Non Equilibrium Electronic Transport in Multilayered Nanostructures.

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Recent advances in strongly correlated materials have produced systems with novel and interesting properties like high Tc superconductors, Mott insulators and others. These novel properties have sparked an interest in industry as well as in academia as new devices are being developed. One such kind of device that can be fabricated is a heterostructure, in which layers of different compounds are stacked in a single direction. Modern deposition techniques like electron beam epitaxy, in which atomic layers of different materials are deposited one at a time creating the device, are capable of fabricating heterostructures with atomic precision. We propose a technique to study heterostructures composed of strongly correlated materials out of equilibrium. By using the Keldysh Green’s function formalism in the dynamical mean field theory (DMFT) framework the properties of a multilayered device are analyzed. The system is composed of infinite dimensional 2D lattices, stacked in the z direction. The first and last planes are then connected to a bulk reservoir, and several metallic planes are used to connect the bulk reservoir to the barrier region. The barrier region is the system of interest, also known as the device. The device is composed of a number of planes where the system correlations have been turned on. The correlations are then model by using the Falicov-Kimball Hamiltonian. The device is then connected to the bulk once again from the opposite side using metallic planes creating a symmetric system. In order to study the non equilibrium properties of the device a linear vector potential \( A(t) = A_0 + tE \) is turned on a long time in the past for a unit of time
and then turned off. This in turn will create a current in the bulk, in effect current biasing the device, as opposed to a voltage bias in which opposite sides of the device are held to a different potential. In this document we will explain the importance of the subject, we will derive and develop the algorithm and we will discuss results and challenges obtained from performing the numerical calculations.

**INDEX WORDS:**  Strongly correlated systems. Dynamical Mean Field Theory. Green’s function formalism. Non equilibrium.
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Richard Hamming was an early pioneer of numerical techniques and computer simulations. In chapter two of his 1997 book "The art of doing science and engineering: learning to learn."[2] he makes the case for the advantages of the digital age. As Hamming points out we are heading towards an information era, in which information is as important as physical goods. The last three decades have seen remarkable accomplishments in the advancement of digital technology. Over such time period the technology industry has been able to continue the trend known as Moore’s law. Moore’s law simply states that the number of transistors per chip will double every eighteen months. This sustain advancement in technology has allowed the proliferation of personal computing. Personal computing have changed our everyday lives, it allows information to be created as well as delivering it. Complex tasks can be carried out with a lower number of mistakes. Initiatives like one laptop per child show the interest in making future generations computer savvy. Computers have also become an essential tool for todays scientists. It is in the spirit of continuing with this advancements in technology that we are interested in novel materials. Minimizing energy consumption while maximizing performance is the industry goal as a whole. We use current technology in order to investigate materials suitable for future applications while keeping this goal in mind.

In 1998, Walter Kohn and John A. Pople won the nobel prize in chemistry[3] for the development of Density Functional Theory (DFT). This was the first time
the Nobel prize was awarded for a technique heavily dependent on computers and simulation. Although it is possible to carry out simple calculations using the basic ideas of DFT using only paper and pencil, the real benefit behind DFT comes from the computational capability of modern computers. DFT from a theoretical point of view will be briefly discussed later in this chapter. Most recently, in 2013, the Nobel prize in chemistry was awarded to Martin Karplus, Michael Levitt, and Ariel Warshel for the development of multiscale simulations used to study chemical and biological processes [4]. They integrated principles of quantum mechanics, molecular mechanics and protein folding together. These techniques have had a huge impact in the understanding of biological systems, with applications in pharmaceutical research. These techniques would not had been possible without the advancement in computer power of the last decades.

It is thus desirable to continue this trend of increasing computing power, while at the same time increasing power efficiency. It is in this vein that the study of new materials becomes an important subject for the development of the industry. From a theoretical point of view, efforts concentrate on determining the properties of a material from first principles. Real materials are being studied starting at the atomic level. Using DFT, the energy structure of the system is obtained from which important characteristics of the system can be determined. This information is used to evaluate the adequacy of the material for any given application. Current research in the areas of energy storage in batteries, solar cells and fuel cells shows the potential of the technique [5][6][7].

More recently there has been strong interest in strongly correlated materials, such as complex oxides in which different phenomena like a super conducting state have been observed. In this limit, the interactions in between pair of electrons is strong and can not be neglected. This creates new interesting quantum phenomena which
can not be easily described using DFT. Therefore, different techniques are required to study strongly correlated devices. Dynamical Mean Field Theory (DMFT) was developed \cite{8} \cite{9} as a means to study the effects of the strong correlations between electrons. Unlike DFT where the starting point is the atomic position of atoms and its electron composition. DMFT works on a lattice, where electron-electron interactions are governed by a model Hamiltonian. Different system characteristics can be simulated by selecting the appropriate Hamiltonian. There are current efforts trying to bring both techniques together, with the objective of extending the reach of both techniques.

1.1 Density Functional Theory

Density functional theory was developed with the objective to solve the many body problem in quantum mechanics by expressing the energy of the system in a density dependent functional form. DFT and similar methods like Hartree-Fock and ab-initio calculations have proven to be successful in the past few decades. Their applications range from drug design to the study of carbon nanotubes. The main advantage of DFT is that it is a straightforward technique that will yield accurate results in real systems. In general DFT is extremely accurate in material properties that depend on energy differences like lattice constants and binding energies. The basic idea behind DFT is to represent the ground state wavefunction of our quantum-mechanical system as a charge density\cite{10}. This is justified by the first Hohenberg-Kohn Theorem \cite{11}. This theorem establish that there is a one to one correspondence between the charge density and an external potential. Therefore; for a given charge density there is a unique external potential that produces such a charge density and vice versa.
The second Hohenberg-Kohn Theorem [11] gives the equivalent of the Schrödinger equation for the charge density. Given any charge density, the functional, \( F[\rho(\vec{r})] \), can be minimized to give an upper bound for the ground state energy.

\[
F[\rho(\vec{r})] = \langle \Psi | \hat{T} + \hat{V}_{\text{e-e}} | \Psi \rangle \quad (1.1)
\]

Where \( F[\rho(\vec{r})] \) is a functional that depends on the density function \( \rho(\vec{r}) \). This expression can be expressed in terms of a variational principle:

\[
E_{V_{\text{ext}}}[\rho'(\vec{r})] = F[\rho'(\vec{r})] + \int V_{\text{ext}}(\vec{r})\rho'(\vec{r})d\vec{r} \geq E_0. \quad (1.2)
\]

At this stage the form of \( F[\rho(\vec{r})] \) still needs to be determined. W. Kohn and L. Sham [12] found a way to approximate this functional. They consider a system of \( N \) electrons where the electrons do not interact with each other. The Schrödinger equation can be solved exactly when no electron-electron interactions are considered; the solution is the \( N \)-electron Slater determinant.

Then \( F[\rho(\vec{r})] \) is broken into parts. The first term is the kinetic energy of the \( N \)-electron non-interacting system. The second term is just the electrostatic energy of a charge density distribution. And the third term is called the exchange correlation functional.

\[
F[n(\vec{r})] = T[n(\vec{r})] + E_H[n(\vec{r})] + E_{xc}[n(\vec{r})] \quad (1.3)
\]

\[
E_H[n(\vec{r})] = \frac{1}{2} \int \int \frac{n(\vec{r}_1)n(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 \quad (1.4)
\]

The exchange correlation functional includes the physics of the many body problem. The interactions between electrons will have a certain energy associated with them.
The exchange correlation term accounts for this energy. While the first two terms are exact, an exact exchange correlation functional is unknown. The first successful approximation proposed for the exchange correlation functional was the local density approximation (LDA) in which the electronic density is assumed to vary slowly, giving a functional of the form.

\[ E^{LD}_{xc} = \int d\vec{r} n(\vec{r}) \epsilon_{xc}[n(\vec{r})] \]  

(1.5)

This functional was later computed using quantum Monte Carlo. A further enhancement for the exchange correlation function is to take into account not only the density but also the gradient of the electronic density. This is known as the generalized gradient approximation.

It is important to notice that, in general, energies calculated using the same exchange correlation function are directly comparable. When calculating properties that depend on the difference of energies we tend to obtain accurate results when compared with experimental data. This can be attributed to the fact that errors introduced in the approximation of the exchange correlation function will partially cancel each other. Each one of these functionals have a corresponding external potential. We can rewrite the problem in terms of the Kohn-Sham Hamiltonian.

\[ \hat{H}_{KS} = -\frac{1}{2} \nabla^2 + V_H(\vec{r}) + V_{xc}(\vec{r}) + V_{ext}(\vec{r}) \]  

(1.6)

The Kohn-Sham Hamiltonian is then solved self-consistently. There are well established software products in the market that allow end users to perform DFT without the hassle of coding their own implementation.
1.2 Strongly correlated materials

A survey about different strongly correlated materials, including complex oxides to be included in here.

1.3 Dynamical Mean Field Theory

Once strong correlations dominate the behavior of the system, DFT starts to fail. This is due to the approximation made for the exchange correlation term $E_{xc}$. Dynamical mean field theory analyzes the problem from a different perspective. As mentioned earlier, DMFT takes into account a model Hamiltonian in a particular lattice. The easiest and most common lattice to work with is the n-dimensional square lattice. In the case of the square lattice each lattice site has two nearest neighboring sites per dimension. This reduces to an equally spaced line in one dimension, a square lattice in two dimensions and the simple cubic lattice in three dimensions. The infinite dimensional case is also of theoretical interest due to simplifications. Other lattices can also be used instead. In literature examples of the honeycomb [17] and Bethe [18] lattices can be found between others.

The model Hamiltonian describes how the electrons interact with each other in the lattice. In the tight binding approximation Fig.(1.1), an electron can hop from site $i$ to site $j$ with an associated energy $t_{ij}$. This energy is given by the hopping integral, or the overlap between to atomic orbitals. The tight binding Hamiltonian [19] can then be written in the second quantization form as

$$\hat{H}_{TB} = - \sum_{ij\sigma} t_{ij} (\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma} + \hat{c}_{j\sigma}^{\dagger}\hat{c}_{i\sigma}), \quad (1.7)$$

where $\hat{c}_{i\sigma}^{\dagger}$ and $\hat{c}_{j\sigma}$ are the creation and annihilation operators respectively. This Hamiltonian describes the kinetic energy of the system. Correlations can then be included
by taking into account electron-electron interactions, or even electron-phonon interactions. The Hubbard model introduced by Hubbard in 1963 [20] is one of the most important models in theoretical physics. It was originally conceived in order to explain the origin of magnetism. The Hubbard Hamiltonian,

\[ \hat{H}_H = - \sum_{ij\sigma} t_{ij} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^{\dagger} \hat{c}_{i\sigma}) + U \sum_i (\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}) \] (1.8)

takes into account electrons with two different spins. Spin up particles and spin down particles interact with an energy \( U \) when located on the same lattice site. Unfortunately an exact solution to the Hubbard model is known only in one dimension and infinite dimensions. While the three dimension solution remains elusive, quantum
Figure 1.2: Hubbard model Hamiltonian. Electrons with positive spin can occupy the same lattice site increasing the energy of the system by $U$. Electrons are allowed to hop to neighboring sites as long as the site doesn’t contain an electron with the same spin on it.

Montecarlo techniques have been applied to the Hubbard model\cite{21} in the cases where there is not a known solution.

A simplification to the problem was proposed by Falicov and Kimball in 1969\cite{22}. The Falicov-Kimball model considers two different bands: A set of conduction $\hat{c}$ electrons and a different set of $\hat{f}$ electrons or localized electrons. Conduction electrons can hop between sites and interact with localized electrons with energy $U$. Localized electrons are frozen in space and interact between themselves with energy $E_f$ when located in the same lattice site. The Hamiltonian for the Falicov-Kimball model can be written as

$$\hat{H}_{FK} = -\sum_{ij} t_{ij} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + E_f \sum_i \hat{f}_i^\dagger \hat{f}_i + U \sum_i \hat{c}_i^\dagger \hat{c}_i \hat{f}_i^\dagger \hat{f}_i.$$ \hspace{1cm} (1.9)
Figure 1.3: Falicov-Kimball model Hamiltonian. Conduction electrons occupy the $\hat{c}$ orbital, there electrons are allowed to hop to neighboring sites. Valence electrons occupied the $\hat{f}$ orbital and they are localized. When both bands are occupy the energy of the system is increased by the onsite energy $U$. 
Other Hamiltonians of current interest include the Ising spin model, the Holstein model and the periodic Anderson model to name a few. The Falicov Kimball model is a good starting point since there is a known solution to the model and it presents a metallic to Mott insulator transition as a function of the parameter value $U$. Finally the effects of the lattice on the model and the effects of the model to the lattice are coupled by using the Dyson Equation; which in turn relates the interacting Green’s function of a system $g$ to the non interaction Green’s function of said system $g_0$ mediated by a self energy $\Sigma$.

$$g(\vec{k},t,t') = g_0(\vec{k},t,t') + g_0(\vec{k},t,t')\Sigma(t,t')g(\vec{k},t,t').$$

(1.10)

In the mean field we approximate the self energy to be independent of momentum. The set of equations is then solved self-consistently, The algorithm in the bulk is depicted in Fig. (1.4) and it goes as follows. First start from a guess to the self energy. Next sum over momentum to obtain the local self energy, this will take into account the geometry of the lattice. We use Dyson equation to find the effective medium. From the effective medium the solution to the Falicov-Kimball model is used to find the impurity Green’s function. Finally this impurity solution is employed to calculate a new guess for the self energy. This loop is iterated until convergence is achieved. This algorithm has been extended to treat the inhomogenous problem in a multilayered system also known as the quantum zipper algorithm. One of the objectives of this thesis is to extend the DMFT algorithm to the multilayer problem but taking into account non equilibrium considerations.
Figure 1.4: The DMFT algorithm is a set of equations that is solved self consistently. Starting from a guess for the self energy, the sum over momentum is determined by the lattice in consideration. The Dyson equation relates the interacting Green’s functions to the non interacting one thru a self energy. The impurity problem solves the model Hamiltonian of the system.
Figure 1.5: Heterostructure device reproduced from [1]. Layers of YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) superconductor material, SrTiO$_3$ (STO), BaZrO$_3$ (BZO) and MgO forming an heterostructure.

Figure 1.6: Multilayered device.
1.4 Heterostructures and the Multilayer Problem

Heterostructures can be tough as an array of layers of alternating compounds in a single dimension. Each compound is independent of each other, and the collective behavior of all the layers determines the properties of a device. Current technology relies in the ability to create processes capable of creating devices with small features. Modern techniques like molecular beam epitaxy [23] allow for the manufacturing of heterostructures with atomic precision. Fig. (1.5) shows such a device. The multilayer problem is formulated such that there is a resemblance to an heterostructure device [24]. At the atomic layer the different elements form a crystalline structure. Since the cross section of the device is large with respect to the width of each individual layer there is the preferential direction of the device. In the multilayer problem this is denoted by the $\hat{z}$ direction. Infinite two dimensional planes are stacked one on top of each other, such that the lattice formed by the aggregate of planes is a simple cubic lattice Fig. (1.6). A number of layers is defined as the barrier region. The barrier is then connected to a bulk via a series of metallic planes. The bulk reservoir imposes the boundary condition of the system. The barrier then can take into a number of configurations dependent on the $U$ values assigned to each plane. If using the Falicov-Kimball model the barrier can be composed of any combination of metallic planes, dirty metals for low $U$, or Mott insulator planes for large $U$. The Falicov-Kimball Hamiltonian in the multilayer problem becomes

$$\hat{H}_{ FK}(t) = - \sum_{\alpha \delta} t_{\alpha \alpha+1}^{\perp} [e^{ieA_{\alpha}(t)} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha+1}^{\dagger} + e^{-ieA_{\alpha}(t)} \hat{c}_{\alpha+1}^{\dagger} \hat{c}_{\alpha}]$$

$$- \sum_{\alpha \delta} t_{\alpha}^{\parallel} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha+\delta} + \sum_{\alpha \delta} (-\mu + U_{\alpha \delta}) \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha}$$

(1.11)

where $t_{\alpha \alpha+1}^{\perp}$ is the hopping for an electron tunneling longitudinally from one plane to another and $t_{\alpha}^{\parallel}$ is the transverse hopping for electrons within the plane. The symbol $\mu$
is the chemical potential and \( U_\alpha \) is the onsite interaction between conduction electrons \( \hat{c} \) and localized electrons whose number operator \( \hat{w}_{\alpha l} = \hat{f}^{\dagger}_{\alpha l} \hat{f}_{\alpha l} \) is a classical variable taking the value of 0 or 1. The hopping \( t \) is restricted to nearest neighbor hopping where the \( \delta \) index sums over nearest neighbors within each plane. In order for the Hamiltonian to remain Hermitian, the hopping from one plane to the next has to be the same in the opposite direction, that is \( t_{\alpha+1,\alpha} = t_{\alpha,\alpha+1} \). The electromagnetic potential \( A_\alpha(t) \) is oriented in the direction of the longitudinal transport. The fact that the phase enters as a complex conjugate for the two longitudinal terms guarantees Hermiticity of the Hamiltonian.

1.5 Beyond linear response

Most interesting applications of the first vacuum tubes as well as today’s modern electronics rely on the nonlinearity of the device. Most research on strongly correlated heterostructures have been performed within linear response\[24\][25]. Some non equilibrium techniques have been applied \[26\][27] to the problem as well but not as intensively.

The difficulty of moving away from equilibrium comes from the fact that the system is no longer time translational invariant. This prevents the Green’s functions to be transformed into a frequency representation. In frequency representation these Green’s functions are simple scalars, but in the time domain they are a continuous matrix which is harder to work with. This will be studied in Chapter 3 where the Keldysh formalism is studied. By imposing the right boundary condition into the system, it is possible to set up the device as a current biased device. This is in contrast to current efforts in the field where a voltage biased device determines the current passing through the device. The formalism will be expanded to show how
this current biased device can be mapped into a frequency representation. Chapter 4 covers the appropriate boundary condition of the current biased device. Chapter 5 discusses the remaining portions necessary to implement a working dynamical mean field theory calculation. Finally results and future areas of research are explored in Chapter 6.
Chapter 2

Spin and exchange coupling for Ti embedded in a surface dipolar network.

The following chapter is a reproduction of the paper published in the Physical Review B journal [28]. This research focuses on studying the atomic properties of single magnetic atoms deposited on a surface. In order to approach the problem theoretically, Density Functional Theory was employed. The theoretical results were then compared to experimental measurements performed using the Scanning Tunneling Microscope (STM). This research was possible thanks to the collaboration between Georgetown University and IBM Almaden Research Center.

2.1 Spin and exchange coupling for Ti embedded in a surface dipolar network

We have studied the spin and exchange coupling of Ti atoms on a Cu$_2$N/Cu(100) surface using density functional theory. We find that individual Ti have a spin of 1.0 (i.e., 2 Bohr Magneton) on the Cu$_2$N/Cu(100) surface instead of spin-1/2 as found by Scanning Tunneling Microscope. We suggest an explanation for this difference, a two-stage Kondo effect, which can be verified by experiments. By calculating the exchange coupling for Ti dimers on the Cu$_2$N/Cu(100) surface, we find that the exchange coupling across a ‘void’ of 3.6Å is antiferromagnetic, whereas indirect (superexchange) coupling through a N atom is ferromagnetic. For a square lattice of Ti on Cu$_2$N/Cu(100), we find a novel spin striped phase.
2.2 Introduction

Atomic-scale magnetic structures on surfaces [29] are of current interest for several reasons. Primarily, they display intriguing physical properties in their own right. Magnetic atoms on surfaces, simple or complex, can display large magnetocrystalline anisotropy which differs from the bulk. The spin can be large, or quenched by electronic effects such as the Kondo effect. And coupling between spins can be via direct overlap, RKKY or superexchange. Secondarily, these systems are compelling because of their parallels with other nano-scale systems – quantum dots, magnetic multilayers, magnetic impurities in thin films, to name just a few. Finally, there are the possible applications to nano-scale magnetic bits and future magnetic devices. A large net spin and magnetic anisotropy are required for atomic-scale magnetic structures to be used as practical nano-scale magnetic bits. A possible way to obtain a large magnetic moment is through a ferromagnetic coupling between transition metal atoms. However, ferromagnetic coupling is rare in transition metal complexes, [30] that is, when the transition metal atom is bonded to a nonmetallic atom. We describe below our studies of such a system.

In a Scanning Tunneling Microscope (STM) measurement [31] of a Ti atom placed on a Cu$_2$N/Cu(100) surface, it was found that the Ti exhibits very different magnetic properties than in gas phase. In the following work, we use density functional theory (DFT) to study the atomic spin of a single Ti atom, and exchange coupling of a dimer of Ti atoms, placed on a single layer of Cu$_2$N on a Cu(100) surface. The Cu$_2$N layer is used as an insulating layer to isolate the spin of a magnetic adatom from the metal electrons of the Cu(100) surface [29, 32]. Hereafter, the Cu$_2$N/Cu(100) surface will be referred to as the CuN surface. We study exchange coupling between Ti atoms in
two different environments: (i) a square lattice of Ti on the CuN surface and (ii) a
dimer of Ti atoms deposited on the CuN surface.

2.3 DFT calculations

We use spin-polarized DFT, as implemented in Quantum-ESPRESSO [33], within a
pseudopotential formalism using a plane wave basis with a cut-off of 30 Ry. A higher
cut-off of 240 Ry was used for the augmentation charges introduced by the ultrasoft
pseudopotential [34]. We use the generalized gradient approximation (GGA) for the
exchange correlation interaction with the functional proposed by Perdew, Burke and
Ernzerhof. [14] An on-site Coulomb interaction (U) for Ti was employed, with U
taken to be 4.7 eV as calculated using a constraint-GGA method [35, 36]. To improve
the convergence, a gaussian smearing of width 0.01 Ry was adopted. Brillouin zone
integrations for the (1×1) surface cell of Cu(100) were carried out using a (16×16×1)
mesh of k-points.

We obtained the bulk lattice parameter for Cu as 3.67 Å, which compares well
with the experimental value of 3.61 Å[37]. To simulate the CuN surface, we use a
symmetric slab of three to five atomic layers of Cu, with a layer of CuN above and
below. Periodic images of the slab were separated by a vacuum of 15 Å along the z
[100] direction.

2.4 CuN surface

The top view of the CuN surface is shown in Fig. 2.1a. The unit cell of the CuN
surface (shown by the black square) consists of two Cu atoms and one N atom. We
find that the N atoms are 0.18 Å above the top Cu atoms in a fully relaxed structure.
The distance between the first and second layers of Cu is 1.97 Å which compares well
with the all-electron result of 1.91 Å \cite{38}. We find that each Cu atom in the surface unit cell loses 0.7 electrons to the N (presumably due to the electronegative nature of N). Thus, Cu and N atoms form a square network of dipoles on the surface, rendering a (nominally) insulating character to the surface. As shown in Fig.2.1a, along the x-axis, two surface Cu atoms are separated by a hollow site and along the y-axis, they are separated by a N-atom. These directions will be referred as hollow-axis and N-axis, respectively. The charge density of the CuN surface along the N- and hollow-axis is shown in Fig.2.1b and (c) respectively. Notice that along the N-axis, charge gets accumulated in the top layer. Similar charge distribution was observed from an all-electron calculation for the same system.

2.5 Spin of Ti on CuN surface

To calculate the spin of Ti on the CuN surface, we first determine the most stable binding site for Ti on the surface. In Fig.2.2, we plot the adsorption energy of Ti at various sites on the CuN surface as a function of Ti coverage, It is computed as $AE(Ti) = E(Ti/CuN) - E(CuN) - E(Ti_{\text{gas}})$, where first, second, and third terms are the total energies of Ti-adsorbed CuN surface, CuN surface, and single Ti atom in gas phase, respectively. Energy of the single Ti atom is calculated using a cubic unit cell of size 19 Å for U equal to 0 and 4.7 eV. Black and red symbols represent the adsorption energies for U=0 and 4.7 eV, respectively. Notice that the adsorption energy decreases as U increases, and, for a given value of U, Ti has the highest binding on top of Cu atoms compared with on top of N or at at hollow sites, in agreement with STM experiments.\cite{31} The total energy difference for the single Ti atom between U=0 and 4.7 eV calculations is found found to be 0.26 eV; the energy at U=4.7 is greater than the energy at U=0 eV. Thus, the difference in adsorption energy for the two values
Figure 2.1: (a) Top view of the CuN on Cu(100) surface; small and big spheres represent N and Cu atoms respectively. Big spheres with symbol “Cu” are the top layer Cu atoms and those without the symbol are the second layer. The black square indicates the c(1 × 1) unit cell of the CuN surface. Along the x-axis, surface Cu atoms are separated by a hollow site (it is marked by ‘H’) and along the y-axis, they are separated by a N atom. Side views of charge density produced by a cut along the (b) N-axis and (c) hollow-axis.

of U is not entirely due to the energy difference for the single Ti atom. When Ti is adsorbed at a hollow site, we find that Ti tends to go deep in the surface (for U=0), thereby distorting the surface significantly. However, as we increase U to 2.5 and 4.7 eV, the surface is not much distorted, but the adsorption energy decreases. Next, we calculate the spin of Ti in (1 × 1), (2 × 2), and (2 × 3) unit cells, i.e., at coverages of 1, 1/4, and 1/6 ML, respectively. These calculations are done for U = 0 and 4.7 eV and the data are plotted in Fig. 2.1. Interestingly, as the coverage of Ti decreases, the spin of Ti nears the experimentally observed value of S = 1/2 for U = 0. Presumably, there are lower coverages of Ti in experiments as the scanning tunneling spectroscopy measurements were conducted on a single Ti atom. However, for U = 4.7 eV, the spin
Figure 2.2: (Color online) Adsorption energy and $S$ of Ti as a function of cell size for $U = 0$ (black) and $U = 4.7$ eV (red). As the cell size increases, coverage of Ti decreases. Filled circles, diamonds, and squares represent the adsorption energy of Ti on top of a Cu atom, on top of a N atom, and at hollow sites, respectively.

of Ti starts at $S = 0.75$ for high coverages and saturates at $S = 1$ for low coverages. Notice that the spin of Ti on top of a N atom or at a hollow site is close to one even at $U = 0$. At one monolayer coverage of Ti, the $(1 \times 1)$ surface unit cell consists of one N atom, one Ti atom and two Cu atoms as shown in Fig. 2.1. A constrained-GGA [35] calculation [36] yields $U = 4.7$ eV for Ti in this configuration. In order to understand the effect of $U$ on the spin of Ti, we do calculations for a range of values of $U$ for the $(1 \times 1)$ unit cell. The results for distances between Ti and its nearest neighbor atoms in the surface, angle subtended by Ti-N-Ti, and the spin of Ti are shown in Table 2.1. We find that Ti-N and Ti-Cu distances increase as $U$ increases, with the net effect of a rising Ti and decreasing (becoming sharper) Ti-N-Ti angle. Most importantly, as $U$ increases the spin of Ti approaches that of the gas phase value of 1. Comparable to the $(1 \times 1)$ unit cell, the distance of Ti from the Cu below in $(2 \times 2)$ is 2.58 Å.
Table 2.1: The Ti-N bond length ($d_{Ti-N}$), the Ti-Cu bond length ($d_{Ti-Cu}$), the Ti-N-Ti angle ($A_{Ti-N-Ti}$) and the spin $S$ of the Ti atom on the CuN surface. The top panel shows these results as a function of Hubbard $U$ (in eV) on Ti, for a ($1 \times 1$) unit cell. The middle panel shows these results for a single Ti atom in ($2 \times 2$), ($2 \times 3$), and ($3 \times 3$) unit cells. The bottom panel shows these results for a dimer of Ti adsorbed along the N- and hollow-axis, respectively. All the bond lengths are given in Angstroms.

<table>
<thead>
<tr>
<th>System</th>
<th>Cell</th>
<th>$U$</th>
<th>$d_{Ti-N}$</th>
<th>$d_{Ti-Cu}$</th>
<th>$A_{Ti-N-Ti}$</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Ti Atom</td>
<td>1 × 1</td>
<td>0.0</td>
<td>1.91</td>
<td>2.49</td>
<td>148.6</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.0</td>
<td>1.95</td>
<td>2.54</td>
<td>141.6</td>
<td>0.6</td>
</tr>
<tr>
<td>Ti Dimer</td>
<td></td>
<td>4.7</td>
<td>2.07</td>
<td>2.58</td>
<td>-</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>N-axis</td>
<td>4.7</td>
<td>2.04</td>
<td>2.65</td>
<td>142.9</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>H-axis</td>
<td>4.7</td>
<td>2.09</td>
<td>2.56</td>
<td>-</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3.0</td>
<td>2.27</td>
<td>2.68</td>
<td>108.4</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>6.0</td>
<td>2.33</td>
<td>2.72</td>
<td>104.2</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>N-axis</td>
<td>4.7</td>
<td>2.07</td>
<td>2.58</td>
<td>-</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>H-axis</td>
<td>4.7</td>
<td>2.04</td>
<td>2.65</td>
<td>142.9</td>
<td>1.0</td>
</tr>
</tbody>
</table>

The Ti-N bond length ($d_{Ti-N}$), the Ti-Cu bond length ($d_{Ti-Cu}$), the Ti-N-Ti angle ($A_{Ti-N-Ti}$) and the spin $S$ of the Ti atom on the CuN surface. The top panel shows these results as a function of Hubbard $U$ (in eV) on Ti, for a ($1 \times 1$) unit cell. The middle panel shows these results for a single Ti atom in ($2 \times 2$), ($2 \times 3$), and ($3 \times 3$) unit cells. The bottom panel shows these results for a dimer of Ti adsorbed along the N- and hollow-axis, respectively. All the bond lengths are given in Angstroms.

Table 2.1: The Ti-N bond length ($d_{Ti-N}$), the Ti-Cu bond length ($d_{Ti-Cu}$), the Ti-N-Ti angle ($A_{Ti-N-Ti}$) and the spin $S$ of the Ti atom on the CuN surface. The top panel shows these results as a function of Hubbard $U$ (in eV) on Ti, for a ($1 \times 1$) unit cell. The middle panel shows these results for a single Ti atom in ($2 \times 2$), ($2 \times 3$), and ($3 \times 3$) unit cells. The bottom panel shows these results for a dimer of Ti adsorbed along the N- and hollow-axis, respectively. All the bond lengths are given in Angstroms.

Table 2.1: The Ti-N bond length ($d_{Ti-N}$), the Ti-Cu bond length ($d_{Ti-Cu}$), the Ti-N-Ti angle ($A_{Ti-N-Ti}$) and the spin $S$ of the Ti atom on the CuN surface. The top panel shows these results as a function of Hubbard $U$ (in eV) on Ti, for a ($1 \times 1$) unit cell. The middle panel shows these results for a single Ti atom in ($2 \times 2$), ($2 \times 3$), and ($3 \times 3$) unit cells. The bottom panel shows these results for a dimer of Ti adsorbed along the N- and hollow-axis, respectively. All the bond lengths are given in Angstroms.

Additionally, it was found that in all three cases of larger unit cells, the spin of Ti is 1 for nonzero values of $U$.

Additional complexity was encountered, as it was found that the initial magnetization of Ti affects the final calculated ground state, indicating a complex energy minimization landscape. Hence we try several initial magnetizations and take the final state corresponding to the lowest energy. For $U=4.7$, we show the data corresponding to two such optimized structures (S-I and S-II) obtained by varying the initial magnetization (Table 2.1). The optimized structure corresponding to S-I is the lowest energy structure (S-I is lower in energy than S-II by 0.3 eV), showing the spin of Ti to be 0.75, indicating possible mixed valent behavior for a monolayer of Ti.
Next, we calculate the spin of Ti in \((2 \times 2)\), \((2 \times 3)\), and \((3 \times 3)\) unit cells, i.e., at coverages of 1/4, 1/6, and 1/9 ML respectively. This data is shown in the middle panel of Table 2.1. Comparable to the \((1 \times 1)\) unit cell, the distance of Ti from the Cu below in \((2 \times 2)\) is 2.58 Å. There is also a similar trend of Ti rising higher above the surface than N, by an amount increasing with increasing U. Most importantly, it was found that in all the three cases of larger unit cells, the spin on Ti is 1. At this point, we note a discrepancy with STM[31] experiments, which see a spin-1/2 Kondo effect. We postulate a resolution of the issue with a two-stage Kondo effect, in which the spin is first compensated from spin-1 to spin-1/2 at a higher temperature, and then seen as a spin-1/2 Kondo effect at the experimentally observed temperature.

2.6 Exchange coupling

To calculate the exchange coupling, we assume a Heisenberg interaction \((H = J S_1.S_2)\), and can relate the value of \(J\) to the energy difference between ferromagnetic and (Ising) antiferromagnetic configurations:

\[
2S^2J = E_{\uparrow\uparrow} - E_{\uparrow\downarrow} \equiv \Delta E
\]  

(2.1)

Here, \(S\) is the magnitude of spin, and \(J\) is the exchange coupling. \(E_{\uparrow\uparrow}\) and \(E_{\uparrow\downarrow}\) are the total energies calculated from DFT when the spins on the magnetic atoms point along the same direction and in opposite directions respectively. Note that Eq. 2.1 holds for all values of quantum spin. The relationship with \(J\) is valid for each \(S^2\) always at full maximal or minimal value (Ising antiferromagnet; colinear spins); for the energy difference with a full quantum antiferromagnetic state, the term \(2S^2J\) would become \((2S+1)SJ\). In this paper, we will mainly concentrate on the energy difference between ferromagnetic (aligned) and antiferromagnetic (antialigned) configurations,
rather than on the value of J. We calculate the exchange coupling for Ti lattices (1ML coverage of Ti) and for two Ti atoms placed on the CuN surface in a large unit cell.

2.6.1 Lattice of Ti atoms on CuN surface

At one monolayer coverage of Ti on CuN surface, Ti forms a square “lattice” on the surface. In this case, the energy of the ferromagnetic configuration \( E_{\text{FM}} \) is the total energy of the \((1 \times 1)\) unit cell since it contains only one Ti atom. However, to obtain \( E_{\uparrow \downarrow} \), we design three different configurations with \((1 \times 2)\), \((2 \times 1)\), and \((\sqrt{2} \times \sqrt{2})\) unit cells as shown in Fig. 2.3(a), (b), and (c) respectively. Arrow signs in the figure indicate relative direction of spins on Ti atoms. Total energies of the three configurations will be referred to as \( E_H \), \( E_N \), and \( E_C \) respectively. Notice that the unit cell size in all three configurations is twice that of the ferromagnetic configuration. Subtracting the total energies of configurations (a), (b), and (c) from two times the energy of the ferromagnetic configuration \((2 \times E_{\text{FM}})\) will give the exchange coupling of Ti atoms along the hollow-axis, along the N-axis, and in the checkerboard configuration, respectively; assuming that there are only nearest neighbor interactions.

Our results for exchange coupling are summarized in Table 2.2. For the lowest energy structure S-I, we find that the exchange coupling along the N-axis is unexpectedly ferromagnetic, i.e., the total energy \( E_{\text{FM}} \) is lower than \( E_N \) by 16.1 meV. However, the exchange coupling across a hollow is antiferromagnetic, i.e., the total energy \( E_H \) is lower than \( E_{\text{FM}} \) by 106.8 meV. Thus, the antiferromagnetic coupling along the hollow-axis is much stronger than the ferromagnetic coupling along the N-axis. The checkerboard pattern (Ising antiferromagnet) is more favored over a pure ferromagnetic state with \( \Delta E \) being 77.8 eV; however, it is less favorable than the hollow-axis antiferromagnetism, presumably due to the energy disadvantage of antiferromagnetic coupling along the N-axis. The overall order, from lowest to highest
Figure 2.3: Schematic diagrams showing spin configurations in Ti lattices. In configuration (a), spins are aligned along the N-axis and antialigned along the hollow-axis; in (b) spins are antialigned along the N-axis and aligned along the hollow-axis. Configuration (c) is a checkerboard configuration with spins antialigned along both the N- and hollow-axis.
energy, is $E_H < E_C < E_{FM} < E_N$. Configuration Fig. 2.3a is the ground state and we term it a spin striped state. These ferromagnetic stripes should be observable in large enough lattices.

In order to understand how structure plays a role in the exchange coupling, we also calculate spin exchange for the structure S-II (Table 2.2). We notice that the exchange coupling for the structure S-II is much lower than that of S-I. This could possibly be due to lower interaction of Ti with the surface (See Table 2.1, Ti-Cu and Ti-N distances are longer in S-II than those in S-I). Spin density plots for the two structures in the ferromagnetic state are shown in Fig 2.4. Notice that the spin density gets stretched out along the hollow-axis for S-I. Also, the N atoms get spin polarized for S-I more than for S-II. This shows that in S-I, there are stronger interactions. The net result is that this structure has the lowest total energy.

### 2.6.2 Dimer of Ti atoms on CuN surface

We have drawn conclusions so far about Ti-Ti coupling based on the calculations in lattices, where the situation is more complicated because one not only has the nearest neighbor (NN) interactions but also has next NN (NNN) interactions and so on. To simulate a Ti-Ti dimer on the surface we use a larger unit cell of $(2 \times 3)$ with two and

<table>
<thead>
<tr>
<th>System</th>
<th>Structure</th>
<th>$E_{FM} - E_N$</th>
<th>$E_{FM} - E_H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice 1 $\times$ 1</td>
<td>S-I</td>
<td>-16.1</td>
<td>106.8</td>
</tr>
<tr>
<td></td>
<td>S-II</td>
<td>6.2</td>
<td>13.9</td>
</tr>
<tr>
<td>Dimer 2 $\times$ 3</td>
<td>-</td>
<td>-16.5</td>
<td>143.9</td>
</tr>
</tbody>
</table>

Table 2.2: The energy differences $\Delta E$ along the N-axis ($E_{FM} - E_N$) and the hollow-axis ($E_{FM} - E_H$) for a lattice of Ti in a $(1 \times 1)$ unit cell, and a dimer of Ti in a $(2 \times 3)$ unit cell.
Figure 2.4: Spin density plot for \((1 \times 1)\) unit cell for lower energy (a) and higher (b) configurations. Different colors (shadings in black and white version) correspond to opposite spins. The Nitrogen atoms appear as small spheres with opposite polarization between the Ti.

three lattice units along the hollow- and N-axis respectively. Interestingly, we find ferromagnetic coupling along the N-axis and antiferromagnetic along the hollow-axis, the same ground states as for the case of \((1 \times 1)\) lattices. Along the N-axis, the energy difference \((\Delta E)\) is -16.5 meV compared to -16.1 meV for the \((1 \times 1)\) case. Along the hollow-axis the energy difference is 143.9 meV compared to 106.8 meV for the \((1 \times 1)\) case. Thus, a Ti lattice and a dimer show a similar trend and strength of coupling. It confirms our assumption of primarily nearest neighbor interactions in a Ti lattice on the CuN surface. Notice that the distance between Ti and the Cu atom below it is 2.56 Å for both the \((1 \times 1)\) case, and the \((2 \times 3)\) case for coupling along the hollow-axis. However, when the dimer is placed along the N-axis the distance between Ti and the
Cu below it increases slightly to 2.65 Å. The Ti-N-Ti angle is 135.6 degrees for the (1 × 1) case which is close to 142.9 degrees for the (2 × 3) case.

In Fig. 2.5 we plot the spin density for the Ti dimer along the N-axis (Fig. 2.5a) and the hollow-axis (Fig. 2.5b). A significant amount of induced spin-polarization around the N atom can be seen from the figure. Ferromagnetic coupling between Ti atoms along the N-axis is established by having an opposite spin N atom both between the Ti atoms and at opposite ends. For anti-aligned spin configuration along the N-axis, the N atom becomes a single-atom antiferromagnet with a net spin of zero. Along the hollow-axis, when spin on both the Ti atoms is aligned, a dramatic anisotropy in the spin polarization of the Ti develops, with a direct overlap established over the hollow site (Fig. 2.5b). The stretching of the Ti bonds in this case case is striking, and suggestive that higher symmetry considerations may be coming into play. However, when spins are antialigned, no such elongation of spin polarization occurs. In both the cases, N atoms on the sides of the two Ti atoms develop a spin polarization opposite to that of the Ti.

The primary sources of exchange coupling between the Ti atoms are superexchange [39], RKKY [40], and direct overlap/direct exchange [37]. The coupling between the adatoms can be direct, if the wave functions should overlap, or RKKY, if the influence of the Cu in the layers below is strong enough. Along the N-axis, the center N atom becomes a natural source for a superexchange coupling between Ti atoms, ruling out RKKY which would need to take an indirect route under the N atom, a much longer route than directly across the N for superexchange. Along the hollow-axis, however, there is no convenient single atom to hop across for superexchange, rather the sea of conduction electrons from the underlying and intervening Cu. (Unless one is to consider superexchange via the second-layer Cu, an unlikely candidate.) In this case RKKY and direct overlap become more likely. Indeed for an aligned spin
configuration, we observe a direct overlap forming, as discussed above. However, the lowest energy state for coupling along the hollow-axis is antiferromagnetic, and we conclude that in this case it is likely due to RKKY coupling. This could be tested experimentally by varying the Ti-Ti distance and measuring the exchange coupling; however, only certain discrete lattice positions would be possible.

2.7 Conclusions

In agreement with experiments,\textsuperscript{32} we find that Ti has the highest adsorption energy when deposited on top of a Cu atom. We find that the spin of Ti atoms varies with the coverage. For low coverages of Ti, the spin of Ti is 0.5, which is an experimentally observed value.\textsuperscript{32} However, the spin of Ti becomes 1 as the value of U is increased even at low coverages.
We find a ferromagnetic coupling along the N-axis and antiferromagnetic along the hollow-axis, for both the lattice and dimer of Ti on the CuN surface. Ti lattice and dimer have a similar trend as well as strength of coupling. This indicates that interactions between Ti atoms in the lattice configuration are local; and a marked spin striped phase is found as the ground state of the lattice. We find a ferromagnetic coupling along the N-axis due to superexchange, with secondary contributions from direct exchange. We also postulate that the antiferromagnetic coupling along the hollow-axis is primarily due to RKKY interactions, with a smaller direct exchange component.
Chapter 3

Non equilibrium Green’s functions

3.1 Keldysh representation

The Keldysh formalism relates directly to the non-equilibrium problem. In general the retarded piece of the Green’s function \( g^R(\vec{k}, \omega) \) relates directly to the density of states of the system in question, in contrast the lesser Green’s function \( g^<(\vec{k}, \omega) \) relates to the population of the density of states. In equilibrium this lesser Green’s have a simple relation to the retarded piece, that is:

\[
g^<_{eq}(\vec{k}, \omega) = -2if(\omega) Im\{g^R(\vec{k}, \omega)\}
\] (3.1)

Where the function \( f(\omega) \) is the usual Fermi-Dirac distribution \( f(\omega) = 1/(1 + \exp(\beta \omega)) \). Away from equilibrium this relation doesn’t hold anymore. In order to calculate the appropriate lesser and retarded Green’s function in the non equilibrium state we start from the definition of the Green’s function. We write the definition in the Heisenberg representation as

\[
g^c(t, t')_{\alpha i \beta j} = -\frac{i}{\hbar} \theta_c(t, t') \langle \hat{c}(t)_{\alpha i} \hat{c}^\dagger_{\beta j}(t') \rangle + \frac{i}{\hbar} \theta_c(t', t) \langle \hat{c}^\dagger(t')_{\beta j} \hat{c}(t)_{\alpha i} \rangle
\] (3.2)

here the definition is given in real space with the indices \( i \) and \( j \) indicating the lattice site in the plane, and indices \( \alpha \) and \( \beta \) indicating the plane. In the Heisenberg representation, the creation and annihilation operators become time dependent, but they can be related to the Schrodinger picture by the unitary time-ordered
product $\hat{U}(t, t_0) = \exp[-i \int_{t_0}^{t} dt' \hat{H}_{FK}(t')/\hbar]$ so the time-dependent creation operator is $\hat{c}(t) = \hat{U}(t, t_0)\hat{c}(t_0)\hat{U}(t, t_0)$. Note that $\hat{U}(t, t_0)$ satisfies $i\hbar \partial_t \hat{U}(t, t_0) = \hat{H}_{FK}(t)\hat{U}(t, t_0)$ with $\hat{H}_{FK}(t)$ the Schrodinger representation for the Hamiltonian. The angle brackets denote a statistical averaging over the density matrix of the original equilibrium distribution that the system is in. The statistical averaging does not enter into the retarded Green’s functions, but does for the Keldysh, or lesser Green’s functions as we will describe in detail below. Because we ultimately work in the steady state for this system, treatment of the averaging over the appropriate density matrix must be handled carefully. This contour-ordered Green’s function is defined on the Keldysh contour, shown in Fig. 4.2. We start at a certain time $t_0$ where the system is in equilibrium and we evolve forward in time. At time $t_{on}$ we turn on a field $E(t) = -dA(t)/dt$ (with $c = 1$). The $U$ operators in the creation and annihilation operators evolve the system forward and backwards in time, and finally it evolves into the imaginary time until $t_0 - i\beta$ where $\beta = 1/T$ is the inverse of the temperature. The times are ordered with respect to the contour. The step function $\theta_c(t, t')$, is also defined with respect to the contour, $\theta_c(t, t')$ equals zero if $t < t'$ and equals one if $t > t'$ on the contour. The derivative with respect to time of the theta function give us a Dirac delta function $d\theta_c(t, t')/dt = \delta_c(t, t')$. We define $\delta_c$ such that $\int_c dt' \delta_c(t, t') = 1$ in the upper branch and $= -1$ in the lower branch. The brackets $\langle \hat{O} \rangle$ denote the expectation value of the operator, $\langle \hat{O} \rangle = Tr\{\exp(-\beta(\hat{H}_{FK}(t \to -\infty) - \mu \hat{N}))\hat{O}\}/Z$. Where $Z$ is the partition function $Tr\{\exp(-\beta(\hat{H}_{FK}(t \to -\infty) - \mu \hat{N}))\}$ and $\hat{N}$ is the particle number operator. We set $\hbar = 1$. Note we will ultimately be interested in the limit of the Green’s functions where $(t + t')/2 = \infty$.

From the definition of the contour ordered Green’s function in Eq. (3.2), we note that the Green’s function depends on two different times. These times can be in either the upper branch or the lower branch of the contour in Fig. 4.2. We will ignore the
imaginary piece of the contour for the time being but it could be included if necessary. We will label the times in the upper branch with the subscript $+$ and the times in the lower branch with the $-$ subscript.

The time variable is a continuous variable, but to do calculations on a computer, we must discretize it and then extrapolate the discretized calculations with $\Delta t \to 0$. In this case, we can think of the Green’s function in a matrix representation with indices $t$ and $t'$. We will notice that there are four different possibilities for the arrangement of the $t$ and $t'$ indices; they either lie in different branches, or in the same branch.

When both lie in the same branch the contour-ordered Green’s function will become time-ordered in the upper branch or anti-time-ordered in the lower branch. We name them $G_{++}$ and $G_{--}$, respectively.

If the two times lie in different time branches, we will either have a lesser $g^<(t, t')$ Green’s function or a greater $g^>(t, t')$ Green’s function depending on which time lies in the upper branch. We will refer to these Green’s functions as $G_{+-}$ for the lesser and $G_{-+}$ for the greater. Our contour-ordered Green’s function can then be written in a matrix representation as follows:

$$g^c(t, t') \rightarrow \tilde{g}^c(t, t') = \begin{pmatrix} G_{++}(t, t') & G_{+-}(t, t') \\ G_{-+}(t, t') & G_{--}(t, t') \end{pmatrix}$$ (3.3)

where $G_{++}(t, t')$, $G_{+-}(t, t')$, $G_{-+}(t, t')$ and $G_{--}(t, t')$ are all square matrices in time of the same size. In this case the time variables are not defined on the contour anymore, but on the real axis instead. We are using a short hand notation in which $G_{++}(t, t') = g^c(t_+, t'_+)$ the plus signs denotes there is a time dependence and such time lies in the upper branch. The same goes for the minus sign, but such a time lies in the lower branch. It was originally shown by Keldysh \[41\] that we could transform this matrix representation of the contour ordered Green’s function into a different representation which depended on the $G_R$, $G_A$ and $G_K$ the retarded, advanced and Keldysh Green’s
functions respectively. We use the transform introduced by Larkin and Ovchinnikov (1975) as discussed by Rammer and Smith.

\[ G(t, t') = L \tau^3 \tilde{g}(t, t') L^\dagger \]  

(3.4)

with

\[ \tau^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]  

(3.5)

and

\[ L = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \]  

(3.6)

We study the general properties of a general matrix \( M \) in the form of the given Green’s function above in appendix B. Notice that the Green’s function follows the same condition imposed on the \( M \) matrix. That is \( G_{++}(t, t') + G_{--}(t, t') = G_{-+}(t, t') + G_{+-}(t, t') \).

Following the results we know the transformed Green’s function becomes

\[ G \rightarrow \begin{pmatrix} g^R & g^K \\ 0 & g^A \end{pmatrix} \]  

(3.7)

Where we have used the following relations between the different Green’s functions;

\[ g^R = G_{++} - G_{+-} = G_{-+} - G_{--} \]  

(3.8)

\[ g^A = G_{++} - G_{-+} = G_{+-} - G_{--} \]  

(3.9)

\[ g^K = G_{++} + G_{--} = G_{-+} + G_{+-} \]  

(3.10)

This representation is of more use to us, since we will calculate the retarded, advanced and Keldysh Green’s functions of our system numerically within DMFT. We need to be careful when translating equations that have been derived from the contour-ordered representation into the matrix representation introduced here. As an example,
we should consider the inverse in the time domain of the contour-ordered Green’s function. The equation is \( \int_{c} d\bar{t} g^c(t, \bar{t}) g^{-1}(\bar{t}, t') = \delta_c(t, t') \), the time variables \( t \) and \( t' \) can be in either branch and the \( \bar{t} \) variable runs over both branches of the contour. This results in four equations, when we separate out the contributions from each piece of the contour.

\[
\int d\bar{t} g^c(t_+, \bar{t}_+) g^{-1}(\bar{t}_+, t'_+) - \int d\bar{t} g^c(t_+, \bar{t}_-) g^{-1}(\bar{t}_-, t'_+) = \delta(t_+, t'_+) \tag{3.11}
\]

\[
\int d\bar{t} g^c(t_+, \bar{t}_+) g^{-1}(\bar{t}_+, t'_-) - \int d\bar{t} g^c(t_+, \bar{t}_-) g^{-1}(\bar{t}_-, t'_-) = 0 \tag{3.12}
\]

\[
\int d\bar{t} g^c(t_-, \bar{t}_+) g^{-1}(\bar{t}_+, t'_+) - \int d\bar{t} g^c(t_-, \bar{t}_-) g^{-1}(\bar{t}_-, t'_+) = 0 \tag{3.13}
\]

\[
\int d\bar{t} g^c(t_-, \bar{t}_+) g^{-1}(\bar{t}_+, t'_-) - \int d\bar{t} g^c(t_-, \bar{t}_-) g^{-1}(\bar{t}_-, t'_-) = -\delta(t_-, t'_-). \tag{3.14}
\]

By setting

\[
\hat{g}^{-1}(t, t') = \begin{pmatrix} G^{-1}_{++}(t, t') & G^{-1}_{+-}(t, t') \\ G^{-1}_{-+}(t, t') & G^{-1}_{--}(t, t') \end{pmatrix}, \tag{3.16}
\]

performing the matrix multiplication between \( g^c \) and \( g^{-1} \), and comparing terms, we note that this equation corresponds to \( \hat{g} \hat{g}^{-1} = I \) with \( I \) the identity matrix. From Appendix B we can write down the inverse of the Green’s function in the new representation

\[
\hat{g}^{-1} = \begin{pmatrix} (G_{++} - G_{+-} G_{--}^{-1} G_{-+})^{-1} & -G_{++}^{-1} G_{+-} (G_{--}^{-1} G_{++}^{-1} + G_{++} G_{+-}^{-1})^{-1} \\ -G_{-+}^{-1} G_{++} (G_{++}^{-1} G_{+-}^{-1} G_{-+})^{-1} & (G_{--}^{-1} G_{-+}^{-1} G_{++}^-1)^{-1} \end{pmatrix} \tag{3.17}
\]

where matrix multiplication is understood between G factors. It’s transform into
the retarded, advanced, Keldysh representation satisfies

\[
G^{-1}(\bar{t}, t') = \begin{pmatrix}
g_R^{-1} & -g_R^{-1} g_{\kappa} g_A^{-1} \\
0 & g_A^{-1}
\end{pmatrix}
\]

(3.18)

which can also be verified directly, via \(GG^{-1} = 1\).

3.1.1 The Dyson Equation

As we did for the inverse Green’s function, we focus next on deriving a matrix representation for the Dyson equation. Recall that the Dyson equation relates the Green’s function to the non-interacting Green’s function and the Green’s function itself via the self-energy. We can try to express the Dyson equation for the contour ordered Green’s function as follows:

\[
g_c(k, t, t') = g_c^0(k, t, t') + \int_c d\bar{t} \int_c d\bar{t}' g_c^0(k, t, \bar{t}) \Sigma_c(\bar{t}, \bar{t}') g_c^c(k, \bar{t}', t'),
\]

(3.19)

where the integral is performed over the contour, \(\Sigma_c\) defines our self-energy, which is momentum independent due to the DMFT approximation and \(g_c^0\) is the non-interacting Green’s function of our system. There will be four pieces to the Dyson equation. One when both times for \(g_c^c(k, t, t')\) are in the upper branch, one when both are in the lower branch and two more when one is in the upper branch and the other one is in the lower branch. The self energy can be rewritten as

\[
\Sigma_c(t, t') = \begin{cases}
\Sigma_{++}(t, t') & \Sigma_{+-}(t, t') \\
\Sigma_{-+}(t, t') & \Sigma_{--}(t, t')
\end{cases}
\]

(3.20)

In order to express the Dyson equation in the matrix representation, we first need to compare the signs obtained by performing the matrix multiplication directly and the corresponding terms from Eq. (3.19) once we have taken into account in which branch of the Keldysh contour the time variable refers to. For example, the first term
where \( t \) and \( t' \) are in the upper branch is:

\[
g_{++}^c(k, t, t') = g_{0,++}^c(k, t, t') + \int_{-\infty}^{\infty} d\bar{t} \int_{-\infty}^{\infty} d\tilde{t} \tilde{g}_{0,++}^c(t, \bar{t}) \Sigma_{++}^c(\bar{t}, \tilde{t}) g_{++}^c(\tilde{t}, t')
- \int_{-\infty}^{\infty} d\bar{t} \int_{-\infty}^{\infty} d\tilde{t} \tilde{g}_{0,+-}^c(t, \bar{t}) \Sigma_{+-}^c(\bar{t}, \tilde{t}) g_{++}^c(\tilde{t}, t')
- \int_{-\infty}^{\infty} d\bar{t} \int_{-\infty}^{\infty} d\tilde{t} \tilde{g}_{0,++}^c(t, \bar{t}) \Sigma_{+-}^c(\bar{t}, \tilde{t}) g_{--}^c(\tilde{t}, t')
+ \int_{-\infty}^{\infty} d\bar{t} \int_{-\infty}^{\infty} d\tilde{t} \tilde{g}_{0,+-}^c(t, \bar{t}) \Sigma_{--}^c(\bar{t}, \tilde{t}) g_{--}^c(\tilde{t}, t')
\tag{3.21}
\]

the minus signs in the second and third line comes from the fact that we are changing
the integration limits to run in the positive direction; when dealing with times in
the lower branch we would integrate from \( \infty \) to \( -\infty \) but we can revert the limits at
the expense of a factor of \( -1 \). We use the same procedure to check the 3 remaining
combinations, we find that in order for the self energy defined in Eq.(3.20) to satisfy
the Dyson equation we need to modify the equation by adding a \( \tau_3 \) to the right of
the self-energy and to the left.

The Dyson equation in the matrix representation becomes

\[
\tilde{g}^c(k, t, t') = \tilde{g}_0^c(k, t, t') + \int d\bar{t} d\tilde{t} \tilde{g}_0^c(k, t, \bar{t}) \tau_3 \tilde{\Sigma}^c(\bar{t}, \tilde{t}) \tau_3 \tilde{g}^c(k, \bar{t}, t')
\tag{3.22}
\]

We apply the same transformation, which corrects Eq.(3.19), in order to get the
Corresponding self energy in the retarded-advanced-Keldysh representation.

\[
L \tau^3 \tilde{g}^c L^\dagger = L \tau^3 \left[ \tilde{g}_0^c + \tilde{g}_0^c \tau_3 \tilde{\Sigma} \tau_3 \tilde{g}_0^c \right] L^\dagger \rightarrow G = G_0 + G_0 L \tau_3 \tilde{\Sigma} L^\dagger G
\]

The transformation for the self energy is thus \( \tilde{\Sigma} = L \tau_3 \tilde{\Sigma} L^\dagger \) and the Dyson equation
conserves the same form in the new representation. We calculate the self-energy in
the retarded-advanced-Keldysh representation

\[
\Sigma = \frac{1}{2} \begin{pmatrix}
\Sigma_{++} + \Sigma_{+-} - \Sigma_{-+} - \Sigma_{--} & \Sigma_{++} + \Sigma_{+-} + \Sigma_{-+} + \Sigma_{--} \\
\Sigma_{++} + \Sigma_{-+} - \Sigma_{--} - \Sigma_{+-} & \Sigma_{++} + \Sigma_{+-} - \Sigma_{-+} + \Sigma_{--}
\end{pmatrix}
\tag{3.24}
\]
Since we have the relation $G_{++} + G_{--} = G_{+-} + G_{-+}$, we prove in Appendix A that the same relation holds for $\Sigma$, that is, $\Sigma_{++} + \Sigma_{--} = \Sigma_{+-} + \Sigma_{-+}$. We next define $\Sigma_R = \Sigma_{++} - \Sigma_{+-}$, $\Sigma_A = \Sigma_{++} - \Sigma_{-+}$ and $\Sigma_K = \Sigma_{++} + \Sigma_{--}$ to yield

$$\Sigma = \begin{pmatrix} \Sigma_R & \Sigma_K \\ 0 & \Sigma_A \end{pmatrix}. \quad (3.25)$$

Performing the matrix multiplication between $G$ and $\Sigma$ we obtain the Dyson equation

$$\begin{pmatrix} g^R & g^K \\ 0 & g^A \end{pmatrix} = \begin{pmatrix} g^0_R + g^0_R \Sigma R g^R & g^0_K + g^0_R \Sigma K g^K + g^0_K \Sigma K g^A + g^0_K \Sigma A g^A \\ 0 & g^A + g^0_A \Sigma A g^A \end{pmatrix}. \quad (3.26)$$

This yields 3 different Dyson equations, the diagonal components correspond to the usual retarded and advanced Dyson equations

$$g^{R,A} = g^{R,A}_0 + g^{R,A}_0 \Sigma^{R,A} g^{R,A}_0 \quad (3.27)$$

or equivalently, by multiplying by the left by $g^{R,A-1}$ and from the left $g^{R,A-1}_0$

$$g^{R,A-1}_0 = g^{R,A-1} + \Sigma^{R,A}. \quad (3.28)$$

Note that the retarded Green’s function depends only on the noninteracting retarded Green’s function and the retarded self energy, while the advanced Green’s function depends only on the advanced equivalents. The Keldysh Green’s function not only depends on the Keldysh components, but also on the retarded and advanced components. The Keldysh piece can be rewritten as follows after multiplying by $g^{R-1}_0$ from the left and $g^{A-1}$ from the right and using the retarded and advanced Dyson equation as:

$$\Sigma^K = g^{R-1}_0 g^K g^{A-1} - g^{R-1}_0 g^K g^{A-1}_0. \quad (3.29)$$
3.2 Impurity Green’s function

The dynamical mean field theory and the quantum zipper algorithms were described in the introduction of this thesis. One of the necessary steps for both algorithms consists of extracting the impurity Green’s function from the non interacting one. Also known as the impurity solution to our model, one of the advantages of using the Falicov-Kimball model as the strongly correlated electron model is the fact that we can solve it exactly. A different model would require a different solver that would add extra time to the numerical calculation. In the case of the Falicov-Kimball model we know the exact solution to be

\[ g_{\text{imp}}(\omega) = (1 - \omega)g_0 + \omega(g_0^{-1} - U\delta_c)^{-1} \]  

(3.30)

where \( g_{\text{imp}} \) is the impurity Green’s function for the Falicov-Kimball model in the contour. Once we express this equation in matrix representation, in the time, anti-time ordered representation the equation doesn’t contain any extra factors of \( \tau_3 \) other than the one introduced by the \( \delta_c \) term. We are now able to find the equivalent expression in the advanced, retarded, Keldysh representation. We apply the transformation

\[ \hat{L}\tau_3 \left[ g_{\text{imp}} = (1 - \omega_1)g_0 + \omega(g_0^{-1} - U\tau_3)^{-1} \right] \hat{L}^\dagger. \]

We have derived the transformation for the first two terms previously. The last term becomes \( \omega_1 \hat{L}\tau_3(g_0^{-1} - U\tau_3)^{-1}\hat{L}^\dagger = \omega_1 \left( \hat{L}(g_0^{-1} - U\tau_3)\tau_3\hat{L}^\dagger \right)^{-1} = \omega_1 \left[ G_0^{-1} - U \right]^{-1} \) where \( G_0^{-1} \) is the inverse of the contour ordered Green’s function in the advance retarded Keldysh representation eq.(3.18).

We are left with the problem of calculating the inverse of \( G_0^{-1} - U \). We follow a similar procedure to find the inverse as the one we used to find the inverse of the contour ordered Green’s function. Multiply the matrix \( G_0^{-1} - U \) to a general 2 by 2 matrix and equate the result to the identity matrix.

\[
\begin{pmatrix} g^{R^{-1}} - U & -g^{R^{-1}}g^{K}g^{A^{-1}} \\ 0 & g^{A^{-1}} - U \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

(3.31)
This yields a set of four equations with four unknowns, from \((g^{A^{-1}} - U)C = 0\) and \((g^{A^{-1}} - U)D = 1\) we find \(C = 0\) and \(D = (g^{A^{-1}} - U)^{-1}\). Using the values of \(C\) and \(D\) we find the values of \(A\) and \(B\) from the remaining two equations, \((g^{R^{-1}} - U)A - (g^{R^{-1}} g^K g^{A^{-1}})C = 1\); \(A = (g^{R^{-1}} - U)^{-1}\) and \((g^{R^{-1}} - U)B - (g^{R^{-1}} g^K g^{A^{-1}})D = 0\) which yields \(B = (g^{R^{-1}} - U)^{-1}(g^{R^{-1}} g^K g^{A^{-1}})(g^{A^{-1}} - U)^{-1}\)

The final impurity solution is given by the following expression

\[
\begin{pmatrix}
g^R_{imp} \\
g^K_{imp} \\
0 \\
g^A_{imp}
\end{pmatrix}
= (1 - \omega_1)
\begin{pmatrix}
g^R_0 \\
g^K_0 \\
0 \\
g^A_0
\end{pmatrix}
+ \omega_1
\begin{pmatrix}
(g^{R^{-1}} - U)^{-1} \\
(g^{R^{-1}} - U)^{-1} g^R_0 g^K_0 g^{A^{-1}} (g^{A^{-1}} - U)^{-1} \\
0 \\
(g^{A^{-1}} - U)^{-1}
\end{pmatrix}
\] (3.32)

This gives the correct retarded and advanced impurity Green’s functions, plus the impurity solution for the Kelydsh Green’s function which becomes

\[
g^K_{imp} = (1 - \omega_1)g^K_0 + \omega_1(g^{R^{-1}} - U)^{-1}g^R_0 g^K_0 g^{A^{-1}} (g^{A^{-1}} - U)^{-1}
\] (3.33)

we can check the limit as the system becomes non-interacting by setting the interacting strength \(U = 0\), the impurity Green’s function becomes the non-interacting Green’s function as it should be the case. Alternatively we can set \(\omega_1 = 1\), and check the equilibrium case of the Keldysh Green’s function. In equilibrium Eq.(3.33) becomes

\[
g^K_{imp} = (2f(\omega) - 1)(g^{R^{-1}} - U)^{-1}(g^{A^{-1}} - g^{R^{-1}})(g^{A^{-1}} - U)^{-1}
\] (3.34)

by adding and subtracting \(U\) to the inverse of the advanced and retarded Green’s functions we find

\[
g^K_{imp} = (2f(\omega) - 1)[(g^{R^{-1}} - U)^{-1} - (g^{A^{-1}} - U)^{-1} + U(g^{R^{-1}} - U)^{-1}(g^{A^{-1}} - U)^{-1} - U(g^{R^{-1}} - U)^{-1}(g^{A^{-1}} - U)^{-1}]
\] (3.35)
The last two terms cancel each other and the remaining term is the correct equilibrium solution for the impurity Keldysh function.

### 3.3 Boundary condition

The next step is to calculate the equation of motion of the Green’s function. This is achieved by taking the derivative of the Green’s function with respect to time. Before proceeding with the calculation of the equation of motion we will consider the boundary conditions of the device. That is we will calculate the Green’s functions in the bulk. This boundary condition is used to drive current into the system.

This problem has been effectively studied in the past. We are interested in determining what is the steady state of the bulk, but in a current carrying state. The solution for the Green’s function away from equilibrium in bulk is [43]

\[
g_{k_z,\text{Bulk}}(k_{\parallel}, t, t') = i \left\{ f \left( \epsilon_{\parallel}(k_{\parallel}) - 2t_{\perp}\cos(k_z) - \mu \right) - \theta_c(t, t') \right\} \times \exp \left\{ -i \left( \epsilon_{\parallel}(k_{\parallel}) - 2t_{\perp}\cos(k_z + A_0) - \mu \right) (t - t') \right\}
\]  

(3.36)

where we have applied a vector potential \( A(t) = -tA_0 \theta(t - t^*) \theta(t^* - t + 1) - A_0 \theta(t - t^* - 1) \) with \( t^* \to -\infty \), this corresponds to turning on a constant field a long time in the past and turning it off after a unit of time. This field will make the system carry a current, but since it was turned and then off a long time in the past it corresponds to a constant shift of the momentum distribution. The momentum \( \vec{k} \) has been split into two components, one in the direction of the current \( k_z \) and another piece perpendicular to the current \( k_{\parallel} \). \( A_0 \) is the electric field magnitude, which is applied in the \( \hat{z} \) direction.
Using the definitions for the retarded, lesser and Keldysh Green’s functions,

\[ g^R(k, t, t') = i\theta(t - t')\langle\{\hat{c}(t), \hat{c}^\dagger(t')\}_+ \rangle \]  
\[ g^<(k, t, t') = i\langle\hat{c}^\dagger(t)c(t')\rangle \]  
\[ g^K(k, t, t') = -i\langle[\hat{c}(t), \hat{c}^\dagger(t)]_-\rangle \]

from Eq (3.36), we can extract the corresponding retarded, lesser and Keldysh Green’s functions to be:

\[ g^R_{kz,\text{Bulk}}(k_\parallel, t_{\text{rel}}) = -i\theta(t_{\text{rel}}) \exp\left\{ -i(\epsilon_\parallel(k_\parallel) - 2t_\perp \cos(k_z + A_0) - \mu)t_{\text{rel}} \right\} \]  
\[ g^{<,K}_{kz-A_0,\text{Bulk}}(k_\parallel, \omega) = -2\pi i\delta(\omega + \mu - \epsilon_\parallel(k_\parallel) + 2t_\perp \cos(k_z)) \times f^{<,K}(\epsilon_\parallel(k_\parallel) - 2t_\perp \cos(k_z - A_0) - \mu) \]

where we have Fourier transformed \( t_{\text{rel}} \) in the lesser and Keldysh Green’s functions. The symbol \( t_{\text{rel}} = t - t' \) is the relative time. All three Green’s functions are time translational invariant, since they depend only on the difference between the two times. We have grouped together the Keldysh and the lesser Green’s functions by using the notation \( f^{<,K}(\omega) \) where \( f^<(\omega) = f(\omega) \) is the usual Fermi-Dirac distribution and \( f^K(\omega) = 2f(\omega) - 1 \).

First we will concentrate on the retarded Green’s function. We will perform a Fourier transformation in the \( t_{\text{rel}} \) variable, to transform it from time space to frequency space. Once we have performed the Fourier transform to frequency space, we will perform a second Fourier transform on the \( k_z \) variable to obtain the Green’s functions in real space for the \( z \) direction, this will allow us to have the bulk Green’s functions in the mixed basis. The Fourier transform to frequency space is

\[ g^R_{kz,\text{Bulk}}(k_\parallel, \omega) = \int dt_{\text{rel}} e^{i\omega t_{\text{rel}}} g^R_{kz,\text{Bulk}}(k_\parallel, t_{\text{rel}}) \]
\[ = -i \int_0^\infty dt_{\text{rel}} \exp\left\{ -i[\epsilon_\parallel(k_\parallel) - 2t_\perp \cos(k_z + A_0) - \mu - \omega]t_{\text{rel}} - \delta^+t_{\text{rel}} \right\} \]
The lower limit comes from the $\theta(t_{rel})$ function, we have set $\omega$ to be $\omega + i\delta^+$ with $\delta^+$ approaching zero from above. The retarded Green’s function in the frequency representation becomes

$$g_{k_z,Bulk}^R(k\parallel, \omega) = \frac{1}{\omega + \mu - \epsilon\parallel(k\parallel) + 2t^\perp \cos(k_z + A_0) + i\delta^+} \quad (3.43)$$

Next we Fourier transform $g^R$ from momentum space in the $z$ direction, $k_z$, to the mixed basis representation. In this mixed basis representation the $z$ variable is given in real space and the $x−y$ plane is treated in momentum space $k\parallel$. The Fourier transform is

$$g_{\alpha\beta}^R(k\parallel, \omega) = \frac{1}{2\pi} \int_0^{2\pi} dk_z g_{k_z}^R(k\parallel, \omega)e^{i(\hat{z}_\alpha - \hat{z}_\beta)\cdot k_z} = \frac{1}{2\pi} \int_0^{2\pi} dk_z \frac{e^{i(\hat{z}_\alpha - \hat{z}_\beta)\cdot k_z}}{\omega + \mu - \epsilon\parallel(k\parallel) + 2t^\perp \cos(k_z + A_0) - i\delta^+} \quad (3.44)$$

we start by performing some variable substitutions, let $z' = \omega + \mu - \epsilon\parallel(k\parallel) - i\delta^+$, $k_z' = k_z + A_0$ and $dk_z' = dk_z$

$$g_{\alpha\beta}^R(k\parallel, \omega) = \frac{1}{2\pi} \int_0^{2\pi} dk_z' \frac{e^{i(\hat{z}_\alpha - \hat{z}_\beta)\cdot k_z}}{2t^\perp(\frac{z'}{2t^\perp} + \cos(k_z'))} \quad (3.45)$$

This integral can be evaluated using calculus of residues. We change the original integral to an integral in the complex plane over the unit circle by rewriting $z = \exp\{i\phi\}$;

$$g_{\alpha\beta}^R(k\parallel, \omega) = \frac{1}{2\pi} \int_0^{2\pi} d\phi \frac{e^{-i(\hat{z}_\alpha - \hat{z}_\beta)\cdot A_0}e^{i(\hat{z}_\alpha - \hat{z}_\beta)\cdot \phi}}{2t^\perp\left(\frac{z'}{2t^\perp} + \cos \phi\right)} = \frac{1}{4\pi t^\perp} \int_{\mu}^1 dz \frac{z\hat{z}_\alpha - \hat{z}_\beta e^{-i(\hat{z}_\alpha - \hat{z}_\beta)\cdot A_0}}{iz^2 + \frac{z'}{t^\perp} + 1} \quad (3.46)$$

We find that that the denominator have two roots. $z_\pm = \frac{z'}{2t^\perp} \pm \frac{1}{2} \sqrt{\left(\frac{z'}{t^\perp}\right)^2 - 4}$, when $\frac{z'}{2t^\perp} < 1$ the argument of the square root becomes negative, and the square root imaginary, the magnitude of $z_\pm$ becomes one for both of the signs, that is both roots lie in the unit circle. For any other values of the argument $|\frac{z'}{2t^\perp}| > 1$ we find that the
root $z_+$ is inside the unit circle with residue

$$e^{-i(z_\alpha - z_\beta) \cdot A_0} \left( \frac{-z'}{2t_\perp} + \frac{1}{2} \sqrt{\left( \frac{z'}{t_\perp} - 4 \right)^2} \right)^{(z_\alpha - z_\beta)} / \sqrt{\left( \frac{z'}{t_\perp} \right)^2 - 4} \quad (3.47)$$

while the root $z_-$ is outside the unit circle.

After replacing back the variable $z$, we get the final expression

$$g_{\alpha\beta, \text{Bulk}}(k_{\parallel}, \omega) =$$

$$e^{-i(z_\alpha - z_\beta) \cdot A_0} \left[ - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}) - i\delta^+) + \sqrt{(\omega + \mu - \epsilon_{\parallel}(k_{\parallel}) - i\delta^+)^2 - 4t_\perp^2} \right]^{(z_\alpha - z_\beta)}$$

$$\frac{(2t_\perp)^{(z_\alpha - z_\beta)}}{\sqrt{(\omega + \mu - \epsilon_{\parallel}(k_{\parallel}) - i\delta^+)^2 - 4t_\perp^2}}$$

$$\quad (3.48)$$

The argument of the square root becomes negative inside the band, since the $\sqrt{\cdots}$ symbol stands for the positive square root of the argument. This equation will produce a negative imaginary part in the local Green’s function which is the correct sign. We repeat the same process to calculate the advanced Green’s function.

This result is quite similar to the one dimensional case result, which is expected since we are transforming only one of the three dimensions of the system, where the $\sqrt{\cdots}$ symbol represents the positive square root. We have to be careful regarding the sign of the square root, the sign is defined by selecting the right pole within the unit circle.

The local form is obtained when $\alpha = \beta$

$$g_{\alpha\alpha, \text{Bulk}}(k_{\parallel}, \omega) = \frac{1}{\sqrt{(\omega + \mu - \epsilon_{\parallel}(k_{\parallel}) - i\delta^+)^2 - 4t_\perp^2}} \quad (3.49)$$

We can also calculate the Green’s function in between neighboring planes that is $g_{\alpha\alpha+1, \text{Bulk}}(k_{\parallel}, \omega) = g_{\alpha-1\alpha, \text{Bulk}}(k_{\parallel}, \omega)$ and $g_{\alpha\alpha-1, \text{Bulk}}(k_{\parallel}, \omega) = g_{\alpha+1\alpha, \text{Bulk}}(k_{\parallel}, \omega)$. The previous relations only hold in the bulk region. The nearest neighbor Green’s functions
are

\[ g^R_{αα+1, Bulk}(k_∥, ω) = e^{-iA_0 2t^⊥} \frac{-(ω + μ - \epsilon_∥(k_∥) - iδ^+)}{\sqrt{(ω + μ - \epsilon_∥(k_∥) - iδ^+)^2 - 4t^⊥^2}} + \frac{\sqrt{(ω + μ - \epsilon_∥(k_∥) - iδ^+)^2 - 4t^⊥^2}} {\sqrt{(ω + μ - \epsilon_∥(k_∥) - iδ^+)^2 - 4t^⊥^2}}^{-1} \] (3.50)

and

\[ g^R_{αα-1, Bulk}(k_∥, ω) = e^{iA_0} \frac{-(ω + μ - \epsilon_∥(k_∥) + iδ^+)}{2t^⊥} \left[ -(ω + μ - \epsilon_∥(k_∥) + iδ^+) + g^{-1}_{αα, Bulk}(k_∥, ω) \right]^{-1} g^R_{αα, Bulk}(k_∥, ω) \] (3.51)

We can also express these equations in terms of the local quantities.

\[ g^R_{αα+1, Bulk}(k_∥, ω) = e^{-iA_0 2t^⊥} \frac{-(ω + μ - \epsilon_∥(k_∥) - iδ^+)}{\sqrt{(ω + μ - \epsilon_∥(k_∥) - iδ^+)^2 - 4t^⊥^2}} + \frac{\sqrt{(ω + μ - \epsilon_∥(k_∥) - iδ^+)^2 - 4t^⊥^2}} {\sqrt{(ω + μ - \epsilon_∥(k_∥) - iδ^+)^2 - 4t^⊥^2}}^{-1} g^{-1}_{αα, Bulk}(k_∥, ω) (3.52)\]

and

\[ g^R_{αα-1, Bulk}(k_∥, ω) = e^{-iA_0} \frac{-(ω + μ - \epsilon_∥(k_∥) + iδ^+)}{2t^⊥} \left[ -(ω + μ - \epsilon_∥(k_∥) + iδ^+) + g^{-1}_{αα, Bulk}(k_∥, ω) \right] g^R_{αα, Bulk}(k_∥, ω) (3.53) \]

In order to obtain the local Green’s function \( g^R_{αα, Bulk}(ω) \), we need to sum over the 2D momentum. We achieve this by integrating over the 2 dimensional density of states for the square lattice, since the only dependence on \( \vec{k}_∥ \) is through \( \epsilon_∥ \). That is

\[ g^R_{αα, Bulk}(ω) = \int d\epsilon_∥(k_∥) \rho^{2D}(\epsilon_∥(k_∥)) g^R_{αα, Bulk}(\epsilon_∥(k_∥), ω) , \] (3.54)

with

\[ \rho^{2D}(\epsilon_∥(k_∥)) = \frac{1}{2π^2 t_∥} K \left( \sqrt{1 - \left( \frac{\epsilon_∥}{2t_∥} \right)^2} \right) , \] (3.55)
where $K(x)$ is the complete elliptic integral of the first kind. We show the density of states for the resulting local Green’s function in Fig. 3.1. It’s expected that by introducing the constant vector potential $A_0$ the lesser Green’s function, that is the distribution of the populated states, will change as a function of $A_0$, while the density of states will remain unaffected.

While in the equilibrium state, $g_{Bulk}$ reduces to the Fermi-Dirac distribution, it doesn’t in our current carrying state. Starting from Eq. (3.41), we calculate the Fourier
transform to the mixed-basis representation,
\[ g^{<,K}_{\alpha\beta,\text{Bulk}}(k_\parallel, \omega) = \frac{1}{2\pi} \int_0^{2\pi} dk_z g^{<,K}_{k_\parallel,\beta}(k_\parallel, \omega) e^{i(z_\alpha - z_\beta)k_z} \]
(3.56)

This can be achieved using the properties of the Dirac delta function \( \int_{-\infty}^{\infty} f(x) \delta(h(x)) dx = \sum_i f(x_i)/|h'(x_i)| \), the delta function is only non-zero at the points when \( \cos(k_z) = (\epsilon_\parallel(k_\parallel) - \omega - \mu)/2t^\perp \), that is \( k_z = \pm \arccos((\epsilon_\parallel(k_\parallel) - \omega - \mu)/2t^\perp) \)

We need to use the following trigonometric identities
\[
\sin(\pm \arccos(\theta)) = \pm \sqrt{1 - \theta^2}, 
\]
(3.57)
\[
\cos(\arccos(\theta) - \phi) = \theta \cos(\phi) + \sqrt{1 - \theta^2} \sin(\phi), 
\]
(3.58)
\[
\cos(- \arccos(\theta) - \phi) = \theta \cos(\phi) - \sqrt{1 - \theta^2} \sin(\phi), 
\]
(3.59)
\[
\exp^{\pm i \arccos(\theta)} = \theta \pm i \sqrt{1 - \theta^2}. 
\]
(3.60)

The argument of the delta function is \( h(k_\parallel) = \omega + \mu - \epsilon_\parallel(k_\parallel) + 2t^\perp \cos(k_z) \), this defines the denominator of the lesser Green’s function \( |h'(k_z)| = \sqrt{4t^\perp} - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2 \).

The lesser and Keldysh Green’s functions in the mix-basis become
\[
g^{<,K}_{\alpha\beta,\text{Bulk}}(k_\parallel, \omega) = 
\frac{ie^{i(z_\alpha - z_\beta)\arccos((\epsilon_\parallel(k_\parallel) - \omega - \mu)/2t^\perp)}}{\sqrt{4t^{\perp2} - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2}} 
\times f^{<,K} \left( \epsilon_\parallel(k_\parallel) - 2t^\perp \cos \left( \arccos \left( \frac{\epsilon_\parallel(k_\parallel) - \omega - \mu}{2t^\perp} \right) - A_0 \right) - \mu \right) 
\frac{ie^{-i(z_\alpha - z_\beta)\arccos((\epsilon_\parallel(k_\parallel) - \omega - \mu)/2t^\perp)}}{\sqrt{4t^{\perp2} - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2}} 
\times f^{<,K} \left( \epsilon_\parallel(k_\parallel) - 2t^\perp \cos \left( \arccos \left( \frac{\epsilon_\parallel(k_\parallel) - \omega - \mu}{2t^\perp} \right) - A_0 \right) - \mu \right) 
\]
(3.61)
which simplifies for \( \alpha = \beta \) to

\[
g_{\alpha \alpha, \text{Bulk}}^{<,K}(k_{\parallel}, \omega) = \\
\frac{\text{if}^{<,K} \left( (\epsilon_{\parallel}(k_{\parallel}) - \mu)(1 - \cos(A_0)) + \omega \cos(A_0) + \sin(A_0) \sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2} \right)}{\sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2}} \\
\frac{\text{if}^{<,K} \left( (\epsilon_{\parallel}(k_{\parallel}) - \mu)(1 - \cos(A_0)) + \omega \cos(A_0) - \sin(A_0) \sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2} \right)}{\sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2}}
\]

(3.62)

In the absence of the field, they reduce to the right equilibrium result

\[
g_{\alpha \alpha, \text{Bulk}}^{<,K}(k_{\parallel}, \omega)_{\text{eq}} = -\frac{2i \text{f}^{<,K}(\omega)}{\sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2}}.
\]

(3.63)

We also calculate the nearest-neighbor lesser and Keldysh Green’s functions \( g_{\alpha \alpha \pm 1, \text{Bulk}}^{<,K}(k_{\parallel}(\epsilon_{\parallel}), \omega) \) and \( g_{\alpha \alpha - 1, \text{Bulk}}^{<,K}(k_{\parallel}(\epsilon_{\parallel}), \omega) \)

\[
g_{\alpha \alpha + 1, \text{Bulk}}^{<,K}(k_{\parallel}(\epsilon_{\parallel}), \omega) = -\left[ \left( \epsilon_{\parallel}(k_{\parallel}) - \omega - \mu \right) - i \sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2} \right]^{-1} \\
\times \frac{2i t_{\perp} f^{<,K} \left( \epsilon_{\parallel}(k_{\parallel}) - 2t_{\perp} \cos \left( \arccos \left( \frac{\epsilon_{\parallel}(k_{\parallel}) - \omega - \mu}{2t_{\perp}} \right) - A_0 \right) - \mu \right)}{\sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2}} \\
- \left[ \left( \epsilon_{\parallel}(k_{\parallel}) - \omega - \mu \right) + i \sqrt{4t_{\perp}^2 - (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2} \right]^{-1} \\
\times \frac{2i t_{\perp} f^{<,K} \left( \epsilon_{\parallel}(k_{\parallel}) - 2t_{\perp} \cos \left( - \arccos \left( \frac{\epsilon_{\parallel}(k_{\parallel}) - \omega - \mu}{2t_{\perp}} \right) - A_0 \right) - \mu \right)}{\sqrt{4t_{\perp}^2 (\omega + \mu - \epsilon_{\parallel}(k_{\parallel}))^2}}
\]

(3.64)
\[ g_{\alpha \alpha -1,\text{Bulk}}(k_\parallel (\epsilon_\parallel), \omega) = - \left( \epsilon_\parallel(k_\parallel) - \omega - \mu \right) - i \sqrt{4t^\perp - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2} \]

\[
\times \frac{i f^{<,K} (\epsilon_\parallel(k_\parallel) - 2t^\perp \cos \left( \arccos \left( \frac{\epsilon_\parallel(k_\parallel) - \omega - \mu}{2t^\perp} \right) - A_0 \right) - \mu)}{2t^\perp \sqrt{4t^\perp - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2}}
\]

\[
- \left( \epsilon_\parallel(k_\parallel) - \omega - \mu \right) + i \sqrt{4t^\perp - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2}
\]

\[
\times \frac{i f^{<,K} (\epsilon_\parallel(k_\parallel) - 2t^\perp \cos \left( - \arccos \left( \frac{\epsilon_\parallel(k_\parallel) - \omega - \mu}{2t^\perp} \right) - A_0 \right) - \mu)}{2t^\perp \sqrt{4t^\perp - (\omega + \mu - \epsilon_\parallel(k_\parallel))^2}}.
\]

These equations are valid only inside the band, that is when \((\omega + \mu - \epsilon_\parallel(k_\parallel)) \leq 2t^\perp\).

### 3.4 Equation of Motion

Once the Green’s function in the bulk is known, we proceed to calculate the equation of motion. By taking the derivative of the Green’s function with respect to time:

\[
\frac{\partial}{\partial t} g^c(t, t')_{\alpha i \beta j} = -i \delta_c(t, t') \langle \hat{c}(t)_{\alpha i} \hat{c}^\dagger_{\beta j}(t') \rangle - i \delta_c(t, t') \langle \hat{c}^\dagger(t')_{\beta j} \hat{c}(t)_{\alpha i} \rangle
\]

\[
- i \theta_c(t, t') \langle \hat{U}^\dagger(t) [\hat{H}_{FK}(t), \hat{c}_{\alpha i}(-\infty)] \hat{U}(t) \hat{c}^\dagger_{\beta j}(t') \rangle + i \theta_c(t, t') \langle \hat{c}^\dagger_{\beta j}(t') \hat{U}^\dagger(t) [\hat{H}_{FK}(t), \hat{c}_{\alpha i}(-\infty)] \hat{U}(t) \rangle
\]

(3.66)

where the Hamiltonian \(\hat{H}_{FK}(t)\) is in the Schrödinger representation which arises from the derivation of the evolution operator. Note the fact that the second term became negative, due to the fact that the time arguments of the step function are inverted.

The first two terms can be grouped together as the anti commutator which yields a Kronecker delta function, \(\{\hat{c}(t)_{\alpha i}, \hat{c}^\dagger_{\beta j}(t)\}_+ = \delta_{\alpha \beta} \delta_{ij}\).
As usual the derivative with respect to time can be replaced by a commutator between the corresponding operator and the full Hamiltonian of the system in the Schrödinger representation:

\[ [\hat{H}_{FK}(t), \hat{c}_{\alpha i}] = [t_{\alpha a+1} e^{ieA_\alpha(t)} \hat{c}_{\alpha+1 i} + t_{\alpha a-1} e^{-ieA_{\alpha-1}(t)} \hat{c}_{\alpha-1 i}] + t_{\alpha} \sum_\delta \hat{c}_{\alpha i+\delta} + \mu \hat{c}_{\alpha i} - U_a \hat{w}_{ai} \hat{c}_{\alpha i}. \] 

(3.67)

Plugging this result into Eq. [3.66], we arrive to the following equation:

\[
\frac{\partial}{\partial t} g(t, t')_{\alpha i \beta j} = -i \delta_{c}(t, t') \delta_{\alpha \beta} \\
- i \theta_{c}(t, t') \left( t_{\alpha a+1} e^{ieA_\alpha(t)} \hat{c}_{\alpha+1 i} \hat{c}_{\beta j}^\dagger(t') + t_{\alpha a-1} e^{-ieA_{\alpha-1}(t)} \hat{c}_{\alpha-1 i} \hat{c}_{\beta j}^\dagger(t') \right) \\
+ t_{\alpha} \sum_\delta \hat{c}_{\alpha i+\delta}(t') \hat{c}_{\beta j}(t') + \mu \hat{c}_{\alpha i}(t) \hat{c}_{\beta j}^\dagger(t') - U_a \hat{w}_{ai} \hat{c}_{\alpha i}(t) \hat{c}_{\beta j}^\dagger(t') \\
+ i \theta_{c}(t', t) \left( t_{\alpha a+1} e^{ieA_\alpha(t)} \hat{c}_{\alpha+1 i}^\dagger(t') \hat{c}_{\beta j}(t) + t_{\alpha a-1} e^{-ieA_{\alpha-1}(t)} \hat{c}_{\alpha-1 i}^\dagger(t') \hat{c}_{\beta j}(t) \right) \\
+ t_{\alpha} \sum_\delta \hat{c}_{\beta j}^\dagger(t') \hat{c}_{\alpha i+\delta}(t) + \mu \hat{c}_{\beta j}(t') \hat{c}_{\alpha i}(t) - U_a \hat{w}_{ai} \hat{c}_{\beta j}(t') \hat{c}_{\alpha i}(t) \right). \] 

(3.68)

Using the definition of the contour-ordered Green’s function in Eq. [3.2], we can rewrite this as:

\[
i \frac{\partial}{\partial t} g(t, t')_{\alpha i \beta j} = -\delta_{c}(t, t') \delta_{\alpha \beta} + t_{\alpha a+1} e^{ieA_\alpha(t)} g_{\alpha+1 i \beta j}(t, t') + t_{\alpha a-1} e^{-ieA_{\alpha-1}(t)} g_{\alpha-1 i \beta j}(t, t') \\
+ t_{\alpha} \sum_\delta g_{\alpha i+\delta \beta j}(t, t') + \mu g_{\alpha i \beta j}(t, t') \\
+ i U_a [\theta_{c}(t, t') \langle \hat{w}_{ai} \hat{c}_{\alpha i}(t) \hat{c}_{\beta j}^\dagger(t') \rangle - \theta_{c}(t', t) \langle \hat{w}_{ai}^\dagger \hat{c}_{\beta j}^\dagger(t') \hat{c}_{\alpha i}(t) \rangle] \] 

(3.69)
Eq. (3.69) is our equation of motion in real space. We use the last term in our equation of motion to define the self-energy of the system. With the Dynamical Mean Field Theory (DMFT) assumption that the self energy is local:

\[
\int_c d\bar{t} \Sigma^{c}_{\alpha i}(t, \bar{t}) g^{c}_{\alpha \beta j}(\bar{t}, t') = U_{\alpha} \{ i \theta_c(t, t') \langle \hat{w}_{\alpha i} \hat{c}_{\alpha i}(t) \hat{c}_{\beta j}^\dagger(t') \rangle - i \theta_c(t', t) \langle \hat{w}_{\alpha i} \hat{c}_{\beta j}^\dagger(t') \hat{c}_{\alpha i}(t) \rangle \} \tag{3.70}
\]

The final equation of motion then becomes

\[
i \frac{\partial}{\partial t} g^{c}_{\alpha \beta j}(t, t') = -\delta_{c}(t, t') \delta_{\alpha \beta} + t_{\alpha \alpha + 1} e^{i eA_{\alpha}(t)} g^{c}_{\alpha + 1 \beta j}(t, t') + t_{\alpha - 1 \alpha} e^{-i eA_{\alpha - 1}(t)} g^{c}_{\alpha - 1 \beta j}(t, t') + t_{\parallel} \sum_\delta g^{c}_{\alpha i + \delta j}(t, t') + \mu g^{c}_{\alpha \beta j}(t, t') + \int_c d\bar{t} \Sigma^{c}_{\alpha i}(t, \bar{t}) g^{c}_{\alpha \beta j}(\bar{t}, t). \tag{3.71}
\]

3.4.1 Mixed basis

As can be seen in Fig. 1.6 the system is translationally invariant in the $\hat{x}$ and $\hat{y}$ directions, since it's a periodic system, the symmetry is only broken in the $\hat{z}$ direction, therefore we would like to perform a Fourier transform on the Green’s functions for the $\hat{x}$ and $\hat{y}$ directions as first shown by Potthoff and Nolting(44). The $\hat{z}$ direction will remain in real space, hence we use a mixed basis. This corresponds to the $t_{\parallel}$ component of the hopping. In order to do so, we use the following relations:

\[
\hat{c}_{\alpha i} = \sum_{\vec{k}_{\parallel}} \hat{c}_{\alpha \vec{k}_{\parallel}} e^{i \vec{k}_{\parallel} \cdot \vec{R}_i} \tag{3.72}
\]

and

\[
\hat{c}_{\beta j}^\dagger = \sum_{\vec{k}_{\parallel}} \hat{c}_{\beta \vec{k}_{\parallel}}^\dagger e^{-i \vec{k}_{\parallel} \cdot \vec{R}_j} \tag{3.73}
\]

as well as

\[
g^{c}_{\alpha \beta}(\vec{k}_{\parallel}, t, t') = \frac{1}{N} \sum_i \sum_j g^{c}_{\alpha i \beta j}(t, t') e^{i \vec{k}_{\parallel} \cdot (\vec{R}_i - \vec{R}_j)}, \tag{3.74}
\]
Where $i$ and $j$ run over the planar sites only and $N$ is the number of sites in a plane. Recall that a sum over plane waves yields a Kronecker delta function $\sum_i \exp[i(\vec{k}|| - \vec{k}'||) \cdot \vec{R}_i]/N = \delta_{\vec{k}||,\vec{k}'||}$, the Fourier transform of the Green’s function becomes

$$
g^{c\beta}_{\alpha}(\vec{k}||,t,t') = -i\theta_c(t,t')\langle \hat{c}_\alpha(\vec{k}||,t)\hat{c}_\beta^\dagger(\vec{k}||,t') \rangle + i\theta_c(t,t')\langle \hat{c}_\beta^\dagger(\vec{k}||,t')\hat{c}_\alpha(\vec{k}||,t) \rangle \quad (3.75)
$$

We perform a Fourier transformation for the two-d kinetic energy piece of the equation of motion following the same procedure, but notice we have an extra factor of $t||$, this will yield the band structure of the plane, in our case a 2D square lattice with $\sum_\delta t||_\delta \exp(i\vec{k}|| \cdot \vec{\delta}) = \epsilon_\alpha(\vec{k}||)$:

$$
t|| \sum_\delta g^{c\alpha+\delta \beta}_{\alpha}(t,t') \rightarrow \sum_{\vec{k}||} -\epsilon(\vec{k}||)g^{c\alpha}_{\alpha\beta}(\vec{k}||,t,t') \quad (3.76)
$$

The final equation of motion in the mixed basis becomes

$$
i\frac{\partial}{\partial t} g^{c}(\vec{k}||,t,t')_{\alpha\beta} = 
- \delta_c(t,t')\delta_{\alpha\beta} + t_{\alpha\alpha+1}^+ e^{ieA_\alpha(t)} g^{c}_{\alpha+1\beta}(\vec{k}||,t,t')
+ t_{\alpha-1\alpha}^- e^{-ieA_{\alpha-1}(t)} g^{c}_{\alpha-1\beta}(\vec{k}||,t,t')
- \epsilon_\alpha(\vec{k}||)g^{c\alpha}_{\alpha\beta}(\vec{k}||,t,t') + \mu g^{c}_{\alpha\beta}(\vec{k}||,t,t')
- \int d\bar{t} \Sigma^c_\alpha(t,\bar{t})g^{c\alpha\beta}_{\alpha\beta}(\vec{k}||,\bar{t},t')
\quad (3.77)
$$

We reorganize this by introducing an integral for all terms with the appropriate Dirac delta function over time

$$
\delta_c(t,t')\delta_{\alpha\beta} = \int d\bar{t} \left\{ \left[ \left( -i\frac{\partial}{\partial \bar{t}} + \mu - \epsilon_\alpha(\vec{k}||) \right) \delta_c(t,\bar{t}) - \Sigma^c_\alpha(t,\bar{t}) \right] g^{c\alpha\beta}_{\alpha\beta}(\vec{k}||,\bar{t},t')
+ \left[ t_{\alpha\alpha+1}^+ e^{ieA_\alpha(t)} g^{c\alpha+1\beta}_{\alpha+1\beta}(\vec{k}||,t,\bar{t})
+ t_{\alpha-1\alpha}^- e^{-ieA_{\alpha-1}(t)} g^{c\alpha-1\beta}_{\alpha-1\beta}(\vec{k}||,t,\bar{t}) \right] \delta_c(\bar{t},t') \right\}
\quad (3.78)
$$

This is our final equation of motion in the mixed basis.
3.4.2 Recurrence relations

From the equation of motion derived above, we turn to calculate the recurrence relations \((L_{\alpha-n}, R_{\alpha+n})\), which we will use in our quantum zipper algorithm. These recurrence relations allow us to determine the Green’s function on a given plane taking into account what the Green’s function is on an adjacent plane.

Our starting point is the equation of motion derived above in Eq. (3.78). The matrix \(g_{c\alpha\beta}(t, t')\) can be thought of as a block matrix in time, that is distributed in a spatial pattern set by the \(\alpha\) and \(\beta\) values. When we take the inverse of the Green’s function, we must do so with respect to both time and spatial indices. To derive a set of recursion relations that are used to solve for the Green’s function, we work with inverses of specific blocks in time, with the spatial indices fixed. One might ask whether such inverses are well defined. They are in equilibrium as they are used in the equilibrium formalism after Fourier transforming to a frequency representation. We will show that the inverses are also well defined here \textit{a posteriori} by examining the final formulas we have, which will include well-defined inverses. For now, we assume this is true and work with inverses that are with respect to the time indices only for each block of fixed alpha and beta. Start by multiplying from the right by the inverse with respect to the time indices of the Green’s function, \(g_{\alpha\beta}^{-1}(\vec{k}_\parallel, t', t''')\), Note that since we are dealing with matrix multiplications, we have to be careful about the multiplication order:

\[
\delta_{\alpha\beta}g_{\alpha\beta}^{-1} c_{\alpha\beta}(k_\parallel, t, t') = \left[ -i\frac{\partial}{\partial t} + \mu - \epsilon(k_\parallel) \right] \delta_{c}(t, t') - \Sigma_{\alpha}(t, t')
\]

\[
+ t_{\alpha+1}^{c} e^{i\epsilon A_\alpha(t)} \int_{c} d\bar{t} g_{\alpha+1\beta}(\vec{k}_\parallel, t, \bar{t}) g_{\beta\alpha}^{-1}(\vec{k}_\parallel, \bar{t}, t')
\]

\[
+ t_{\alpha-1}^{c} e^{-i\epsilon A_{\alpha-1}(t)} \int_{c} d\bar{t} g_{\alpha-1\beta}(\vec{k}_\parallel, t, \bar{t}) g_{\beta\alpha}^{-1}(\vec{k}_\parallel, \bar{t}, t')
\]

(3.79)
Here \( \int_t dt' \) is used for matrix multiplication of the time indices. Now let \( \beta \to \alpha \) with \( \alpha \to \alpha - n \), and \( n > 0 \), to give

\[
0 = \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}_\parallel) \right] \delta_c(t, t') - \Sigma_{\alpha-n}(t, t')
+ t^\perp_{\alpha-n\alpha-n+1} e^{ieA_{\alpha-n}(t)} \int_c d\vec{t} g_{\alpha-n+1\alpha}(\vec{k}_\parallel, t, \vec{t}) g_{\alpha-n\alpha}(\vec{k}_\parallel, \vec{t}, t')
+ t^\perp_{\alpha-n-1\alpha-n} e^{-ieA_{\alpha-n-1}(t)} \int_c d\vec{t} g_{\alpha-n-1\alpha}(\vec{k}_\parallel, t, t') g_{\alpha-n\alpha}(\vec{k}_\parallel, \vec{t}, t') \tag{3.80}
\]

Now define the left function \( L^c_{\alpha-n} \) via

\[
L^c_{\alpha-n}(\vec{k}_\parallel, t, t') = -t^\perp_{\alpha-n\alpha-n+1} e^{ieA_{\alpha-n}(t)} \int_c d\vec{t} g_{\alpha-n+1\alpha}(\vec{k}_\parallel, t, \vec{t}) g_{\alpha-n\alpha}(\vec{k}_\parallel, \vec{t}, t') \tag{3.81}
\]

We can rewrite Eq. (3.80) in terms of the \( L_\alpha \) function. To do this, we must calculate the inverse of \( L^c_{\alpha-n-1} \) with respect to the time indices for fixed spacial indices. Recall the inverse relation \( (AB)^{-1} = B^{-1}A^{-1} \) for square invertible matrices. This then yields

\[
L^{-1}_{\alpha-n-1}(\vec{k}_\parallel, t, t') = -t^\perp_{\alpha-n-1\alpha-n} \int_c d\vec{t} g_{\alpha-n-1\alpha}(\vec{k}_\parallel, t, t') g_{\alpha-n\alpha}(\vec{k}_\parallel, \vec{t}, t') e^{-ieA_{\alpha-n-1}(t')} \tag{3.82}
\]

in which the multiplicative inverse of the \( e \) and Green’s functions factors have to be inverted in order as well. From Eq. (3.80), we find

\[
L^c_{\alpha-n}(\vec{k}_\parallel, t, t') = \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}_\parallel) \right] \delta_c(t, t') - \Sigma^c_{\alpha-n}(t, t')
- t^\perp_{\alpha-n-1\alpha-n} e^{-ieA_{\alpha-n-1}(t)} L^{-1}_{\alpha-n-1}(\vec{k}_\parallel, t, t') e^{ieA_{\alpha-n-1}(t')} \tag{3.83}
\]

Using the same procedure we find the right recurrence relation \( R_{\alpha+n} \). We start from the equation of motion and we let \( \alpha \to \alpha + n \) and \( \beta \to \alpha \) with \( n > 0 \). Then the right function is defined by

\[
R^c_{\alpha+n}(\vec{k}_\parallel, t, t') = -t^\perp_{\alpha+n-1\alpha+n} \int_c d\vec{t} e^{-ieA_{\alpha+n-1}(t)} g_{\alpha+n-1\alpha}(\vec{k}_\parallel, t, t') g_{\alpha+n\alpha}(\vec{k}_\parallel, \vec{t}, t') \tag{3.84}
\]

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thus

\[ R_{\alpha+n}^c(\vec{k}_\parallel, t, t') = \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}_\parallel) \right] \delta_c(t, t') - \Sigma_{\alpha+n}^c(t, t') - t_{\alpha+n}^{c+1} e^{ieA_{\alpha+n}(t)} R_{\alpha+n+1}^c(\vec{k}_\parallel, t, t') e^{-ieA_{\alpha+n}(t')} \] (3.85)

Finally, we examine the case with \( \alpha = \beta \) in the equation of motion:

\[ g^{-1}(\vec{k}_\parallel, t, t')_{\alpha\alpha} = \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}_\parallel) \right] \delta_c(t, t') - \Sigma_{\alpha}(t, t') - L_{\alpha}(\vec{k}_\parallel, t, t') - R_{\alpha}(\vec{k}_\parallel, t, t') \] (3.86)

We know that our Green’s functions will approach their bulk values as we get far away from the barrier. These bulk values are needed to form the boundary condition of our calculation. We need to calculate our recursion relations in that limit, that is \( L_{-\infty} \) and \( R_{\infty} \) in the limit as the plane number approaches \( \infty \), we won’t see variations in our recursion relations anymore and Eqs. (3.83) and (3.85) become quadratic matrix equations, since \( L_{\alpha}^c = L_{\alpha-n}^c \) and \( R_{\alpha}^c = R_{\alpha+n}^c \). The quadratic equation for the left recurrence relation becomes

\[ 0 = \int_{c} d\tilde{t} L_{-\infty}^c(\vec{k}_\parallel, t, \tilde{t}) e^{-ieA_{-\infty}(\tilde{t})} L_{-\infty}^c(\vec{k}_\parallel, \tilde{t}, t') e^{ieA_{-\infty}(t')} \]

\[ -\int_{c} d\tilde{t} \left\{ \left[ -i \frac{\partial}{\partial \tilde{t}} + \mu - \epsilon(\vec{k}_\parallel) \right] \delta_c(\tilde{t}, \tilde{t}) - \Sigma_{-\infty}^c(\tilde{t}, \tilde{t}) \right\} e^{-ieA_{-\infty}(\tilde{t})} L_{-\infty}^c(\vec{k}_\parallel, \tilde{t}, t') e^{ieA_{-\infty}(t')} + t_{-\infty}^{c+2} \delta_c(t, t') \] (3.87)

with a similar equation for the \( R \) recurrence. As we did for the Dyson equation, we will rewrite this set of equations into matrix form. Starting from the definition of the left function Eq. (3.81), after writing down the equations in the contour and comparing signs becomes

\[ \bar{L}_{\alpha-n}^c(\vec{k}_\parallel, t, t') \tau_3 = -t_{\alpha-na-n+1}^{c+1} \int_{c} d\tilde{t} e^{ieA_{\alpha-n}(\tilde{t})} g_{\alpha-n+1\alpha}^c(\vec{k}_\parallel, t, \tilde{t}) \tau_3 g_{\alpha-na}^{-1}(\vec{k}_\parallel, \tilde{t}, t') \tau_3 \] (3.88)

With

\[ \bar{L}_{\alpha-n}^c(\vec{k}_\parallel, t, t') \rightarrow \begin{pmatrix} L_{\alpha-n,++}^c(\vec{k}_\parallel, t, t') & L_{\alpha-n,+}^c(\vec{k}_\parallel, t, t') \\ L_{\alpha-n,+}^c(\vec{k}_\parallel, t, t') & L_{\alpha-n,-}^c(\vec{k}_\parallel, t, t') \end{pmatrix} \] (3.89)
Applying the transformation $\hat{L}_\tau$ from the left and $\tau_3 \hat{L}^\dagger$ from the right we find
\begin{equation}
L^{c}_{\alpha-n}(\vec{k}_\parallel, t, t') = -t_{\alpha-n+1}^{\dagger}(t) \int d\vec{r} e^{ieA_{\alpha-n}(t)} G^{c}_{\alpha-n+1}(\vec{k}_\parallel, t, \bar{t}) G^{c-1}_{\alpha-n}(\vec{k}_\parallel, \bar{t}, t') \tag{3.90}
\end{equation}
where $L^{c}_{\alpha-n}$ is upper diagonal
\begin{equation}
L^{c}_{\alpha-n}(\vec{k}_\parallel, t, t') = \begin{pmatrix}
L^{R}_{\alpha-n}(\vec{k}_\parallel, t, t') & L^{K}_{\alpha-n}(\vec{k}_\parallel, t, t') \\
0 & L^{A}_{\alpha-n}(\vec{k}_\parallel, t, t')
\end{pmatrix} \tag{3.91}
\end{equation}

Eq. (3.82) in matrix form then becomes
\begin{equation}
\tau_3 \bar{L}^{\dagger-1}_{\alpha-n-1}(\vec{k}_\parallel, t, t') \tau_3 = -t_{\alpha-n-1}^{\dagger-1} \int d\vec{r} \bar{g}^{c-1}_{\alpha-n-1}(\vec{k}_\parallel, t, \bar{t}) \bar{g}^{c-1}_{\alpha-n}(\vec{k}_\parallel, \bar{t}, t') \tau_3 e^{ieA_{\alpha-n-1}(t')} \tag{3.92}
\end{equation}
and after applying the same transformation as above $\hat{L}_\tau$ from the left and $\hat{L}^\dagger$ from the right we obtain the inverse of the left function in the retarded-advanced-Keldysh form
\begin{equation}
\bar{L}^{-1}_{\alpha-n-1}(\vec{k}_\parallel, t, t') = \begin{pmatrix}
L_{\alpha-n-1}^{R}(-1)(\vec{k}_\parallel, t, t') & -L_{\alpha-n-1}^{R}(-1)(\vec{k}_\parallel, t, t') L_{\alpha-n-1}^{K}(\vec{k}_\parallel, t, t') L_{\alpha-n-1}^{A-1}(\vec{k}_\parallel, t, t') \\
0 & L_{\alpha-n-1}^{A-1}(\vec{k}_\parallel, t, t')
\end{pmatrix} \tag{3.93}
\end{equation}
as one might have expected. The same holds for the right function.

Now we solve the recurrence relation in the bulk. In the bulk we are far away from the barrier so $L_\infty = R_\infty$. Also there is no $U$ interaction since the bulk is metallic and we are sufficiently far away so that the barrier region doesn’t have any effect on the leads. The self energy is zero as well.

We write the local Green’s function in Eq. (3.97) in the matrix form, after setting $\Sigma_\alpha = 0$ and $L_\alpha = R_\alpha$ and we apply the transformation $\hat{L}$ from the left and $\tau_3 \hat{L}^\dagger$ from the right
\begin{equation}
\hat{L} \left[ \bar{g}^{c-1}(\vec{k}_\parallel, t, t')_{-\infty-\infty} \right] \tau_3 \hat{L}^\dagger = \hat{L} \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}_\parallel) \right] \tau_3 - 2\tau_3 L_\infty(\vec{k}_\parallel, t, t') \tau_3 \hat{L}^\dagger \tag{3.94}
\end{equation}
after performing the transformation, since $G^c$ is upper diagonal and the $\tau_3$ term is diagonal we find that $L_{-\infty}$ is upper diagonal, therefore, the relationship $L_{-\infty,++} + L_{-\infty,--} = L_{-\infty,+-} + L_{-\infty,-+}$ holds. Since $L_{-\infty}$ is upper diagonal, as we go along the structure applying it consecutively to $G^c$ (which is also upper diagonal) the recursion relation will remain upper diagonal.

In order to solve the quadratic recurrence relation, we write Eq. (3.87) in matrix form

$$\int d\bar{t} L_{-\infty}^c(\vec{k}, t, \bar{t}) e^{-iA_{-\infty}(t)} \tau_3 L_{-\infty}^c(\vec{k}, t, t') \tau_3 e^{iA_{-\infty}(t')}$$

$$- \int d\bar{t} \left\{ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}) \right\} \delta(t, \bar{t}) - \Sigma^c_{-\infty}(t, \bar{t}) \right\} e^{-iA_{-\infty}(t)} \tau_3 L_{-\infty}^c(\vec{k}, t, t') \tau_3 e^{iA_{-\infty}(t')}$$

$$+ t^2_{-\infty} \delta(t, t') = 0. \quad (3.95)$$

We next transform to the Keldysh representation by applying $\hat{L}\tau_3$ from the left and $\tau_3\hat{L}^\dagger$ from the left.

$$\int d\bar{t} L_{-\infty}^c(\vec{k}, t, \bar{t}) e^{-iA_{-\infty}(t)} \tau_3 L_{-\infty}^c(\vec{k}, t, t') e^{iA_{-\infty}(t')}$$

$$- \int d\bar{t} \left\{ -i \frac{\partial}{\partial t} + \mu - \epsilon(\vec{k}) \right\} \delta(t, \bar{t}) - \Sigma^c_{-\infty}(t, \bar{t}) \right\} e^{-iA_{-\infty}(t)} \tau_3 L_{-\infty}^c(\vec{k}, t, t') e^{iA_{-\infty}(t')}$$

$$+ t^2_{-\infty} \delta(t, t') = 0. \quad (3.96)$$

If we restrict the potential $A_\alpha(t) = A_0 + tE_\alpha$ to be linear in time we find that the time dependencies in Eq. (3.96) as well as in equations (3.83), (3.85) and (3.86) reduces to dependencies on $t_{rel} = (t - t')$ only. This allow us to Fourier transform to frequency space each one of those equations. The local Green’s function Eq.(3.86) becomes

$$g^{-1}_c(\vec{k}, \omega)_{\alpha\alpha} = \left[ \omega + \mu - \epsilon(\vec{k}) \right] 1 - \Sigma^c_\alpha(\omega) - L^c_\alpha(\vec{k}, \omega) - R^c_\alpha(\vec{k}, \omega) \quad (3.97)$$
which is identical to the equilibrium case, while the recursion relations Eq. (3.83) and Eq. (3.85) become

\[
L_{\alpha-n}(\vec{k}_\parallel, \omega) = \left[ \omega + \mu - \epsilon(\vec{k}_\parallel) \right] \mathbb{1} - \sum_{\alpha-n}^c(\omega) - t_{1\alpha-n-1\alpha-n}^2 L_{\alpha-n-1}(\vec{k}_\parallel, \omega + eE_{\alpha-n-1})
\]

(3.98)

\[
R_{\alpha+n}(\vec{k}_\parallel, \omega) = \left[ \omega + \mu - \epsilon(\vec{k}_\parallel) \right] \mathbb{1} - \sum_{\alpha+n}^c(\omega) - t_{1\alpha+n\alpha+n+1}^2 R_{\alpha+n+1}(\vec{k}_\parallel, \omega - eE_{\alpha+n})
\]

(3.99)

These formulas are the generalization of the equilibrium result to the case when there is a field present. In equilibrium, the vector potential vanishes and so \( E_\alpha = 0 \) and the equilibrium result holds. Note that when an electric field is present, the recursion shifts the frequency values from one plane to the next.

And finally our quadratic recurrence relation Eq. (3.96) is Fourier transformed to

\[
L_{\infty}(\vec{k}_\parallel, \omega)L_{\infty}(\vec{k}_\parallel, \omega + eE_{\infty})
- \left[ \omega + \mu - \epsilon(\vec{k}_\parallel) \right] \mathbb{1} - \sum_{\infty}^c(\omega) \right] L_{\infty}(\vec{k}_\parallel, \omega + eE_{\infty}) + t_{\perp}^2 \mathbb{1} = 0 \quad (3.100)
\]

we look at the advanced and retarded components of this equation which have similar components, notice that in the bulk the electric field will vanish and the equation will become a quadratic equation in \( L_{\infty} \)

\[
L_{\infty}(\vec{k}_\parallel, \omega)L_{\infty}(\vec{k}_\parallel, \omega + eE_{\infty})
- \left( \omega + \mu - \epsilon(\vec{k}_\parallel) - \Sigma_{\infty}(\omega) \right) L_{\infty}(\vec{k}_\parallel, \omega + eE_{\infty}) + t_{\perp}^2 \mathbb{1} = 0 \quad (3.101)
\]

This formula would hold if we had interacting leads and is hard to solve. When there are no interactions \( \Sigma_{\infty} = E_{\infty} = 0 \) and it becomes a quadratic equation that can be easily solved.

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We solve this quadratic equation via

\[ L_{-\infty}^{RA}(\vec{k}_\parallel, \omega) = \frac{\omega + \mu - \epsilon(\vec{k}_\parallel)}{2} \pm \frac{1}{2} \sqrt{\left(\omega + \mu - \epsilon(\vec{k}_\parallel)\right)^2 - 4t_{-\infty}^2} \]  

which corresponds to the equilibrium result. We must choose the correct sign for the square root. We choose the sign such that the magnitude of \( L_{-\infty}^{R} \) is larger than \( t_{-\infty} \). In contrast, the third equation, which corresponds to the Keldysh piece of the recurrence relation doesn’t yield a quadratic equation, but it does depends on the advanced and retarded recurrence relations as well as in the retarded and advanced self energies. The Keldysh piece is

\[
L_{-\infty}^{R}(\vec{k}_\parallel, \omega)L_{-\infty}^{K}(\vec{k}_\parallel, \omega + eE_{-\infty}) + L_{-\infty}^{K}(\vec{k}_\parallel, \omega)L_{-\infty}^{A}(\vec{k}_\parallel, \omega + eE_{-\infty})
- \left(\omega + \mu - \epsilon(\vec{k}_\parallel) - \Sigma_{-\infty}^{R}(\omega)\right) L_{-\infty}^{K}(\vec{k}_\parallel, \omega + eE_{-\infty})
+ \Sigma_{-\infty}^{K}(\omega) L_{-\infty}^{A}(\vec{k}_\parallel, \omega + eE_{-\infty}) = 0
\]  

We cannot use this equation to solve for \( L_{-\infty}^{K} \) in the bulk because once we set \( \Sigma_{-\infty} = 0 \) and \( E_{-\infty} = 0 \) we find \( 0 = 0 \).

We need to derive the Keldysh right and left relations instead from the Keldysh Green’s function in the bulk in order to be able to calculate the Keldysh piece of \( L \) and \( R \). From the definition of the left function. We obtain

\[ L_{\alpha}^{RA}(\vec{k}, \omega) = -t_{\alpha}^{\perp} g_{\alpha+1\alpha}(\vec{k}, \omega) / g_{\alpha\alpha}(\vec{k}, \omega) \]  

(3.104)

for the retarded and advanced parts and

\[ L_{\alpha}^{K}(\vec{k}, \omega) = -t_{\alpha}^{\perp} \left( -g_{\alpha+1\alpha}(\vec{k}, \omega) g_{\alpha\alpha}(\vec{k}, \omega) + g_{\alpha+1\alpha}(\vec{k}, \omega) / g_{\alpha\alpha}(\vec{k}, \omega) \right). \]  

(3.105)

Hence,

\[ L_{\alpha}^{K}(\vec{k}, \omega) = L_{\alpha}^{R}(\vec{k}, \omega) g_{\alpha\alpha}(\vec{k}, \omega) / g_{\alpha\alpha}(\vec{k}, \omega) - L_{\alpha}^{A}(\vec{k}, \omega) g_{\alpha+1\alpha}(\vec{k}, \omega) / g_{\alpha+1\alpha}(\vec{k}, \omega) \]  

(3.106)
Likewise we use the definition of the right recurrence relation to find the Keldysh part in terms of the retarded and advanced right recurrence relations

\[ R^K_\alpha(\vec{k}, \omega) = R^R_\alpha(\vec{k}, \omega) \frac{g^{K}_{\alpha\alpha}(\vec{k}, \omega)}{g^{R}_{\alpha\alpha}(\vec{k}, \omega)} - R^A_\alpha(\vec{k}, \omega) \frac{g^{K}_{\alpha-1\alpha}(\vec{k}, \omega)}{g^{A}_{\alpha-1\alpha}(\vec{k}, \omega)} \quad (3.107) \]

where

\[ g^K_{\alpha\alpha}(\vec{k}, \omega) = f^K(x_+ \vec{k}) g^R_{\alpha\alpha}(\vec{k}, \omega) + f^K(x_- \vec{k}) g^R_{\alpha\alpha}(\vec{k}, \omega) \quad (3.108) \]

with

\[ x_\pm = (\epsilon_{||}(k||) - \mu) (1 - \cos(A_0)) + \omega \cos(A_0) \pm \sin(A_0) \sqrt{4t^2_{\perp} - (\omega + \mu - \epsilon_{||}(k||))^2} \quad (3.109) \]

In the case where the constant vector potential vanishes, both arguments become identical and \( L^K_\alpha = R^K_\alpha \). This would correspond to the equilibrium recurrence relations and no current would be carried through. In order to get this result we have used the fact that \( L^{A-1}_\alpha = L^{R}_\alpha \) and \( L^{R-1}_\alpha = L^{A}_\alpha \) and we have used the local retarded Green’s function in the bulk

\[ g^{R}_{\alpha\alpha} = -i \frac{-i}{\sqrt{4t^2_{\perp} - (\omega + \mu - \epsilon_{||}(k||))^2}} \quad (3.110) \]

to rewrite the local Keldysh Green’s function with and the nearest neighbors retarded, advanced and Keldysh, Green’s functions

\[ g^{R}_{\alpha+1\alpha}(\vec{k}, \omega) = -\frac{1}{t^{\perp}_\alpha} L^{A}_\alpha(\vec{k}, \omega) g^{R}_{\alpha\alpha}(\vec{k}, \omega) \quad (3.111) \]

\[ g^{R}_{\alpha-1\alpha}(\vec{k}, \omega) = -t^{\perp}_\alpha R^{R}_\alpha(\vec{k}, \omega) g^{R}_{\alpha\alpha}(\vec{k}, \omega) \quad (3.112) \]

\[ g^{K}_{\alpha+1\alpha}(\vec{k}, \omega) = -\frac{1}{t^{\perp}_\alpha} L^{A}_\alpha(\vec{k}, \omega) f^K(x_+ \vec{k}) g^{R}_{\alpha\alpha}(\vec{k}, \omega) - \frac{1}{t^{\perp}_\alpha} L^{R}_\alpha(\vec{k}, \omega) f^K(x_- \vec{k}) g^{R}_{\alpha\alpha}(\vec{k}, \omega) \quad (3.113) \]

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\[ g_{\alpha-1\alpha}(\vec{k}, \omega) = -t^\perp_\alpha R^R_\alpha(\vec{k}, \omega) f^K(x_+) g^{R\alpha}_\alpha(\vec{k}, \omega) - t^\perp_\alpha R^A_\alpha(\vec{k}, \omega) f^K(x_-) g^{R\alpha}_\alpha(\vec{k}, \omega) \] (3.114)

From these results we can extract the Keldysh piece for the right and left functions.

\[ L^K_\alpha(\vec{k}, \omega) = \sqrt{4t^2_\perp - (\omega + \mu - \epsilon(\vec{k}))^2 f^K(x_+)} \] (3.115)
\[ R^K_\alpha(\vec{k}, \omega) = \sqrt{4t^2_\perp - (\omega + \mu - \epsilon(\vec{k}))^2 f^K(x_-)} \] (3.116)

where the left function depends only on the distribution function \( f^K \) evaluated at the positive displacement \( x_+ \) created by the vector potential and the right relation depends only on the negative displacement \( x_- \).

### 3.4.3 Consistency check for the recurrence relations

We summarize this section by writing down the main result for the recurrence relations in the retarded, advanced, Keldysh, representation.

\[ L^{R,A}_{-\infty}(\vec{k}_\parallel, \omega) = R^{R,A}_{-\infty}(\vec{k}_\parallel, \omega) \]
\[ = \frac{1}{2} \left( \omega + \mu - \epsilon(\vec{k}_\parallel) \right) \pm \frac{1}{2} \sqrt{\left( \omega + \mu - \epsilon(\vec{k}_\parallel) \right)^2 - 4t^2_\perp} \] (3.117)
\[ L^K_\alpha(\vec{k}_\parallel, \omega) = \sqrt{4t^2_\perp - (\omega + \mu - \epsilon(\vec{k}_\parallel))^2 f^K(x_+)} \] (3.118)
\[ R^K_\alpha(\vec{k}_\parallel, \omega) = \sqrt{4t^2_\perp - (\omega + \mu - \epsilon(\vec{k}_\parallel))^2 f^K(x_-)} \] (3.119)

These recursion relations have to satisfy Eq. (3.86) once written in the Keldysh representation.

\[ G^{c^{-1}}(\vec{k}_\parallel, \omega)_{\alpha\alpha} = \left[ \omega + \mu - \epsilon(\vec{k}_\parallel) \right] \mathbb{1} - \Sigma^{c}_\alpha(\omega) - L^{c}_\alpha(\vec{k}_\parallel, \omega) - R^{c}_\alpha(\vec{k}_\parallel, \omega) \] (3.120)
In the bulk this equation becomes,

\[
\begin{pmatrix}
g_{\text{Bulk}}^{-1}(\vec{k}, \omega) & -g_{\text{Bulk}}(\vec{k}, \omega)g_{\text{Bulk}}^K(\vec{k}, \omega)g_{\text{Bulk}}^{-1}(\vec{k}, \omega) \\
0 & g_{\text{Bulk}}^{-1}(\vec{k}, \omega)
\end{pmatrix}
\begin{pmatrix}
g_{\text{Bulk}}^{-1}(\vec{k}, \omega) \\
0
\end{pmatrix}
= \begin{pmatrix}
\omega + \mu - \epsilon(\vec{k}) - L^R_{-\infty}(\vec{k}, \omega) - R^R_{-\infty}(\vec{k}, \omega) \\
0
\end{pmatrix}
\begin{pmatrix}
\omega + \mu - \epsilon(\vec{k}) - L^A_{-\infty}(\vec{k}, \omega) - R^A_{-\infty}(\vec{k}, \omega)
\end{pmatrix}.
\]

(3.121)

We can verify directly that the recurrence relations above satisfies all the elements in the matrices above. We find

\[g_{\text{Bulk}}^{-1}(\vec{k}, \omega) = \sqrt{(\omega + \mu - \epsilon(\vec{k}))^2 - 4t^\perp^2} \quad (3.122)\]

\[g_{\text{Bulk}}^{-1}(\vec{k}, \omega) = -\sqrt{(\omega + \mu - \epsilon(\vec{k}))^2 - 4t^\perp^2} \quad (3.123)\]

and

\[g_{\text{Bulk}}^K(\vec{k}, \omega) = |g_{\text{Bulk}}^{-1}(\vec{k}, \omega)|^2(L^K_{-\infty}(\vec{k}, \omega) + R^K_{-\infty}(\vec{k}, \omega)) = g_{\text{Bulk}}^R(\vec{k}, \omega)(f^K(x_+) + f^K(x_-)) \quad (3.124)\]

which corresponds to local Keldysh Green’s function in Eq. (3.63).
Chapter 4

Current biasing a multilayered device as a boundary condition for inhomogeneous nonequilibrium dynamical mean-field theory

Recently, nonequilibrium dynamical mean-field theory was developed as a new technique to solve the bulk nonequilibrium many-body problem. The computational effort needed to solve the nonequilibrium problem in the bulk is similar to the efforts needed to solve the inhomogeneous multilayered problem for current flow perpendicular to the planes. Because the leads provide the appropriate boundary conditions for the open system, one can directly solve for the steady state within a frequency representation, and thereby obtain the current-voltage relation for the device. Here we discuss the problem of determining the boundary condition for the Green’s functions, which can be used to determine the so-called self-energy of the leads, which is a critical step needed in this problem.

4.1 Introduction

Nearly all useful electronic devices rely on nonlinear behavior in the current-voltage relation for the device in order to operate. Examples include semiconductor transistors, tunnel diodes, Josephson junctions, and so on. Recently, motivated by the creation of two-dimensional electron gases at the interfaces of band/Mott-insulating devices, interest has focused on devices made from strongly correlated materials because the strong correlation effects have the potential to be more easily tuned than
in more conventional devices. To date, these strongly correlated multilayered devices have been described primarily in linear response [24, 25, 44, 46, 47], although there has been some work completed in nonequilibrium [27, 48]. But the fundamental problem of determining the current-voltage relation has remained elusive. Here we show how one can use ballistic metal leads and current biasing to determine the appropriate boundary condition for describing the steady-state behavior of these devices.

Figure 4.1: (Color online) Schematic of the multilayered device. On the top and the bottom, the system is attached to bulk leads which carry current in the longitudinal direction. Each plane is labeled by a Greek index $\alpha$, while Roman indices are used to describe the planar sites. For an interacting device, the ballistic metal leads are attached to the barrier region in the center, which is where the scattering occurs. In this region, an electric field needs to be applied to guarantee current conservation through the device.
A schematic picture of such a device is given in Fig. 4.1. The metallic leads are chosen to be ballistic metals because they can be easily current biased. We imagine the system starts in the infinite past in equilibrium at a temperature \( T \). An electric field is turned on for a finite period of time to generate current flow and then is turned off. We describe the field with the Peierls substitution in the vector-potential-only gauge \[49\]. After the field is turned off, the vector potential is equal to \(-A_0\) for large positive and large negative values of the \( z \) coordinate. This generates a constant current flow in the ballistic metal leads. In order to maintain current conservation throughout the device, we need to create local electric fields over a finite number of planes, where the current falls below the value in the ballistic metal (due to scattering or due to proximity to the barrier region). For these planes, we can describe the vector potential with a simple linear function \( A_\alpha(t) = -A_0 - E_\alpha t \), which yields an electric field of \( E_\alpha \) in the \( z \)-direction at the \( \alpha \)th plane (we choose units such that \( \hbar = c = e = a = 1 \), with \( a \) the lattice spacing). Because the vector potential is linear in time, the system as a whole will satisfy time translation invariance and can be described by taking a Fourier transform from time to frequency and employing a frequency representation for all relevant functions. This provides a huge simplification of the problem, as one can determine the steady state using a similar formalism as is used in equilibrium and thereby calculate the current-phase relation.

The system is an open system since particles and heat are carried by the current that flows through the leads to the active region of the device and back to the leads. In such systems, the effect of the leads on the transport within the active region of the device can be fully encoded in a term that acts like an extra self-energy for the active region of the device and is called the self-energy of the leads \[50\]. Since electrons cannot be created or destroyed, we must enforce charge current conservation for the current flow through each longitudinal plane. We assume the current density
is uniform on each plane, as the planes are chosen to be homogeneous. Within this formalism, one can very simply modify the algorithm used in equilibrium to calculate the retarded Green’s functions and the many-body density of states (DOS). It ends up being identical in form to the equilibrium case except for a shift of the energy by the local electric field for the recurrence relation which determines the self-energy of the leads; in the bulk region of the leads, the electric field vanishes and the DOS in the presence of current flow remains the same as the DOS in equilibrium, as one might expect since the quantum states remain the same, only their occupancy is changed to create current flow. Within this approach, heat current need not be conserved. Indeed, current flow through the active region creates Joule heat which is carried with the particle current, and also transferred to an “effective reservoir” in the regions near the interfaces of the device.

It is the Keldysh or lesser component of the Green’s function that determines the occupancy of the states, and since their Dyson equation is homogeneous, one needs an appropriate boundary condition to calculate them in the active region of the device. This boundary condition arises from the behavior of the bulk system under constant current flow, which is a problem that can be solved exactly. In this contribution, we show how to exactly solve the bulk problem and to use it to solve for the self-energy of the leads, which provides this necessary boundary condition.

The remainder of the paper is organized as follows: In Sec. II, we describe the formalism used to determine the lead self-energy, in Sec. III, we present the numerical results, and in Sec. IV, we provide our conclusions.
4.2 Formalism

There are a few different theoretical methods used to describe a finite open system attached to metallic leads. Probably the most popular method is to assume the left lead and the right are attached to separate reservoirs, one at voltage $V/2$ and the other at voltage $-V/2$. Then the hopping between the leads and the device are slowly turned on and the system is allowed to reach the steady state \[51\]. One calculates the current flow in this steady state, and uses that with the voltage applied across the device to determine the current-voltage relation. This approach corresponds to a voltage-biased device and it is probably the most commonly used technique in calculations. We propose to use a different method which should yield completely equivalent results, but works in a very different fashion. Here, the device and the leads are connected initially and the system is equilibrated at a temperature $T$. Next an electric field is turned on for a short period of time to establish a current flow through the device. If the leads are ballistic metals, then the field can be turned off, and the leads will continue to have constant current flow for all time. Additional constant electric fields are then turned on within the finite region of the device, where scattering occurs, in order to maintain particle current conservation. The system is let to evolve to the steady state, which is then used to determine the current-voltage relation by calculating the voltage by integrating the electric field that is required to guarantee current conservation.

The many-body formalism begins with the so-called contour-ordered Green’s function, defined by \[41, 52, 53\]

$$g^{c}_{\alpha i \beta j}(t, t') = -\frac{i}{\mathcal{Z}} \text{Tr} \left[ T_c e^{-\beta \mathcal{H}(-\infty)} c_{\alpha i} (t) c^{\dagger}_{\beta j} (t') \right],$$

(4.1)

where $\mathcal{H}(-\infty)$ is the initial equilibrium Hamiltonian, $\mathcal{Z} = \text{Tr} \exp[-\beta \mathcal{H}(-\infty)]$ is the initial equilibrium partition function, $T_c$ is the contour-ordering operator, which orders
Figure 4.2: Kadanoff-Baym-Keldysh contour used to calculate the contour-ordered Green’s function. The system starts in equilibrium at time $t_0$ and $\beta = 1/T$ is the inverse temperature for the initial equilibrium state. The electric field is turned on at time $t_{on}$, and then the system evolves to the steady state. In the calculational method described here, both $t_0$ and $t_{on}$ are taken in the limit where they approach $-\infty$. This evolution can be explicitly calculated for the noninteracting leads, which then form the boundary condition for the interacting problem to be solved. In this limit, one can also ignore the imaginary branch of the contour, since the steady state does not maintain any correlations with the initial equilibrium state.

The times according to their order along the contour, and $c_{\alpha i}(t)$ [$c_{\alpha i}^\dagger(t)$] are the annihilation [creation] operators for a spinless electron in the Heisenberg representation with respect to the time-dependent Hamiltonian $\mathcal{H}(t)$ on plane $\alpha$ at planar site $i$; these operators satisfy the usual fermionic anticommutation relations when evaluated at the same time. This representation in terms of spatial components only is inconvenient for dealing with multilayered systems, so we perform a partial Fourier transform with respect to the planar indices, since the system is translationally invariant in every plane, to define the mixed-basis Green’s function

$$g_{\alpha \beta}^c(k_\parallel; t, t') = -\frac{i}{Z} \text{Tr} \left[ \mathcal{T}_c e^{-\beta \mathcal{H}(-\infty)} c_{\alpha k_\parallel}(t) c_{\beta k_\parallel}^\dagger(t') \right], \quad (4.2)$$
where $k^\parallel$ is the two-dimensional planar momentum.

We ignore specific details of the Hamiltonian in our current discussion, because the results are general and hold for all Hamiltonians with local interactions. The equilibrium Hamiltonian is, however, assumed to have a nearest-neighbor hopping term determined by hopping integrals $t^\parallel_\alpha$ for hopping within the $\alpha$th plane and $t^\perp_{\alpha\alpha+1}$ for hopping between the $\alpha+1$st plane and the $\alpha$th plane. Because the system has either a constant vector potential or a constant electric field applied across it, the nonequilibrium Hamiltonian is described with a longitudinal hopping integral that satisfies

$$t^\perp_{\alpha,\alpha+1}(t) = t^\perp_{\alpha+1,\alpha}(t) e^{iA_\alpha(t)},$$

$$t^\perp_{\alpha+1,\alpha}(t) = t^\perp_{\alpha,\alpha+1}(t) e^{-iA_\alpha(t)},$$

(4.3)

since $t^\perp_{\alpha,\alpha+1} = t^\perp_{\alpha+1,\alpha}$ when the system is in equilibrium. Here, the vector potential always has a constant shift, but also can have a linear term in time when there is an electric field at the $\alpha$th plane. The two hopping terms are complex conjugates as is required for a Hermitian Hamiltonian. Note that the parallel hopping remains time independent when current only flows perpendicular to the planes. It is convenient to introduce the planar bandstructure $\epsilon^\parallel(\mathbf{k}^\parallel)$ to describe the band dispersion within each plane ($\mathbf{k}^\parallel$ is the two-dimensional planar momentum). We let $\delta$ denote the nearest neighbor translation vector within each plane, then $\epsilon^\parallel_\alpha(\mathbf{k}^\parallel) = -t^\parallel_\alpha \sum_\delta \exp(i\mathbf{k}^\parallel \cdot \delta)$.

It is a straightforward calculation to determine the equation of motion for the contour-ordered Green's function under the assumption of a local self-energy (which is required by nonequilibrium dynamical mean-field theory). Defining the contour-ordered delta function in the standard way such that

$$\int_c dt' \delta_c(t, t') f(t') = f(t),$$

one
\[ \int_{t_c} dt \left\{ \left[ \left( -i \frac{\partial}{\partial t} + \mu - \epsilon^\parallel_p (k^\parallel) \right) \delta_c(t, \bar{t}) - \Sigma^c_\alpha(t, \bar{t}) \right] g^c_{\alpha\beta}(k^\parallel; \bar{t}, t') \ight. \\
+ \left. \left[ t^\perp_{\alpha+1} e^{iA_\alpha(t)} g^c_{\alpha+1\beta}(k^\parallel; t, \bar{t}) + t^\perp_{\alpha-1} e^{-iA_{\alpha-1}(t)} g^c_{\alpha-1\beta}(k^\parallel; t, \bar{t}) \right] \delta_c(\bar{t}, t') \right\} = \delta_c(t, t') \delta_{\alpha\beta}. \] (4.4)

Here \( \Sigma^c_\alpha(t, t') \) is the local contour-ordered self-energy for the Green’s function at the \( \alpha \)-th plane.

This equation is of the form \( g^{-1}g = I \), which allows us to find \( g \) by taking the matrix inverse of \( g^{-1} \), as is usually done when solving the Dyson equation. Here, we must think of the matrix for \( g^{-1} \) as a series of double time blocks that are sparsely distributed in a spatial pattern given by \( \alpha \) and \( \beta \) that includes a diagonal and the two subdiagonals, and is in the form of a block tridiagonal matrix. The inverse of such a matrix can be found by employing a series of recursion relations \[24, 25, 44, 54\]. To derive these, we imagine our system as a set of equations for all possible \( \alpha \) and \( \beta \) indices, and we work with matrix inverses with respect to the time blocks only. One might ask whether such inverses are well defined. They clearly are in equilibrium, as they are used to solve the problem in frequency space. Here, we show that they also are well defined \( a \ posteriori \) after assuming that they are and showing that the results of all of the recursions remain well defined. Hence, we start by multiplying Eq. (4.4) from the right by the inverse of the block matrix \( g^{-1}_{\alpha\beta}(k^\parallel; t, t') \) where the inverse is only with respect to the time indices of the matrix for a fixed \( \alpha \) and \( \beta \). Next, we let
\[ \beta \to \alpha \text{ and } \alpha \to \alpha - n \text{ for } n > 0, \text{ to yield} \]

\[
0 = \left[ -i \frac{\partial}{\partial t} + \mu - e^\parallel(k) \right] \delta_c(t, t') - \Sigma^c_{\alpha-n}(t, t') \quad (4.5)
\]

\[
+ t^\perp_{\alpha-na-n+1} e^{iA_{\alpha-n}(t)} \int d\bar{t} \bar{g}^c_{\alpha-n+1\alpha}(k^\parallel; t, \bar{t}) \times g^{c-1}_{\alpha-na}(k^\parallel; t, t')
\]

\[
+ t^\perp_{\alpha-n-1-a-n} e^{-iA_{\alpha-n-1}(t)} \int d\bar{t} g^c_{\alpha-n-1\alpha}(k^\parallel; t, \bar{t}) \times g^{c-1}_{\alpha-na}(k^\parallel; \bar{t}, t').
\]

Next, we define the contour-ordered left function \( L^c_{\alpha-n} \) via

\[
L^c_{\alpha-n}(k^\parallel; t, t') = -t^\perp_{\alpha-na-n+1} e^{iA_{\alpha-n}(t)} \times \int d\bar{t} \bar{g}^c_{\alpha-n+1\alpha}(k^\parallel; t, \bar{t}) g^{c-1}_{\alpha-na}(k^\parallel; \bar{t}, t').
\]

Using this definition, we can rewrite Eq. \((4.5)\) in terms of the \( L^c \) function. To do this, we need the inverse of the \( L^c \) function with respect to the time indices. If we recall that \((AB)^{-1} = B^{-1}A^{-1}\), then we find

\[
L^c_{\alpha-n}(k^\parallel; t, t') = \left[ -i \frac{\partial}{\partial t} + \mu - e^\parallel(k^\parallel) \right] \delta_c(t, t') - \Sigma^c_{\alpha-n}(t, t') \quad (4.7)
\]

\[-t^\perp_{\alpha-n-1-a-n} e^{-iA_{\alpha-n-1}(t)} L^c_{\alpha-n-1}(k^\parallel; t, t') e^{iA_{\alpha-n-1}(t')}.
\]

One can perform a similar procedure to determine the contour-ordered right functions. Once again, we start from Eq. \((4.4)\) and let \( \alpha \to \alpha + n \) and \( \beta \to \alpha \), with \( n > 0 \).

The contour-ordered right function \( R^c_{\alpha+n} \) is defined via

\[
R^c_{\alpha+n}(k^\parallel; t, t') = -t^\perp_{\alpha+n-1-a+n} e^{-iA_{\alpha+n-1}(t)} \times \int d\bar{t} \bar{g}^c_{\alpha+n-1\alpha}(k^\parallel; t, \bar{t}) g^{c-1}_{\alpha+n\alpha}(k^\parallel; \bar{t}, t').
\]

The corresponding recursion relation becomes

\[
R^c_{\alpha+n}(k^\parallel; t, t') = \left[ -i \frac{\partial}{\partial t} + \mu - e^\parallel(k^\parallel) \right] \delta_c(t, t') - \Sigma^c_{\alpha+n}(t, t') \quad (4.9)
\]

\[-t^\perp_{\alpha+n-1-a+n} e^{-iA_{\alpha+n}(t)} R^c_{\alpha+n+1}(k^\parallel; t, t') e^{-iA_{\alpha+n+1}(t')}.
\]
Finally, if one examines the equation of motion in Eq. (4.4) for $\alpha = \beta$ and uses the definitions for the left and right functions in Eqs. (4.7) and (4.8), respectively, one finds

$$
g_{\alpha\alpha}^{c\pm 1}(k^\parallel; t, t') = \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon^\parallel_{\alpha}(k^\parallel) \right] \delta_c(t, t') - \Sigma^c_{\alpha}(t, t') \hspace{1cm} (4.10)$$

$$
- t_{a-1a}^{\pm 12} e^{-iA_{a-1}(t)} L_{a-1}^{c\pm 1}(k^\parallel; t, t') e^{iA_{a-1}(t')} \\
- t_{a+1a}^{\pm 12} e^{iA_{a}(t)} R_{a+1}^{c\pm 1}(k^\parallel; t, t') e^{-iA_{a}(t')} .
$$

Note that this result is the diagonal time-block element of the full inverse of the contour-ordered Green’s function, and not just the inverse of the time block. Clearly, one can see that the sum of the inverses of the left and the right functions can be thought of as an extra contribution to the self-energy for the system, which we call the self-energy of the leads. This formula remains a bit unwieldy, so it is customary to iterate the $L$ and $R$ recursion relations one more time to determine $L_{\alpha}$ and $R_{\alpha}$. Then, the diagonal element of the Green’s function becomes

$$
g_{\alpha\alpha}^{c\pm 1}(k^\parallel; t, t') = \left[ -i \frac{\partial}{\partial t} + \mu - \epsilon^\parallel_{\alpha}(k^\parallel) \right] \delta_c(t, t') + \Sigma^c_{\alpha}(t, t') + L_{\alpha}^{c}(k^\parallel; t, t') + R_{\alpha}^{c}(k^\parallel; t, t'),
$$

which agrees with the form used in equilibrium calculations.

Now, to see that the system can be solved in a frequency representation, we assume that we have reached a steady state, where the contour-ordered self-energy $\Sigma^\alpha_{\alpha}(t, t')$ is time-translation invariant, and depends only on the relative time $t - t'$. Since we will derive below the $L$ and $R$ functions in the bulk, and show that they depend only on the relative time when there is constant current flow, then all of the terms in the two recursion relations given in Eqs. (4.7) and (4.9) depend on the relative time only, since the vector potential is at most a linear function in time, so the exponential
factors combine and become a function only of $t - t'$. Hence, the $L$ and $R$ functions will depend only on the relative time as will the local Green’s function.

It is not so simple to use the contour-ordered objects in the full algorithm used to solve the problem, so we now separate out the retarded, advanced, and Keldysh (or lesser) components \[41, 42, 53\]. Since the retarded and advanced functions are related to each other in a simple way, we really need to solve for only two sets of functions: (i) the retarded ones and (ii) the Keldysh (or lesser) ones. The strategy to do this is straightforward, but quite tedious. To start, we rewrite the contour-ordered Green’s function $g^c$, which is defined for two times on the contour, as a matrix-valued function, with both times on the real axis. We use $+$ and $-$ signs to indicate that the real time lies on the upper (outward) branch or the lower (inward) branch. Hence we perform the transformation \[41\]

$$
g^c \rightarrow \bar{g}^c(t, t') = \begin{pmatrix}
G^{++}(t, t') & G^{+-}(t, t') \\
G^{-+}(t, t') & G^{--}(t, t')
\end{pmatrix}
$$

where the overbar indicates the $2 \times 2$ matrix representation. These four components are overdetermined, because only three of them are independent. One can transform the Green’s function from this $2 \times 2$ representation to the so-called Larkin-Ovchinnikov representation, which is a set of matrix transformations which convert $\bar{g}^c$ to the upper triangular form \[42\]

$$
\bar{g}^c \rightarrow G = \begin{pmatrix}
g^R(t, t') & g^K(t, t') \\
0 & g^A(t, t')
\end{pmatrix}
$$

where the retarded Green’s function satisfies $g^R = G^{++} - G^{+-}$, the advanced Green’s function satisfies $g^A = G^{++} - G^{-+}$, and the Keldysh Green’s function satisfies $g^K = G^{++} + G^{--}$. Explicitly writing out these definitions yields

$$
g^R_{\alpha\beta}(k||; t, t') = -\frac{i}{\mathcal{Z}} \theta(t - t') \text{Tr} e^{-\beta \mathcal{H}(-\infty)} \{c_{\alpha k\parallel}(t), c^\dagger_{\beta k\parallel}(t')\}^+, \quad \text{(4.14)}
$$

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for the retarded Green’s function,
\[ g^A_{\alpha\beta}(k^\parallel; t, t') = \frac{i}{Z} \theta(t' - t) \text{Tr} e^{-\beta \mathcal{H}(-\infty)} \{ c_{\alpha k\parallel}(t), c^\dagger_{\beta k\parallel}(t') \}^+, \tag{4.15} \]
for the advanced Green’s function, and
\[ g^K_{\alpha\beta}(k^\parallel; t, t') = -\frac{i}{Z} \text{Tr} e^{-\beta \mathcal{H}(-\infty)} [c_{\alpha k\parallel}(t), c^\dagger_{\beta k\parallel}(t')]^-, \tag{4.16} \]
for the Keldysh Green’s function. One can immediately see that the following identity holds between retarded and advanced Green’s functions, while for the Keldysh Green’s function, we have
\[ g^K_{\alpha\beta}(k^\parallel; t, t') = -g^K_{\beta\alpha}(k^\parallel; t', t). \tag{4.18} \]
When we Fourier transform to frequency, we find the identities become
\[ g^R^*_{\alpha\beta}(k^\parallel; \omega) = g^A_{\beta\alpha}(k^\parallel; \omega) \tag{4.19} \]
and
\[ g^K^*_{\alpha\beta}(k^\parallel; \omega) = -g^K_{\beta\alpha}(k^\parallel; \omega), \tag{4.20} \]
which implies that the local Keldysh Green’s function is purely imaginary in frequency space.

It sometimes is convenient to use the so-called lesser Green’s function to evaluate observables. The lesser Green’s function is defined by
\[ g^<_{\alpha\beta}(k^\parallel; t, t') = \frac{i}{Z} \text{Tr} e^{-\beta \mathcal{H}(-\infty)} c^\dagger_{\beta k\parallel}(t') c_{\alpha k\parallel}(t). \tag{4.21} \]
After Fourier transforming to the frequency domain, it can be found from the retarded, advanced, and Keldysh Green’s functions via
\[ g^<_{\alpha\beta}(k^\parallel; \omega) = \frac{1}{2} \left[ g^K_{\alpha\beta}(k^\parallel; \omega) - g^K_{\beta\alpha}(k^\parallel; \omega) + g^A_{\alpha\beta}(k^\parallel; \omega) \right]. \tag{4.22} \]
Using this upper triangular representation, one can go through some tedious algebra to transform the left and right recurrence relations to this upper triangular form. In addition, one can Fourier transform from the relative time representation to the frequency representation. Reading off the diagonal and off-diagonal components, we find the recursion relations become

\[
L_{\alpha-n}(k^\parallel; \omega) = \omega + \mu - \epsilon_{\alpha-n}(k^\parallel) - \Sigma_{\alpha-n}^R(\omega) \frac{t_{\alpha-n\alpha-n-1}^{\perp/2}}{L_{\alpha-n-1}^R(k^\parallel; \omega + E_{\alpha-n-1})}.
\] (4.23)

Here, \(E_\alpha\) is the electric field at plane \(\alpha\). It is easy to see that the advanced function satisfies \(L^A = L^{R*}\). The advanced recursion relation has precisely the same form as in Eq. (4.23) except all \(R\) superscripts are replaced by \(A\) superscripts. Since the retarded and advanced self-energies are related by complex conjugates, as are the initial (bulk) \(L_{-\infty}\) starting values, the two recursions are complex conjugates of each other, and hence so are \(L^R_\alpha\) and \(L^A_\alpha\) for all \(\alpha\). The Keldysh recursion relation then becomes

\[
L^K_{\alpha-n}(k^\parallel; \omega) = -\Sigma^K_{\alpha-n}(\omega) + \frac{t_{\alpha-n\alpha-n-1}^{\perp/2}L^K_{\alpha-n-1}(k^\parallel; \omega + E_{\alpha-n-1})}{|L^R_{\alpha-n-1}(k^\parallel; \omega + E_{\alpha-n-1})|^2}.
\] (4.24)

The similar equations for the right functions are as follows: (i) for the retarded right functions we have

\[
R^R_{\alpha+n}(k^\parallel; \omega) = \omega + \mu - \epsilon_{\alpha+n}(k^\parallel) - \Sigma_{\alpha-n}^R(\omega) - \frac{t_{\alpha+n\alpha+n+1}^{\perp/2}}{R^R_{\alpha+n+1}(k^\parallel; \omega - E_{\alpha+n})},
\] (4.25)

(with \(R^{R*} = R^A\)) and (ii) for the Keldysh right functions we have

\[
R^K_{\alpha+n}(k^\parallel; \omega) = -\Sigma^K_{\alpha+n}(\omega) + \frac{t_{\alpha+n+1\alpha+n}^{\perp/2}R^K_{\alpha+n+1}(k^\parallel; \omega - E_{\alpha+n})}{|R^K_{\alpha+n+1}(k^\parallel; \omega - E_{\alpha+n})|^2}.
\] (4.26)

One can immediately see that the retarded (and advanced) recursions are independent of the Keldysh functions, so they can be solved separately from the Keldysh case (which depends on all three types of functions). To begin, we must determine \(L^R_{-\infty}\) and \(R^R_{\infty}\). The recursion for the left functions starts for negative \(\alpha\) and moves
up through positive $\alpha$ and for the right function it is the reverse. The starting point for both recursions is found from the recursion relations for the ballistic metal, where $\Sigma_{\pm\infty}(\omega) = 0$, $\epsilon_{\pm\infty}(k_{\parallel}) = \epsilon^l(k_{\parallel})$ and $t_{\alpha\alpha-1}^\perp = t^\perp$ for $\alpha \to \pm\infty$. Then the equation for $L_{-\infty}^R$ satisfies

$$L_{-\infty}^{R2}(k_{\parallel}; \omega) - [\omega + \mu - \epsilon^l(k_{\parallel})]L_{-\infty}^R(k_{\parallel}; \omega) + t^{\perp 2} = 0 \quad (4.27)$$

with solution

$$L_{-\infty}^R(k_{\parallel}; \omega) = \frac{\omega + \mu - \epsilon^l(k_{\parallel})}{2} \pm \frac{1}{2} \sqrt{[\omega + \mu - \epsilon^l(k_{\parallel})]^2 - 4(t^{\perp})^2}. \quad (4.28)$$

When the square root is imaginary, we choose the sign so that the imaginary part of $L^R$ is greater than zero (this may seem odd for a retarded object, but it happens because of how the $L^R$ function enters into determining the retarded Green’s function). When the square root is real, we choose the sign such that $L^R$ is larger in magnitude than $t^\perp$. This solution is identical to what was used in equilibrium, as we anticipated, since the current carrying state has no electric field over it, so the states are unchanged, just their occupancy differs from that in the bulk. Direct calculation also shows that $R^R_R(\infty; k_{\parallel}; \omega) = L_{-\infty}^R(k_{\parallel}; \omega)$.

The dynamical mean-field theory proceeds via an iterative solution [25]. One starts with a guess for the self-energies on all of the planes. Then we compute the local Green’s functions from Dyson’s equation, which requires us to use the $L$ and $R$ functions. Next, one uses the Dyson equation for the impurity problem to extract the effective medium. The impurity problem is solved for this effective medium, and then the self-energy is extracted from the Dyson equation for the impurity problem again. This then produces the new self-energy guess for the next iteration. In this work, we focus on the bulk system, so we do not describe the details for how to solve the impurity problem, which will be done elsewhere.
In a real calculation, we work with a finite number of planes. In equilibrium, this typically was thirty planes on each side of the barrier region plus the number of planes in the barrier. One then sets the \( L^R \) functions equal to \( L^R_{-\infty} \) up to the first plane that is being simulated in the finite system. From there, we use the recursion relations in Eq. (4.23) to determine all of the \( L^R_\alpha \) functions. The right functions proceed similarly.

We fix \( R^R \) at the value \( R^R_\infty \) until we get to the first simulated plane from the top, and then we use the recursion relations in Eq. (4.25) to find all of the \( R^K_\alpha \) functions. From these two results, we find the local retarded Green’s function for each plane. Taking complex conjugates then gives all of the advanced functions.

Unfortunately, one cannot use the same procedure for the Keldysh functions that we used to find the retarded functions. This is because the recursion relations for the Keldysh case are homogeneous equations when the Keldysh self-energy vanishes, and hence they can be manipulated into an identity that reduces to \( 0 = 0 \) and does not allow one to solve for the \( L^K \) or \( R^K \) functions in the bulk limit. Instead, we go back to the original definitions of the \( L \) and \( R \) functions and manipulate them to determine the Keldysh functions in the bulk. To begin, we note that

\[
L^R_{\alpha-1}(k^\parallel;\omega) = -t^\perp_\alpha e^{-iA_0} \frac{g^R_{\alpha\alpha}(k^\parallel;\omega)}{g^R_{\alpha-1\alpha}(k^\parallel;\omega)} \tag{4.29}
\]

for the retarded function and

\[
L^K_{\alpha-1}(k^\parallel;\omega) = -t^\perp_\alpha e^{-iA_0} \left[ -\frac{g^K_{\alpha\alpha}(k^\parallel;\omega)g^K_{\alpha-1\alpha}(k^\parallel;\omega)}{g^K_{\alpha-1\alpha}(k^\parallel;\omega)} + \frac{g^K_{\alpha\alpha}(k^\parallel;\omega)}{g^K_{\alpha-1\alpha}(k^\parallel;\omega)} \right]. \tag{4.30}
\]

Using Eq. (4.29), we rewrite Eq. (4.30) as

\[
L^K_{\alpha-1}(k^\parallel;\omega) = -L^R_{\alpha-1}(k^\parallel;\omega) \frac{g^K_{\alpha-1\alpha}(k^\parallel;\omega)}{g^K_{\alpha-1\alpha}(k^\parallel;\omega)} - t^\perp_\alpha e^{-iA_0} \frac{g^K_{\alpha\alpha}(k^\parallel;\omega)}{g^K_{\alpha-1\alpha}(k^\parallel;\omega)}. \tag{4.31}
\]

Performing the same type of analysis for the right functions yields

\[
R^K_{\alpha+1}(k^\parallel;\omega) = -R^K_{\alpha+1}(k^\parallel;\omega) \frac{g^K_{\alpha+1\alpha}(k^\parallel;\omega)}{g^K_{\alpha+1\alpha}(k^\parallel;\omega)} - t^\perp_\alpha e^{iA_0} \frac{g^K_{\alpha\alpha}(k^\parallel;\omega)}{g^K_{\alpha+1\alpha}(k^\parallel;\omega)}. \tag{4.32}
\]
These two relations now provide a pathway to calculate the $L^K$ and $R^K$ functions in the bulk by simply calculating the local and nearest-neighbor Green’s functions in the bulk using the mixed basis. This is what we do next.

To begin, we must calculate the retarded Green’s function in nonequilibrium. We start the system in equilibrium at time $t_0$ and turn the field on at time $t_{on}$ and leave it on for one unit of time, where the vector potential decreases from 0 to $-A_0$. We take the limit where both $t_0$ and $t_{on}$ approach $-\infty$. Since the Hamiltonian commutes with itself at different times, even when the field is on, the Green’s function is simple to determine in momentum space $[k = (k^\parallel, k_z)$ is the three-dimensional momentum$] (55)$

$$
g^R(k; t, t') = -i\theta(t - t')e^{-i(\epsilon^\parallel(k^\parallel) - 2t^\perp \cos(k_z + A_0) - \mu)(t - t')} \quad (4.33)
$$

when both $t$ and $t'$ are much larger than $-\infty$ and $k_z$ is the $z$-component of the momentum. Taking the Fourier transform to the frequency representation yields

$$
g^R(k; \omega) = \frac{1}{\omega + \mu - \epsilon^\parallel(k^\parallel) + 2t^\perp \cos(k_z + A_0) + i0^+} \quad (4.34)
$$

In order to show that this result yields the same self-energy of the leads as found in Eq. (4.28), we need to Fourier transform $k_z$ to real space in order to represent the Green’s function in the mixed basis. Let $z_\alpha$ denote the $z$-component of the $\alpha$th plane. Then the mixed-basis Green’s function is found from

$$
g^R_{\alpha\beta}(k^\parallel; \omega) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_z e^{-i(z_\alpha - z_\beta)k_z} g^R(k; \omega). \quad (4.35)
$$

We substitute Eq. (4.34) into Eq. (4.35) and use the notation $\omega + \mu - \epsilon^\parallel(k^\parallel) - i0^+ = 2t^\perp \gamma$ and $k_z' = k_z + A_0$ to get

$$
g^R_{\alpha\beta}(k^\parallel; \omega) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_z' e^{-i(z_\alpha - z_\beta)(k_z' - A_0)} \quad (4.36)
$$

This integral can be evaluated via a contour integration and the residue theorem. We convert the integral over $k'_z$ to an integral over the unit circle with $Z = \exp(ik'_z)$. This
gives
\[ g_{\alpha\beta}^{R}(k\parallel; \omega) = \frac{e^{i(z_{\alpha}-z_{\beta})A_{0}}}{2\pi i t^{\perp}} \oint dZ \frac{Z^{-z_{\alpha}+z_{\beta}}}{Z(2\gamma + Z + 1/Z)} \] (4.37)
with the integral over the unit circle, evaluated in the standard counter clockwise direction. The poles lie at the roots of \( Z^{2} + 2\gamma Z + 1 = 0 \), or \( Z_{\pm} = -\gamma \pm \sqrt{\gamma^{2} - 1} \).

If \(|\gamma| > 1\), then the two roots are real, and since their product is one, one root lies outside the unit circle and one root inside. If \(|\gamma| < 1\), then the two roots are complex, with opposite signs of their imaginary parts. There also can be a pole at \( Z = 0 \) if \( z_{\alpha} - z_{\beta} > 0 \). We assume that \( z_{\alpha} - z_{\beta} < 0 \) for now. Then if we let \( Z_{in} \) denote the root inside the unit circle and \( Z_{out} \) denote the root outside the unit circle, then the integral becomes
\[ g_{\alpha\beta}^{R}(k\parallel; \omega) = \frac{e^{i(z_{\alpha}-z_{\beta})A_{0}}}{i t^{\perp}} \frac{Z_{in}^{-z_{\alpha}+z_{\beta}}}{Z_{in} - Z_{out}}, \] (4.38)

In particular, the local Green’s function satisfies
\[ g_{\alpha\alpha}^{R}(k\parallel; \omega) = \frac{1}{\pm\sqrt{[\omega + \mu - \epsilon^{\parallel}(k\parallel) - i0^{+}]^{2} - 4t^{2}}} \] (4.39)
where the plus or minus sign is chosen according to which root lies within the unit circle. One can also choose the sign according to causality \emph{a posteriori}: when the Green’s function is complex, it must have a negative imaginary part and analyticity determines how it behaves when it is real. For a fixed \( k\parallel \) this is the local retarded Green’s function for a one-dimensional system, as one expects. Indeed, if we evaluate the frequency representation of Eq. (4.9) and examine the retarded component, then substituting in the results in the bulk limit, including Eq. (4.28), yields the result in Eq. (4.39), which is a good check that this approach works correctly.

Using this result for the local Green’s function, we can combine it with the Fourier transform of Eq. (4.11) to determine what the equilibrium \( L^{K} \) function is. We know the Keldysh component of the diagonal Green’s function is \( g_{\alpha\alpha}^{K}(k\parallel; \omega) \) and the Keldysh component of the inverse local Green’s function is schematically given
by \((g^{-1})^K = -(g^R)^{-1}g^K(g^A)^{-1}\), so we find, because \(L^K = R^K\) in equilibrium, that 
\[
L^K = -g^K/(2|g^R|^2).
\]
But \(g^K = -2ifK\text{Im}g^R\), with the equilibrium Keldysh distribution function defined just below Eq. (4.43). Within the band, which is the only place that \(K\) functions are nonzero, \(g^R\) is pure imaginary, so we get

\[
L_{-\infty, \text{eq.}}(k; \omega) = -ifK(\omega)\sqrt{4(t^+)^2 - [\omega + \mu - \epsilon(k)]^2}, \quad (4.40)
\]

where the square root is the positive root.

We also need to evaluate the nearest-neighbor Green’s functions in this mixed basis. When \(\beta = \alpha + 1\), the result simply follows from the above integration, where we find

\[
g^R_{\alpha \alpha + 1}(k; \omega) = e^{-iA_0} - \frac{\omega + \mu - \epsilon(k)}{2t^+} \pm \sqrt{\frac{[\omega + \mu - \epsilon(k)]^2}{4t^+} - 1} \pm \sqrt{[\omega + \mu - \epsilon(k)] - i0^+}^2 - 4t^+^2, \quad (4.41)
\]

and the plus or minus sign is chosen according to the discussion given above. For the other nearest-neighbor Green’s function \((\alpha \alpha - 1)\), it looks like one has to work harder since there is an extra pole at \(Z = 0\). But this isn’t the case. If \(z_\alpha - z_\beta > 0\), then we can factor out the exponential term in Eq. (4.36) that depends on \(A_0\) and then we let \(k'_z \rightarrow -k'_z\), which is the equivalent of interchanging \(\alpha\) and \(\beta\) in the remaining integral. Hence the integral is independent of the sign of \(z_\alpha - z_\beta\) and we find

\[
g^R_{\alpha \alpha - 1}(k; \omega) = e^{iA_0} - \frac{\omega + \mu - \epsilon(k)}{2t^+} \pm \sqrt{\frac{[\omega + \mu - \epsilon(k)]^2}{4t^+} - 1} \pm \sqrt{[\omega + \mu - \epsilon(k)] - i0^+}^2 - 4t^+^2. \quad (4.42)
\]

For example, using Eqs. (4.39) and (4.41) in Eq. (4.29), then gives the result in Eq. (4.28), as it must. The general formula for Eq. (4.38) is then to replace the exponent of \(Z_m\) in the numerator by \(|z_\alpha - z_\beta|\).

Our next step is to calculate the Keldysh (or lesser) Green’s functions in the bulk. Both of these functions can be written as

\[
g^K,<(k; t, t') = if^{K,<}[\epsilon(k) - 2t^+ \cos(k_z) - \mu] \\
\times e^{-i[\epsilon(k) - 2t^+ \cos(k_z + A_0) - \mu](t-t')}, \quad (4.43)
\]
in the large-time limit, where the distribution function \( f(x) \) satisfies \( f^<(x) = 1/[1 + \exp(\beta x)] \) and \( f^K(x) = 2f^<(x) - 1 \). Fourier transforming to frequency space yields

\[
g^K,<(k; \omega) = 2\pi i f^K,<[\epsilon^\parallel(k^\parallel) - 2t^\perp \cos(k_z) - \mu] \times \delta[\omega + \mu - \epsilon^\parallel(k^\parallel) + 2t^\perp \cos(k_z + A_0)].
\] (4.44)

Next, we Fourier transform with respect to \( k_z \) to get the mixed-basis Green’s functions

\[
g^K,\alpha\beta(k^\parallel; \omega) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_z e^{-i(z_\alpha - z_\beta)k_z} g^K,<(k; \omega),
\] (4.45)

which can be immediately done because the integrand is proportional to a delta function. One needs to note that there are two roots where the argument of the delta function vanishes, and that we must divide the integrand by the absolute value of the derivative of the argument of the delta function, evaluated at each root. Note that the Keldysh (lesser) Green’s function is nonzero only when we are within the band, implying

\[
\left|\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp}\right| \leq 1.
\] (4.46)

The end result is

\[
g^K,\alpha\beta(k^\parallel; \omega) = i \left\{ \begin{aligned}
&f^K,<[\omega \cos(A_0) - (\mu - \epsilon^\parallel(k^\parallel))(1 - \cos(A_0)) - \sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2} \sin(A_0)]
\times \left[ -\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} - i \sqrt{1 - \left(\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp}\right)^2} \right]^{z_\alpha - z_\beta} \\
+ &f^K,<[\omega \cos(A_0) - (\mu - \epsilon^\parallel(k^\parallel))(1 - \cos(A_0)) + \sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2} \sin(A_0)]
\times \left[ -\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} + i \sqrt{1 - \left(\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp}\right)^2} \right]^{z_\alpha - z_\beta} \\
\times &\frac{1}{\sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2}} e^{i(z_\alpha - z_\beta)A_0}.
\end{aligned} \right\}
\] (4.47)
If we define $\omega \pm$ by
\[
\omega^{\pm}(k^\parallel; A_0) = \omega \cos(A_0) - (\mu - \epsilon^\parallel(k^\parallel))(1 - \cos(A_0)) \\
\pm \sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2 \sin(A_0)},
\] (4.48)
then we have the local Green’s function satisfies
\[
g^{K,<}_{\alpha\alpha}(k^\parallel; \omega) = i \frac{f^{K,<}[\omega^+(k^\parallel; A_0)] + f^{K,<}[\omega^-(k^\parallel; A_0)]}{\sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2}},
\] (4.49)
and the nearest-neighbor Green’s functions are
\[
g^{K,<}_{\alpha\alpha+1}(k^\parallel; \omega) = i \left\{ f^{K,<}[\omega^+(k^\parallel; A_0)] \left[ -\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} - i \sqrt{1 - \left( \frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} \right)^2} \right] \\
+ f^{K,<}[\omega^-(k^\parallel; A_0)] \left[ -\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} + i \sqrt{1 - \left( \frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} \right)^2} \right] \right\} \\
\times \frac{e^{-iA_0}}{\sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2}}
\] (4.50)
and
\[
g^{K,<}_{\alpha+1\alpha}(k^\parallel; \omega) = i \left\{ f^{K,<}[\omega^+(k^\parallel; A_0)] \left[ -\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} + i \sqrt{1 - \left( \frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} \right)^2} \right] \\
+ f^{K,<}[\omega^-(k^\parallel; A_0)] \left[ -\frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} - i \sqrt{1 - \left( \frac{\omega + \mu - \epsilon^\parallel(k^\parallel)}{2t^\perp} \right)^2} \right] \right\} \\
\times \frac{e^{iA_0}}{\sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2}}
\] (4.51)
where, in all cases, these Green’s functions vanish when the argument of the square root becomes negative. When $A_0 = 0$, these results reduce to the known equilibrium result; in particular,
\[
g^{K,<}_{\alpha\alpha}(k^\parallel; \omega) = \frac{2i f^{K,<}(\omega)}{\sqrt{4(t^\perp)^2 - (\omega + \mu - \epsilon^\parallel(k^\parallel))^2}}.
\] (4.52)

as expected.
Now we have all the information needed to calculate the boundary functions \( L^K \) and \( R^K \) in Eqs. (4.31) and (4.32). The result is, after some long algebra,

\[
L^K_{\infty} (k; \omega) = -i f^K (k; A_0) \sqrt{4(t^\perp)^2 - [\omega + \mu - \epsilon(k)]^2}
\]

and

\[
R^K_{\infty} (k; \omega) = -i f^K (k; A_0) \sqrt{4(t^\perp)^2 - [\omega - \mu - \epsilon(k)]^2}.
\]

(4.53) (4.54)

Obviously, both of these results also become the equilibrium result in Eq. (4.40) when \( A_0 = 0 \).

The results for the lesser Green’s functions are identical to those for the Keldysh Green’s functions except for a simple change in the distribution function.

This then concludes the derivation of the formalism. To work out the full results with a strongly correlated active region of the device requires one to also self-consistently determine the electric field to maintain current conservation. We don’t discuss these issues further here, as our goal was to determine the boundary conditions which lead to the so-called “self-energy of the leads” and this is now complete.

4.3 Numerical Results

The current is easy to calculate within this formalism. For the bulk case, with a constant shift of the vector potential by \(-A_0\) in the \(z\)-direction, one has

\[
J_z(t, A_0) = -i \sum_k v_k + A_0 g^< (k; t, t)
\]

(4.55)

where \( v_k = d\epsilon(k)/dz = 2t^\perp \sin(k) \) is the band velocity. Using, \( g^<(k; t, t) = i f^<(\epsilon(k) - \mu) \) gives

\[
J_z(t, A_0) = \sum_k 2t^\perp \sin(k_z + A_0) f^<(\epsilon(k) - \mu).
\]

(4.56)
If we work in a homogeneous system, where \( t^\parallel = t^\perp = t \), then we can rewrite the current (which doesn’t depend on time once the field is turned off) as

\[
J_z(A_0) = -\frac{1}{3} \sum_k \epsilon(k) f^<(\epsilon(k) - \mu) \sin(A_0).
\]  

This shows that the amplitude of the current is proportional to the negative of the average kinetic energy in the initial equilibrium state and has a simple sinusoidal dependence on the amplitude of the vector potential. This result is plotted in Fig. 4.3.

In Figs. 4.4 and 4.5 we plot the local lesser Green’s function versus the density of states when the system is carrying current for a low and for a high temperature. The lesser Green’s function is found from Eq. (4.22), and the imaginary part divided by \( 2\pi \) corresponds to the local density of states multiplied by a current-dependent effective distribution function. This distribution function has a simple form only for \( A_0 = 0 \),
Figure 4.4: (Color online) Local lesser Green's function for an initial equilibrium temperature given by $T = 0.1t$ and with perpendicular current flow corresponding to a constant vector potential shift given by $A_0$ as labeled in the different curves. Panel (a), shows how higher energy states initially increase their occupation versus the equilibrium result. Panel (b) continues increasing $A_0$ until the current vanishes again at $A_0 = \pi$. Further increasing the vector potential makes the current go negative, and the local lesser Green’s function is identical to the result with $A_0 = 2\pi - A'_0$. The bulk density of states is also shown as a reference.
Figure 4.5: (Color online) Local lesser Green’s function for an initial equilibrium temperature given by $T = t$ and with perpendicular current flow corresponding to a constant vector potential shift given by $A_0$ as labeled in the different curves. Panel (a), shows how higher energy states initially increase their occupation versus the equilibrium result. Panel (b) continues increasing $A_0$ until the current vanishes again at $A_0 = \pi$. Further increasing the vector potential makes the current go negative, and the local lesser Green’s function is identical to the result with $A_0 = 2\pi - A_0'$. The bulk density of states is also shown as a reference.
where it becomes the Fermi-Dirac distribution function \( f^< (\omega - \mu) \). In all other cases, the distribution function changes with the parallel momentum and hence one has to perform a weighted average over the two-d momentum, or equivalently one performs an integration over the 2d density of states. The net distribution function ends up looking more like the sum of two effective Fermi-Dirac distributions, but even then, the exact shape is somewhat different. Note that as more current flows through the system, higher energy states are occupied, but the system never gets into a negative temperature situation because the field is applied only in one axial direction rather than along the diagonal. One can also see that for a large \( A_0 \), the initial temperature plays a smaller role in determining the distribution function.

These results prepare us to calculate the fully correlated case, where there is an active region. This will be done elsewhere.

4.4 Summary

In this work, we have presented the formal groundwork for how to determine the current-voltage relation of a strongly correlated multilayered device with inhomogeneous dynamical mean-field theory. Unlike conventional nonequilibrium dynamical-mean-field theory, which requires a formalism in the time domain, the steady state can be solved for in the frequency domain, as long as one can calculate the boundary conditions given by the ballistic leads of the system which are current biased. This is done here, which sets the stage for the solution of the full strongly correlated problem. The only issues that we did not describe in detail are how to solve the relevant impurity problems and how to find the self-consistent electric fields through the device. These results will be presented elsewhere. We believe that solving the full problem will
provide insight into the nonlinear behavior of strongly correlated devices, especially those constructed from Mott insulators.
Now we are able to formulate our numerical algorithm. We work with the quantum zipper algorithm which is an extension of the dynamical mean field theory algorithm. The main difference in between the two algorithms lies in the system in consideration. While DMFT deals with bulk materials, the quantum zipper algorithm couples together a set of two dimensional planes thru the recurrence relations derived earlier.

The quantum zipper algorithm is a self consistent iterative method, we start with a guess for the self energy at each plane, next we find the local Green’s function using this guess for the self energy. This relationship is given by Eq.(3.86), we first calculate all the $L$ and $R$ recurrence relations, by starting in the Bulk where we know the solution to the homogenous Green’s function Eq.(3.36). Recall that we have to calculate the advanced, retarded and Keldysh pieces for each recurrence relation.

Next we use the Dyson equation to extract the effective medium Eq.(3.26). Once again this have to be done for each plane and for the retarded advanced and Keldysh representations. For the retarded representation we use the equation $g_{0,\alpha}^{R^{-1}} = g_{\alpha}^{R^{-1}} + \Sigma_{\alpha}^{R}$ with an identical equation for the advanced part. We obtain an equivalent expression for the Keldysh piece.

$$g_{0,\alpha}^{R^{-1}} g_{0,\alpha} g_{0,\alpha}^{A^{-1}} = g_{\alpha}^{R^{-1}} g_{\alpha}^{K} g_{\alpha}^{A^{-1}} - \Sigma_{\alpha}^{K} \quad (5.1)$$

The next step is to calculate the solution to the impurity problem, Eq.(3.33). We do this for each plane. Finally we use the Dyson equation one more time to find an
updated self energy at each plane. We repeat this loop self-consistently until we reach convergence or we have reached a maximum number of iterations. Fig(5.1) depicts the quantum zipper algorithm self consistent loop.

Finally we use the converged self energy to find the local Green’s function of the system and the nearest neighbor Green’s function. The nearest neighbor Green’s func-
tion will be required to calculate the current flowing through the device. The algorithm can be separated into two independent pieces, one corresponding to the retarded and advanced pieces of the contour Green’s function and another piece for the Keldysh one. While the retarded and advanced pieces don’t depend on the Keldysh piece these steps can be done independently of the steps necessary to calculate the Keldysh piece. In the other hand, the Keldysh component for the left and the right recurrence relations depends on the retarded and advances pieces, so we will need to complete these calculations first before proceeding with the Keldysh part. Next we follow the same algorithm to calculate the Keldysh Green’s functions with similar expressions. We summarize all the equations required to perform the calculation in the following table.
<table>
<thead>
<tr>
<th>Equation (Step)</th>
<th>Retarded/Advanced</th>
<th>Keldysh</th>
</tr>
</thead>
<tbody>
<tr>
<td>left function (1)</td>
<td>[ L^R_A(\vec{k}_p,\omega) = \frac{\omega + \mu - \epsilon(\vec{k}_p)}{2} \pm \frac{1}{2} \sqrt{(\omega + \mu - \epsilon(\vec{k}<em>p))^2 - 4t</em>{\infty}^2} ]</td>
<td>[ L_K^{\infty} = f^K(x_\pm) \sqrt{4(t_\perp^L)^2 - (\omega + \mu - \epsilon^\parallel(k_\parallel))^2} ]</td>
</tr>
<tr>
<td>left recursion (1)</td>
<td>[ L_{\alpha-n}^{R,A}(\vec{k}<em>\parallel,\omega) = \omega + \mu - \epsilon(\vec{k}</em>\parallel) - \Sigma_{\alpha-n-1}^{R,A}(\omega) - t_{\alpha-n-1}^2 L_{\alpha-n-1}^{R,A}(\vec{k}<em>\parallel,\omega + eE</em>{\alpha-n-1}) ]</td>
<td>[ x_\pm = (\epsilon^\parallel(k_\parallel) - \mu) (1 - \cos(A_0)) + \omega \cos(A_0) \pm \sin(A_0) \sqrt{4t_\perp^2 - (\omega + \mu - \epsilon^\parallel(k_\parallel))^2} ]</td>
</tr>
<tr>
<td>g local</td>
<td>[ g_{\alpha\alpha}^{R,A^{-1}}(\vec{k}<em>\parallel,\omega) = \omega + \mu - \epsilon(\vec{k}</em>\parallel) ]</td>
<td>[ g_{\alpha\alpha}(\vec{k}<em>\parallel,\omega) = g</em>{\alpha\alpha}^R(\vec{k}_\parallel,\omega) ]</td>
</tr>
<tr>
<td>sum over $\vec{k}_\parallel$ (2)</td>
<td>[ g_{\alpha\alpha}^{R,A,K}(\omega) = \int d\epsilon_\parallel \rho_{\alpha}^{2D}(\epsilon_\parallel) g_{\alpha\alpha}^{R,A,K}(\epsilon_\parallel,\omega), \quad \rho_{\alpha}^{2D}(\epsilon_\parallel(k_\parallel)) = \frac{1}{2\pi i \epsilon_\parallel} \sum_{\vec{k}<em>\parallel} K \left( \sqrt{1 - \left( \frac{\epsilon</em>\parallel}{2\epsilon_\parallel} \right)^2} \right) ]</td>
<td>[ \times \Sigma_{\alpha}^{K}(\vec{k}<em>\parallel,\omega) + L</em>{\alpha}^{K}(\vec{k}<em>\parallel,\omega) + R</em>{\alpha}^{K}(\vec{k}_\parallel,\omega) ]</td>
</tr>
<tr>
<td>Dyson Eq. (3,5)</td>
<td>[ g_{\alpha\alpha}^{R,A^{-1}}(\omega) = g_{\alpha\alpha}^{R,A^{-1}}(\omega) + \Sigma_{\alpha}^{R,A}(\omega) ]</td>
<td>[ -g_{\alpha\alpha}^{R^{-1}}(\omega) g_{\alpha\alpha}^{K}(\omega) g_{\alpha\alpha}^{A^{-1}}(\omega) = -g_{\alpha\alpha}^{R^{-1}}(\omega) g_{\alpha\alpha}^{K}(\omega) g_{\alpha\alpha}^{A^{-1}}(\omega) + \Sigma_{\alpha}^{K}(\omega) ]</td>
</tr>
<tr>
<td>Impurity (4)</td>
<td>[ g_{\text{imp},\alpha\alpha}(\omega) ]</td>
<td>[ g_{\text{imp}}^{K}(\omega) = (1 - \omega_1) g_{\alpha\alpha}(\omega) + \omega_1 (g_{\alpha\alpha}^{R^{-1}}(\omega) - U)^{-1} ]</td>
</tr>
</tbody>
</table>

\[ g_{\text{imp},\alpha\alpha}(\omega) = (1 - \omega_1) g_{\alpha\alpha}^{R,A}(\omega) + \omega_1 \left( g_{\alpha\alpha}^{R,A^{-1}}(\omega) - U \right)^{-1} \]
5.1 Observables of interest

5.1.1 Number current

To calculate the number current operator $\hat{J}$, we use the polarization operator as in the bulk case $\vec{P}_{\alpha j} = \vec{R}_{\alpha j} \hat{c}_{\alpha j} \hat{c}_{\alpha j}$. Note that the polarization operator now depends on two indeces the lattice site $j$ and the plane number $\alpha$. The current operator is thus defined as the derivative with respect to time of the polarization operator $\vec{J}(\vec{r}, t) = \partial/\partial t \vec{P}_{\alpha j}(\vec{r}, t) = i \sum_{\alpha j}[\hat{H}_{FK}(t), \hat{P}_{\alpha j}]$. In order to calculate the current we need to calculate the commutator between the polarization operator and our Hamiltonian defined in Eq.(1.11). Since both the polarization operator and the potential part of the Hamiltonian depend only on the number operator they commute with each other and only the kinetic part contributes to the current. The involved commutators are

$$\left[ \hat{c}_{\gamma}^{\dagger} \hat{c}_{\gamma+1l}, \vec{R}_{\alpha j} \hat{c}_{\alpha j} \right] = \vec{R}_{\alpha j} (\hat{c}_{\gamma}^{\dagger} \hat{c}_{\alpha j} \delta_{\gamma+1alj} - \hat{c}_{\alpha j}^{\dagger} \hat{c}_{\gamma} \delta_{\gamma+1alj})$$

$$\left[ \hat{c}_{\gamma+1l}^{\dagger} \hat{c}_{\gamma l}, \vec{R}_{\alpha j} \hat{c}_{\alpha j} \right] = \vec{R}_{\alpha j} (\hat{c}_{\gamma+1l}^{\dagger} \hat{c}_{\alpha j} \delta_{\gamma+1alj} - \hat{c}_{\alpha j} \hat{c}_{\gamma+1l} \delta_{\gamma+1alj})$$

$$\left[ \hat{c}_{\gamma l}^{\dagger} \hat{c}_{\gamma l+\delta}, \vec{R}_{\alpha j} \hat{c}_{\alpha j} \right] = \vec{R}_{\alpha j} (\hat{c}_{\gamma l}^{\dagger} \hat{c}_{\alpha j} \delta_{\gamma+1alj} - \hat{c}_{\alpha j} \hat{c}_{\gamma l+\delta} \delta_{\gamma+1alj})$$

Summing over $\alpha$ and $j$ we obtain

$$\hat{J} = i \left\{ -t_\perp \sum_{\gamma l} (e^{ieA_\gamma(t)} \vec{R}_{\gamma+1l} \hat{c}_{\gamma+1l} - e^{-ieA_\gamma(t)} \vec{R}_{\gamma l} \hat{c}_{\gamma+1l}^{\dagger}) + e^{-ieA_\gamma(t)} \vec{R}_{\gamma l} \hat{c}_{\gamma+1l}^{\dagger} \hat{c}_{\gamma l} - e^{-ieA_\gamma(t)} \vec{R}_{\gamma l} \hat{c}_{\gamma+1l}^{\dagger} \hat{c}_{\gamma l} - t_\parallel \sum_{\gamma l \delta} (\vec{R}_{\gamma l+\delta} \hat{c}_{\gamma l+\delta}^{\dagger} - \vec{R}_{\gamma l} \hat{c}_{\gamma l}^{\dagger} \hat{c}_{\gamma l+\delta}) \right\}. \quad (5.2)$$

The delta vector corresponds to $\delta = \vec{R}_{\gamma l+\delta} - \vec{R}_{\gamma l}$ the nearest-neighbor lattice translation vector for sites in the same plane, also define another delta vector $\delta'$ to be
the nearest-neighbor lattice translation vector between lattice sites in adjacent planes
\( \vec{\delta} = \vec{R}_{\gamma l} - \vec{R}_{\gamma + 1l} \). Usually \(|\vec{\delta}| = |\vec{\delta}'|\) but in the general case it doesn’t have to. The total current is

\[
\hat{J} = i \{ -t_{\perp} \sum_{\gamma l} \vec{\delta}(e^{ieA_{\gamma}(t)}\hat{c}_{\gamma l}^\dagger\hat{c}_{\gamma + 1l} + e^{-ieA_{\gamma}(t)}\hat{c}_{\gamma + 1l}^\dagger\hat{c}_{\gamma l}) - t_{\parallel} \sum_{\gamma l} \vec{\delta}_{\gamma l}^\dagger\hat{c}_{\gamma + \delta l} \} \tag{5.3}
\]

We are only interested in the perpendicular expectation value of the current \( \langle \hat{J}_\perp \rangle \), thereof we ignore the second term in the equation above.

### 5.1.2 Expectation value of the kinetic energy

We would like to calculate the expectation value of the kinetic energy, in order to do so we first need to consider the kinetic part of our Hamiltonian.

\[
\hat{T} = -t_{\parallel} \sum_{\gamma l} \hat{c}_{\gamma l}^\dagger\hat{c}_{\gamma + \delta l} - t_{\perp} \sum_{\gamma l} [e^{ieA_{\gamma}(t)}\hat{c}_{\gamma l}^\dagger\hat{c}_{\gamma + 1l} + e^{-ieA_{\gamma}(t)}\hat{c}_{\gamma + 1l}^\dagger\hat{c}_{\gamma l}] \tag{5.4}
\]

Rewrite the kinetic energy in momentum space using Eq. (14)-(15)

\[
\hat{T} = \sum_{\gamma \vec{k}_{||}} \epsilon(\vec{k}_{||})\hat{c}_{\gamma l}^\dagger(\vec{k}_{||})\hat{c}_{\gamma l}(\vec{k}_{||}) - t_{\perp} \sum_{\gamma \vec{k}_{||}} [e^{ieA_{\gamma}(t)}\hat{c}_{\gamma l}^\dagger(\vec{k}_{||})\hat{c}_{\gamma + 1l}(\vec{k}_{||}) + e^{-ieA_{\gamma}(t)}\hat{c}_{\gamma + 1l}^\dagger(\vec{k}_{||})\hat{c}_{\gamma l}(\vec{k}_{||})] \tag{5.5}
\]

Evaluate the expectation value using the definition of the lesser Green’s function

\[
g_{\alpha\beta}(\vec{k}_{||}, t = 0^+) = (i/\hbar)\langle \hat{c}_\alpha(\vec{k}_{||})\hat{c}_\beta(\vec{k}_{||}) \rangle
\]

\[
\hat{T} = -i \sum_{\gamma \vec{k}_{||}} \epsilon(\vec{k}_{||})g_{\gamma\gamma}(\vec{k}_{||}, t = 0) - t_{\perp} \sum_{\gamma \vec{k}_{||}} [e^{ieA_{\gamma}(t)}g_{\gamma\gamma + 1}(\vec{k}_{||}, t = 0) + e^{-ieA_{\gamma}(t)}g_{\gamma + 1\gamma}(\vec{k}_{||}, t = 0)] \tag{5.6}
\]

### 5.1.3 Double occupancy

In order to calculate the double occupancy at each plane we will use the definition of the self energy derived previously Eq. (3.70). The double occupancy is simply given by
the expectation value of having both a conduction and a valence electron in the same lattice site. That is \( \langle DO \rangle = \langle \hat{f}^{\dagger}_{\alpha i} \hat{f}_{\alpha i} \hat{c}^{\dagger}_{\alpha i} \hat{c}_{\alpha i} \rangle \). In order to find the double occupancy we start by evaluating Eq. (3.70) at equal sites \( \alpha i = \beta j \) and equal times \( t = t' \) but with the caveat that the time \( t \) lies in the upper branch of the Keldysh contour and the time \( t' \) lies in the lower branch. This yields

\[
\int_{-\infty}^{\infty} dt \Sigma_{\alpha i}(t_+, \tilde{t}_+) g^c_{\alpha i}(\tilde{t}_+, t_-) - \int_{-\infty}^{\infty} dt \Sigma_{\alpha i}(t_+, \tilde{t}_-) g^c_{\alpha i}(\tilde{t}_-, t_-) = -iU_\alpha \langle \hat{f}^{\dagger}_{\alpha i} \hat{f}_{\alpha i} \hat{c}^{\dagger}_{\alpha i} \hat{c}_{\alpha i} \rangle
\]

(5.7)

This is given in the time ordered formalism, we translate into the Keldysh formalism using the usual relationship for the Green’s functions and the self energies. These relationships are summarized in Eq. (B.20). The double occupancy in the Keldysh formalism becomes,

\[
\langle DO \rangle = \frac{i}{4U_\alpha} \left[ \left( \Sigma^R_{\alpha i} + \Sigma^A_{\alpha i} + \Sigma^K_{\alpha i} \right) (-g^R_{\alpha i} + g^A_{\alpha i} + g^K_{\alpha i}) \right.

\left. - \left( \Sigma^R_{\alpha i} + \Sigma^A_{\alpha i} + \Sigma^K_{\alpha i} \right) (-g^R_{\alpha ai} - g^A_{\alpha ai} + g^K_{\alpha ai}) \right] \quad (5.8)
\]

where we have omitted the time dependencies and the integral over the contour is implicit. After some simplification the final equation for the double occupancy becomes.

\[
\langle DO \rangle = \frac{i}{2U_\alpha} \left[ \left( \Sigma^A_{\alpha i} + \Sigma^K_{\alpha i} \right) g^A_{\alpha i} + \Sigma^R_{\alpha i} (-g^R_{\alpha i} + g^K_{\alpha i}) \right] \quad (5.9)
\]
Chapter 6

Results

The inhomogeneous dynamical mean field theory algorithm derived in previous chapters is implemented using the Fortran programming language as well as Python scripts to process and analyze the output data. A typical calculation starts with setting the constant parameters of the calculation:

- The number of layers in the structure. We refer to the planes in which the strong interactions are turned on as the barrier region and to the metallic planes as the leads. The results presented in the rest of this chapter are for a barrier consisting of a single Falicov Kimball plane. The code however is capable of handling any number of barriers with any combination of $U_\alpha$ values. We use 30 metallic layers at each side of the barrier for a total of 61 layers. These metallic layers are used to ensure that Green's functions relax to the bulk result.

- The temperature of the device. For the results presented below the device temperature is equal to one tenth of the hopping energy. This is equivalent to room temperature.

- Falicov-Kimball filling. This determines the filling of the system. We work with the Falicov-Kimball model at half filling which provides particle-hole symmetry.

- The vector potential $A_0$ at the bulk leads. This will impose a current-carrying state to the metallic leads in the interface. Due to the lack of scattering we
expect this current to carry through the device. The retarded and advanced pieces of the formalism are independent of $A_0$. Additionally is also possible to assign different vector potentials to different sides of the device, $A_0^R$ from the right and $A_0^L$ from the left. This is mechanism that we are currently exploring.

- We are free to vary the electric field at the barrier plane $E_{\text{barrier}}$. The electric field at the barrier and the vector potential $A_0$ will have a unique relation that will determine the current-voltage characteristics of our device. The way the algorithm is implemented allows us to calculate the Green’s functions for any arbitrary combination of $A_0$ and $E_{\text{barrier}}$. We are left with is the task of finding the correct combination of $A_0$ to $E_{\text{barrier}}$.

The Quantum zipper algorithm is first performed to obtain the retarded and advanced Green’s functions. Once convergence has been achieved on the retarded Green’s functions the quantum zipper algorithm is performed again but this time for the Keldysh Green’s functions. Once convergence has been achieved, it’s possible to calculate the quantities of interest by integrating over the appropriate Green’s functions, for example integrating over the local lesser Green’s function for the filling or the nearest neighbors lesser Green’s function to obtain the current. We will discuss the current limitations of the technique and discuss possible problems and solutions.

6.1 Retarded Green’s Function

We begin by examining the retarded and advanced Green’s functions. This can be done for any range of $U_{\text{barrier}}$ and $E_{\text{barrier}}$ parameters. The local retarded Green’s functions $G_{aa}^R(\omega)$ will not depend on the value of the vector potential $A_0$. This is the case since the vector potential only affects the distribution of states and doesn’t directly affect the density of states of the system. We consider three different cases
of onsite interaction $U_{\text{barrier}}$. For a dirty metal a low onsite interaction is required, and the value of $U_{\text{barrier}} = 1.0$ is chosen for the calculations. Near the Mott insulator transition the retarded Green’s function develops a dip in the density of states. The behavior right before the transition occurs is modeled by using an onsite interaction of $U_{\text{barrier}} = 4.0$. Finally the Mott insulating phase is characterized by the formation of a gap around zero frequency in the density of states. A large onsite interaction is required to obtain a large gap. We use $U_{\text{barrier}} = 16.0$ to achieve the Mott insulating state. In Fig.(6.1) we compare the retarded Green’s function for the three different values of $U_{\text{bulk}}$ vs the retarded Green’s function at the barrier plane with the same onsite interaction $U_{\text{barrier}}$ once the quantum zipper algorithm has achieved convergence. We notice the retarded Green’s functions share the overall behavior in bulk as well as the barrier. In the multilayered system the features of the Green’s function become sharper. For $U = 16$ we also observe that in the bulk there is a clearly defined gap near zero frequency. In contrast once we have a single insulating plane there is a small density of states around zero frequency. This effect is due to the neighboring metallic planes.

Once the quantum zipper algorithm has converged we can examine the retarded Green’s function at individual planes as well as the self energy at the barrier. The self energy is found to be zero in all the metallic planes connecting the barrier to the bulk reservoir as expected. In Fig.(6.2) we examine the local Green’s function at different plane numbers. From right to left we find the density of states at the barrier plane previously shown, the density of states one plane before the barrier, two planes before the barrier and finally at the first plane of the nano structure. For all values of $U$ a peak can be seen one plane before the barrier, and then two peaks two planes away from the barrier. This pattern repeats for each plane after and before the barrier.
Figure 6.1: Local density of states for different values of $U$. a) Result for calculations performed in the bulk for a 3D cubic lattice. b) Result for a single impurity plane in the multilayered nano structure. The density of states presented is the density of states at the barrier plane, which is connected to metallic leads and ultimately to a bulk reservoir at both ends of the device.

producing a new peak at each plane we get away from the barrier. The appearance of these peaks is a product of the disturbance in the electric charge caused by the barrier. These are known as Friedel oscillations. If we were to zoom in the region around zero frequency in the density of states for the first plane we would notice the the Green’s function is not smooth as it is in the bulk case, but there are many small oscillations. This is akin to representing a function by its Fourier series but truncating higher frequency terms.

There is no potential at the barrier in the previous results, and these results agree with previously published results [25]. Next we include an electric field at the barrier plane $E_{\text{barrier}}$ in order to observe the effect caused by the electric field. We set the
Figure 6.2: Local density of states for different values of $U_{\text{barrier}}$ at different planes near the barrier region. a) Density of states two planes before the barrier plane. b) Density of states one plane before the barrier plane. c) Density of states at the barrier plane. A strong insulating plane causes the bandwidth of the adjacent metallic planes to widen but this effect is rapidly lost in subsequent planes.

Figure 6.3: Local density of states for different values of $U_{\text{barrier}}$ at the first plane of the multilayered device. The retarded Green’s function had enough planes to relax back to the bulk result and the effects of the barrier can only be seen by the Friedel oscillations caused by it. Inset shows a closer look to the Friedel oscillations.
field to be slightly lower than half of the onsite interaction $U$. Fig.(6.4) and Fig.(6.5) summarizes the new local Green’s functions at different planes in the heterostructure. As we increase the electric field $E_{\text{barrier}}$ we observed an asymmetry developing in the density of states. They are symmetrical with respect to the y axis at $E_{\text{barrier}} = 0$, but there is a shift towards lower frequencies when $E_{\text{barrier}} > 0$ for planes to the left of the barrier, and a symmetric shift to the higher frequencies for the planes to the right. This is the case because of the mirror symmetry of the heterostructure.
Figure 6.4: Local density of states for different values of $U_{\text{barrier}}$ at different planes near the barrier region. a) Density of states two planes before the barrier plane. b) Density of states one plane before the barrier plane. c) Density of states at the barrier plane. There is an applied $E_{\text{barrier}} \neq 0$ at the barrier plane. For $U_{\text{barrier}} = 1$, $U_{\text{barrier}} = 4$ and $U_{\text{barrier}} = 16$ the field applied is $E_{\text{barrier}} = 0.4$, $E_{\text{barrier}} = 1.8$ and $E_{\text{barrier}} = 7.5$ respectively. Note the asymmetry in the density of states caused by the field.

Figure 6.5: Local density of states for different values of $U_{\text{barrier}}$ at the first plane of the multilayered device when an electric field $E_{\text{barrier}}$ has been applied. There are no major differences with the case where there is no electric field applied.
6.2 Lesser Green’s function

Once the retarded Green’s function has been determined for a given set of parameters we can calculate the different lesser Green’s functions using the quantum zipper algorithm. Since the retarded Green’s function doesn’t depend on $A_0$ we are free to calculate the lesser Green’s functions for different values of $A_0$ without having to calculate the retarded Green’s functions again. Any adjustment in the $E_{\text{barrier}}$ parameter on the other hand will require a new run of the quantum zipper algorithm once again for the retarded piece of the Green’s functions. First we will observe the effects of changing $A_0$ when there is no $E_{\text{barrier}}$. In Fig(6.6) we calculate the lesser Green’s function when the vector potential $A_0 = 0$, the result obtained by the quantum zipper algorithm matches exactly with the known theoretical result in equilibrium. Once $A_0$ is different from zero in Fig(6.7) we obtain a much more complex behavior and the relation $G_\alpha^\omega(\omega) = -2if(\omega)\text{Im}\{G^R_{\alpha\alpha}(\omega)\}$ doesn’t hold anymore.

We would expect the lesser Green’s function to relax to its bulk value the same way the retarded Green’s function does. Unfortunately this is not the case. This is an artifact of forcing a current to pass through the device due to the initial condition in the bulk but at the same time not allowing a voltage to develop in the device ($E_{\text{barrier}} = 0$). This can be seen by looking at the lesser Green’s function in the first and last plane in Fig.(6.8) and comparing to the bulk result for the lesser Green’s function. It is also noted that the difference is more pronounced as we increase the value of the onsite interaction $U_{\text{barrier}}$. We make use of the lesser Green’s function first sum rule to quantify the error in the calculation when there is no potential. The first sum rule for the lesser Green’s function gives the electron filling at each plane; that is $\int d\omega G_\alpha^\omega(\omega)/(2\pi) = \rho_\alpha^e = 1/2$ since we are working at half filling. We calculate
Figure 6.6: Lesser Green’s function for different values of $U_{\text{barrier}}$ at different planes near the barrier region for $A_0 = 0$. a) Lesser Green’s function two planes before the barrier plane. b) Lesser Green’s function one plane before the barrier plane. c) Lesser Green’s function at the barrier plane. This corresponds to the known equilibrium solution.

This quantity for the different values presented in Fig.(6.8) at the first and the last plane of the nanostructure and tabulate the results in Table(6.2). We can see that the charge is transferred from one side of the barrier to the other. The extra charge in plane 0 corresponds exactly to the missing charge in the last plane. Once we introduce the $E_{\text{barrier}}$ in the calculations the filling in the metallic planes varies. In general all planes far away to the right of the barrier share the same value while all the planes far away to the left of the barrier share a different value such that the sum of both values equals one. There is a bigger variation in the filling near the barrier.

We would like the filling to be conserved in all planes of the heterostructure at the same time. Also the lesser Green’s function should converge back to the bulk value when far away from the barrier. We intend to achieve this by adjusting $E_{\text{barrier}}$ until the first and last planes fillings equal one half each. Fig(6.9) shows the filling minus
Figure 6.7: Lesser Green’s function for different values of $U_{\text{barrier}}$ and $A_0$ for planes near the barrier. As the vector potential $A_0$ increases there is a broadening of the lesser Green’s function near zero frequency. This effect is similar to an increase in temperature in the equilibrium case.
Figure 6.8: Lesser Green’s function for different values of $U_{\text{barrier}}$ as well as the bulk solution at the first and last plane of the heterostructure when $E_{\text{barrier}} = 0$. Notice as the $U_{\text{barrier}}$ increases the lesser Green’s function at the first and last plane diverge from the bulk result. This is an abnormality of the lack of voltage at the insulating barrier while still carrying a current through the barrier.
### Table 6.1: $G^<$ first sum rule at the end planes of the multilayered device.

<table>
<thead>
<tr>
<th>$\pi A_0$</th>
<th>$U = 1$</th>
<th>$U = 4$</th>
<th>$U = 16$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>first plane</td>
<td>last plane</td>
<td>first plane</td>
</tr>
<tr>
<td>0</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>$4\pi$</td>
<td>0.509</td>
<td>0.491</td>
<td>0.571</td>
</tr>
<tr>
<td>$8\pi$</td>
<td>0.516</td>
<td>0.484</td>
<td>0.621</td>
</tr>
<tr>
<td>$12\pi$</td>
<td>0.507</td>
<td>0.493</td>
<td>0.566</td>
</tr>
</tbody>
</table>

one half at the first plane for different values of $A_0$ when $U_{\text{barrier}} = 1$ as a function of applied $E_\alpha$. We begin with $U_{\text{barrier}} = 1$ since it has the lowest discrepancy on filling when $E_{\text{barrier}} = 0$. For small values of $A_0$ Fig. (6.9) shows a linear dependence on the filling in the first plane vs applied $E_{\text{barrier}}$. We implement a Newton-Raphson root finding algorithm to find the value of $E_{\text{barrier}}$ which ensures filling conservation through the device. As the value of $A_0$ increases a quadratic dependence is developed for the filling with respect to the applied $E_{\text{barrier}}$ and we can not find the root anymore. In the cases where convergence is achieved we calculate the nearest neighbor’s lesser Green’s functions using left and right functions calculated earlier. The integral with respect to frequency of the lesser Green’s function will yield the current from one plane to the next. We show in Fig. (6.10) the current as a function of plane number for $U_{\text{barrier}} = 1$ for the different values of $A_0$ at which we found a root in the filling with respect to $E_{\text{barrier}}$. We use the corresponding $E_{\text{barrier}}$ that guarantees filling conservation. As it can be seen by the plot as the value of $A_0$ increases not only the $E_{\text{barrier}}$ increases but the value of current from one plane from the next as well.

As can be seen from Fig. (6.10) the current oscillates around the barrier and finally drops to a lower conductivity for planes after the barrier. There might be a couple
Figure 6.9: Filling minus one half at the first plane of the heterostructure vs $E_{\text{barrier}}$ for different values of $A_0$. All the planes before the barrier have the same filling. Planes after the barrier have a different filling $\rho_{e2}$ such that $\rho_e + \rho_{e2} = 1.0$. Notice a root exists only for small values of $A_0$.

of methods to solve this issue. One of the proposed methods would require to adjust the potential $E_\alpha$ not only at the barrier plane but in adjacent metallic planes as well this would minimize the oscillations observed in the current as well as the oscillations observed in the filling around the barrier. A different possible solution that could address the drop in current after the barrier is to allow the vector potential $A_0$ to be different at the different leads of the device. $A_0^R$ when coming from the right and $A_0^L$ when coming from the left. At the moment these two techniques have not been fully implemented. We finalize this section by recording the values of $E_{\text{barrier}}$ for which we have filling conservation when $U_{\text{barrier}} = 1$ in Table (6.2).
Table 6.2: Calculated $E_{\text{barrier}}$ using Newton-Raphson method in order to have conservation of charge in all the planes. For values of $A_0$ above $5\pi/20$ there is no charge conservation by just adjusting $E_{\text{barrier}}$

<table>
<thead>
<tr>
<th>$A_0$</th>
<th>$\pi/20$</th>
<th>$2\pi/20$</th>
<th>$3\pi/20$</th>
<th>$4\pi/20$</th>
<th>$5\pi/20$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{\text{barrier}}$</td>
<td>-.0414</td>
<td>-.0894</td>
<td>-.1520</td>
<td>-.2626</td>
<td>NA</td>
</tr>
</tbody>
</table>

Figure 6.10: Current through the heterostructure for different values of $A_0$, and the corresponding $E_{\text{barrier}}$ such that the filling is conserved. $U_{\text{barrier}} = 1$. The current is fairly constant far away from the barrier, but there is a certain amount of perturbations near the barrier. There is also a drop in the total current being carried as the current crosses the barrier. The unphysical behavior might be addressed by allowing the vector potential $A_0$ to be different at the opposite sides of the device.
6.3 Conclusions and future areas of interest

The physics of quantum systems out of equilibrium is a vast topic with strong interest in which this research takes ideas and collaborates to. In this thesis we have developed a formalism to study heterostructures in which the materials are highly correlated. In order to study the non linear behavior of the systems we expanded the quantum zipper algorithm, used to obtain the density of states of the system, by utilizing the Keldysh formalism. This technique allows us to study the dynamics of the system out of equilibrium by calculating not only the retarded piece to the Green’s function but the Keldysh piece as well. We show the effects of introducing a vector potential in the bulk which is a novel result and it is key in determining the boundary conditions of the system. We also show the effect of introducing an electric field on a single layer of the heterostructure, and its effect in the density of states near the layer in which the field is applied. This in turns allows us to determine the unique relationship between current and electric field in the device. Now the only challenge standing is finding the correct optimization scheme that will allow us to determine the correct combination of parameters such that all the physical properties of a real device will hold. As an example we show how by adjusting the electric field we can enforce the filling to be conserved in all the planes. In the same way we expect to be able to vary the vector potential at both ends of the device individually in order to achieve current conservation. Once we have achieved current and filling conservation we can say we have a physical device and other properties of the device could be studied. The results of the physical devices will be publish at a later time.

Finally we believe that once the major challenge of parameter optimization has been addressed this tool will provide novel and interesting results.
Appendix A

Self Energy Relation

Here, we prove that \( \Sigma_{++} + \Sigma_{--} = \Sigma_{+-} + \Sigma_{-+} \). Begin by writing the Dyson equation
\[
G = G_0 + G_0 \Sigma G
\]
in matrix form and perform the multiplication in the last term.

\[
G_0 \Sigma G = \begin{pmatrix}
G_{0,++} \Sigma_{++} G_{++} - G_{0,-+} \Sigma_{+-} G_{++} & G_{0,++} \Sigma_{++} G_{+-} - G_{0,-+} \Sigma_{+-} G_{+-} \\
-G_{0,++} \Sigma_{+-} G_{++} + G_{0,-+} \Sigma_{-+} G_{++} & -G_{0,++} \Sigma_{+-} G_{+-} + G_{0,-+} \Sigma_{-+} G_{+-} \\
G_{0,-+} \Sigma_{++} G_{++} - G_{0,-+} \Sigma_{+-} G_{+-} & G_{0,-+} \Sigma_{++} G_{+-} - G_{0,-+} \Sigma_{-+} G_{+-} \\
-G_{0,-+} \Sigma_{+-} G_{++} + G_{0,-+} \Sigma_{-+} G_{++} & -G_{0,-+} \Sigma_{+-} G_{+-} + G_{0,-+} \Sigma_{-+} G_{+-}
\end{pmatrix}
\]

(A.1)
since \( G_{++} + G_{--} = G_{+-} + G_{-+} \) on the left side of the equation, it has to be true on
the right side as well, therefore the sum of the diagonal elements equals the sum of
the off-diagonal elements. Regrouping such that the \( \Sigma_{++} \) and \( \Sigma_{--} \) are on one side of
the equation and \( \Sigma_{+-} \) and \( \Sigma_{-+} \) are on the other, we obtain,

\[
(G_{0,++} - G_{0,-+}) \Sigma_{++} (G_{0,++} - G_{0,-+}) + (G_{0,-+} - G_{0,++}) \Sigma_{+-} (G_{0,-+} - G_{0,++}) =
(G_{0,++} - G_{0,-+}) \Sigma_{+-} (G_{0,-+} - G_{0,++}) + (G_{0,++} - G_{0,-+}) \Sigma_{-+} (G_{0,++} - G_{0,-+})
\]

(A.2)
after some factorization. Using the relation for the \( Gs \), we can change the second term
on each side of the identity to factorize the \( \Sigma s \) together

\[
(G_{0,++} - G_{0,-+}) (\Sigma_{++} + \Sigma_{--}) (G_{0,++} - G_{0,-+}) = (G_{0,++} - G_{0,-+}) (\Sigma_{+-} + \Sigma_{-+}) (G_{0,-+} - G_{0,++})
\]

(A.3)
One more time using the relation of the $G$s, we change the last term in the right side of the equation from $G_{0,-+} - G_{0,--}$ to $G_{0,++} - G_{0,+-}$. The $G$s cancel each other and we are left with the symmetry relation for the self energy $\Sigma_{++} + \Sigma_{--} = \Sigma_{+-} + \Sigma_{-+}$. 
Appendix B

Matrix representation.

Consider a general matrix $M(t, t')$ where the time dependencies are defined within the Keldysh contour and are discretized with respect to the time variables. These times can be in either the upper branch of the contour or the lower branch of the contour,

$$M(t, t') = \begin{pmatrix} m_{11}(t, t') & m_{12}(t, t') \\ m_{21}(t, t') & m_{22}(t, t') \end{pmatrix} \quad (B.1)$$

where $m_{11}$, $m_{12}$, $m_{21}$ and $m_{22}$ are square matrices of the same size. We have split the big matrix $M$ into four sub matrices of smaller size. We also impose the following restriction $m_{11}(t, t') + m_{22}(t, t') = m_{12}(t, t') + m_{21}(t, t')$. In the following sub sections we will develop a few relationships for this general matrix.

Inverse of $M$

We start by finding the inverse of the matrix $M$, we find $M^{-1}$ such that $MM^{-1} = I$, with $I$ being the identity matrix. $M$ is invertible as long as $m_{11}$ and $m_{22}$ are invertible themselves. We must be careful since $m_{12}$ and $m_{21}$ might not be invertible even if $M$ is invertible. Give $M^{-1}$ the general form

$$M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad (B.2)$$
Performing the matrix multiplication between $M$ and $M^{-1}$ yields four different equations:

\[
\begin{align*}
    m_{11}A + m_{12}C &= 1 	ag{B.3} \\
    m_{21}A + m_{22}C &= 0 	ag{B.4} \\
    m_{11}B + m_{12}D &= 0 	ag{B.5} \\
    m_{21}B + m_{22}D &= 1 	ag{B.6}
\end{align*}
\]

We solve for $C$ from the second equation and for $B$ from the third equation. We find $C = -m_{22}^{-1}m_{21}A$ and $B = -m_{11}^{-1}m_{12}D$. We substitute the value of $B$ and $C$ in the first and fourth equation to get $(m_{11} - m_{12}m_{22}^{-1}m_{21})A = 1$ and $(m_{22} - m_{21}m_{11}^{-1}m_{12})D = 1$. Therefore the inverse is

\[
M^{-1} = \begin{pmatrix}
    (m_{11} - m_{12}m_{22}^{-1}m_{21})^{-1} & -m_{11}^{-1}m_{12}(m_{22} - m_{21}m_{11}^{-1}m_{12})^{-1} \\
    -m_{22}^{-1}m_{21}(m_{11} - m_{12}m_{22}^{-1}m_{21})^{-1} & (m_{22} - m_{21}m_{11}^{-1}m_{12})^{-1}
\end{pmatrix}
\]  

(B.7)

It is straightforward to now show $MM^{-1} = I$, the inverse should also be true, that is we will show that $M^{-1}M = I$ in the next subsection.

\[M^{-1}M = I \text{ PROOF}\]

in order to prove that $MM^{-1} = I$, we start with the following equality

\[
m_{12} - m_{12}m_{22}^{-1}m_{21}m_{11}^{-1}m_{12} = m_{12} - m_{12}m_{22}^{-1}m_{21}m_{11}^{-1}m_{12} \tag{B.8}
\]

we can either group terms from the right or from the left, since we are dealing with matrix multiplications the way we arrange things matter. Factorize from the right in one side of the equation and from the left in the other side of the equation.

\[
m_{12}m_{22}^{-1}(m_{22} - m_{21}m_{11}^{-1}m_{12}) = (m_{11} - m_{12}m_{22}^{-1}m_{21})m_{11}^{-1}m_{12} \tag{B.9}
\]
now we can multiply the whole equation by \((m_{11} - m_{12}m^{-1}_{22}m_{21})\) from the left and by 
\((m_{22} - m_{21}m^{-1}_{11}m_{12})\) from the right. We find the following identity.

\[
(m_{11} - m_{12}m^{-1}_{22}m_{21})^{-1}m_{12}m^{-1}_{22} = m^{-1}_{11}m_{12}(m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1} \tag{B.10}
\]

The same procedure is followed to find the second identity, but we start with the expression \(m_{21} - m_{21}m^{-1}_{11}m_{12}m^{-1}_{22}m_{21}\) equals to itself. Factorize from the right in one side and from the left in the other and multiply by the appropriate inverses to get our second identity.

\[
(m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1}m_{21}m^{-1}_{11} = m^{-1}_{22}m_{21}(m_{11} - m_{12}m^{-1}_{22}m_{21})^{-1} \tag{B.11}
\]

Now we can perform the matrix multiplication of \(M^{-1}M\) which equals

\[
\begin{pmatrix}
(m_{11} - m_{12}m^{-1}_{22}m_{21})^{-1}m_{22} & (m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1}m_{21} \\
-m^{-1}_{11}m_{12}(m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1}m_{21} & -m^{-1}_{11}m_{12}(m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1}m_{22} \\
(m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1}m_{21} & (m_{22} - m_{21}m^{-1}_{11}m_{12})^{-1}m_{22} \\
-m^{-1}_{22}m_{21}(m_{11} - m_{12}m^{-1}_{22}m_{21})^{-1}m_{11} & -m^{-1}_{22}m_{21}(m_{11} - m_{12}m^{-1}_{22}m_{21})^{-1}m_{12}
\end{pmatrix} \tag{B.12}
\]

For the first diagonal element, use the second identity Eq.\([B.11]\) in the second term and factorize

\[
(1 - m^{-1}_{11}m_{12}m^{-1}_{22}m_{21})(m_{11} - m_{12}m^{-1}_{22}m_{21})^{-1}m_{11} = 1 \tag{B.13}
\]

likewise the second diagonal element will equal one using the first identity equation. Using Eqs.(B.10) and (B.11) the off-diagonal elements become zero, giving as a result the identity matrix.
\( \hat{L}\tau_3 M\hat{L}^\dagger \) TRANSFORM

Next we use the definition of \( \tau_3 \) and \( \hat{L} \) to transform \( M \) into an upper diagonal matrix, this becomes

\[
\begin{align*}
\mathcal{M} = \hat{L}\tau_3 M\hat{L}^\dagger = & \frac{1}{2} \begin{pmatrix}
 m_{12} - m_{22} + m_{11} - m_{21} & m_{11} + m_{12} + m_{21} + m_{22} \\
 m_{11} + m_{22} - m_{12} - m_{21} & m_{12} - m_{22} + m_{11} - m_{21}
\end{pmatrix} \\
\end{align*}
\]

(B.14)

and we define

\[
\begin{align*}
 m^R &= m_{11} - m_{12} = m_{21} - m_{22} \quad \text{(B.15)} \\
 m^A &= m_{11} - m_{21} = m_{12} - m_{22} \quad \text{(B.16)} \\
 m^K &= m_{11} + m_{22} = m_{12} + m_{21} \quad \text{(B.17)}
\end{align*}
\]

the matrix \( \mathcal{M} \) becomes an upper diagonal matrix

\[
\begin{align*}
\mathcal{M} = \begin{pmatrix}
 m^R & m^K \\
 0 & m^A
\end{pmatrix}
\end{align*}
\]

(B.18)

TRANSFORMATION OF \( M^{-1} \)

Now we use the equation \( MM^{-1} = I \) to find the transformation of the inverse of \( M^{-1} \).

Apply the \( L\tau^3 \) from the right and \( \tau^3\hat{L}^\dagger \) from the left. The right side of the equation is just the same identity matrix since \( \tau_3\tau_3 = I \) and \( \hat{L}\hat{L}^\dagger = I \) the left side becomes \( \hat{L}\tau_3 MM^{-1}\tau_3\hat{L}^\dagger \), introduce a term \( \hat{L}^\dagger\hat{L} \) in between the two matrices. The resulting equation is

\[
\begin{align*}
\hat{L}\tau_3 MM^{-1}\tau_3\hat{L}^\dagger = I \\
\end{align*}
\]

(B.19)

We find \( \mathcal{M}^{-1} = \hat{L}M^{-1}\tau_3\hat{L}^\dagger \) and \( MM^{-1} = I \).
In order to calculate $M^{-1}$ we use the following relations

\begin{align*}
m_{11} &= \frac{1}{2}(m^R + m^A + m^K) \quad \text{(B.20)} \\
m_{22} &= \frac{1}{2}(-m^R - m^A + m^K) \quad \text{(B.21)} \\
m_{12} &= \frac{1}{2}(-m^R + m^A + m^K) \quad \text{(B.22)} \\
m_{21} &= \frac{1}{2}(m^R - m^A + m^K) \quad \text{(B.23)}
\end{align*}

which follow from our definitions of $m^R$, $m^A$ and $m^K$. Replacing these equations into Eq.(B.7) and after some simplification we find:

\[ M^{-1} = L \begin{pmatrix} A' & -D' - G_A^{-1} \\ -A' + G_A^{-1} & D' \end{pmatrix} L^\dagger \]  

(B.24)

with

\begin{align*}
A' &= \frac{1}{2}(m^A^{-1} + m^R^{-1} - m^R^{-1} m^K m^A^{-1}) \quad \text{(B.25)} \\
D' &= -\frac{1}{2}(m^A^{-1} + m^R^{-1} + m^R^{-1} m^K m^A^{-1}) \quad \text{(B.26)}
\end{align*}

Now we can calculate $M^{-1}$ to be

\[ M^{-1} = \begin{pmatrix} A' + (-D' - G_A^{-1}) & (-A' + G_A^{-1}) - D' & A' - (-D' - G_A^{-1}) - (-A' + G_A^{-1}) + D' \\ A' + (-D' - G_A^{-1}) + (-A' + G_A^{-1}) + D' & A' - (-D' - G_A^{-1}) + (-A' + G_A^{-1}) - D' \end{pmatrix} \begin{pmatrix} m^{R-1} & -m^{R-1} m^K m^{A-1} \\ 0 & m^{A-1} \end{pmatrix} \]  

(B.27)


