# Chapter 4

# Green's function formalism

Having a numerical representation of the system in terms of a tight-binding model, one still needs a mathematical framework within which different physical properties can be calculated. Green's functions can be a valuable tool in this respect. One of their advantages is the relative ease with which they can be calculated, compared to a direct numerical solution of the Schrödinger equation. In particular, a very efficient recursive method is available for obtaining the Green's functions necessary for the evaluation of the transmission coefficients in the Landauer-Büttiker formalism [2, 31]. This method will be discussed in some detail in the current chapter, where parts of the discussion will follow Refs. [2, 31]. We will also show how to extend this standard recursive technique, allowing for an extra set of Green's functions to be calculated with the same high efficiency. With this larger set of Green's functions, a wider range of physical properties comes in our reach, but it will also allow us to do certain calculations in the next chapters more efficiently.

## 4.1 Green's functions: The basics

In quantum physics, the single-particle Green's function operator $\widehat{G}(E)$ of a system described by a Hamiltonian $\widehat{H}$ can be defined as the solution to the operator equation [2, 31, 46]

$$\left[E - \widehat{H}\right] \widehat{G}(E) = 1, \tag{4.1}$$

A formal solution to this equation would be given by $\widehat{G}(E) = (E - \widehat{H})^{-1}$. However, such a solution is not well defined for values of $E$ corresponding to the eigenvalues of the Hamiltonian. This subtlety can be appreciated more when going to the position-spin representation of Eq. (4.1):

$$\left[E - H(\mathbf{x})\right] G(\mathbf{x}, \mathbf{x}', E) = \delta(\mathbf{x} - \mathbf{x}'). \tag{4.2}$$

The vector $\mathbf{x}$ contains both the position and spin variables $\mathbf{x} = (\mathbf{r}, \sigma)$, and the function

$$G(\mathbf{x}, \mathbf{x}', E) = \langle\, \mathbf{x} | \widehat{G}(E) | \mathbf{x}' \,\rangle \tag{4.3}$$

is called the Green's function of the system. From Eq. (4.2), it can be seen that the Green's function can be considered as a wavefunction at $\mathbf{r}$ resulting from a unit excitation at $\mathbf{r}'$. But on the other hand, $G$ can also be considered as the source for such an excitation. Both solutions satisfy Eq. (4.2), but they correspond to different boundary conditions: if $H$ would be the Hamiltonian for a particle moving in a constant potential, then the first solution would correspond to an outgoing wave from the point $\mathbf{r}'$, while the second solution would be an incoming wave. In order to incorporate such boundary conditions into a unique definition for the Green's function, one adds an infinitesimal imaginary variable into the energy, which leads to the following definitions:

$$G^{\pm}(\mathbf{x}, \mathbf{x}', E) \equiv \lim_{\eta \to 0^+} G(\mathbf{x}, \mathbf{x}', E \pm \mathrm{i}\eta), \tag{4.4}$$

where the functions $G^{\pm}$ satisfy

$$\left[E \pm \mathrm{i}\eta - H(\mathbf{x})\right] G^{\pm}(\mathbf{x}, \mathbf{x}', E) = \delta(\mathbf{x} - \mathbf{x}'). \tag{4.5}$$

The functions $G^+$ and $G^-$ are called respectively the retarded and advanced Green's function. In the example given above, the retarded Green's function would correspond to the outgoing wave and the advanced Green's function to the incoming wave. More generally, when Fourier transforming the functions $G^{\pm}$ to the time domain using a closed contour integration in the complex plane, they would correspond to causal and anticausal solutions [47].

In the operator language, the retarded and advanced Green's function operators are defined uniquely for all real values of $E$ by the relation

$$\widehat{G}^{\pm}(E) \equiv \lim_{\eta \to 0^+} \frac{1}{E \pm \mathrm{i}\eta - \widehat{H}}, \tag{4.6}$$

and they can thus essentially be calculated by inverting the Hamiltonian.

In the next sections, we will stop writing the hat in $\widehat{G}$ to denote an operator. It will be clear from the context whether $G$ stands for a function (or a matrix in a discrete system) or an operator. We will also drop the subscript $\pm$ for distinguishing between the retarded or advanced Green's function: $G$ will always stand for a retarded Green's function. From Eq. (4.6), it is clear that the advanced Green's function corresponds to the hermitian conjugate of the retarded one, i.e., $G^- = (G^+)^\dagger \equiv G^\dagger$.

## 4.2 Transmission coefficients and the Green's function

In the Landauer-Büttiker formalism presented in Chap. 2, a central device is connected to perfect leads, and its current-voltage characteristics can be expressed in terms of transmission coefficients between those leads. These transmission coefficients can be related to the Green's function of the central device, thereby justifying the effort we will make in the next sections to find this Green's function. We will

suffice with merely stating this relation here, since it is standard nowadays, and since a thorough derivation would take us too far[1]. In a tight-binding representation of the system, the transmission coefficient between leads $p$ and $q$ is given by [2, 49]:

$$T_{pq} = \mathrm{Tr}\Big[\Gamma_p G_{pq} \Gamma_q G_{pq}^\dagger\Big]. \tag{4.7}$$

The Green's function $G_{pq}$ in this expression is a submatrix of the Green's function $G$ of the whole system: it contains only the elements of $G$ between sites in the central device that connect to leads $p$ and $q$: in particular, if $\mathcal{P}_{p(q)}$ is a projection operator onto the sites of the central device to which lead $p$ ($q$) is connected, then

$$G_{pq} = \mathcal{P}_p \, G \, \mathcal{P}_q. \tag{4.8}$$

The matrix $\Gamma_p$ in Eq. (4.7) is the so-called broadening function of lead $p$. It is given in terms of what is known as the self-energy $\Sigma_p$ of the lead:

$$\Gamma_p = \mathrm{i}\big(\Sigma_p - \Sigma_p^\dagger\big). \tag{4.9}$$

This self-energy is related to elements of the Green's function between sites at the surface of the lead. The exact definition, and a more detailed discussion of these self-energies will be given in the next section [see Eq. (4.13].

## 4.3 Lattice Green's function method

One could have the impression that all has been said already about the Green's function technique: one just derives the tight-binding Hamiltonian of the system, writes it out in matrix form, and calculates the Green's function by inverting the matrix $E + \mathrm{i}\eta - H$. Physical quantities, like the transmission coefficients of the Landauer-Büttiker formalism, can then be calculated by expressing them in terms of this Green's function.

However, since we are concerned with an open system (there are semiinfinite leads connected to the sample), the tight-binding Hamiltonian matrix describing the complete system has infinite dimension and cannot be inverted numerically. Furthermore, even if one is able to truncate the Hamiltonian matrix, its direct inversion turns out to be numerically very expensive. These issues will be addressed in the current section. During the discussion, we will use quite often the notation $G_{nn'}$ to denote a submatrix of the total Green's function matrix $G$. $G_{nn'}$ "connects" sites of columns $n$ and $n'$, i.e.,

$$\langle\, m, \sigma | G_{nn'}(E) | m', \sigma' \,\rangle = G_{nm\sigma, n'm'\sigma'}(E) = \langle\, nm\sigma | G(E) | n'm'\sigma' \,\rangle, \tag{4.10}$$

where $(m, n)$ label the sites in the tight-binding lattice, and $\sigma, \sigma'$ are the spin indices.

[1] The interested reader can find such a derivation in Ref. [48].

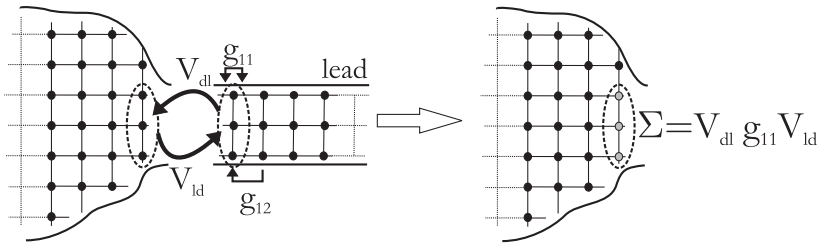


**Figure 4.1:** The influence of a lead can be described by adding its self-energy to the Hamiltonian of the device.

### 4.3.1 Semiinfinite leads: Self-energy description

Within the Landauer-Büttiker formalism, the system is composed of a central device connected to leads (see Fig. 2.1), and its Hamiltonian can therefore be subdivided as:

$$H = H_{cd} + \sum_i \left(H_l^i + V_{ld}^i + V_{dl}^i\right). \tag{4.11}$$

$H_{cd}$ is the Hamiltonian for the central device, and $H_l^i$ the Hamiltonian for lead $i$. The coupling between lead and device is described by $V_{ld}^i$ (and its hermitian conjugate $V_{dl}^i$). A direct inversion $\left[E + \mathrm{i}\eta - H\right]^{-1}$ to obtain the Green's function is numerically impossible, since every $H_l^i$ has infinite dimension.

The standard way to resolve this problem consists of describing the lead influence by a self-energy term: it can be shown (see, e.g., Refs. [2, 31]) that the central device, including the influence of the leads on it, is described by a *finite-dimensional* Hamiltonian

$$\mathcal{H}_{cd} = H_{cd} + \sum_i \Sigma^i, \tag{4.12}$$

where $\Sigma^i$ is called the (retarded) self-energy[2] of lead $i$:

$$\Sigma^i = V_{dl}^i \, g_l^i \, V_{ld}^i. \tag{4.13}$$

The quantity $g_l^i$ in this expression is the Green's function of the isolated semiinfinite lead: $g_l^i = [E + \mathrm{i}\eta - H_l^i]^{-1}$. At first sight it seems that the problem is just shifted, since now the calculation of $g_l^i$ will involve the inversion of the infinite-dimensional Hamiltonian $H_l^i$. However, since a nearest-neighbor tight-binding model is used, the matrices $V_{dl}^i$ and $V_{ld}^i$ have nonzero elements only between sites on the surface of the lead and their neighboring sites in the device. This means that only the surface Green's function $(g_l^i)_{11}$ is needed in Eq. (4.13) (see also Fig. 4.1), and

[2] In many-body physics, self-energy terms are sometimes introduced to describe coupling of the system to phonons or to describe many-body interactions [47]. In these cases, the self-energies are usually only calculated up to some order in perturbation theory, so that the Hamiltonian one obtains is only an approximation. However, in our case the truncation of the device Hamiltonian by describing the influence of the leads by their self-energies is exact: no approximations whatsoever are made.

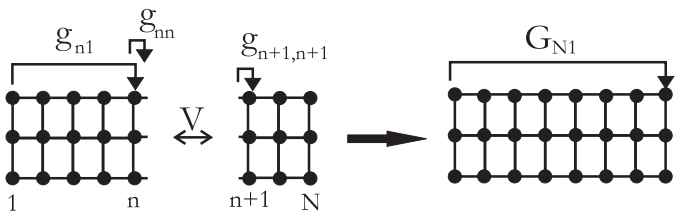


**Figure 4.2:** Attaching two isolated sections with Dyson's equation to obtain Green's functions for the connected system.

the point is that several methods are at our disposal for calculating this Green's function: in the absence of a magnetic field it is known analytically [2], while in the case of a magnetic field one can resort to several numerical methods (see, e.g., Refs. [50, 51]). The particular method we have used will be explained in Appendix B, in order not to drown the reader into a too dense technical discussion at this point.

Now, if the central device comprises $C$ lattice sites, the Hamiltonian $\mathcal{H}_{cd}$ in Eq. (4.12) can be represented by a $2C \times 2C$ matrix (the factor 2 arises from spin) and the corresponding Green's function can in principle be obtained from

$$G_{cd} = \left[E + \mathrm{i}\eta - \mathcal{H}_{cd}\right]^{-1}. \tag{4.14}$$

Nevertheless, the number of floating point operations necessary to invert a $2C \times 2C$ matrix scales as $(2C)^3$, and therefore the inversion in Eq. (4.14) puts heavy constraints on the numerically reachable system size. Fortunately, more efficient recursive methods exist for obtaining $G_{cd}$, and these will form the subject of the next sections.

### 4.3.2 Recursive technique: Standard method

Recursive methods for the evaluation of Green's functions are based upon the division of the device in smaller sections of which the Green's functions can be calculated easily. These sections are then "glued together" by using the so-called Dyson's equation [47],

$$G = g + g\,V\,G, \tag{4.15}$$

which allows to relate the Green's function $g$ of two disconnected subsystems to the Green's function $G$ of the connected system, where V describes the hopping between the subsystems.

Before embarking upon a detailed discussion of the recursive Green's function technique, we will illustrate the use of Dyson's equation with an example, depicted in Fig. 4.2. Consider a system consisting of two parts, and suppose that we have access to the Green's function $g$ describing the *isolated* parts. Now we would like to obtain $G_{N1}$, i.e., elements of the Green's function between the first and last column

of the *coupled* device. This can be done by projecting Eq. (4.15) between columns $N$ and 1:

$$\begin{aligned} G_{N1} &= \langle\, N|G|1\,\rangle && \text{(4.16a)} \\ &= \langle\, N|g|1\,\rangle + \sum_{|\alpha\,\rangle,|\beta\,\rangle} \langle\, N|g|\alpha\,\rangle\langle\, \alpha|V|\beta\,\rangle\langle\, \beta|G|1\,\rangle && \text{(4.16b)} \\ &= \langle\, N|g|n\,\rangle\, \langle\, n|V|n+1\,\rangle\, \langle\, n+1|G|1\,\rangle && \text{(4.16c)} \\ &= g_{Nn}\, V_{n,n+1}\, G_{n+1,1}. && \text{(4.16d)} \end{aligned}$$

Equation (4.16c) is obtained by noting that the hopping matrix $V$ between the disconnected systems has only nonzero elements between columns $n$ and $n+1$ in our nearest neighbor tight-binding model. Furthermore, we have $g_{N1} = 0$ since $g$ is for the disconnected system only. We can proceed now to find the unknown $G_{n+1,1}$ in Eq. (4.16d) by taking again the appropriate matrix elements of Dyson's equation. This procedure can be continued until we have found a closed set of equations. We immediately write down the resulting equations:

$$\begin{aligned} G_{n+1,1} &= g_{n+1,n+1}\, V_{n+1,n}\, G_{n1}, \quad \text{with} && \text{(4.17a)} \\ G_{n1} &= g_{n1} + g_{nn}\, V_{n,n+1}\, G_{n+1,1}. && \text{(4.17b)} \end{aligned}$$

From these equations, we obtain:

$$G_{n+1,1} = \Big[1 - g_{n+1,n+1}\, V_{n+1,n}\, g_{nn}\, V_{n,n+1}\Big]^{-1} g_{n+1,n+1}\, V_{n+1,n}\, g_{n1}. \qquad (4.18)$$

Substituting this in Eq. (4.16d), we will get an expression for $G_{N1}$ in terms of Green's functions for the isolated sections, which was our initial goal.

We now have enough technical luggage to proceed to the recursive Green's function technique [31, 52]. In the following, we will consider a central device discretized on a rectangular tight-binding lattice consisting of $M$ rows and $N$ columns (Fig. 4.3). The influence of the leads that are attached to this central device will be described by their self-energy, giving rise to a finite-dimensional Hamiltonian $\mathcal{H}_{cd}$ for the device, as discussed in the preceding section. It will be assumed that all leads are attached at the left and right edges of the central device so that their self-energies only influence sites of the first and last column of the device (depicted gray in the figures). If this would not be the case, self-energy terms could introduce an effective hopping between lattice columns that are not nearest neighbors, and in this case the recursive technique cannot be applied: in the example above, $V$ would have nonzero contributions between columns different from $n$ and $n+1$, leading to much more complicated expressions in Eq. (4.16c).

A wide range of physical quantities of such a system can be written in terms of the small subset of Green's function matrices that is depicted in Fig. 4.3: it concerns elements of the Green's function between the first/last column of the device and any intermediate column. The first step towards calculating these consists of separating

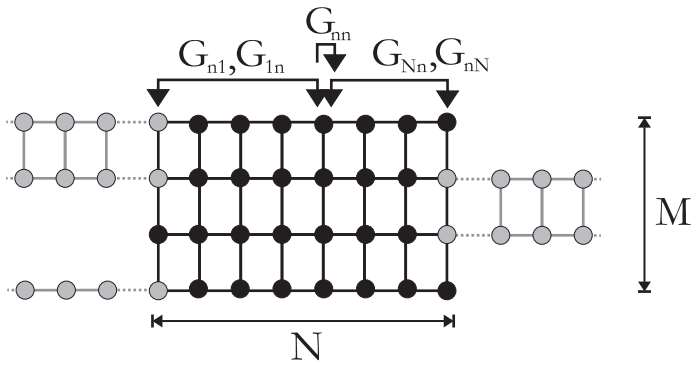


**Figure 4.3:** Subset of device Green's functions needed for calculating the physical quantities of interest. Leads attached to the central device are depicted in gray.

the device in isolated columns, and calculating the Green's function $G_{ii}^{\text{isol}}$ for every isolated column $i = 1, 2, ..., N$ by doing a direct inversion:

$$G_{ii}^{\text{isol}} = \Big[E + \mathrm{i}\eta - \langle\, i|\mathcal{H}_{cd}|i\,\rangle\Big]^{-1}, \tag{4.19}$$

where $\langle\, i|\mathcal{H}_{cd}|i\,\rangle$ is the tight-binding Hamiltonian of column $i$. This step is depicted in Fig. 4.4(a).

The next step consists of assembling the complete device by gluing together the columns one by one, as shown in Fig. 4.4(b). Suppose we already have the Green's functions $G_{n1}^L$, $G_{1n}^L$, $G_{nn}^L$ of a strip of $n$ columns connected together. The superscript $L$ is added to denote the fact that they only represent a part of the device (namely a strip of $n$ columns), not the whole device. The Green's functions $G_{n+1,1}^L, G_{1,n+1}^L$, and $G_{n+1,n+1}^L$ for a section of $n+1$ columns can then be derived by projecting Dyson's equation [Eq. (4.15)] between the appropriate columns, in a similar way to what has been done in the simple example discussed above. We will only state the end result here:

$$G_{n+1,n+1}^L = \Big[1 - G_{n+1,n+1}^{\text{isol}}\, V_{n+1,n}\, G_{n,n}^L\, V_{n,n+1}\Big]^{-1} G_{n+1,n+1}^{\text{isol}}, \tag{4.20a}$$

$$G_{n+1,1}^L = G_{n+1,n+1}^L\, V_{n+1,n}\, G_{n,1}^L, \tag{4.20b}$$

$$G_{1,n+1}^L = G_{1n}^L\, V_{n,n+1}\, G_{n+1,n+1}^L. \tag{4.20c}$$

Starting from the leftmost column $n = 1$ with $G_{1,1}^L = G_{1,1}^{\text{isol}}$, one can proceed in this way through the whole sample and calculate the $G_{n1}^L$, $G_{1n}^L$ and $G_{nn}^L$ for all $n$. After connecting the last column, one obtains the Green's function submatrices $G_{N1}^L = G_{N1}$ and $G_{1N}^L = G_{1N}$ connecting the first and last column of the complete device. These steps complete the *standard* recursive Green's function method [31, 52], and they suffice for describing transport quantities within the Landauer-Büttiker formalism. Indeed, all leads are connected to the left or right edge of the system,

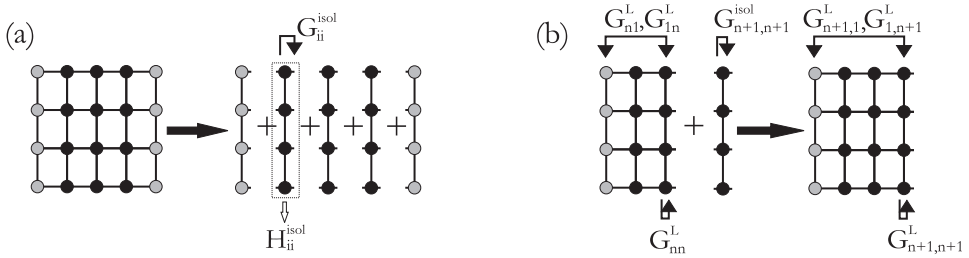


**Figure 4.4:** Standard recursive technique. The device is divided into its separate columns (a), and Dyson's equation is used to glue them together and to find the relevant Green's functions (b).

and the relation in Eq. (4.7) thus expresses the transmission coefficients in terms of the Green's functions $G_{N1}$ or $G_{1N}$.

Looking back at the Eqs. (4.19)-(4.20), one can see that the computational operations necessary for obtaining the final Green's functions are either products or inversions of $2M \times 2M$ matrices, and the total amount of such operations is proportional the length $N$ of our system. Since the computational effort for a matrix product or inversion scales as $(2M)^3$ in the number of floating point operations, the total numerical effort for the recursive technique scales as $M^3N$ for large systems ($N \gg 1$). In this way, we gain a factor of $N^2$ in efficiency compared to the direct inversion of the complete $(2MN) \times (2MN)$ matrix $E + \mathrm{i}\eta - \mathcal{H}_{cd}$, which scaled as $M^3N^3$. The price one has to pay for the increased efficiency is that one can only calculate a smaller subset of Green's functions (direct inversion would give us $G_{nn'}$ for all $n, n'$).

### 4.3.3 Recursive technique: An extension

We have extended the standard recursive technique in order to obtain the additional Green's functions $G_{Nn}$, $G_{nN}$, $G_{n1}$, $G_{1n}$ and $G_{nn}$ depicted in Fig. 4.3. Having such functions available will prove to be convenient in the next chapters.

We proceed as follows. After having completed the standard technique, we start over from the Green's functions of the isolated columns, and glue them together as we did previously on the basis of Dyson's equation, but now beginning from the right column. This is depicted in Fig. 4.5(a). The Green's functions we calculate with every step are $G^R_{Nn}$, $G^R_{nn}$ and $G^R_{nN}$. They can be given in terms of the $G^R_{N,n+1}$, $G^R_{n+1,n+1}$ and $G^R_{n+1,N}$ as:

$$G^R_{nn} = \left[1 - G^{\text{isol}}_{nn}\, V_{n,n+1}\, G^R_{n+1,n+1}\, V_{n+1,n}\right]^{-1} G^{\text{isol}}_{nn}, \tag{4.21a}$$

$$G^R_{Nn} = G^R_{N,n+1}\, V_{n+1,n}\, G^R_{n,n}, \tag{4.21b}$$

$$G^R_{nN} = G^R_{nn}\, V_{n,n+1}\, G^R_{n+1,N}. \tag{4.21c}$$

Starting from $G^R_{NN} = G^{\text{isol}}_{NN}$, one can obtain $G^R_{Nn}$, $G^R_{nN}$ and $G^R_{nn}$ for all $n =$

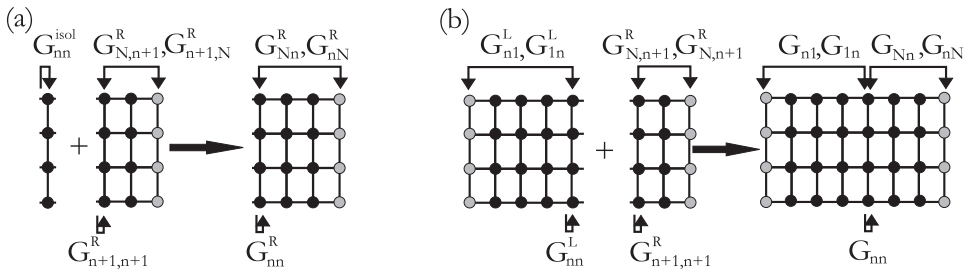


**Figure 4.5:** Extension of the standard recursive technique. The isolated columns are glued together, but now starting from the righthand side (a). The final step consists of adding these strips of columns to the ones calculated in Fig. 4.4 (b).

$N-1, N-2, ..., 1$. Again, the superscript $R$ has been added to denote that these are Green's functions for a subsection of the complete device.

The final step consists of attaching the previously calculated Green's functions $G^L$ and $G^R$ in pairs, as illustrated in Fig. 4.5(b). One attaches a strip of connected columns 1 to $n$ (with known Green's functions $G^L_{n1}$ and $G^L_{nn}$) to the strip of columns $n+1$ to $N$ (with Green's functions $G^R_{N,n+1}$ and $G^R_{n+1,n+1}$), and this is done for all $n = 1, ..., N$. Again, projection of Dyson's equation leads to the relevant mathematical expressions:

$$G_{n1} = \left[1 - G^L_{nn}\, V_{n,n+1}\, G^R_{n+1,n+1}\, V_{n+1,n}\right]^{-1} G^L_{n1}, \tag{4.22a}$$

$$G_{1n} = G^L_{1n} + G^L_{1n}\, V_{n,n+1}\, G^R_{n+1,n+1}\, V_{n+1,n}\, G_{nn}, \tag{4.22b}$$

$$G_{nn} = \left[1 - G^L_{nn}\, V_{n,n+1}\, G^R_{n+1,n+1}\, V_{n+1,n}\right]^{-1} G^L_{nn}, \tag{4.22c}$$

$$G_{Nn} = G^R_{N,n+1}\, V_{n+1,n}\, G_{n,n}, \tag{4.22d}$$

$$G_{nN} = G_{nn}\, V_{n,n+1}\, G^R_{n+1,N}, \tag{4.22e}$$

Both these additional steps consist of doing a number of matrix multiplications and inversions that scales linear in $N$. The numerical computation of the extra Green's functions with our extended recursive method thus has the same efficiency as the standard technique.

Having access to these extra Green's functions will prove to be very convenient in the following chapters: it will allow us to obtain quantities like the current density distribution, and furthermore, certain calculations can be done with greater efficiency than with the standard Green's functions $G_{N1}$ and $G_{1N}$ alone.