n,n} = g'_n (\mathbb{1} + h_{n,n+1}G'_{n+1,n+1}h_{n+1,n}g'_n)
\]

(3.60)

which is valid for \( n < N \). Thus, we now have the true diagonal of the Green’s function. To find the element of the Green’s function at \((1, N)\), we use the recursion relation

\[
G'_{n,N} \bigg|_{n<N} = -g'_n h_{n,n+1} G'_{n+1,N}
\]

(3.61)

which after \( N - 1 \) iterations give us the necessary element of the Green’s function to solve Eq. (3.54).

We would also like to note that a full calculation of the diagonal elements of the Green’s function is not necessary to determine the element \( G'_{1,N} \). However, the diagonal elements contain information on the total density of states of the system. These are related by

\[
\nu(E) = -\frac{1}{\pi} \text{Im}[tr(G'(E))]
\]

(3.62)

where \( \nu \) is the density of states at energy \( E \), \( tr \) stands for the trace, and \( \text{Im}[] \) means the imaginary part.
3.4 Example: One-Dimensional Single Site Anderson Hamiltonian

To illustrate these equations, we will apply this technique to a one-site basis Anderson Hamiltonian (Eq. (3.14)) where all block matrices are size 1 × 1 with
\[ t = h_{n,n+1} = h_{n+1,n} \text{ and } \epsilon_n = h_{n,n} \] which contains the disorder of the system. This gives us a matrix form of
\[
[G^r]^{-1} = \begin{pmatrix}
\omega - \epsilon_1 - \Sigma^L & t & 0 & \ldots & 0 & 0 \\
t & \omega - \epsilon_2 & t & \ldots & 0 & 0 \\
0 & t & \omega - \epsilon_3 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & t & 0 \\
0 & 0 & 0 & 0 & t & \omega - \epsilon_{N-1} \\
0 & 0 & 0 & 0 & 0 & t & \omega - \epsilon_N - \Sigma^R \\
\end{pmatrix}.
\]
(3.63)

The first partial inverse is
\[
g^r = (\omega - \epsilon_1 - \Sigma^L)^{-1}
\]
(3.64)
with the general partial inverse recursion given as
\[
g^r_n = (\omega - \epsilon_n - t^2 g^r_{n-1})^{-1}
\]
(3.65)
with final case
\[
G^r_{N,N} = g^r_N = (\omega - \epsilon_N - \Sigma^R - t^2 g^r_{N-1})^{-1}.
\]
(3.66)
The diagonal is given by
\[
G^r_{n-1,n-1} = g^r_{n-1}(1 + t^2 G^r_{n,n} g^r_{n-1})
\]
(3.67)
with \( G^r_{1,N} \) found through the recursion of
\[
G^r_{m,N} \bigg|_{m<N} = -t g^r_m G^r_{m+1,N}
\]
(3.68)
which after \( N - 1 \) iterations give us the necessary element.
To test this routine, we will first compare our results with the density of states of a clean system. For one-dimension, the density of states is defined as

\[
\nu(E) = \frac{2 \pi}{E} \frac{1}{dk}
\]

(3.69)

where we have previously determined the energy for this system analytically in Sec. 2.2.1. If we use the energy that we calculated in Eq. (2.33), we find the density of states to be

\[
\nu(E) = \frac{2}{\pi i t \sqrt{4 - (E/t)^2}}.
\]

(3.70)

We compare this analytic result to the results from our numeric routines in Fig. 3.4 and find perfect agreement.

Figure 3.4: Density of states versus energy for a clean single atomic chain. Here, \( \epsilon_n = 0 \) which indicates the lack of disorder. The black dots correspond to numerical calculation while the red curve is the theoretical predicted density of states given in Eq. (3.70).

Next, we add in an uncorrelated disorder component to the Hamiltonian. For this, we randomly choose values for \( \epsilon_n \) from a Gaussian disorder distribution with average \( \mu = 0 \) and standard deviation \( \sigma = 1 \). We compare the disordered density of states with the clean system and plot the results in Fig. 3.5. We see that the divergence of the density of states at \( E = \pm 2 \) is blurred away and states with energy \( |E/t| > 2 \) begin to appear.
Figure 3.5: Density of states for a uncorrelated disorder distributions (black dots). The red line is the density of states of the clean system as given in Eq. (3.70).
4 POWER-LAW SPECTRAL CORRELATED DISORDER DISTRIBUTIONS IN ONE-DIMENSION

4.1 Long-Range $1/\kappa^\alpha$ Correlations

For spectral densities of $S(\kappa) \sim 1/\kappa^\alpha$ with $\alpha > 0$, it is not trivial to find the correlation function by the usual definition of the Fourier transform of the spectral density. The reason being that the integral

$$\int_0^\infty \frac{e^{ix\kappa}}{\kappa^\alpha} d\kappa$$

(4.1)

is undefined due to the divergence at $\kappa = 0$. If we try to remove this discontinuity by introducing a short range cutoff, for example

$$S(k) = \frac{1}{(1 + |k|)^\alpha}$$

(4.2)

we find that the correlation function, for $\alpha > 1$, has the form[31]

$$\Gamma(x) \approx e^{-c|x/a|^{1-\alpha}} \quad \text{for} \quad x >> a.$$  

(4.3)

where $c$ is a positive constant, $a$ is the lattice spacing. When $\alpha < 1$, the correlation takes the form

$$\Gamma(x) \sim \frac{1}{x^{1-\alpha}}$$

(4.4)

which corresponds to scale-free disorder distributions that will be discussed in chapter. 5. For all values of $\alpha$, the correlation function rapidly goes to zero in the thermodynamic limit which, by Kotani theory (Sec. 2.8), implies that all eigenstates must be localized. The resolution of this contradiction is the purpose of this chapter.

By introducing a short-range cutoff, we are essentially removing the longest ranged contributors to the correlation function. A straightforward way to analyze the correlation function would be to calculate the function numerically. However, the difficulty is that it is system size dependent as was demonstrated in Ref. [96]. To sidestep these issues, we
will present a method to find the exact correlation function without the aid of a short-range cutoff while avoiding computational difficulties.

4.2 The Exact Correlation Function

The correlation function is defined as

$$\Gamma(i, j) = \frac{\sigma_{i,j}}{\sigma^2}$$ (4.5)

where $\sigma$ is the variance of the disorder distribution and $\sigma_{i,j}$ is the covariance defined as

$$\sigma_{i,j} = \langle (\epsilon_i - u)(\epsilon_j - u) \rangle$$ (4.6)

with $u$ being the average of the disorder distribution and $\langle ... \rangle$ implying the expectation value. If $u = 0$, we are left with the expression

$$\Gamma(i, j) = \frac{\langle \epsilon_i \epsilon_j \rangle}{\langle \epsilon_i^2 \rangle}. \quad (4.7)$$

The typical numerical method\[19\] used to generate the random on-site variables $\epsilon_i$ in the Anderson Hamiltonian, Eq. (2.35), stems from work on colored noise models that produce temporally correlated signals that follow a power spectrum of $P(\omega_k) = \omega_k^{-\alpha}$ where the frequency $\omega_k = k\Delta \omega$ with $k$ an integer and $\Delta \omega = 2\pi/T$ with $T$ being the total time interval[69, 32]. A random variable $X(t_j)$, with $t_j$ being time and $j$ an integer, is given by the discrete Fourier transform

$$X(t_j) = \sum_{k=1}^{N/2} \left[ a_k \cos(\omega_k t_j) + b_k \sin(\omega_k t_j) \right]$$ (4.8)

where $N = T/\Delta t$, $\Delta t = (t_{j+1} - t_j)$, and Fourier components $a_k = \sqrt{P(\omega_k)\Delta \omega} \cos(\phi_k)$ and $b_k = -\sqrt{P(\omega_k)\Delta \omega} \sin(\phi_k)$ with $\phi_k$ a random independent variable chosen from 0 to $2\pi$. We place the values of the Fourier components into the above expression to find

$$X(t_j) = \sum_{k=1}^{N/2} \sqrt{\omega_k^{-\alpha} \Delta \omega} \cos(\omega_k t_j + \phi_k). \quad (4.9)$$
We can now map the above expression to a real space model by using the position $x_j$ in place of $t_j$ and subsequently the reciprocal variable, or momentum, $\kappa_k$ in place of $\omega_k$:

$$X(x_j) = \sum_{k=1}^{N/2} \sqrt{k^{-\alpha} \Delta \kappa} \cos(\kappa_k x_j + \phi_k). \quad (4.10)$$

In this case, $N = L/a$ with $L$ being the system size, $\kappa_k = 2\pi k/L$, $\Delta \kappa = 2\pi/L$, and $x_j = ja$. Placing these values into the above equation we arrive at

$$\epsilon_j = \sum_{k=1}^{N/2} \left| \frac{2\pi}{L} \right|^{(1-\alpha)/2} \kappa^{-\alpha/2} \cos \left( \frac{2\pi jk N}{N} + \phi_k \right) \quad (4.11)$$

where we have used $\epsilon_j$ to emphasize that this is the on-site disorder distribution for the Anderson tight-binding model. This is the precise disorder expression that is used to calculate the on-site energies in the numerical work where an Anderson transition was observed[19].

Since $\phi_k$ is the only random value associated with this generation method, it is straightforward to calculate the disorder average of this quantity

$$\langle \epsilon_i \rangle = \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{(1-\alpha)/2} \kappa^{-\alpha/2} \langle \cos \left( \frac{2\pi ik N}{N} + \phi_k \right) \rangle \quad (4.12)$$

$$= \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{(1-\alpha)/2} \langle \cos \phi_k \rangle \cos \left( \frac{2\pi ik N}{N} \right) - \langle \sin \phi_k \rangle \sin \frac{2\pi ik N}{N}. \quad (4.13)$$

The expectation values are simply solved by integrating over a uniform distribution between 0 and $2\pi$ which yield

$$\langle \cos \phi_k \rangle = \int_0^{2\pi} d\phi_k \cos \phi_k = 0 \quad (4.14)$$

$$\langle \sin \phi_k \rangle = \int_0^{2\pi} d\phi_k \sin \phi_k = 0. \quad (4.15)$$

Substituting these into the previous equation we find that the average value of the disorder distribution is

$$\langle \epsilon_i \rangle = 0 \quad (4.16)$$
Since the average is 0, the correlation function will be given by Eq. (4.7). Thus, we can evaluate the correlation function by calculating the covariance

\[
\langle \epsilon_i \epsilon_j \rangle = \frac{N}{2} \sum_{q=1}^{N/2} \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{1-\alpha} (qk)^{-\alpha/2} \langle \cos \left( \frac{2\pi k}{N} + \phi_k \right) \cos \left( \frac{2\pi q}{N} + \phi_q \right) \rangle. \tag{4.17}
\]

If \( k \neq q \), the expectation value can be separated as \( \phi_k \) and \( \phi_q \) are independent variables.

\[
\langle \epsilon_i \epsilon_j \rangle = \sum_{q=1}^{N/2} \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{1-\alpha} (qk)^{-\alpha/2} \langle \cos \left( \frac{2\pi k}{N} + \phi_k \right) \cos \left( \frac{2\pi q}{N} + \phi_q \right) \rangle. \tag{4.18}
\]

We would like to point out that the expectation value \( \langle \cos \left( \frac{2\pi k}{N} + \phi_k \right) \rangle \) has already been evaluated when we determined the average value of the disorder distribution which was found to be 0. Thus, the only surviving terms are those where \( k = q \). This removes one of the sums, leaving the expression

\[
= \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{1-\alpha} k^{-\alpha} \langle \cos \left( \frac{2\pi k}{N} + \phi_k \right) \cos \left( \frac{2\pi k}{N} + \phi_k \right) \rangle \tag{4.19}
\]

which can be simplified to yield a correlation function of

\[
\langle \epsilon_i \epsilon_j \rangle = \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{1-\alpha} k^{-\alpha} \pi \cos \frac{2\pi (i-j)k}{N}. \tag{4.20}
\]

The variance can be determined from Eq. (4.20) by setting \( i = j \) leaving

\[
\langle \epsilon_i^2 \rangle = \sum_{k=1}^{N/2} \left| \frac{2\pi}{N} \right|^{1-\alpha} k^{-\alpha}. \tag{4.21}
\]

Since the value of the correlation function only depends on the difference of positions \( i \) and \( j \), we define a distance \( n = |i-j| \). Using this along with Eqs. (4.7), (4.20) and (4.21) we find

\[
\Gamma(\alpha, n) = \frac{\sum_{k=1}^{N/2} k^{-\alpha} \cos \frac{2\pi nk}{N}}{\sum_{k=1}^{N/2} k^{-\alpha}}. \tag{4.22}
\]

which is a size dependent correlation function.

The thermodynamic limit \( (N \to \infty) \) must be taken with care as \( n \in [0, N/2] \).

Therefore, we will define a new variable \( \gamma = 2n/N \) which has a range of \([0, 1]\). In this way,
we have removed the system size dependence from the argument of both sums while our new variable $\gamma$ represents the separation between two sites in terms of a percentage of the system size (e.g. $\gamma = 0.5$ always denotes a separation distance of a quarter of the system size). This new variable was first introduced in Ref. [96].

With the system size dependence effectively removed, we are now free to take the upper limit of the sum to infinity

$$\Gamma(\alpha, \gamma) = \frac{\sum_{k=1}^{\infty} k^{-\alpha} \cos \pi \gamma k}{\sum_{k=1}^{\infty} k^{-\alpha}}. \quad (4.23)$$

To simplify the expression further, we must evaluate the summations. However, care must be taken as the series in the denominator diverges as or more quickly than a harmonic series for any value of $\alpha < 1$. We will thus split the derivation into two sections, one dealing with $\alpha > 1$ and one dealing with $\alpha < 1$.

### 4.2.1 $\alpha < 1$

We begin with Eq. (4.23) where we must evaluate the convergence of the numerator and denominator. The denominator is easily seen to be divergent as the series converges more slowly than the harmonic series for any values of $\alpha < 1$. The numerator however, is a series with an irregular sign change. The convergence of the numerator can be seen by applying the Dirichlet convergence test which guarantees the convergence of an infinite series provided the elements of the series can be written as

$$r_k = a_k b_k \quad (4.24)$$

with \{a_k\} being a set of real numbers and \{b_k\} a set of complex numbers that satisfy the conditions

$$a_k \geq a_{k+1} > 0 \quad (4.25)$$

$$\lim_{k \to \infty} a_k = 0 \quad (4.26)$$
and
\[ \left| \sum_{k=1}^{N} b_k \right| \leq M \quad \text{for every positive integer } N \quad (4.27) \]

where \( M \) is a constant. If these conditions hold, the series
\[ \sum_{k=1}^{\infty} r_k \quad (4.28) \]
converges.

To apply this test, let
\[ r_k = \frac{e^{\pm i \pi \gamma k}}{k^\alpha} \quad (4.29) \]
where
\[ a_k = \frac{1}{k^\alpha} \quad (4.30) \]
and
\[ b_k = e^{\pm i \pi \gamma} \quad (4.31) \]

Using these definitions, the conditions in Eqs. (4.25) and (4.26) are trivially seen to be satisfied for \( 0 < \alpha < 1 \). Furthermore, the summation of \( b_k \) given in the left hand side of Eq. (4.27) is a finite geometric series and can be written as
\[ \left| \sum_{k=1}^{N} b_k \right| = \left| \frac{1 - e^{\pm i N \pi \gamma}}{1 - e^{\pm i \pi \gamma}} \right| \quad (4.32) \]
and after some algebra,
\[ = \sqrt{\frac{1 - \cos N \pi \gamma}{1 - \cos \pi \gamma}} \quad (4.33) \]
where \( 1 - \cos \pi \gamma \neq 0 \) except for when \( \gamma = 0 \). For any other \( \gamma \), the largest possible value that this equation can take is when \( \cos(N \pi \gamma) = -1 \). Thus, if we choose our \( M \) such that
\[ M = \sqrt{\frac{2}{1 - \cos \pi \gamma}} \quad (4.34) \]
the condition of Eq. 4.27 will always be satisfied which proves the convergence of the series in Eq. (4.29).
Finally, by breaking the numerator of Eq. (4.23) into imaginary exponential functions, we can apply our results from Eq. (4.29) to conclude that it also converges as the sum of two convergent series is also convergent. Thus, for all values of $\gamma > 0$ the correlation function is 0 since the numerator converges and the denominator diverges to $\infty$. We note that at $\gamma = 0$, the numerator and denominator are equal and the correlation function gives the value 1. Furthermore, for $\alpha = 0$, the numerator is bounded between $[0, 2/(1 - \cos \pi \gamma)]$ which means that the correlation function is also zero for $\alpha = 0$ and $\gamma \neq 0$. Thus, the correlation function for $\alpha \leq 1$ is given by

$$
\Gamma(\alpha, \gamma) = \begin{cases} 
1 & \text{if } \gamma = 0 \\
0 & \text{otherwise} 
\end{cases}.
$$

(4.35)

From these results, the reason why no transition was observed for these values of $\alpha$ is due to the fact that the disorder potential is non-deterministic (as in the sense discussed in Sec. 2.8) due to weak correlations present in the system. We will now turn our attention to the more interesting case of $\alpha > 1$.

**4.2.2 $\alpha > 1$**

For this range of $\alpha$, both the summations of the numerator and denominator converge and $N$ can be taken to infinity without worry. Thus, we can simplify Eq. (4.23), by rewriting the cosine into imaginary exponential functions as

$$
\Gamma(\alpha, \gamma) = \frac{\sum_{k=1}^{\infty} k^{-\alpha} (e^{i\pi \gamma})^k + \sum_{k=1}^{\infty} k^{-\alpha} (e^{-i\pi \gamma})^k}{2 \sum_{k=1}^{\infty} k^{-\alpha}}.
$$

(4.36)

The terms in the numerator are the definition of the polylogarithm functions $Li_\alpha(z)$ while the denominator is the Riemann-Zeta sum $\zeta(\alpha)$. This gives our key expression for $\alpha > 1$

$$
\Gamma(\alpha, \gamma) = \frac{Li_\alpha(e^{i\pi \gamma}) + Li_\alpha(e^{-i\pi \gamma})}{2\zeta(\alpha)}.
$$

(4.37)
For general values of $\alpha$, Eq. (4.37) cannot be simplified further. However, a simplified solution exists at the critical value[19] of $\alpha = 2$ where the Anderson transition first occurs. This comes from a relationship between the polylogarithm functions in the numerator and the Bernoulli polynomials through the identity

$$Li_n(e^{i\pi\gamma}) + (-1)^n Li_n(e^{-i\pi\gamma}) = -\frac{(i2\pi)^n}{n!} B_n(\gamma/2)$$

where $n = 1, 2, 3, \ldots$, and $B_n(\gamma/2)$ is the order $n$ Bernoulli polynomial. For $\alpha = n = 2$ we have

$$\Gamma(\alpha = 2, \gamma) = \pi^2 \frac{B_2(\gamma/2)}{\zeta(2)}$$

where $\zeta(2) = \pi^2/6$ and the second order Bernoulli polynomial is $B_2(x) = x^2 - x + 1/6$. Using these identities we find the simple expression

$$\Gamma(\alpha = 2, \gamma) = \frac{3}{2} \gamma^2 - 3\gamma + 1.$$

This expression is the red solid line that is plotted in Fig. 4.1. We have also plotted Eq. (4.37) for a few values of $\alpha$ above and below the critical $\alpha$. Three surprising features appear from these expressions that are not expected from the general Fourier transform:

1.) The function is linear near $\gamma \sim 0$ for the critical value of $\alpha = 2$ while the behavior is convex for $\alpha > 2$ and concave for $\alpha < 2$.

2.) The correlation function goes negative for $\alpha > 1$.

3.) The correlation function converges to a non-zero value at the thermodynamic limit of $\gamma = 1$ and yields a value of $-1/2$ at the critical value, $\alpha = 2$.

Features 1.) and 2.) occur for smaller values of $\gamma$ and should be considered as short-range effects. 3.), however, is the value of the correlation between the two most distant points when $N \to \infty$ and is the most important factor governing the Anderson transition. The appropriate sufficient condition for an Anderson transition for this correlation is thus $\Gamma(\gamma = 1) < -1/2$. 
Figure 4.1: Plot of the correlation function as a function of the dimensionless quantity $\gamma$. The red solid line corresponds to the critical value of $\alpha = 2$ which is given by Eq. (4.40). The other curves correspond to various values of $\alpha$ from Eq. (4.37).

If we look specifically at the correlation function at it’s largest separation distance, $\gamma = 1$, we can rewrite Eq. (4.37) as

$$\Gamma(\alpha, \gamma = 1) = \frac{Li_{\alpha}(-1)}{\zeta(\alpha)}$$  \hspace{1cm} (4.41)

where $Li_{\alpha}(-1) = -\eta(\alpha)$ with $\eta(\alpha)$ being the Dirichlet-eta function. We can relate $\eta(\alpha)$ to the Riemann-zeta function through the relationship $\eta(\alpha) = (1 - 2^{1-\alpha})\zeta(\alpha)$. Thus, we have

and expression for the longest range correlations in the system

$$\Gamma(\alpha, \gamma = 1) = 2^{1-\alpha} - 1$$  \hspace{1cm} (4.42)

which is plotted in Fig. 4.2.

Though the correlations are negative, this still implies a very strong relation between infinitely separated sites. For positive correlations, two sites that are greatly separated are more likely to have similar energies. For negative correlations, these sites are more likely
Figure 4.2: Plot of the correlation for the largest separation distance, \( \gamma = 1 \), of the function \( \Gamma \). The origin corresponds to the critical value of \( \alpha = 2 \) and yields a correlation of \(-1/2\). For larger values of \( \alpha \), the correlation becomes more negative and results in a larger region of extended states[19].

to have energies with opposite signs. Due to this correlation, an overarching sinusoidal structure begins to develop in the disorder realizations and allows low energy states to extend for values of \( \alpha \geq 2 \). An example of this smoothening can be seen in Fig. 4.3. Thus, we have shown that there is no inconsistency between the numerical results for \( \sim 1/\kappa^\alpha \) correlations and the results of Kotani theory.

4.3 Comparison to the Random Dimer Model

In order to gain some insight into the effect of long-range negative correlations, we numerically calculate the correlation function of the random dimer model (Reviewed in Sec. 2.9) for comparison. We found that for \( \epsilon_A = t \) and \( \epsilon_B = -t \), which are the two possible values of the on-site energy where extended states first occur, the correlation between any two points is \( \sim 0.3 \). Again we see that these results are consistent with Kotani’s theory but different from the correlation from spectral disorder as they do not take on negative
Figure 4.3: Typical disorder realization of a $1/k^\alpha$ spectral correlation. In this figure, $N = 1000$ and the same set of random numbers $\{\phi_k\}$ for $\alpha = 2$ (solid, blue), $\alpha = 4$ (dotted, red), and $\alpha = 10$ (dashed, black) have been used. Energy is normalized such that $\langle \epsilon^2 \rangle = 1$. Plots show tendency for strong correlations that induce a sinusoidal structure in the disorder distribution.

values. Note that one of the key distinctions between the results of the random dimer model and long-range spectral correlations is that the former produces a discrete number of extended states while the latter produces a true mobility edge. Comparing our results for long-range spectral correlations to the random dimer model, this suggests that the cross over to negative correlations in the thermodynamic limit may be necessary for a band of extended states.

4.4 On-going Projects Related to Correlation Driven Anderson Transitions

In this chapter, we have seen that a one-dimensional Anderson transition can occur if the correlations in the disorder distribution are extended enough to correlate sites on opposite ends of the system. Along with this, we have noticed that short-range features of the correlation function change as we pass through the critical value of $\alpha$. While we believe these short-range features cannot create an Anderson transition alone, they may
Figure 4.4: A numerical calculation of the random dimer model for $N = 1000$, $\epsilon_A = t$ and $\epsilon_B = -t$. As the system size is increased, the correlation function approaches a constant values of 0.3 for all $\gamma$.

have a direct impact on the amount of correlation needed between sites separated on the order of the system size. With this in mind, we have begun exploring the idea of creating a correlation function with independently adjustable short-range and long-range parameter.
5 Scale-Free Correlated Disorder in One-Dimension

5.1 Experimental Observation of Matter Wave Localization

We are now in a position to study the localization of eigenstates in one-dimensional atomic chains with correlated disorder. Since Anderson localization is predicted to be a phenomenon associated with wave mechanics[4], the first attempts to study this effect came from micro-cavity and other light based experiments[88, 18, 93, 12, 13, 85, 2, 82, 51]. These results confirmed the predictions of the simple one-dimensional Anderson model that we presented in Sec. 2.6. Localization has also been observed in sound waves through ultrasound experiments[91, 37].

For matter waves, a novel and promising technique has recently been developed to study Anderson localization by directly imaging the disorder induced wavefunctions through optically trapped Bose-Einstein condensates (BEC).[77, 8, 73] In the experiment, lasers are positioned along the x, y, and z directions and the intensity and frequency of the laser are adjusted to create an artificial crystal. In the case of 1D localization, the x and y lasers are run at high intensity to confine the condensate while the z-directional laser is low intensity to simulate the periodicity of a 1D crystal. The z-directional laser is turned off at time $t = 0$ and the dynamics are dominated by a repulsive interaction until a later time when the diffusive states nearly decouple into a set of plane waves that correspond to the periodicity of the now turned off confining potential[77]. Up to this point, no disorder has been added to the system and we have plane-wave propagating matter-waves. The disorder is now introduced by lasing a small plate of crushed glass causing diffraction through the plate which creates a random intensity pattern over the propagating plane waves. This intensity pattern mimics a random spatial disorder, similar to that of the Anderson model, and is termed a speckle potential. The nearly decoupled plane waves feel this speckle potential and localize as per the usual Anderson localization.
mechanism[8, 73]. A very interesting feature of this disorder potential generation method is that it naturally creates correlations in the disorder distribution that are directly tunable by adjusting the grain-size of the diffusing plate. By these methods, it may be possible in the near future to probe the effects of correlations on Anderson localized states.

With this in mind, we would like to discuss our analysis of one common correlation that naturally occurs in many physical systems such as percolation models[39, 89], nucleotide sequencing[71], heartbeat dynamics (which is a temporal correlation)[40], and is closely related to the previously mentioned speckle potentials[8]: the \(1/r^\alpha\) correlation or scale-free correlation.

5.2 Validity of Single Parameter Scaling Hypothesis

Existing between the class of short-range and long-range correlated models lies the scale-free correlated disorder model of \(\sim 1/r^\alpha\). This case is of particular interest as it does not contain a typical length scale, as is the case in other short-range correlated models[43], yet does not have "enough" correlation to satisfy Kotani theory and generate extended states. This correlation has been the subject of intensive theoretical research[75, 74, 64, 17], yet some basic questions still remain, such as the validity of the SPS hypothesis.

From Kotani theory, Sec. 2.8, we can conclude that a metal/insulator transition does not exist for these correlations and that all states will be localized. This is due to the fact that the correlation function goes to zero in the thermodynamic limit. Nevertheless, the properties of the localized states themselves are useful for experimental comparison and will also help to define the role of correlations. Furthermore, several works[75, 74, 17] have studied the effects of scale-free correlations which makes this case a solid test-bench for our numerical routines.
We begin with a study of the SPS hypothesis, Sec. 2.6, by calculating the dimensionless conductance. Through this, we have a straightforward way to compare experimental data (when available) and test the reach of the single parameter scaling hypothesis (as a reminder, validation of SPS implies the complete localization of all eigenstates while violations prove neither extension or localization[1, 16]). In the following, we analyze this hypothesis by calculating the conductance as per the prescription outlined in Sec. 3.4. For our statistics, we will use the geometric average $\langle \ln G \rangle$ of the conductance opposed to the arithmetic average $\langle G \rangle$ due to the large variations in $G$.

The numerical procedure goes as follows:

1.) Set the correlation parameter $\alpha$, system size $N$, hopping energy $t$, energy $E$, and number of disorder configurations $D$.

2.) Calculate the spectral density $S(k)$ using Eq. (3.10).

3.) Calculate the self-energies from the recursion method in Sec. 3.3.1 with Eqs. (3.52) and (3.53) along with $\Gamma_{L,R}$ from Eq. (3.37).

4.) Generate a disorder distribution from the procedure in Sec. 3.1.

5.) Find the Green’s function across the conductor from the method in Sec. 3.3.2.

6.) Calculate $\ln G$ for each energy from Eq. (3.54) and store the output.

7.) Repeats steps 4 – 7 for all disorder realizations.

8.) Take the average and variance of $\ln G$ using Eqs. (2.37) and (2.38) for $n = 2$.

5.2.1 1st Cumulant

To check the scaling of the $\beta$-function with the typical conductance, we first must show that $\langle \ln G \rangle$ is the only relevant scaling variable for the function

$$\beta(G) = \frac{d\langle \ln G \rangle}{d \ln L}.$$  (5.1)
Figure 5.1: (Top) Plot of the typical conductance versus system size. Different symbol shapes represent different values of disorder strength with $W/t = 1.0$ (triangles), 0.5 (squares), and 0.2 (circles). Different colors correspond to $\alpha = 0.25$ (Red), 1.00 (Black), and 1.50 (Blue). Finally, different sizes correspond to energies $E = 0$ (Large Filled), 1.0 (Large Hollow), and 1.8 (Small Solid). (Bottom) Same data as top figure except that $L$ is rescaled for each data set by $\xi$ to cause a data collapse which confirms SPS.

Using the aforementioned procedure, we generate $\langle \ln G \rangle$ which is plotted versus the system size in Fig. 5.1. Each parameter set gives a strong linear behavior with a slope of 1 and parameter dependent shift in the y-direction. Since the data is plotted on logarithmic
axes and the slope of the lines is 1, the data in Fig. 5.1 is described by

\[ \ln(-\ln \mathcal{G}) = \ln L - \ln \xi(E, W, \alpha) \]  
(5.2)

which can be simplified to

\[ \langle -\ln \mathcal{G} \rangle = \frac{L}{\xi(E, W, \alpha)} . \]  
(5.3)

If we place Eq. (5.3) into Eq. (5.1) we find that

\[ \beta(\mathcal{G}) = \langle \ln \mathcal{G} \rangle \]  
(5.4)

which agrees with the SPS hypothesis as \( \beta \) is only a function of the geometric average of the conductance. We would like to point out that the value of \( \xi \) is irrelevant for the scaling of the \( \beta \)-function. Thus, we are at liberty to rescale \( \xi \) as we please without affecting the scaling results. This leads us to another way of seeing the \( \beta \)-function scaling through a data collapse. This data is the bottom plot in Fig. 5.1.

To cause the data collapse, we used the parameter set of \( E/t = 0, W/t = 1 \), and \( \alpha = 1 \) as a reference point and rescaled the length scale of all other parameter sets such that they collapse on the reference data set. This choice of collapse is arbitrary as the scaling of the \( \beta \)-function does not depend on the reference. However, the length scale \( \xi \) is not without meaning and is in fact proportional to the localization length, \( \lambda \), of each data set. This can be seen through the definition of the lowest Lyapunov exponent[6, 22]

\[ \tilde{\lambda}(L) = \frac{1}{2L} \ln \left(1 + \frac{1}{\mathcal{G}}\right) = \frac{1}{2L} \left( \ln(1 + \mathcal{G}) - \ln \mathcal{G} \right) . \]  
(5.5)

If \( L \) is large, then \( \frac{1}{L} \ln(1 + \mathcal{G}) \sim 0 \) as the conductance is bound between the values of 0 and 1 making \( \ln(1 + \mathcal{G}) \) exist between 0 and \( \ln 2 \). Using this we can rewrite the above equation as

\[ -\ln \mathcal{G} = 2L\tilde{\lambda}(L) . \]  
(5.6)
Likewise, the average value of the inverse Lyapunov exponent converges to the localization length in the limit of large $L$. Thus we have

$$\langle -\ln G \rangle = \frac{2L}{\lambda}$$

(5.7)

where $\lambda$ is the localization length. Comparing this to Eq. (5.3) gives the relationship $\lambda \propto \xi$.

Figure 5.2: Plot of the ratio of first and second cumulant as a function of $E/t$. Colors correspond to $\alpha = 0.5$ (Red), 1.0 (Black), and 1.5 (Blue) while shapes correspond to $W/t = 1.0$ (Triangles), 0.5 (Squares), and 0.2 (Circles). The dashed black line is the expected ratio of Eq. (5.8). Note that each data set diverges at some energy which we refer to as $E_{sps}$. For $\alpha = 0.5$, $W/t = 1.0$, all energies violate this condition which we represent by $E_{sps} = 0$.

### 5.2.2 2nd Cumulant

As stated in Sec. 2.6, an analysis of the single parameter scaling hypothesis is just as dependent upon the fluctuations of the dimensionless conductance as the average. For strong disorder, even uncorrelated systems have been shown to violate the SPS hypothesis, requiring a second scaling parameter[16]. For weak disorder, it has been shown[6] that the
first two cumulants are related by

\[ \frac{C_2}{2\langle -\ln G \rangle} = 1. \]  \hspace{1cm} (5.8)

To test this condition, we take the sample variance

\[ C_2 = \frac{1}{D} \sum_{i=1}^{D} (\ln G_i - \langle -\ln G \rangle)^2 \]  \hspace{1cm} (5.9)

for each parameter set where \( D \) is the total number of disorder configurations. We plot these results in Fig. 5.2. From these plots, a clear divergence from Eq. (5.8) can be seen for each set of parameters. The energy where this divergence first occurs will be referred to as \( E_{sps} \) or the SPS violation energy. Thus, the SPS hypothesis is upheld for all energies \( |E| < E_{sps} \) and violated for \( |E| > E_{sps} \).

To systematically study this energy from our simulations, we numerically calculate the ratio of the cumulants in Eq. (5.8). We characterize \( E_{sps} \) as the energy when this ratio first becomes greater than 1.1, (i.e. a 10% deviation from the expected value). We chose this value as we expect roughly 5 – 10% error from our numeric calculations. We plot the analysis of this ratio for multiple disorder strengths in Fig. 5.3.

At first glance, \( E_{sps} \) would seem to depend on the variables \( \alpha \) and \( W/t \) independently. However, if we rescale the disorder strength by \( \alpha \), we induce a data collapse. Thus, we propose that \( E_{sps} \) is only a function of the ratio \( W/t\alpha \). We plot our \( E_{sps} \) results versus this new variable in Fig. 5.5 and find that all data collapse onto a single trajectory.

These results imply that for any given disorder strength satisfying \( \alpha > W/t \), a range of energies exist around the band center that confirm the SPS hypothesis and implies the exponential localization of these states. Furthermore, it is possible to violate SPS for all energies by choosing a correlation parameter that satisfies the condition \( W/t \geq \alpha \). Since smaller values of \( \alpha \) correspond to longer range correlations, we conclude that given any disorder strength, a correlations exists such that SPS will be violated for all energies.
Figure 5.3: Plot of the SPS violation energy versus $\alpha$ for multiple disorder strength. The shapes and colors correspond to disorder strengths of $w/t = 1/3$ (red triangles), $1/5$ (purple squares), $1/8$ (orange circles), $1/10$ (blue rectangles), $1/15$ (green up-side-down triangles), and $1/20$ (black stars). These values were determined from systems of size $2^{17}$ sites and 1000 disorder distributions. The error associated with each points is between $5 - 10\%$ with the error bars omitted for clarity.

Naively, these results seem to suggest a simple rescaling of the disorder strength by $\alpha$. This would be inline with the results for uncorrelated disordered systems which show increasingly large disorder strengths lead to two-parameter scaling. However, this interpretation is not consistent with results for the localization length as we will show in the following sections.

5.3 Previous Scaling Results for the Localization Length

Previous work[41] has shown that the localization length can be written in terms of the spectral density of the disorder distribution as

$$\lambda^{-1} = \frac{(W/t)^2 S(k)}{8 \sin^2 k}$$  \hspace{1cm} (5.10)

with

$$E = 2t \cos ka$$  \hspace{1cm} (5.11)
Figure 5.4: Plots of $E_{sps}$ versus the ratio $\frac{W}{t\alpha}$. Data is extracted from all permutations of $\alpha = 0.50, 0.75, 1.00, 1.25, 1.50$ and $W/t = 1.00, 0.50, 0.33, 0.25, 0.20$. Solid line is a guide to the eye. (Top) Linear scale. (Bottom) Logarithmic scale.

where $W$ is the standard deviation of the disorder distribution, $k$ is the momentum, and $S(k)$ the spectral density. This result stems from a second order perturbation expansion which is valid in the weak disorder ($W/t \ll 1$) limit and for $0 < |E/t| < 2$. The energy restriction comes from the anomalous scaling of the localization length around $E/t = 0$. 
and $E/t = \pm 2$ which are referred to as the band center and edge anomalies\[44, 20, 80, 81, 21\]. From this, we see that the disorder strength can be completely decoupled from $E$ and $\alpha$ and universally scales with the disorder strength as $\lambda \sim (W/t)^{-2}$. For this case, the effect of the correlation resides in the function $S(k)$ which is a multiplicative factor of the disorder strength, similar to our rescaled disorder strength variable of $W/t\alpha$ from the $E_{sp}$ energy.

### 5.4 Scale-Free Correlation at the Band Edge

Since Eq. (5.10) applies to all correlated disorder models, the only appearance of a new type of scaling region would be at the band edge. Previous results have shown\[75\] through a renormalization scheme that the localization length scales with the disorder strength as

$$
\lambda \propto \left(\frac{W}{t}\right)^{-2/(4-\alpha)} \equiv \lambda_0
$$

near the band edge when scale-free correlations are present and $\alpha < 1$. For $\alpha > 1$ we have

$$
\lambda \propto \left(\frac{W}{t}\right)^{-2/(3)}.
$$

Thus, the localization length now scales with the disorder strength raised to an $\alpha$ dependent exponent and converges to the uncorrelated value of $2/3$ when $\alpha \geq 1$. This result was expanded\[74\] for states around the band edge by using $\lambda_0$ as a starting point. The analysis is based off results for uncorrelated potentials where the localization length scales with a function $f(x)$ as

$$
\lambda/\lambda_0 = f(x)
$$

where $x$ depends on the distance from the band edge as well as the band edge localization length $\lambda_0$. The variable $x$ is defined as

$$
x = (2 - E/t)\lambda_0^2
$$
Figure 5.5: Plots of the inverse localization length versus energy. The different colored curves correspond to numerical results calculated from transfer matrix methods for $W/t = 1/3$ (blue), $W/t = 1/5$ (red), and $W/t = 1/10$ (yellow) with the vertical dark lines indicating the values of $E_{sp}$, with the leftmost line correspond to the blue curve and the rightmost to the yellow. The dashed black curves are calculated from Eq. (5.10). (Top) $\alpha = 0.5$ (Bottom) $\alpha = 1.0$.

where $\lambda_0$ is given by Eq. (5.12). While no general expression for $f(x)$ exists, it has been shown[20, 44] to possess the following limiting behavior

$$f(x) = \begin{cases} 
\text{const} & \text{if } x \ll 1 \\
x & \text{if } x \gg 1 
\end{cases}$$

(5.16)
for uncorrelated disorder. In Ref. [74], numerical calculations for the localization length in the presence of scale-free disorder reported that the function $f(x) \to f_\alpha(x)$ and takes the form

$$f(x) = \begin{cases} 
\text{const} & \text{if } x \ll 1 \\
 x^{(3-\alpha)/2} & \text{if } x \gg 1
\end{cases} \quad (5.17)$$

for states near the band edge.

For the small $x$ limit, we can solve Eq. (5.17) for the localization length using Eqs. (5.12), (5.14), and (5.15) to find

$$\lambda \sim \left( \frac{W}{t} \right)^{-2/(4-\alpha)} \quad (5.18)$$

Since $x \ll 1$, this result corresponds to a strong disorder limit, i.e. $\frac{W}{t} \gg (2 - E)^{(4-\alpha)/4}$. For large $x$, we can use the same set of equations to find

$$\lambda \sim \left( \frac{W}{t} \right)^{-2} \quad (5.19)$$

which is identical to the scaling function outlined in Sec. 5.3. This region corresponds to a weak disorder limit i.e. $\frac{W}{t} \ll (2 - E/t)^{(4-\alpha)/4}$. However, these results could also be interpreted in terms of states very near to the band edge and state. In the following section, we will address the reason for these two possible interpretations.

### 5.5 Extension of Band Edge Scaling Results

We calculate the Lyapunov exponent using the method described in Sec. 3.2 in conjunction with the disorder generation method outlined in Sec. 3.1. We calculate the lowest Lyapunov exponent for various $\alpha$’s, $E$’s, and hopping energies $t$. For all runs we set the disorder strength $W = 1$ and lattice constant $a = 1$ effectively defining our energy and length unit. Thus, the disorder strength is set by the value of $t$ because the only relevant variable is the ratio of $W/t$. Finally, we average over 1000 disorder configurations for each parameter set.
Figure 5.6: Raw localization length data plotted versus $x$ and scaled with $\lambda_0$ for systems of size $L = 2^{17}$ (red circles), $2^{18}$ (purple triangles), $2^{19}$ (blue squares), and $2^{20}$ (green diamonds). The black stars represent the extrapolated value of the localization length, $L \to \infty$, with the line being a guide to the eye.

Using the raw data for the lowest Lyapunov exponent we extrapolate the localization length through the fitting function

$$\tilde{\lambda} = m \frac{1}{L} + \lambda^{-1}$$

(5.20)

where $\tilde{\lambda}$ is the lowest Lyapunov exponent, $m$ is a fitting parameter, $L$ is the system size, and $\lambda$ is the localization length. A sample of our data for the lowest Lyapunov exponent as well as the extrapolated localization length is plotted in Fig. 5.6.

The extrapolated localization and the variable $x$ are functions of the three parameters $\alpha$, $E$, and $t$. To determine the scaling of the localization length with disorder strength, through the variable $x$, we will fix the values of $\alpha$ and $E$ for each data set and change $x$ by varying the hopping energy $t$ which effectively changes the disorder strength ratio $W/t$. A sample of this data is plotted in Fig. 5.7. From this figure, we can clearly see a linear region appearing for values of $x \gg 1$. 
Figure 5.7: Plot of the extrapolated localization length versus $x$ for $x > 1$. Data is coded by color and shape and corresponds to $E/t = 0.01$ (red circles), 1.01 (blue squares), and 1.81 (black triangles) with different symbol sizes corresponding to $\alpha = 0.5$ (large solid), 1.0 (large open), and 1.5 (small solid). Each set exhibits a linear behavior when $x >> 1$.

We confirm the linear scaling, Eq. (5.17), of $\lambda/\lambda_0$ versus $x$ that is seen on logarithmic axes through the fitting function

$$\ln\left(\frac{\lambda}{\lambda_0}\right) = \gamma \ln x + \ln \Delta.$$  \hspace{1cm} (5.21)

or in simplified terms

$$\lambda/\lambda_0 = \Delta x^\gamma.$$ \hspace{1cm} (5.22)

Our results for the fitting parameter $\gamma$ are plotted in Fig. 5.8 and clearly show the validity of Eq. (5.17) for all energies in the large $x$ limit. A similar analysis for small $x$ confirms the predicted constant behavior for small energies.

This analysis implies that $x$ is the quantity that defines the regions of weak and strong disorder with $x \gg 1$ corresponding to the scaling region where $\lambda \sim (W/t)^{-2}$ and $x \ll 1$ corresponding to the regions where $\lambda \sim (W/t)^{-2/(4-\alpha)}$. It should be noted that there is not a sharp transition at $x = 1$ but a broad crossover region around $x \sim 1$. 
Figure 5.8: The slope of the linear region when \( x \gg 1 \) as exemplified in Fig. 5.7. The different data sets correspond to, from top to bottom, \( \alpha = 0.25, 0.50, 0.75, 1.00, 1.25, 1.50, \) and 2.00. The solid line running through each data set is given by the anticipated value of \( \gamma = (3 - \alpha)/2 \).

### 5.6 The Crossing Energy

If we examine the localization length in the region \( x \sim 1 \), we notice that an energy exists where the localization length becomes independent of \( \alpha \). As this energy resides between the two distinct scaling regions, we will refer to this point as a crossing energy \( E_c \). For clarity, we will plot our results as the inverse localization length versus energy, unlike our previous analysis. A sample of this data is shown in Fig. 5.9.

From this data, two distinct regions can be seen. In the region below the crossing energy, \( E < E_c \), the localization length increases \((\lambda^{-1} \to 0)\) as the correlation increases \((\alpha \to 0)\) while \( E > E_c \) shows a decreasing localization length with increasing correlations. The value of \( E_c \) is found for various disorder strengths and it’s dependence on \( W/t \) is shown in the inset of Fig. 5.9.

Given the appearance of a crossing energy, previous results for band edge scaling in correlated disordered systems, it would appear that the quantity \( E_c \) is signifying a change in scaling behavior from Eq. (5.10) to Eq. (5.18). This energy appears in the region...
Figure 5.9: The inverse localization length $\lambda$ for three values of $\alpha$ at disorder strength $w/t = 1$. Data is extrapolated to $L \to \infty$ from systems of size $L = 2^{17} - 2^{20}$ and averaged over 1000 disorder configurations. This figure presents two distinct regions in energy. For states near the band center, the localization length increases as correlations increase while at the edge, the localization length decreases as correlations increase. The energy where the change of behavior occurs is $E_c$. (Inset) The crossing energy $E_c$ for various disorder strengths.

around $x \sim 1$. This change in scaling is reminiscent of our $E_{sps}$ results and it is natural to wonder if they are related. If we compare the expression for $x = 1$ and an approximate form of $E_{sps}$, we have the two equations

$$E_c \sim 2 - \left(\frac{W}{t}\right)^{4/(4-\alpha)}$$  \hspace{1cm} (5.23)

and

$$E_{sps} \sim 2 - \left(\frac{W}{t\alpha}\right).$$  \hspace{1cm} (5.24)

We plot these two functions for a few values of $\alpha$ in Fig. 5.10 and find that both decrease with increasing disorder strength yet have different scaling behaviors, even near $W/t \sim 0$. 

Figure 5.10: The scaling for $E_c$ (black) and $E_{sps}$ (blue) as given by Eqs. (5.23) and (5.24) respectively. The different lines correspond to the values of $\alpha = 0.1$ (dashed), $\alpha = 0.5$ (solid), and $\alpha = 1.0$ (dotted) respectively.


6 Disordered Rashba Spin-Orbit Interaction in Graphene

6.1 Graphene

For the final section of this document, we would like to discuss an ongoing project related to the study of random spin-orbit interactions in graphene, which is a single atomic layer of carbon atoms that form a honeycomb structure. Due to each carbon having three nearest neighbors, covalent $sp^2$ bonds form as a result of the mixing of the 2s, 2xp, and 2yp orbitals. These are referred to as $\sigma$ bonds. These bonds are remarkably strong and are responsible for graphene’s high structural integrity. The remaining electrons form $\pi$ bonds from neighboring 2zp orbitals and are perpendicular to the lattice plane. The $\pi$ bonds are much weaker than the sigma bonds and are the states responsible for conduction.

A tight-binding model, using a two site-basis of A and B as shown in Fig. 6.1, can be used to calculate the band structure of the $\pi$ band analytically; (see appendix C for a detailed derivation). The energy bands are given by

$$E/t = \pm \sqrt{1 + 4 \cos^2 \frac{\sqrt{3}aK_x}{2} + 4 \cos \frac{\sqrt{3}aK_x}{2} \cos \frac{3aK_y}{2}}$$

and are plotted in Fig. 6.2 where we can see the formation of cones above and below the Fermi energy, located at $E = 0$ for undoped graphene, where the conduction and valence band touch. Of the six points plotted, only two of the points are unique, which are defined as the $K$ and $K'$ points with the rest connected by a reciprocal lattice vector. Slightly away from $E = 0$, the cones have a linear energy dispersion of $E \sim |k|$ and result in a Fermi velocity, $v_f = dE/dk$, that is constant regardless of energy and wave vector $k$. $v_f$ is estimated to be $v_f = c/300$ where $c$ is the speed of light, even at room temperature. This independence of $v_f$ with $E$ is reminiscent of photons, were the speed of light remains constant with energy. Due to this similarity, along with being a spin 1/2 particle, the carriers in graphene can be described by a massless fermion model.
Furthermore, the two-site basis structure introduces another quantum number associated with the chirality of the state. This can take only two values and is mathematically identical to a quantum spin. This pseudo-spin, along with the zero mass, make this model mappable to the massless neutrino Dirac equation with the speed of light becoming $v_f$ and the real spin replaced by the pseudo-spin. Hence, the carriers in graphene are usually referred to massless Dirac fermions.

Scientific interest in this material has increased dramatically due to its first stable experimental fabrication\[67\]. While the theoretical band structure of graphene was known for quite some time\[90\], experimental exploration of these systems was thought impossible due to the consequences of the Mermin-Wagner theorem\[57\] which implies no long-range order can exist in one or two dimensional systems. While the discovery of graphene was originally viewed as a contradiction, the experimental discovery\[58\] and numerical confirmation\[29\] of corrugations (or ripples) that effectively introduce a third dimension by slightly shifting sites perpendicular to the lattice plane validated\[29\] the Mermin-Wagner theorem and illuminated an inherent correlated disorder.

Experimental measurements highlight the outstanding electronic properties of graphene showing electronic mobilities exceeding that of silicon by an order of magnitude with ballistic electronic transport over several micrometers\[67\].

6.1.1 Graphene Nanoribbons

Due to graphene’s fantastic electronic properties, long spin lifetimes, extraordinary durability, and natural material abundance, it is only natural to ask if we can create circuits composed of graphene. Experimental studies have demonstrated that graphene nanoribbons (GNRs) can been fabricated chemically from unzipped carbon nanotubes\[47\] and etched from large graphene flakes through electron beam lithography\[10\]. While
Figure 6.1: The graphene lattice. This geometry requires the use of a two site basis that we label A and B with the highlighted area being the smallest possible unit cell.

Figure 6.2: The $\pi$ band for graphene. The red and green dots correspond to the $K$ and $K'$ points. This is an extended zone scheme to show the hexagonal symmetry (i.e. we are plotting points that are equivalent up to a translation in $K$) with the only unique values between $aK_x \sqrt{3}/2 \in [0, \pi)$ and $aK_x 3/2 \in [0, \pi)$. The $K$ and $K'$ are located at $(\pi/3, 0)$ and $(2\pi/3, 0)$. 
Figure 6.3: The zigzag and armchair edge geometries and width characterization scheme. The width is determined by the number of dimer pairs that make up the GNR unit cell (shaded regions with alternating blue and green regions highlighting the different dimer pairs). This armchair width is insulating as \( M = 3m - 1 \) cannot be satisfied for any value of \( m \).

these techniques can create ribbons as narrow as a few tens of nanometers, the edge geometry is highly volatile and has prominent effects on the electronic properties. The two most widely considered geometries are the so called zigzag and armchair edges shown in Fig. 6.3. In the case of zigzag boundaries, the nanoribbon is metallic, regardless of the width of the ribbon, and a large number of degenerate states appear at \( E = 0 \). For armchair boundaries, the ribbons are metallic if the width of the ribbon satisfies the condition

\[
M = 3m - 1,
\]

(6.2)

where \( m \) is any positive integer. For any other width, an armchair GNR is insulating. The band structure for a few armchair GNR’s are plotted in Fig. 6.4 which we obtained by a direct diagonalization of the tight-binding Hamiltonian. We will address the band structure for zigzag ribbons in the following sections.
Figure 6.4: The band structure for different width armchair GNRs. (Top) $M = 4$. (Middle) $M = 8$. (Bottom) $M = 10$. For the top and bottom plots, a band gap exists between the conductance and valence band. For the middle plot, $M = 8$ satisfies the condition $M = 3m - 1$ and the bands touch at $K = 0$. 
6.2 Spin Coherence in Graphene

Along with its amazing electronic properties, graphene was predicted to have a long spin lifetime $\tau_s$\cite{87}. This quantity implies that an electron injected into graphene with a well-defined spin will completely decohere after a time $\tau_s$. However, experimental results\cite{35,94} so far indicate a much smaller relaxation time than predicted theoretically. In general, there are four common spin relaxation mechanisms that are common to all metals and semiconductors. These are the Elliot-Yafet mechanism, D’yakonov-Perel mechanism, Bir-Aronov-Pikus mechanism, and hyperfine interaction (see Ref. [100] for detailed explanation of all mechanisms). For graphene, the Bir-Aronov-Pikus mechanism and hyperfine-interaction can be ignored as the nuclear magnetic moment for carbon is minuscule. These typically manifest in heavier elements that have been doped\cite{68}.

The D’yakonov-Perel (DP) mechanism appears when the inversion symmetry of the lattice is broken which is unavoidable for graphene due it’s dual site basis. The Elliot-Yafet (EY) mechanism on the other hand couples the spin degree of freedom to the momentum which allows spin relaxation by ordinary momentum scattering. The typical defining difference between these two mechanisms is the relationship of the spin relaxation time $\tau_s$ with the momentum scattering time (average time between momentum scattering events) $\tau_p$. For EY, $\tau_s \propto \tau_p$ with an inverse relation for DP as $\tau_s \propto 1/\tau_p$\cite{70}.

Recent theoretical work has suggested that neither EY or DP mechanisms are solely responsible for the experimentally observed lifetimes and suggests a different mechanism at work\cite{68}.

Among other possible mechanisms for the dramatic difference in spin relaxation time is the effect of a random Rashba field (RRF) that appears due to ripples or other similar inversion symmetry breaking defects\cite{38,26,97,42}. The effects of RRFs on the electronic properties of graphene are just starting to be explored with recent work highlighting some consequences related to the spin Hall effect\cite{25}.
The word Rashba in an RRF stems from the Rashba effect which indicates a breaking of the degeneracy between spin bands through a momentum scattering term

\[ H_r = \Delta_r (\vec{\sigma} \times \vec{p}) \cdot \hat{z}. \] (6.3)

The random field in this case refers to the disorder introduced into the factor \( \Delta_r \) which can be tuned through added impurities, substrate interactions, or electric fields. Since this term couples the momentum states of the system and appears due to broken inversion symmetry in the direction perpendicular to the graphene sheet, this term can lead to either DP or EY mechanisms.

In preparation for introducing a random Rashba field, we will now present a detailed reproduction of work done on uniform Rashba fields in GNRs as well as transmission calculations. This work will serve the dual purpose of highlighting the role of the Rashba spin-orbit interaction as well as providing a solid proving ground for our numerical routines.

### 6.3 Rashba Spin-Orbit Interaction

In the previous chapters, we have assumed that no spin-orbit interactions were present in our model Hamiltonians. This means that our Hamiltonian was diagonal in spin space and each eigenvalue had a degeneracy of 2. A spin full representation of the Hamiltonian for an infinite graphene sheet is given by the block matrix

\[ H = \begin{pmatrix} H_{\uparrow\uparrow} & H_{\uparrow\downarrow} \\ H_{\downarrow\uparrow} & H_{\downarrow\downarrow} \end{pmatrix} \] (6.4)

where \( \uparrow\downarrow \) refer to the z-components of spin which we choose to be perpendicular to the graphene sheet. The diagonal elements of this matrix are the standard nearest neighbor tight-binding Hamiltonian, Eq. (2.22),

\[ H_0 = H_{\uparrow\uparrow} + H_{\downarrow\downarrow} = t \sum_{(i,j)} \sum_s c_{i,s}^\dagger c_{j,s} + h.c. \] (6.5)
where $s$ represents either $\uparrow$ or $\downarrow$.

The off-diagonal parts of the matrix are related by $H_{\uparrow\downarrow} = H_{\downarrow\uparrow}^\dagger$ due to Hermiticity. These elements represent the Rashba spin-orbit interaction term which is defined as

$$H_r = H_{\uparrow\downarrow} + H_{\downarrow\uparrow} = \sum_{(i,j)} \sum_{s,s'} ic_{i,s}^\dagger (u_{i,j}^s \cdot \vec{\sigma}) c_{j,s'} + h.c. \quad (6.6)$$

with $\vec{\sigma} = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}$ with $\sigma_i$ representing the $i^{th}$ Pauli matrix, and $u_{i,j}^s$ given by

$$u_{i,j}^s = -\frac{\Delta_r}{a} \hat{z} \times \vec{\delta}_k \quad (6.7)$$

with $\Delta_r$ the strength of the Rashba interaction and $\vec{\delta}_k$ is the two-dimensional displacement vector between nearest neighbor points $i$ and $j$.

![Figure 6.5: Diagram of a graphene ribbon with the three displacement vectors $\delta_i$ defined in Eqs (6.8)-(6.10). The solid points represent the $A$ sublattice while the hollow points represent the $B$ sublattice. The Rashba term in Eq. (6.12) is defined as a summation over the $A$ sublattice only.](image)

The three possible nearest-neighbor displacement vectors are shown in Fig. 6.5. These vectors are defined in terms of the lattice constant as

$$\delta_1 = a \hat{y} \quad (6.8)$$

$$\delta_2 = a \frac{\sqrt{3}}{2} \hat{x} - a \frac{1}{2} \hat{y} \quad (6.9)$$

and

$$\delta_3 = -a \frac{\sqrt{3}}{2} \hat{x} - a \frac{1}{2} \hat{y} \quad (6.10)$$
Using the above equations, we can rewrite the diagonal term of the Hamiltonian as a summation over the \( A \) sublattice points with \( \vec{r} \) being the position of any site on the \( A \) sublattice. The diagonal element in spin space is given by

\[
H_0 = t \sum_{\vec{r}} (c_{\vec{r},\uparrow}^\dagger d_{\vec{r}+\delta_1,\uparrow} + c_{\vec{r},\uparrow}^\dagger d_{\vec{r}+\delta_2,\uparrow} + c_{\vec{r},\uparrow}^\dagger d_{\vec{r}+\delta_3,\uparrow} + c_{\vec{r},\downarrow}^\dagger d_{\vec{r},\downarrow} + d_{\vec{r},\uparrow}^\dagger c_{\vec{r}+\delta_1,\uparrow} + d_{\vec{r},\downarrow}^\dagger c_{\vec{r}+\delta_2,\downarrow} + d_{\vec{r},\downarrow}^\dagger c_{\vec{r}+\delta_3,\downarrow} + h.c.)
\]

(6.11)

where we have introduced a new creation/annihilation operator \( d \) that acts on the \( B \) sublattice for clarity. Likewise, the Rashba term of the Hamiltonian is

\[
H_r = \Delta_r \sum_{\vec{r}} (e^{i\frac{\pi}{2}} c_{\vec{r},\uparrow}^\dagger d_{\vec{r}+\delta_1,\downarrow} + e^{i\frac{\pi}{2}} c_{\vec{r},\downarrow}^\dagger d_{\vec{r}+\delta_2,\downarrow} - e^{i\frac{\pi}{2}} c_{\vec{r},\uparrow}^\dagger d_{\vec{r}+\delta_3,\downarrow} - e^{i\frac{\pi}{2}} c_{\vec{r},\downarrow}^\dagger d_{\vec{r}+\delta_1,\downarrow} + h.c.)
\]

(6.12)

where the phase factors are due to the imaginary factor in the definition of the Rashba term as well as the combinations of Pauli matrices. The total Hamiltonian can be written as

\[
H = H_0 + H_r.
\]

(6.13)

### 6.4 Zigzag Boundaries and Rashba Interaction

To apply the above formula to a GNR, we would need to add in hard-wall boundary conditions along the width of the ribbon with periodic boundary conditions along the length. The generation of these conditions will depend on the desired geometry. In this section, we will apply these boundary conditions to zigzag nanoribbons and calculate the band structure and conductance.

#### 6.4.1 Band Structure Calculation

It is convenient for our calculation to define the position of each \( A \) sublattice point as

\[
\vec{r} = a \sqrt{3} n \hat{x} + \vec{b}_m
\]

(6.14)
for all integers \( n \in [0, N] \) and vector \( \vec{b}_m \) given by

\[
\vec{b}_m = \begin{cases} 
\frac{a\sqrt{3}}{4} \left[ 1 - (-1)^{\frac{n}{2}} \right] \hat{x} + \frac{a(3m - 1)}{4} \hat{y}, & \text{if } m \text{ even} \\
\frac{a\sqrt{3}}{4} \left[ 1 - (-1)^{\frac{m-1}{2}} \right] \hat{x} + \frac{a(3m - 1)}{4} \hat{y}, & \text{if } m \text{ odd}
\end{cases}
\]

(6.15)

for any integer \( m \in [1, 2M] \) where \( M \) is the width of ribbon as indicated in Fig. 6.3. The reason for the even and odd distinction is due to the definition of the width of the ribbon.

As we pointed out previously, the width is defined in dimer pairs of \( A \) and \( B \) sublattice sites. This means that the total number of sites in a unit cell are \( 2M \). By using this description, we can uniquely define every site in the unit cell through the integers \( n \) and \( m \) which define the position of each site along the ribbon. This allows us to change the summations in Eqs. (6.11) and (6.12) from a summation over \( \vec{r} \) to two summations over \( n \) from \( 0 \to N - 1 \) and \( m \) from 1 to \( 2M \).

![Figure 6.6: A zigzag GNR of width M=4. The green box represented the repeated unit cell used in the band structure calculation. The translational distance between each unit cell is \( a\sqrt{3} \) as indicated.](image)

The positions we define in Eq. (6.14) are ideal for representing a hardwall boundary zigzag GNR with the repeated unit cell indicated by the green box in Fig. 6.6. Due to the periodicity in the \( \hat{x} \)-direction, we can represent the creation and annihilation operators in the Hamiltonian as the Fourier transform in the \( \hat{x} \)-direction as (note that this applies for the
operators as well.)

\[ c_{n,m,s} = \sum_{p=0}^{N-1} \tilde{c}_{m,K_p} e^{iK_p \mathbf{r} \cdot \mathbf{e}_x}. \]  

(6.16)

Since we have periodic boundary conditions along \( n \), this means that

\[ c_{n=0,m,s} = c_{n=N-1,m,s} \]  

(6.17)

which, by replacing in Eq. (6.16), gives

\[ \sum_{p=0}^{N-1} \tilde{c}_{m,K_p} e^{iK_p \mathbf{b}_m \cdot \mathbf{e}_x} = \sum_{p=0}^{N-1} \tilde{c}_{m,K_p} e^{iK_p (a \sqrt{3}N + \mathbf{b}_m \cdot \mathbf{e}_x)}. \]  

(6.18)

The only way for this expression to be valid is if we have an equivalency between like terms i.e.

\[ c_{m,K_p} e^{iK_p \mathbf{b}_m \cdot \mathbf{e}_x} = \tilde{c}_{m,K_p} e^{iK_p (a \sqrt{3}N + \mathbf{b}_m \cdot \mathbf{e}_x)}. \]  

(6.19)

If we now compare this expression to the Bloch condition, we find that

\[ e^{iK_p a \sqrt{3}N} = 1 \]  

(6.20)

which implies that the argument of the exponent must be equal to \( 2\pi p \) where \( p \) is an integer. Simplifying this expression gives us the value of the wave vector \( k \) as

\[ K_p = \frac{2\pi p}{a \sqrt{3}N}. \]  

(6.21)

In the Hamiltonian, the creation and annihilation operators appear in pairs of \( A \) and \( B \) sublattice operators. If we replace a pair of these operators by their Fourier transforms in Eq. (6.16), we find that for each pair

\[ \tilde{c}_{n,m,s} d_{n,m',s'} = \sum_{p,p'=0}^{N} \tilde{c}_{p,m,s} \tilde{c}_{p',m',s'} e^{iK_p \mathbf{r} \cdot \mathbf{e}_x} e^{iK_{p'} \mathbf{r}' \cdot \mathbf{e}_x}. \]  

(6.22)

The dot products in the exponent can be written as

\[ \mathbf{r} \cdot \mathbf{e}_x = a \sqrt{3}n + b_m \cdot \mathbf{e}_x \]  

(6.23)
which simplifies Eq. (6.22) to
\[ c_{n,m,s}^\dagger d_{n,m',s'} = \sum_{p,p' = 0}^{N} \tilde{c}_{p,m,s}^\dagger \tilde{c}_{p',m',s'} e^{ia \sqrt{3} n (K_p - K_{p'})} e^{i(K_p b_m - K_{p'} b_{m'})} \hat{x}. \]  
(6.24)
Recall that we replaced the sum over \( \vec{r} \) by sums over \( m \) and \( n \). If we take into account the sum over \( n \), we arrive at
\[ \sum_{n = 0}^{N} c_{n,m,s}^\dagger d_{n,m',s'} = \sum_{p,p' = 0}^{N} \tilde{c}_{p,m,s}^\dagger \tilde{c}_{p',m',s'} e^{i(K_p b_m - K_{p'} b_{m'})} \hat{x} \sum_{n = 0}^{N} e^{ia \sqrt{3} n (K_p - K_{p'})} \]  
(6.25)
which can be simplified using the properties of discrete Fourier transforms and Eq. (6.21) to find
\[ \sum_{n = 0}^{N} e^{ia \sqrt{3} n (K_p - K_{p'})} = \delta_{p,p'} \]  
(6.26)
where \( \delta_{p,p'} \) is the Kronecker delta function. This leaves us with the expression
\[ \sum_{n = 0}^{N} c_{n,m,s}^\dagger d_{n,m',s'} = \sum_{p = 0}^{\infty} \tilde{c}_{p,m,s}^\dagger \tilde{c}_{p,m',s'} e^{i(K_p b_m - K_{p'} b_{m'})} \hat{x} \]  
(6.27)
Thus, by replacing this result for every term in the Hamiltonian, we find that the system is diagonal in \( p \)-space.

This has simplified the problem to the diagonalization of a \( 4M \times 4M \) matrix where a factor 2 comes from the two site basis representation and another factor of 2 comes from the spin degree of freedom. This matrix can be divided into \( 2M \times 2M \) spin space sub-blocks as shown in Eq. (6.4) with the positional label \( m \) labeling each site’s designated column and row in all following spin-block matrices (e.g. the site at \( m = 3 \) will be represented in row and column 3). Finally, the diagonal sub-blocks are related by \( H_{\uparrow,\uparrow} = H_{\downarrow,\downarrow} \) and the off-diagonal by \( H_{\uparrow,\downarrow} = H_{\downarrow,\uparrow}^\dagger \).

For the case of \( M = 2 \), the spin-block matrices are
\[
H_{\uparrow,\uparrow} = 2t \begin{pmatrix}
0 & \cos \frac{m}{N} & 0 & 0 \\
\cos \frac{m}{N} & 0 & \frac{1}{2} & 0 \\
0 & \frac{1}{2} & 0 & \cos \frac{m}{N} \\
0 & 0 & \cos \frac{m}{N} & 0
\end{pmatrix}
\]  
(6.28)
and

\[ H_{\uparrow, \downarrow} = 2i\Delta_r \begin{pmatrix} 0 & \sin \pi \left( \frac{n}{N} - \frac{1}{6} \right) & 0 & 0 & 0 \\ \sin \pi \left( \frac{n}{N} + \frac{1}{6} \right) & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & \sin \pi \left( \frac{n}{N} - \frac{1}{6} \right) & 0 \\ 0 & 0 & \sin \pi \left( \frac{n}{N} + \frac{1}{6} \right) & 0 & 0 \\ 0 & 0 & 0 & 0 & \sin \pi \left( \frac{n}{N} + \frac{1}{6} \right) \end{pmatrix}. \] (6.29)

For the case of \( M = 3 \), we need to increase the size of both matrices by two columns and rows. However, only four new non-zero elements appear along the tridiagonal. The \( M = 3 \) matrices are thus

\[ H_{\uparrow, \downarrow} = 2t \begin{pmatrix} 0 & \cos \frac{mn}{N} & 0 & 0 & 0 & 0 \\ \cos \frac{mn}{N} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \cos \frac{mn}{N} & 0 & 0 \\ 0 & 0 & \cos \frac{mn}{N} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & \cos \frac{mn}{N} \\ 0 & 0 & 0 & 0 & \cos \frac{mn}{N} & 0 \end{pmatrix}. \] (6.30)

and

\[ H_{\uparrow, \downarrow} = 2i\Delta_r \begin{pmatrix} 0 & \sin \pi \left( \frac{n}{N} - \frac{1}{6} \right) & 0 & 0 & 0 & 0 \\ \sin \pi \left( \frac{n}{N} + \frac{1}{6} \right) & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & \sin \pi \left( \frac{n}{N} - \frac{1}{6} \right) & 0 & 0 \\ 0 & 0 & \sin \pi \left( \frac{n}{N} + \frac{1}{6} \right) & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & \sin \pi \left( \frac{n}{N} - \frac{1}{6} \right) \\ 0 & 0 & 0 & 0 & \sin \pi \left( \frac{n}{N} + \frac{1}{6} \right) & 0 \end{pmatrix}. \] (6.31)

If the width of the ribbon is increased again (\( M = 4 \)), another two columns and rows would be added along with the same non-zero matrix elements along the tridiagonal. This procedure can be extrapolated out to any desired ribbon width.
In Fig. 6.7, we plot the band structure for ribbons of length $M = 2, 3, \text{ and } 4$ with the Rashba interaction energy turned off and with it set to $\Delta_r/t = 0.4$. We compare our results to Refs. [95, 62]. Our results perfectly reproduce reported values.

Figure 6.7: Zigzag GNR with added Rashba spin-orbit interaction. The plots show the band structure of ribbons of width $W = 2, 3, \text{ and } 4$ without and with Rashba spin-orbit interaction. This term breaks the degeneracy of the spin-$\uparrow$ and spin-$\downarrow$ bands as can be seen from the $\Delta_r/t = 0.4$ plots. Note: we have only plotted $1/4$ of the full band structure as it is mirror symmetric around energy as well as $K$. Finally, notice a flat band region around $E = 0$ with and without Rashba. These are the conducting states of the zigzag GNR.
6.4.2 Conductance Calculation

Next, we would like to compare these band structure calculations to transmission calculations using the Recursive Green’s function method outlined in Ref. 3.3. One of the advantages of using this method, compared to the diagonalization routine described previously, is that we do not need to rewrite the real-space Hamiltonian in momentum space. Using a real space basis will allow us, later on, to easily add disorder into the Rashba interaction term and create a random Rashba field.

To implement the Green’s function method, we need to construct the intra-cell interaction Hamiltonian $h_0$ as well as the inter-cell interaction Hamiltonian $h_1$. Similar to the previous method, each of these Hamiltonians will be matrices of size $4M \times 4M$ which is the total number of states in the unit cell. These matrices will contain both spin components with rows/columns $1 \rightarrow 2M$ representing the spin-up states for sites at position $m = 1, 2, 3, \ldots, 2M$ and rows/columns $2M + 1 \rightarrow 4M$ representing the spin-down for sites at position $m = 1, 2, 3, \ldots, 2M$.

Using Eqs. (6.11) and (6.12) we find the intra-cell interaction Hamiltonian for $M = 2$ to be

$$h_0 = \Delta_r \begin{pmatrix}
0 & \frac{t}{\Delta_r} & 0 & 0 & 0 & e^{-i\frac{\pi}{6}} & 0 & 0 \\
\frac{t}{\Delta_r} & 0 & \frac{t}{\Delta_r} & 0 & e^{i\frac{5\pi}{6}} & 0 & e^{-i\frac{\pi}{6}} & 0 \\
0 & \frac{t}{\Delta_r} & 0 & \frac{t}{\Delta_r} & 0 & e^{i\frac{5\pi}{6}} & 0 & e^{-i\frac{\pi}{6}} \\
0 & 0 & \frac{t}{\Delta_r} & 0 & 0 & 0 & e^{i\frac{\pi}{6}} & 0 \\
0 & e^{-i\frac{5\pi}{6}} & 0 & 0 & 0 & \frac{t}{\Delta_r} & 0 & 0 \\
e^{i\frac{\pi}{6}} & 0 & e^{-i\frac{\pi}{6}} & 0 & \frac{t}{\Delta_r} & 0 & \frac{t}{\Delta_r} & 0 \\
0 & e^{i\frac{5\pi}{6}} & 0 & e^{-i\frac{5\pi}{6}} & 0 & \frac{t}{\Delta_r} & 0 & \frac{t}{\Delta_r} \\
0 & 0 & e^{i\frac{5\pi}{6}} & 0 & 0 & \frac{t}{\Delta_r} & 0 & 0
\end{pmatrix} \quad (6.32)$$
and the inter-cell interaction Hamiltonian to be

\[
\begin{pmatrix}
0 & \frac{i}{\Delta_r} & 0 & 0 & 0 & e^{-i\frac{5\pi}{6}} & 0 & 0 \\
\frac{i}{\Delta_r} & 0 & 0 & 0 & e^{i\frac{5\pi}{6}} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{i}{\Delta_r} & 0 & 0 & 0 & e^{-i\frac{5\pi}{6}} \\
0 & 0 & \frac{i}{\Delta_r} & 0 & 0 & 0 & e^{i\frac{5\pi}{6}} & 0 \\
e^{i\frac{5\pi}{6}} & 0 & 0 & 0 & \frac{i}{\Delta_r} & 0 & 0 & 0 \\
0 & 0 & 0 & e^{-i\frac{5\pi}{6}} & 0 & 0 & 0 & \frac{i}{\Delta_r} \\
0 & 0 & e^{i\frac{5\pi}{6}} & 0 & 0 & 0 & \frac{i}{\Delta_r} & 0 
\end{pmatrix}
\]

(6.33)

In order to test these equations numerically, we will calculate the density of states using Green’s function methods through the summation of imaginary diagonal Green’s function elements (See Eq. (3.62)). We can compare this result to the density of states calculated from the band structure calculations in Sec. 6.4.1. To transform the numerically calculated band structure into a density of states representation, we count the amount of states \(n_E\) within a small window \(E - \eta_E\) to \(E + \eta_E\) where we choose \(\eta\) to be arbitrarily small. Dividing \(n_E\) by the total number of states in the band structure will give us the density of states at energy \(E\). Repeating this procedure for all energies gives us the total density of states. We plot some of these results in Fig. 6.8.

Now that we have verified the density of states, we will look at the conductance calculation for these systems. Some results are shown in Fig. 6.9 where we can clearly see the appearance of conductance plateaus. The height of each plateau is equivalent to the amount of conducting channels at that energy. This point can be illustrated when we compare the conductance with the band structures from Fig. 6.7. In Fig. 6.9, we have superimposed the rotated band structure on the conductance results for easy comparison. From this we can see that the number of times a band crosses at the energy \(E\) is equivalent to the conductance. Thus, this verifies that our numerical Green’s function routines deliver
Figure 6.8: Density of states for a (top) $M = 4$ and (bottom) $M = 8$ zigzag GNR with added Rashba spin-orbit interaction of $\Delta_r / t = 0.4$. The red dots correspond to the calculation of the density of states through the Green’s function method while the black line corresponds to the density of states calculated from the band structure in Sec. 6.4.1

the expected density of states and conductance as compared with external results and parallel methods.
Figure 6.9: Conductance for a (top) $M = 4$ and (bottom) $M = 8$ zigzag GNR with added Rashba spin-orbit interaction of $\Delta_r/t = 0.4$ compared to the band structure. The Blue curves correspond to the conductance $G$ with respect to the energy. We can see clear conductance plateaus that are related to the number of conducting channels available. To emphasize this, we have plotted the band structure (purple curves) from Fig. 6.7 (which has been rotated 90 degrees such that the momentum states are on the y-axis and the energy on the x-axis). For each energy, the conductance is equal to the number of times a band crosses the chosen energy. To illustrate this, in the top figure a dashed line through $E/t = 1.6$, with all band crosses circled, illustrates this point.

6.5 Random Rashba Field

We would like to end this section with a brief discussion on future work related to RRF fields.
Similar to the generation method used for the on-site disorder in the previous section, we can include a disordered Rashba interaction by randomly generating the coupling parameter $\Delta_r$. The first step would be to study the case of uncorrelated disorder which to our knowledge has yet to be addressed in detail.

A more realistic model would incorporate correlations into the RRF. To do this, we would need to modify the disorder generation method presented in Sec. 3.1 to incorporate a two-dimensional correlation. In this case, we would need to generate a random variable for each bond between neighboring atoms as the Rashba term is in essence a hopping term. Since each site contains 3 bonds, the number of bonds per unit cell for a zigzag ribbon will be given by $b = 3M - 1$. Furthermore, the scaling of the order of operation of a conductance calculation is given by $\sim N(4M)^3$, which limits us to narrow GNR. Because of these reasons, early attempts to implement correlated variable generation have resulted in highly inefficient and expensive routines. Further research is needed to improve the efficiency and make this study practically viable.

In a recent experimental work by the group of K. Kern (brought to our attention by private communications), has shown that intercolated Au clusters on top of epitaxially grown graphene appears to introduce a strong spin-orbit coupling that results in increased resistances. This result implies changes to the localization behavior of the electronic states. We are interested in studying this localization behavior using our present routines.

As a toy model, we plan to consider a zigzag GNR that consists of three constant spin-orbit coupling parameters between C-C bonds, C-Au Bonds, and Au-Au bonds. In the aforementioned experiment, the amount of gold particles introduced is small and it can be assumed that the distribution of Au clusters is uncorrelated. Thus, we can randomly choose a few sites on the GNR as nucleation points for the Au clusters from a simple uncorrelated distribution. Finally, we can generate a random radius for the gold cluster and assign the appropriate spin-orbit coupling parameters between sites. Since this
method requires solely the use of uncorrelated variable generation methods, we can more efficiently study these systems while creating new algorithms pertaining to random Rashba fields.
7 Discussion and Conclusions

Throughout this document we have presented a detailed analysis of the effects of various long-range correlated disorder model on the electronic states of one-dimensional systems. This study shows that correlations can not only drive a metal-insulator quantum phase transition through the Anderson localization phenomena, but can also critically affect the individual electronic phases, specifically the insulating case where all eigenstates are spatially localized.

By comparing numeric results with mathematical theorems related to one-dimensional stochastic Schrödinger operators, we have demonstrated quantitatively not only the need for long-range correlations, but the need for extensive long-range correlations for the existence of an Anderson transition. We applied our analysis to the case of $\sim 1/k^\alpha$ spectral density correlations, $\sim 1/r^\alpha$ real space correlations, as well as to the random dimer model and noticed distinct difference among these. Furthermore, we find different behaviors in the short-range components of these correlations. This observation highlights the importance of the interplay between the short and long ranged components of the correlation function and their combined effect on the Anderson metal-insulator transition.

Furthermore, we conducted a detailed analysis on $\sim 1/r^\alpha$ correlations which, besides being practically important due to their frequent appearance in natural systems, are conceptually interesting as they reside in a region between short- and infinite-ranged correlated disorder models and do not introduce disorder length scale. We calculated the $\beta$ scaling function and confirmed standard localization physics for a range of energies $E < W/t\alpha$ by verifying the single parameter scaling hypothesis. For $E < W/t\alpha$, we argued that, though states remain localized, the divergence from the single parameter scaling hypothesis indicates the presence of non-typical localization phenomena that likely result
from an extension of the band edge anomaly that is presented for uncorrelated disordered systems.

This interpretation is given further proof when examining the localization length for different values of the correlation parameter $\alpha$. In this, we find a crossover energy $E_c$ that separates regions of enhanced localization, near the band edge, and suppressed localization, near the band center, with increasing correlation. This crossing is supported by analytic results in the weak disorder limit. We argued as well that this energy separates two different scaling regions near the band edge and center.

Finally, we outlined a problem pertaining to random spin-orbit coupling in a two-dimensional graphene nanoribbon. We reviewed common numerical methods and reproduced several previous results as well as showed consistency between two different generation methods nonequivalent physical quantities. Finally, we discuss current efforts to generate a disordered Rashba field as well as a way to model gold intercalated graphene nanoribbons.
REFERENCES


Appendix A: Participation Ratio

Near a critical point, the fluctuations in the wavepacket distributions can become increasingly large and make an analysis of the localization length difficult. To study these fluctuations, it is common to study the the mean 4th power of the wavefunction amplitude which determines the percentage of sites that contribute to the state[86]. We define the participation ratio

\[ A_k = \frac{1}{L} \left( \frac{\int_0^L |\psi_k(x)|^2 dx}{\int_0^L |\psi_k(x)|^4 dx} \right)^2 \]  

(A.1)

for each energy state \( k \) with system size \( L \) and amplitude \( \psi_k(x) \). If the state is localized, the participation ratio will approach zero as the system size increases. If all sites contribute equally with \( |\psi_k(x)| = 1 \) or a periodic amplitude is assumed such as \( |\psi_k(x)| = \cos(kx) \), the participation ratio evaluates to 1 and 2/3 respectively in the thermodynamic limit. Though the exact value of the participation ratio depends on the form of the amplitude, any finite valued \( A_k \) provides evidence for wavefunction delocalization. This argument can be extended to higher dimensions in both the discrete and continuous case. As an example, if the amplitude in the continuous case is \( \cos(k^x x) \cos(k^y y) \) or \( \cos(k^x x) \cos(k^y y) \cos(k^z z) \), \( A_k \) approaches 4/9 and 8/27 respectively.

Furthermore, for any exponentially localized state, the participation ratio obeys an asymptotic limit of

\[ A_k(L) \sim \frac{1}{L^d} \text{ for } L \gg \lambda_k \]  

(A.2)

where \( d \) is the dimensionality of the system, \( L \) is the system size, and \( \lambda \) is the localization length of state \( k \). When the participation ratio of a critical state is analyzed, due to the intense fluctuations at criticality, it is found that it follows a similar form of Eq. (A.2) with \( d \) replaced by a fractal dimension \( D \).
For a numeric study, it is more useful to work with the discrete definition of the participation ratio

\[ A_k = \frac{1}{N} \left( \frac{\sum_{n=0}^{N-1} |\psi_k(x_n)|^2}{\sum_{n=0}^{N-1} |\psi_k(x_n)|^4} \right)^2 \]  

(A.3)

where \( k \) is now an integer and \( x \) is replaced by the integer \( n \) which labels the site number. Numerically calculating Eq. (A.3) requires that we find the full wave solution for the disordered Hamiltonian. Thus, a full matrix diagonalization is required. We employed two independently developed matrix diagonalization routines and both yielded identical results. However, due to the resource intensive cost associated with a full matrix diagonalization (operations grow as \( \sim N^3 \)), we could only reach system sizes of the order \( N \sim 10^3 \). For the study of long-range correlations, these systems sizes are inadequate for weak disorder strengths where the localization length is comparable, or greater, to the system size.

In the case of strong disorder, the localization length is one or two orders of magnitude smaller than the system size, however in this region the eigenstates are localized due to large potential fluctuations rather than the typical Anderson destructive interference mechanism. Nevertheless, we conducted a study of the fractal exponent for strongly disordered systems with scale-free correlation. We plot some of our results for the participation ratio and extract the "fractal" dimension \( D \). For all energies and correlations, we see that \( D = d = 1 \) which indicates the absence of Anderson transition as expected.
Figure A.1: The participation ratio exponent $D$ as a function of energy for systems with scale-free disorder correlations. The colors correspond to $\alpha = 0.5$ (blue), $\alpha = 1.0$ (red), and $\alpha = 1.5$ (yellow). These results are extracted from system sizes of $N = 200 – 1000$ and confirm the absence of a critical point.
Appendix B: Anomalous Diffusion of a Wavepacket

The dynamics of an electronic wavepacket through a disordered system can provide valuable information about the localization or extension of eigenstates. Along with providing a unique view of the particle’s trajectory, the critical exponents associated with an Anderson transition can be extracted.[79]

The most straightforward numerical algorithm for this type of calculation is a simple matrix diagonalization. From this, we can extract the coefficients of the eigenstates

$$\eta_{n,k} = \langle n|k \rangle$$

(B.1)

where we use the integers $n$ to represent the discrete real space and $k$ to represent reciprocal space. There is a degree of arbitrariness in the selection of initial states as we only require a state with a high degree of localization. Thus, for simplicity, we choose our initial state to be confined at a single site denoted $|n_0\rangle$. This along with the definition of the position and squared position operators

$$\hat{X}|n\rangle = x_n$$

(B.2)

and

$$\hat{X}^2|n\rangle = x_n^2$$

(B.3)

leads to the formulas

$$\langle X(\tau) \rangle = \sum_{k,q,n} \eta_{n_0,k}^{\dagger} \eta_{n,q}^{\dagger} \eta_{n_0,q} \eta_{n,k} \exp \left[ \frac{i\tau(E_k - E_q)}{\hbar} \right] x_n$$

(B.4)

and

$$\langle X^2(\tau) \rangle = \sum_{k,q,n} \eta_{n_0,k}^{\dagger} \eta_{n,q}^{\dagger} \eta_{n_0,q} \eta_{n,k} \exp \left[ \frac{i\tau(E_k - E_q)}{\hbar} \right] x_n^2$$

(B.5)

with $E_k$ being the energy of state $k$ and $\tau$ being the time. These quantities directly relate to the standard deviation by

$$\sigma(\tau) = \sqrt{\langle X^2(\tau) \rangle - \langle X(\tau) \rangle^2}$$

(B.6)
which can be used to extract the critical parameters and summarize the spread of the wavepacket.

For small times, we can gain some insight into the diffusion through the Heisenberg representation and an expansion of the time-evolution operator. By using fermionic anti-commutation relations \( \{ c^\dagger_i, c_j \} = \delta_{i,j} \) and \( \{ c_i, c_j \} = \{ c^\dagger_i, c^\dagger_j \} = 0 \) and the general Heisenberg representation for an operator

\[
\hat{A}_H = \hat{A} - i\tau[H, \hat{A}] - \frac{\tau^2}{2!}[H, [H, \hat{A}]] + ... \tag{B.7}
\]

we can find the time dependent expectation value of the operators

\[
\langle \hat{X}_H \rangle = 0 \tag{B.8}
\]

and

\[
\langle \hat{X}_H^2 \rangle = 2\tau^2(at)^2 - 2\tau^4(\langle \epsilon_i - \epsilon_{i+1} \rangle)^2(at)^2 + ... \tag{B.9}
\]

Note that if the disorder were constant, i.e. \( \epsilon_i = \epsilon \), or time is small, we arrive at the well known diffusion equation

\[
\sigma(t) = \tau \sqrt{2}(at) \tag{B.10}
\]

From the original work on Anderson localization [4], we know that localization suppresses the diffusion of a wavepacket which leads to a constant value for \( \sigma \) at long times. We will define this saturation value as the localization length \( \xi(E) \). Taking into account these two limits, we propose the scaling function

\[
\overline{\sigma^2_E}(\tau) = D^2\tau^2F\left(\frac{D^2\tau^2}{\xi(E)^2}\right) \tag{B.11}
\]

with limits

\[
\lim_{\tau\to0}\overline{\sigma^2_E}(\tau) = D^2\tau^2 \tag{B.12}
\]

\[
\lim_{\tau\to\infty}\overline{\sigma^2_E}(\tau) = \xi(E)^2. \tag{B.13}
\]
If an Anderson transition exists, we know that we can characterize the phase transition between localized and extended states through the exponent $\nu$ defined by the universal scaling behavior

$$\xi \sim E^{-\nu}. \quad (B.14)$$

by putting this into Eq. (B.11) and performing a change of variables to the dimensionless variable $u$, we arrive at

$$\sigma^2(\tau) = \frac{D^{2-1/\nu} \tau^{2-1/\nu}}{2\nu} \int u^{-1/\nu} F(u) du. \quad (B.15)$$

Thus, we have extracted the time from the integral and now are left with

$$\sigma(t) \sim \tau^{1-1/2\nu}. \quad (B.16)$$

with the exponent $\theta = 1 - 1/2\nu$ describing a region of anomalous diffusion. We can relate $\theta$ to the standard deviation of the wavepacket by

$$\theta = \frac{d \log \sigma}{d \log \tau}. \quad (B.17)$$

If an anomalous region exists, there will be a time interval where $\theta(\tau) = \theta$.

We attempted to apply this method to $\sim 1/r$ correlations to test the appearance of anomalous extended states but without success. Without the appearance of a true quantum phase transition, an anomalous diffusive region cannot be identified. We plot a typical data set in Fig. B.1.

The main limitation of the above algorithm is the scaling of operations with system size. As an example, a typical matrix diagonalization routine that uses an LU decomposition algorithm takes an order of $\sim N^3$ operations to complete. Once the matrix is diagonalized, for each point in time it takes another $\sim N^3$ operations to calculate the standard deviation. With these limits, it is difficult to realize systems of more than 10000
sites which pales in comparison to the transfer matrix and recursive Green’s function methods. 

Recently, we have found literature that provides a highly efficient time-evolution algorithm that uses an expanded time evolution operator in terms of Chebychev polynomials[28, 46]. Preliminary results suggest these methods can be used to study larger systems as the algorithm requires less memory. However, this method maybe well suited to study the role of short-range correlation in wavepacket dynamics.
APPENDIX C: DERIVATION OF GRAPHENE BAND STRUCTURE

Figure C.1: Diagram of a graphene ribbon with the three displacement vectors $\delta_i$. The solid points represent the A sublattice while the hollow points represent the B sublattice.

Consider an infinite graphene sheet as shown in Fig. C.1 with the three possible nearest-neighbor displacement vectors given by

\[ \delta_1 = a\hat{y} \]  \hspace{1cm} (C.1)
\[ \delta_2 = a\frac{\sqrt{3}}{2}\hat{x} - a\frac{1}{2}\hat{y} \]  \hspace{1cm} (C.2)
and
\[ \delta_3 = -a\frac{\sqrt{3}}{2}\hat{x} - a\frac{1}{2}\hat{y} \]  \hspace{1cm} (C.3)

The nearest-neighbor tight-binding Hamiltonian can be written in terms of the A and B sublattice creation/annihilation operators $c_{\vec{r}}$ and $d_{\vec{r}}$, which act on the real space states $|A; \vec{r}\rangle$ and $|B; \vec{r}\rangle$ respectively, as

\[ H = -t \sum_{\vec{r}} \sum_{j=1}^{3} (c_{\vec{r} + \delta_j}^+ d_{\vec{r} + \delta_j} + h.c.) \]  \hspace{1cm} (C.4)

where the summation is over the position of each point in the A sublattice.

Using Bloch’s theorem, we can construct the Fourier components of the creation/annihilation operators as

\[ c_{\vec{k}}^+ = \frac{1}{N} \sum_{\vec{r}} e^{-i\vec{k} \cdot \vec{r}} c_{\vec{r}}^+ \]  \hspace{1cm} (C.5)
and
\[ d_{\vec{r}+\vec{e}_j} = \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{e}_j} e^{i\vec{q}\cdot\vec{r}} \vec{d}_{\vec{q}} \]  
(C.6)

which act on the states \(|A; \vec{k}\rangle\) and \(|B; \vec{k}\rangle\) respectively.

Placing these components into the Hamiltonian we arrive at
\[ H = -\frac{t}{N^2} \sum_{\vec{q}, \vec{k}} \sum_{j=1}^{3} (\tilde{c}_{\vec{k}}^\dagger \tilde{d}_{\vec{q}} e^{i\vec{q}\cdot\vec{e}_j} + \text{h.c.}) \sum_{\vec{r}} e^{i(\vec{q}-\vec{k})\cdot\vec{r}} \]  
(C.7)

with the sum over \(\vec{r}\) evaluates to
\[ \sum_{\vec{r}} e^{i(\vec{q}-\vec{k})\cdot\vec{r}} = N^2 \delta_{\vec{q},\vec{k}} \]  
(C.8)

with \(\delta_{\vec{q},\vec{k}}\) being a Kronecker delta function. This further simplifies the Hamiltonian to
\[ H = -t \sum_{\vec{k}} (\tilde{c}_{\vec{k}}^\dagger \tilde{\mathcal{L}}_{\vec{k}} \sum_{j=1}^{3} [e^{i\vec{k}\cdot\vec{e}_j}] + \text{h.c.}). \]  
(C.9)

Using the definitions of the displacement vectors, we can find the summation over \(j\), which we will define as \(\phi\), to be
\[ \phi = \sum_{j=1}^{3} e^{i\vec{k}\cdot\vec{e}_j} = e^{i\vec{k}\cdot\vec{a}} \left( 1 + 2e^{-i3ak_y/2} \cos \frac{\sqrt{3}ak_x}{2} \right) \]  
(C.10)

which makes the Hamiltonian
\[ H = -t \sum_{\vec{k}} (\phi \tilde{\mathcal{L}}_{\vec{k}}^\dagger \tilde{d}_{\vec{k}} + \text{h.c.}). \]  
(C.11)

To find the energy, we are left to diagonalize a \(2 \times 2\) Hamiltonian in the A-B sublattice basis which can be represented in matrix format as
\[ H = \begin{pmatrix} 0 & \phi \\ \phi^* & 0 \end{pmatrix} \]  
(C.12)

which, when diagonalized, yields the eigenvalues
\[ E/t = \pm|\phi| = \pm \sqrt{1 + 4 \cos^2 \frac{\sqrt{3}ak_x}{2} + 4 \cos \frac{\sqrt{3}ak_x}{2} \cos \frac{3ak_y}{2}} \]  
(C.13)