Chapter 4

Quantum transport

Before beginning the final chapter on our efforts to engineer a quantum spin Hall state in graphene, we take a detour to describe the techniques required to simulate the transport phenomena encountered in Section 5.4

4.1 Landauer formalism and Fisher-Lee relation

The theoretical tools commonly used for dealing with transport in mesoscopic devices were developed by Landauer-Buttiker, and we aim here to briefly introduce the technique. For a more in depth review we turn the interested reader towards Ferry and Goodnick or Datta,[81, 82] but below we try to include enough detail to keep this manuscript self contained. Throughout this section, and the rest of the chapter, we have also benefitted greatly from the efforts by Georgo Metalidis and Petra Dietl, [35, 83] to distill the treatments found in the textbooks and follow their approach quite closely.

The standard treatment is to have the central mesoscopic device hooked up to electron reservoirs via leads, and the current through the device is then directly related to the probability that an electron has been transmitted through it. The leads are considered to be free from defects and translationally invariant in the direction of propagation, although their finite width will yield quantized modes in the transverse direction. If these channels are labelled by an index m the result for the conductance looks as follows

$$G = \frac{2e^2}{h} \sum_m T_n(E) \qquad (4.1)$$

If we had a uniform electron gas travelling at speed v with n electrons per unit length, then we would have a current equal to env. In our case, the transverse modes from the leads will each have a dispersion relation $E_m(k)$ and if the modes are occupied according to the Fermi distribution function

$f(E)$, then we can write for the current

$$I_{1\to2} = \frac{2e}{L} \sum_{m,k} T_m(E)v(k)f(E - \nu_1) \tag{4.2}$$

where $v(k)$ is the group velocity, ν_1 is the chemical potential in lead 1 and we have used the constant electron density $1/L$ for a single mode propagating along a wire of length L. The overall current can then be found by subtracting the contribution from the second lead, with chemical potential ν_2, giving

$$I = \frac{2e}{L} \sum_{m,k} T_m(E)v(k)\left[f(E - \nu_1) - f(E - \nu_2)\right] \tag{4.3}$$

Using the rule for converting a discrete sum in k-space to an integral

$$\sum_k \to \frac{L}{2\pi} \int dk \tag{4.4}$$

and the expression for the group velocity

$$v(k) = \frac{1}{h}\frac{dE}{dk} \tag{4.5}$$

allows us to rewrite the above as an integral over the energy

$$I = \frac{2e}{L} \sum_m \int dE\, T_m(E)\left[f(E - \nu_1) - f(E - \nu_2)\right] \tag{4.6}$$

For low temperatures, and low voltages, $eV = \nu_1 - \nu_2$, so that we're in the linear response regime, we can then employ the Taylor exapansion

$$f(E - \nu_1) - f(E - \nu_2) \approx \delta(E - E_F)(\nu_1 - \nu_2) \tag{4.7}$$

giving us the desired expression

$$G = \frac{I}{V} = \frac{2e^2}{h} \sum_m T_m(E) \tag{4.8}$$

So to calculate the transport properties of our device, we will need these transmission amplitudes. However, Instead of calculating the scattering amplitude directly, it is common practice to find the Green's function, which can then be used to find the transmission coefficient. The so called Fisher-Lee

relations accomplish this task,[84] which we introduce in the next section.

4.2 Introduction to Green's functions

For a system described by Hamiltonian H, the time-independent Schrödinger equation reads

$$[E - H] \Psi (r) = 0, \tag{4.9}$$

and the Green's function operator can then be defined as

$$[E - H] G(E) = \mathbb{1}, \tag{4.10}$$

in this case giving the response of the system to a delta function perturbation. So long as E is not an eigenvalue of H the solution is given by

$$G(E) = [E - H]^{-1} \tag{4.11}$$

To remedy the fact that the expression is not well defined for all energies, we introduce the so called retarded and advanced Green's functions

$$G^{\pm}(E) = \lim_{\eta \to 0^+} [E \pm i\eta - H]^{-1} \tag{4.12}$$

and as they are related by hermitian conjugation, we shall use G for the retarded function and drop the $\pm$ notation for the remainder of the chapter. We shall also require the spectral function, which is defined as

$$A = i \left(G - G^{\dagger} \right) \tag{4.13}$$

However, we shall need to use it in one of its other guises, and thus introduce the expansion of the Green's function in terms of the eigenbasis:

$$G = \frac{1}{E + i\eta - H} = \sum_k \frac{|k\rangle \langle k|}{E + i\eta - \epsilon_k} \tag{4.14}$$

where the $|k\rangle$'s are all eigenvectors of H with the corresponding eigenvalues

ϵ_k. Expanding the spectral function in the eigenbasis yields

$$A \;=\; i\left(\frac{1}{E + i\eta - H} - \frac{1}{E - i\eta - H}\right) \tag{4.15}$$

$$=\; i\sum_k |k\rangle\langle k|\left(\frac{1}{E + i\eta - \epsilon_k} - \frac{1}{E - i\eta - \epsilon_k}\right) \tag{4.16}$$

$$=\; \sum_k |k\rangle\langle k|\frac{2\eta}{\left(E - \epsilon_k\right)^2 + \eta^2} \tag{4.17}$$

and letting η go to zero then gives

$$A \;=\; 2\pi\sum_k \delta\left(E - \epsilon_k\right)|k\rangle\langle k|, \tag{4.18}$$

the desired expression.

In order to motivate the effort below where we go on to calculate the Green's function, we also introduce the Fisher-Lee relation for the transmission coefficient

$$T_{12} = Tr\left[\Gamma_1 G_{12}\Gamma_2 G_{12}^\dagger\right] \tag{4.19}$$

where

$$\Gamma_{1(2)} = i\left[\Sigma_{1(2)} - \Sigma_{1(2)}^\dagger\right] \tag{4.20}$$

and the so called self-energies $\Sigma_{1(2)}$ can be thought of as effective Hamiltonians describing the interaction between the device and leads, with G_{12} a matrix of Green's function elements connecting the first column of the central device to the last.

The expression, 4.19, actually turns out to be intractable if H is of infinite dimension, which will occur if we take the semi-infinte leads into consideration. However, it is often possible to find the self energy analytically for clean leads in a simple geometry, leading to a finite Hamiltonian, or alternatively using a numerical iteration procedure. This is the method we shall use and introduce later in section 4.6 after first deriving an expression for the self energies.

4.3 Semi Infinite leads-Self energy description

We start by writing full Hamiltonian of our system, consisting of two leads and the central device, in the following block form

$$H = \begin{pmatrix} H_L & V_{LC} & 0 \\ V_{LC}^\dagger & H_C & V_{RC}^\dagger \\ 0 & V_{RC} & H_R \end{pmatrix}, \tag{4.21}$$

where H_L, H_C, and H_R are Hamiltonians for the left lead, the central device, and the right lead, and the off-diagonal terms, V_{LC} and V_{RC} contain the coupling terms between the device and the leads. The Hamiltonian is, of course, hermitian, and so the following relations are true

$$V_{CL} = V_{LC}^\dagger, \quad V_{CR} = V_{RC}^\dagger. \tag{4.22}$$

The Green's function can be subdivided in a similar fashion, and Eq. (4.10) can then be written as

$$\begin{pmatrix} \epsilon - H_L & -V_{LC} & 0 \\ -V_{LC}^\dagger & \epsilon - H_C & -V_{RC}^\dagger \\ 0 & -V_{RC} & \epsilon - H_R \end{pmatrix} \begin{pmatrix} G_L & G_{LC} & 0 \\ G_{CL} & G_C & G_{CR} \\ 0 & G_{RC} & G_R \end{pmatrix} = \mathbb{1}, \tag{4.23}$$

where we introduce $\epsilon = (E+i\eta)\mathbb{1}$. We need to solve for G_C, and so expanding the matrix equation above we find the series of equations (4.23)

$$(\epsilon - H_L) G_{LC} - V_{LC} G_C = 0, \tag{4.24}$$

$$-V_{LC}^\dagger G_{LC} + (\epsilon - H_C) G_C - V_{RC}^\dagger G_{RC} = \mathbb{1}, \tag{4.25}$$

$$-V_{RC} G_C + (\epsilon - H_R) G_{RC} = 0. \tag{4.26}$$

From the first and the third equations we have

$$G_{LC} = (\epsilon - H_L)^{-1} V_{LC} G_C, \tag{4.27}$$

$$G_{RC} = (\epsilon - H_R)^{-1} V_{RC} G_C, \tag{4.28}$$

and substituting into the second equation we then find

$$(\epsilon - H_C - \Sigma) G_C = \mathbb{1}, \tag{4.29}$$

where we have introduced the self energy, $\Sigma = \Sigma_1 + \Sigma_2$, having the form

$$\Sigma = \underbrace{V_{LC}^\dagger \left(\epsilon - H_L\right)^{-1} V_{LC}}_{\Sigma_1} + \underbrace{V_{RC}^\dagger \left(\epsilon - H_R\right)^{-1} V_{RC}}_{\Sigma_2}, \qquad (4.30)$$

And so for a central device coupled to two leads the Green's function can be found by solving the following equation

$$G_C(E) = \left[(E + i\eta)\mathbb{1} - H_C - \Sigma\right]^{-1}, \qquad (4.31)$$

where the effects of the leads are included through the self-energy.

It is also worth noting that the self-energy, (4.30), is determined solely by the coupling Hamiltonians and the retarded Green's functions of the isolated leads $G_i = (\epsilon - H_i)^{-1}$ $(i = L, R)$. And so the self-energy is independent of the state of the central device itself.

As was noted earlier, although we have managed to successfully account for the leads through the self-energy term, the solution still involves the inversion of an infinite matrix, and so some further step is required to find a tractable alternative. However, because we are limiting ourselves to nearest-neighbour hopping from lead to device, the matrices V_{LC} and V_{RC} in Eqn. 4.30 will only have nonzero elements between the sites on the surface of each lead and their neighbouring sites in the central device. Therefore only the surface Green's functions, G_L^{11} and G_R^{11} are required, which we solve for in section 4.6.

Lastly, to show that the self energy terms described above are equivalent to the ones found in the Fisher-Lee relation, Eqn. 4.19, we now aim to calculate the current through the system in a complementary fashion to section 4.1. We assume, as before, that the leads are in equilibrium, and there is small voltage V applied between them. It is usually necessary to use the nonequilibrium Green function method, as utilized below for the local current, but as this is a non-interacting system, we can get by with a simplified approach, following Paulsson. [85]

So, we start by writing the Schrödinger equation, Eqn. 4.9, in the following block form

$$\begin{pmatrix} H_L & V_{LC} & 0 \\ V_{LC}^\dagger & H_C & V_{RC}^\dagger \\ 0 & V_{RC} & H_R \end{pmatrix} \begin{pmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{pmatrix} = E \begin{pmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{pmatrix}, \qquad (4.32)$$

where Ψ_L, Ψ_C, and Ψ_R are vector wave functions of the left lead, the central device, and the right lead respectively.

We then proceed by assuming we have an incoming wave in the left lead, Ψ_L^0, that is known, and use the ansatz $\Psi_L = \Psi_L^0 + \Psi_L^1$, where the reflected component Ψ_L^1, as well as Ψ_C, and Ψ_R, appear only as a result of the interactions between the subsystems. The other necessary condition is that we find a retarded solution.

With these conditions, we solve for equation (4.32) yielding

$$\Psi_L^1 = \left(1 + G_L^0 V_{LC} G_C V_{LC}^\dagger\right)\Psi_L^0, \tag{4.33}$$

$$\Psi_R = G_R^0 V_{RC} G_C V_{LC}^\dagger \Psi_L^0, \tag{4.34}$$

$$\Psi_C = G_C V_{LC}^\dagger \Psi_L^0. \tag{4.35}$$

where G_C is the full green's function of the central device including the contribution from the self energies of the leads. Assuming we are in steady-state, the probability to find an electron in the device, $|\psi_C|^2$, will be conserved, and therefore

$$0 = \frac{\partial |\psi_C|^2}{\partial t} = \frac{\partial \psi_C^\dagger}{\partial t}\psi_C + \psi_C^\dagger \frac{\partial \psi_C}{\partial t}. \tag{4.36}$$

Using this condition, and the time-dependent Schrodinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \tag{4.37}$$

we find

$$\frac{\partial \psi_C}{\partial t} = -\frac{i}{\hbar}\left(V_{LC}^\dagger \psi_L + H_C \psi_C + V_{RC}^\dagger \psi_R\right), \tag{4.38}$$

with a similar expression for the hermitian conjugate. Substituting back into Eqn. 4.36 then results in an expression of the form

$$j = j_L + j_R \tag{4.39}$$

where

$$j_{i=L,R} = \frac{i}{\hbar}\left(\Psi_i^\dagger V_{iC}\Psi_C - \Psi_C^\dagger V_{iC}^\dagger \Psi_i\right), \tag{4.40}$$

which we interpret as probability currents coming from the left and right leads. The electrical current then follows from multiplying through by the charge e.

To find the current in terms of the green's functions we'll now substitute in our expressions for the wave functions above (Eqn. 4.33-4.35)). Starting with the right lead,

$$
\begin{aligned}
I_{R \to L} &= \frac{ie}{\hbar} \left(\Psi_R^\dagger V_{RC} \Psi_C - \Psi_C^\dagger V_{RC}^\dagger \Psi_R \right) \\
&= \frac{ie}{\hbar} \left(\Psi_L^{0\dagger} V_{LC} G_C^\dagger V_{RC}^\dagger \left(G_R^{0\dagger} - G_R^0 \right) V_{RC} G_C V_{LC}^\dagger \Psi_L^0 \right) \\
&= -\frac{e}{\hbar} \left(\Psi_L^{0\dagger} V_{LC} G_C^\dagger \Gamma_R G_C V_{LC}^\dagger \Psi_L^0 \right).
\end{aligned}
\tag{4.41}
$$

The full current of all possible left eigenstates is given by

$$
I = \sum_\lambda j_\lambda = \sum_\lambda \frac{e}{\hbar} \left(\Psi_{L\lambda}^{0\dagger} V_{LC} G_C^\dagger \Gamma_R G_C V_{LC}^\dagger \Psi_{L\lambda}^0 \right) f_L(E_\lambda),
\tag{4.42}
$$

the distribution function $f_L(E_\lambda)$ describes the population of the left states, the distribution function of the right lead is absent here, because we consider only the current from the left to the right.

The same current is given by the Landauer formula through the transmission function $\bar{T}(E)$

$$
I = \frac{e}{h} \int_{-\infty}^{\infty} \bar{T}(E) f_L(E) dE.
\tag{4.43}
$$

If one compares these two expressions for the current, the transmission function at some energy is obtained as

$$
\begin{aligned}
\bar{T}(E) &= 2\pi \sum_\lambda \delta(E - E_\lambda) \left(\Psi_{L\lambda}^{0\dagger} V_{LC} G_C^\dagger \Gamma_R G_C V_{LC}^\dagger \Psi_{L\lambda}^0 \right) \\
&= 2\pi \sum_\lambda \sum_\delta \delta(E - E_\lambda) \left(\Psi_{L\lambda}^{0\dagger} V_{LC} \Psi_\delta \right) \left(\Psi_\delta^\dagger G_C^\dagger \Gamma_R G_C V_{LC}^\dagger \Psi_{L\lambda}^0 \right) \\
&= \sum_\delta \left(\Psi_\delta^\dagger G_C^\dagger \Gamma_R G_C V_{LC}^\dagger \left(2\pi \sum_\lambda \delta(E - E_\lambda) \Psi_{L\lambda}^0 \Psi_{L\lambda}^{0\dagger} \right) V_{LC} \Psi_\delta \right) \\
&= \mathrm{Tr} \left(\Gamma_L G_C^\dagger \Gamma_R G_C \right)
\end{aligned}
\tag{4.44}
$$

which is equivalent to the Fisher-Lee relation. As advertised, to evaluate the sum in brackets we used the eigenfunction expansion (4.18) for the left contact.

4.4 Local current

The expression for the local current relies on the non equilibrium Green's function (NEGF) formalism, which is significantly more involved than the simple result used in the simulations. To go in depth here would take us quite far off track, so we will attempt to give a brief derivation following Jiang et al. [86] A more complete treatment of the NEGF formalism can be found in the textbooks by Ferry and Goodnick and Datta, [81, 82] as well as the more recent textbook by Di Ventra. [87]

So, for a model on the lattice, the local current originating from site **i** to **j** is given as the expectation value of the time rate of change of the local charge at that point, which is then expanded using the Heisenberg equation of motion:

$$
\begin{aligned}
J_{i \to j} &= e \left\langle \dot{N}_i \right\rangle \\
&= \frac{ie}{\hbar} \left\langle \left[H, \sum_{\alpha} N_{i\alpha} \right] \right\rangle \\
&= -\frac{e}{\hbar} \sum_{\alpha,\beta} \left[H_{i\alpha,j\beta} G^<_{i\alpha,j\beta}(t,t) - H_{j\alpha,i\beta} G^<_{i\alpha,j\beta}(t,t) \right]
\end{aligned}
\tag{4.45}
$$

where

$$
G^<_{i\alpha,j\beta}(t,t') = i \left\langle c^\dagger_{i\alpha}(t,t') c_{j\beta}(t,t') \right\rangle
\tag{4.46}
$$

is the Keldysh Green's function and α, β represent the state of the system. Taking the Fourier transform of the above, so that we go from time to energy representation, yields

$$
J_{i \to j} = -\frac{2e}{h} \sum_{\alpha,\beta} \int_{-\infty}^{\infty} Re \left[H_{i\alpha,j\beta} G^<_{i\alpha,j\beta}(E) \right]
\tag{4.47}
$$

For small applied voltages and in the zero temperature limit, which is the regime we are working in, applying the Keldysh equation

$$
G^< = G^r \left(i\Gamma_L f_L + i\Gamma_R f_R \right) G^a
\tag{4.48}
$$

allows us to split up the integral above such that

$$
\begin{aligned}
J_{i \to j} =& \frac{2e}{h} \sum_{\alpha,\beta} \int_{-\infty}^{eV_R} Im\left[G^r \left(\Gamma_L + \Gamma_R\right) G^a\right] \\
& + \frac{2e^2}{h} Im[\sum_{\alpha\beta} H_{\mathbf{i}\alpha,\mathbf{j}\beta} G^n_{\mathbf{j}\beta\mathbf{i}\alpha}(E_F)](V_L - V_R)
\end{aligned}
\tag{4.49}
$$

where V_L, V_R are the voltages at the *Lead*-L,R. α, β denote the state indices. $G^n(E_F) = G^r \Gamma_L G^a$ is electron correlation function with the line width function $\Gamma_\alpha(E_F) = i[\Sigma^r_\alpha(E_F) - (\Sigma^r_\alpha(E_F))^+]$, the Green function $G^r(E_F) = [E_F - H_{cen} - \Sigma^r_L(E_F) - \Sigma^r_R(E_F)]^{-1}$ and the Hamiltonian in the central region denoted as H_{cen}.

Because of time reversal symmetry, the first part of the equation above vanishes and thus we are left with the expression

$$
J_{\mathbf{i} \to \mathbf{j}} = \frac{2e^2}{h} Im[\sum_{\alpha,\beta} H_{\mathbf{i}\alpha,\mathbf{j}\beta} G^n_{\mathbf{j}\beta,\mathbf{i}\alpha}(E_F)](V_L - V_R)
\tag{4.50}
$$

4.5 Recursive Green's function technique

It is possible to solve Eqn. 4.31 directly, once the effects of the leads have been made finite, but this is computationally expensive and would limit the lattice sizes one can study, while also being inefficient as only part of this information is needed to find the conductance via Eqn. 4.19.

So in lieu of finding the entire Green's function in one step, we introduce the recursive Green's function technique, where the lattice is divided into smaller sections which can be computed exactly and then 'glued' together using Dyson's equation,

$$
G = g + gVG
\tag{4.51}
$$

Here, g is the Green's function of the isolated columns, which are known, V contains the hopping terms between columns and can be thought of as the perturbation, and G is the full Green's function of the connected system we are interested in.

Starting at one end of the sample then, it is possible to proceed through the entire lattice by adding one column at a time, arriving at the full Green's function for the system once the opposite end has been attached. To begin,

like Dietl, we illustrate the technique using the simplest possible case, a system consisting of just two sections (illustrated in Fig. 4.1) which we would like to connect using Dyson's equation as above. Once it is clear how to connect these two pieces, we can then move on to finding the full set of equations for the recursive Green's function technique applied to an arbitrary number of sections. So, in the basis of eigenstates for the columns, we start by projecting Dyson's equation between the first and last columns, 1 and N of the system
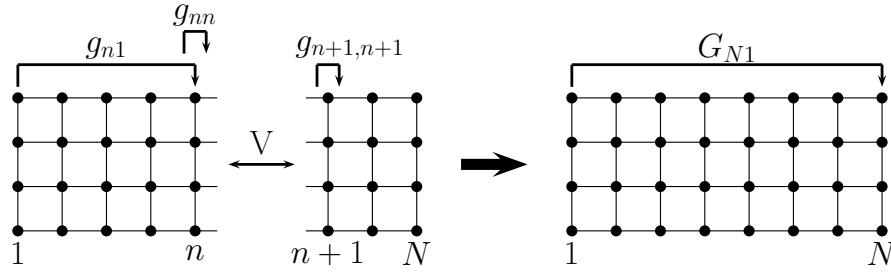

Figure 4.1: Schematic illustrating how two separate sections are joined together using Dyson's equation to give the full connected Green's function

$$
\begin{aligned}
G_{N1} &= \langle N|G|1\rangle \\
&= \langle N|g|1\rangle + \sum_{|\alpha\rangle,|\beta\rangle} \langle N|g|\alpha\rangle\langle\alpha|V|\beta\rangle\langle\beta|G|1\rangle \\
&= \langle N|g|n\rangle\langle n|V|n+1\rangle\langle n+1|G|1\rangle \\
&= g_{Nn}V_{n,n+1}G_{n+1,1}
\end{aligned}
\tag{4.52}
$$

Complete sets of lattice site states have been inserted, and we have used the fact that V has only non-zero elements between columns n and $n+1$ because we are only considering nearest neighbour hopping. Since g is only available for the disconnected system, we have also set $g_{N1} = 0$. Implied above is the splitting of the two separate pieces from 1 to n and then from $n+1$ to N. To proceed, we can repeat the above procedure to find the unknown Green's function $G_{n+1,1}$ and then again to find the closed set of equations:

$$G_{n+1,1} = g_{n+1,n+1}V_{n+1,n}G_{n1}, \qquad (4.53)$$

$$G_{n1} = g_{n1} + g_{nn}V_{n,n+1}G_{n+1,1} \qquad (4.54)$$

Substituting the second into the first and re-arranging we then have:

$$G_{n+1,1} = [1 - g_{n+1,n+1}V_{n+1,n}g_{nn}V_{n,n+1}]^{-1} g_{n+1,n+1}V_{n+1,n}g_{n1} \qquad (4.55)$$

which we can then substitute back into Eqn. 4.52 to get an expression for G_{N1} in terms of the known Green's functions for the isolated columns as desired.

With this in hand, we can now proceed to derive the full blown technique for use on an arbitrarily large system in two dimensions. For convenience, we consider a rectangular tight binding lattice with M rows and N columns, but this will be perfectly compatible with the required honeycomb lattice used for our simulations, where each column will be constructed from graphene unit cells instead of just the individual sites. The effect of the leads attached to the device is accounted for through their self energies, which will yield a finite Hamiltonian, as shown in section 4.6, and is applicable so long as the leads are attached only to the left and right edges. If they were attached centrally, then one could end up with hopping terms that were not nearest neighbour and thus the current technique would break down.

The first step is to divide the system into isolated columns, and for each of these from $i = 1, 2 ...., N$ we calculate green's function using direct inversion:

$$g_{ii}^{isol} = \left[(E + i\eta)\,\mathbb{1} - \langle i|H_D + \sum_{p=L,R} \Sigma_p |i\rangle \right]^{-1} \qquad (4.56)$$

where for the first and last columns, we have included the self-energy of the leads. We then start adding the columns one by one from the left to build the complete device, as shown in Fig. 4.2.

If we imagine that the first n columns have been attached and we have the Green's functions G_{n1}^L and G_{nn}^L, the Green's functions $G_{n+1,1}^L$ and $G_{n+1,n+1}^L$ can then be derived by projecting Dyson's equation (Eqn. 4.51) between the appropriate columns as shown above. The results are as follows:
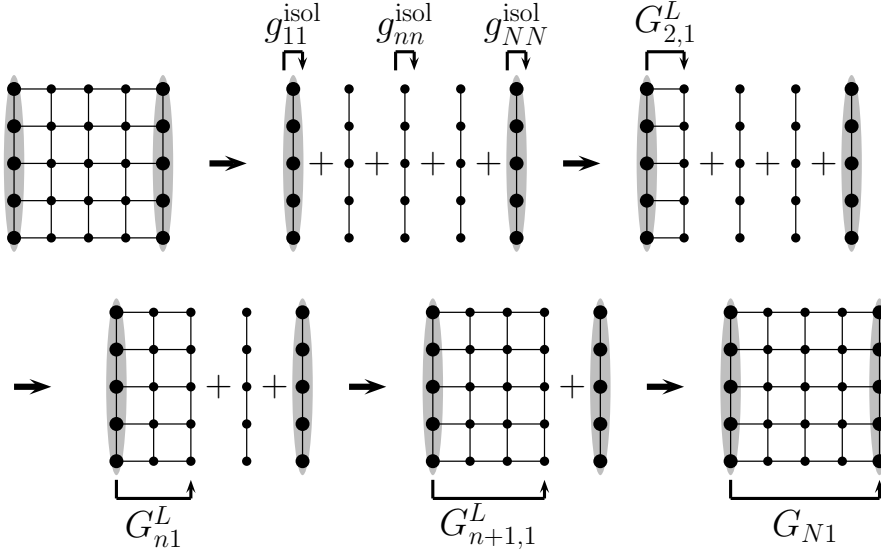
Figure 4.2: Schematic illustrating the full recursive Green's function technique where the device is stitched together from left to right until the propagator between the first and last columns is obtained.

$$G^L_{n+1,n+1} = \left[\mathbb{1} - g^{isol}_{n+1,n+1} V_{n+1,n} G^L_{n,n} V_{n,n+1} \right]^{-1} g^{isol}_{n+1,n+1}$$
$$G^L_{n+1,1} = G^L_{n+1,n+1} V_{n+1,n} G^L_{n,1}$$

Starting from the far left side with $n = 1$ and $G^L_{1,1} = g^{isol}_{1,1}$, it is then possible to proceed through the entire sample in this manner. After the last column has been connected we have $G^L_{N1} = G_{N1}$, and our work is done. These set of steps give us all that is required to describe transport phenomena within the Landauer-Buttiker formalism.

To deal with describing the current across a sample, we'll require an extension on this technique, which we now address. Above, we have found only G_{N1}, which was all we needed for the overall conductance. However, for local properties we'll require G_{n1} for any n, as can be seen from Eqn. 4.50 below.

The procedure starts from the right side of the device, stitching the Green's functions for the isolated columns together with Dyson's equation

as was done above. At each step, G_{nn}^R is given in terms of $G_{n+1,n+1}^R$ as follows:

$$G_{nn}^R = \left[\mathbb{1} - g_{nn}^{isol} V_{n,n+1} G_{nn}^R V_{n+1,n}\right]^{-1} g_{nn}^{isol} \qquad (4.57)$$

To start off, we set $G_{NN}^R = G_{NN}^{isol}$, and then apply the above for all $n = N - 1, N - 2, ..., 1$. From here, we can find the final set of Green's functions by stitching together the G^L and G^R in pairs, attaching a strip of connected columns 1 to n with known Green's functions G_{n1}^L and G_{nn}^L to the strip of columns $N + 1$ to N with known Green's functions $G_{n+1,n+1}^R$. Again, this is done for all $n = 1, ..., N$ leading to the expression

$$G_{n1} = \left[\mathbb{1} - G_{nn}^L V_{n,n+1} G_{n+1,n+1}^R V_{n+1,n}\right]^{-1} G_{n1}^L \qquad (4.58)$$

4.6 Surface Green's function

As discussed in section 4.3, to incorporate the effect of the leads we need to find the surface Green's functions. Finding the analytic solution is possible in most cases, but we will rely on a numeric technique to achieve the same end. For an isolated lead, the total retarded Green's function looks the same as Eqn. 4.10

$$g(E) = \left[(E + i\eta)\mathbb{1} - H_l\right]^{-1} \qquad (4.59)$$

The fact that these leads are perfect conductors in the Landauer-Buttiker formalism, and thus translationally invariant, means we can write the Hamiltonian in block diagonal form

$$(E + i\eta)\mathbb{1} - H_l = \begin{pmatrix} d & -A & 0 & 0 & \cdots \\ -B & D & -A & 0 & \cdots \\ 0 & -B & D & -A & \cdots \\ \vdots & 0 & -B & D & \ddots \\ & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \qquad (4.60)$$

where d, D, A and B are all $2M \times 2M$ matrices, with M being the width of the lead and the factor of 2 coming from spin. The matrix D contains the hoppings for a single isolated column, with A and B providing the hopping between neighbouring columns. The matrix d has been singled out because it contains the hoppings for the surface of the lead, but it is identical to D. If the total Green's function is then partitioned in a similar way, consisting

of $2M \times 2M$ submatrices, we can re-write the above as follows:

$$\begin{pmatrix} d & -A & 0 & 0 & \cdots \\ -B & D & -A & 0 & \cdots \\ 0 & -B & D & -A & \cdots \\ \vdots & 0 & -B & D & \ddots \\ & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \cdot \begin{pmatrix} g_{11} & g_{12} & g_{13} & \cdots \\ g_{21} & g_{22} & g_{23} & g_{24} & \cdots \\ g_{31} & g_{32} & g_{33} & g_{34} & \cdots \\ \vdots & g_{42} & g_{43} & g_{44} & \ddots \\ & \vdots & \vdots & \ddots & \ddots \end{pmatrix} = \mathbb{1} \quad (4.61)$$

If we then focus on the first column of the matrix product, we end up with an infinite set of equations for g_{11}, the surface Green's function:

$$dg_{11} = 1 + Ag_{21}, \quad (4.62)$$

$$Dg_{p1} = Bg_{p-1,1} + Ag_{p+1,1}, \quad \forall p \geq 2. \quad (4.63)$$

Thus, it appears that in order to find g_{11} we would need to know all matrices g_{p1} with $p \geq 2$. However, using the second equation, we can express the Green's functions g_{p1} with even indices $p = 2r$ ($r = 1, 2, ...$) as a function of the Green's functions with odd indices:

$$g_{2r,1} = D^{-1}Bg_{2r-1,1} + D^{-1}Ag_{2r+1,1} \quad (4.64)$$

Inserting this expression back into Eqn. 4.62, we can then write g_{11} as a function of only the g_{p1} with p odd:

$$\left(d - AD^{-1}B\right) g_{11} = 1 + \left(AD^{-1}A\right) g_{31} \quad (4.65)$$

$$\left(D - AD^{-1}B - BD^{-1}A\right) g_{2r+1,1} = \left(BD^{-1}B\right) g_{2r-1,1} + \left(AD^{-1}A\right) g_{2r+3,1} \quad (4.66)$$

Comparing these equations with the original expressions in Eqn. 4.62, they can be seen to have the same form if we define the following set of

renormalized matrices:

$$d' = d - AD^{-1}B,$$
$$D' = D - AD^{-1}B - BD^{-1}A,$$
$$A' = AD^{-1}A, \tag{4.67}$$
$$B' = BD^{-1}B,$$
$$g'_{r,1} = g_{2r-1,1}, \quad r = 2, 3...$$

And so it is possible to iterate this procedure again and again, which will eventually allow us to arrive at an approximation for the surface Green's function as the effective interaction A' becomes vanishingly small. The equation for g_{11} after n iterations looks as follows:

$$d_n g_{11} = 1 + A_n g_{2^n+1,1} \tag{4.68}$$

and once A_n vanishes for sufficiently large n, we have the approximation for the surface Green's function:

$$g_{11} \approx d_n^{-1} \tag{4.69}$$