From S. Datta,
Electronic Transport in Mesoscopic systems, Cambridge 1997

3.3 Green's functions: a brief introduction

The S-matrix tells us the response at one lead due to an excitation at another. The Green's function is a more powerful concept that gives us the response at any point (inside or outside the conductor) due to an excitation at any other. For non-interacting transport, the only excitations we need to worry about are those due to waves incident from the leads. For such excitations, the Green's function and the S-matrix are related concepts and what we use is largely a matter of taste (we will derive their relationship in Section 3.4). The real power of Green's functions is evident when we try to include the effect of interactions (electron–electron or electron–phonon), as we will do in Chapter 8. Such interactions give rise to excitations within the conductor, and cannot be described by simple S-matrices.

In this chapter we will restrict our discussion to non-interacting transport. For non-interacting transport, the language of Green's function is really not necessary and our main purpose in introducing it is that it provides a useful practical tool for computing the S-matrix of arbitrarily shaped conductors (Section 3.5). Besides it is useful in relating the scattering viewpoint to other viewpoints that are widely used in the literature (Sections 3.6–3.8).

In this section we will briefly summarize some properties of the Green's function that we will need for our discussion. The concept of Green's functions appears in many physical contexts including circuit theory, electrostatics and electromagnetics. Whenever the response R is related to the excitation S by a differential operator D_{op}

$$\mathrm{D}_{\mathrm{op}} R = S$$

we can define a Green's function and express the response in the form

$$R = \mathrm{D}_{\mathrm{op}}^{-1} S = GS \quad \text{where} \quad G \equiv \mathrm{D}_{\mathrm{op}}^{-1}$$

Our problem can be expressed in the form

$$\left[E - H_{\mathrm{op}}\right]\Psi = S$$

where Ψ is the wavefunction and S is an equivalent excitation term due to a wave incident from one of the leads. The corresponding Green's function can be written as

$$G = \left[E - H_{\mathrm{op}}\right]^{-1} \tag{3.3.1}$$

where H_{op} is the Hamiltonian operator (see Eq.(1.2.2), the subband energy E_s has been included as part of the potential $U(x,y)$):

$$H_{\mathrm{op}} \equiv \frac{(\mathrm{i}\hbar\nabla + e\mathbf{A})^2}{2m} + U(\mathbf{r}) \tag{3.3.2}$$

Retarded and advanced Green's functions

The inverse of a differential operator is not uniquely specified till we specify the boundary conditions. It is common to define two different Green's functions (retarded and advanced) corresponding to two different boundary conditions. The difference is best appreciated with a simple example.

Consider a simple one-dimensional wire with a constant potential energy U_0 and zero vector potential. From Eqs.(3.3.1) and (3.3.2) we can write

$$G = \left[E - U_0 + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]^{-1}$$

that is,

$$\left(E - U_0 + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right) G(x,x') = \delta(x - x') \tag{3.3.3}$$

This looks just like the Schrödinger equation

$$\left(E - U_0 + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi(x) = 0$$

except for the source term $\delta(x - x')$ on the right. We could view the Green's function $G(x,x')$ as the wavefunction at x resulting from a unit excitation applied at x'. Physically we expect such an excitation to give rise to two waves traveling outwards from the point of excitation, with amplitudes A^+ and A^- as shown in Fig. 3.3.1.

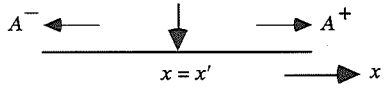

Fig. 3.3.1. Retarded Green's function for an infinite 1-D wire.

We can write

$$G(x,x') = A^+ \exp\left[ik(x-x')\right], \quad x > x'$$
$$G(x,x') = A^- \exp\left[-ik(x-x')\right], \quad x < x' \tag{3.3.4}$$

where $k = [2m(E-U_0)]^{1/2}/\hbar$. Regardless of what A^+ and A^- might be, this solution satisfies Eq.(3.3.3) at all points other than $x = x'$. In order to satisfy Eq.(3.3.3) at $x = x'$, the Green's function must be continuous

$$\left[G(x,x')\right]_{x=x'^+} = \left[G(x,x')\right]_{x=x'^-} \tag{3.3.5a}$$

while the derivative must be discontinuous by $2m/\hbar^2$.

$$\left[\frac{\partial G(x,x')}{\partial x}\right]_{x=x'^+} - \left[\frac{\partial G(x,x')}{\partial x}\right]_{x=x'^-} = \frac{2m}{\hbar^2} \tag{3.3.5b}$$

Substituting for $G(x,x')$ from Eq.(3.3.4) into Eq.(3.3.5), we obtain

$$A^+ = A^- \quad \text{and} \quad ik\left[A^+ + A^-\right] = \frac{2m}{\hbar^2}$$

Hence
$$A^+ = A^- = -\frac{\mathrm{i}}{\hbar v} \quad \text{where} \quad v \equiv \frac{\hbar k}{m} \tag{3.3.6}$$

and the Green's function is given by

$$G(x,x') = -\frac{\mathrm{i}}{\hbar v}\exp\left[ik\left|x-x'\right|\right]$$

It is important to note that there is another solution

$$G(x,x') = +\frac{\mathrm{i}}{\hbar v}\exp\left[-ik\left|x-x'\right|\right]$$

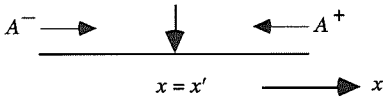

Fig. 3.3.2. Advanced Green's function for an infinite 1-D wire.

which satisfies Eq.(3.3.3) just as well. This solution consists of incoming waves that disappear at the point of excitation (Fig. 3.3.2) rather than outgoing waves that originate at the point of excitation (Fig. 3.3.1). The two solutions are referred to as the advanced Green's function (G^{A}) and the retarded Green's function (G^{R}):

$$G^{\mathrm{R}}(x,x') = -\frac{\mathrm{i}}{\hbar v}\exp\left[ik\left|x-x'\right|\right] \tag{3.3.7}$$

and
$$G^{\mathrm{A}}(x,x') = +\frac{\mathrm{i}}{\hbar v}\exp\left[-ik\left|x-x'\right|\right]$$

where
$$k \equiv \frac{\sqrt{2m(E-U_0)}}{\hbar} \quad \text{and} \quad v \equiv \frac{\hbar k}{m}$$

Both these solutions satisfy the same equation (Eq.(3.3.3)) but they correspond to different *boundary conditions*: the retarded function corresponds to outgoing waves while the advanced function corresponds to incoming waves (far away from the source).

The infinitesimal η

One way to incorporate the boundary conditions into the equation itself is to add an infinitesimal imaginary part to the energy. Instead of Eq.(3.3.3) we write ($\eta > 0$)

$$\left(E - U_0 + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \mathrm{i}\eta\right) G^{\mathrm{R}}(x,x') = \delta(x-x')$$

for the retarded function. The small imaginary part of the energy introduces a positive imaginary component to the wavenumber.

$$k' = \frac{\sqrt{2m(E+\mathrm{i}\eta-U_0)}}{\hbar} = \frac{\sqrt{2m(E-U_0)}}{\hbar}\sqrt{1+\frac{\mathrm{i}\eta}{E-U_0}}$$
$$\approx \frac{\sqrt{2m(E-U_0)}}{\hbar}\left[1+\frac{\mathrm{i}\eta}{2(E-U_0)}\right] \equiv k(1+\mathrm{i}\delta)$$

This imaginary part makes the advanced function grow indefinitely as we move away from the point of excitation. This makes the retarded function the only acceptable solution, since a proper solution must be bounded.

Similarly the advanced function is the only acceptable solution of the equation ($\eta > 0$)

$$\left(E - U_0 + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - i\eta\right) G^{A}(x,x') = \delta(x-x')$$

In general the retarded Green's function is defined as (cf.Eq.(3.3.1))

$$G^{R} = \left[E - H_{op} + i\eta\right]^{-1} \quad (\eta \to 0^{+}) \tag{3.3.8a}$$

while the advanced Green's function is defined as

$$G^{A} = \left[E - H_{op} - i\eta\right]^{-1} \quad (\eta \to 0^{+}) \tag{3.3.8b}$$

From hereon we will generally refer to the retarded Green's function as just the 'Green's function'.

Green's function for a multi-moded wire

Next let us look at the Green's function for an infinite multi-moded wire (Fig. 3.3.3). The Green's function $G^{R}(x,y;x',y')$ represents the wavefunction

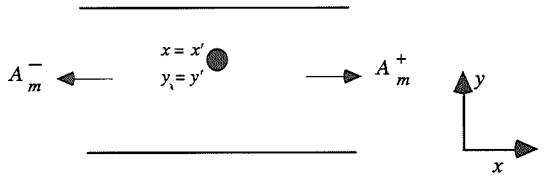

Fig. 3.3.3. Green's function for an infinite multi-moded wire.

at (x,y) due to an excitation at $x = x'$, $y = y'$. We would expect such an excitation to give rise to outgoing waves in different modes as shown. We could write the Green's function in the form

$$G^{R}(x,x') = \sum_m A_m^{\pm}\chi_m(y)\exp\left[ik_m|x-x'|\right] \tag{3.3.9}$$

where the A_m^+ and A_m^- are the amplitudes of the different modes that propagate away from the source. The transverse mode wavefunctions, $\chi_m(y)$ satisfy the equation (see Eq.(1.6.3) with B = 0)

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + U(y)\right]\chi_m(y) = \varepsilon_{m,0}\chi_m(y) \tag{3.3.10}$$

where $U(y)$ is the transverse confining potential in the y-direction. These functions are orthogonal

$$\int \chi_n(y)\chi_m(y)dy = \delta_{nm} \tag{3.3.11}$$

since they satisfy the same equation with different eigenvalues. We will assume that these functions $\chi_m(y)$ are real.

To calculate the mode amplitudes A_m^+ and A_m^-, we proceed as we did for the 1-D wire and obtain (cf.Eq.(3.3.5))

$$\begin{aligned}&\left[G^{R}(x,x')\right]_{x=x'+} = \left[G^{R}(x,x')\right]_{x=x'-}\\ &\left[\frac{\partial G^{R}(x,x')}{\partial x}\right]_{x=x'+} - \left[\frac{\partial G^{R}(x,x')}{\partial x}\right]_{x=x'-} = \frac{2m}{\hbar^2}\delta(y-y')\end{aligned} \tag{3.3.12}$$

Substituting from Eq.(3.3.9) into (3.3.12) we obtain

$$\begin{aligned}&\sum_m A_m^+\chi_m(y) = \sum_m A_m^-\chi_m(y)\\ &\sum_m ik_m\left[A_m^+ + A_m^-\right]\chi_m(y) = \frac{2m}{\hbar^2}\delta(y-y')\end{aligned} \tag{3.3.13}$$

Multiplying Eq.(3.3.13) by $\chi_n(y)$, integrating over y and using the orthogonality relation (Eq.(3.3.11)) we obtain

$$A_m^+ = A_m^- \quad \text{and} \quad ik_m\left[A_m^+ + A_m^-\right] = \frac{2m}{\hbar^2}\chi_m(y')$$

Hence the mode amplitudes are given by

$$A_m^+ = A_m^- = -\frac{i}{\hbar v_m}\chi_m(y') \tag{3.3.14}$$

As we might expect, the amplitude A_m of mode m is proportional to the transverse wavefunction at the point of excitation, $\chi_m(y')$. Substituting Eq.(3.3.14) into Eq.(3.3.9) we obtain the Green's function:

$$G^{R}(x,y;x',y') = \sum_m -\frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')\exp\left[ik_m|x-x'|\right] \tag{3.3.15}$$

where $$k_m \equiv \frac{\sqrt{2m(E-\varepsilon_{m,0})}}{\hbar} \quad \text{and} \quad v_m \equiv \frac{\hbar k_m}{m}$$

Eigenfunction expansion

We end this section by deriving a result that is often used to calculate Green's functions. The basic idea is that for any structure, if we know the eigenfunctions of the Hamiltonian operator

$$H_{\rm op}\psi_\alpha(\mathbf{r}) = \varepsilon_\alpha\psi_\alpha(\mathbf{r}) \tag{3.3.16}$$

then we can calculate the Green's function by performing the following summation:

$$G^{\rm R}(\mathbf{r},\mathbf{r}') = \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{E-\varepsilon_\alpha+i\eta} \tag{3.3.17}$$

We could have used this result to calculate the Green's function that we just obtained (Eq.(3.3.15)). However, the mathematics involves contour integration and is less transparent (see Exercise E.3.2 at the end of this chapter).

To derive Eq.(3.3.17), we first note that the eigenfunctions form a complete orthonormal set

$$\int\psi_\beta^*(\mathbf{r})\psi_\alpha(\mathbf{r})d\mathbf{r} = \delta_{\beta\alpha} \tag{3.3.18}$$

so that we can expand the Green's function in the form

$$G^{\rm R}(\mathbf{r},\mathbf{r}') = \sum_\alpha C_\alpha(\mathbf{r}')\psi_\alpha(\mathbf{r}) \tag{3.3.19}$$

where the coefficients C_α have to be determined appropriately. Next we substitute Eq.(3.3.19) into the equation for the Green's function

$$(E-H_{\rm op}+i\eta)G^{\rm R}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$

and make use of Eq.(3.3.16) to obtain (note that $H_{\rm op}$ acts only on $\mathbf{r}$, not $\mathbf{r}'$)

$$\sum_\alpha (E-\varepsilon_\alpha+i\eta)C_\alpha\psi_\alpha(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}')$$

Multiplying by $\psi_\alpha^*(\mathbf{r})$, integrating over $\mathbf{r}$ and making use of the orthogonality relation (Eq.(3.3.18)) we obtain the coefficients C_α:

$$C_\alpha = \frac{\psi_\alpha^*(\mathbf{r}')}{E-\varepsilon_\alpha+i\eta}$$

Substituting back into Eq.(3.3.19) we obtain the result stated earlier (Eq.(3.3.17)). Similarly we can show that

$$G^{\rm A}(\mathbf{r},\mathbf{r}') = \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{E-\varepsilon_\alpha-i\eta} \tag{3.3.20}$$

From Eqs.(3.3.17) and (3.3.20) it is straightforward to show that

$$G^{\rm A}(\mathbf{r},\mathbf{r}') = \left[G^{\rm R}(\mathbf{r}',\mathbf{r})\right]^* \;\rightarrow\; G^{\rm A} = \left[G^{\rm R}\right]^+ \tag{3.3.21}$$

so that the advanced function is the Hermitian conjugate of the retarded function.

3.4 *S*-matrix and the Green's function

With this brief introduction to Green's functions, we are ready to discuss the Fisher–Lee relation which expresses the elements of the S-matrix in terms of the Green's function (see D. S. Fisher and P. A. Lee (1981), *Phys. Rev. B*, **23**, 6851). Consider a conductor connected to a set of leads. For convenience, we use a different coordinate system in each lead as shown in Fig. 3.4.1. The interface between lead p and the conductor is

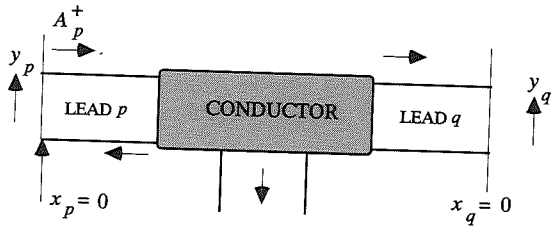

Fig. 3.4.1. A unit impulse in lead p generates an incident wave which is partially transmitted to each of the other leads.

defined by $x_p = 0$. We will use the symbol $G^{\rm R}_{qp}$ to denote the Green's function between a point lying on the plane $x_p = 0$ and another point lying on $x_q = 0$:

$$G^{\rm R}_{qp}(y_q;y_p) \equiv G^{\rm R}(x_q=0,y_q;x_p=0,y_p) \tag{3.4.1}$$

Let us try to write this quantity in terms of the S-matrix element connecting the two leads. This is easy to do if we neglect the transverse dimension (y) of the leads and treat them as one-dimensional. We know that the unit excitation at $x_p = 0$ gives rise to a wave of amplitude A_p^- away from the conductor (not shown in the Figure) and a wave of amplitude A_p^+ toward the conductor. The wave traveling toward the conductor is scattered by the conductor into different leads. Hence we can write

$$G^{\rm R}_{qp} = \delta_{qp}A_p^- + s'_{qp}A_p^+ \tag{3.4.2}$$

But we know that (see Eq.(3.3.6))

$$A_p^+ = A_p^- = -\frac{\mathrm{i}}{\hbar v_p}$$

Also, $s'_{qp} = s_{qp}\sqrt{v_p/v_q}$ (see Eq.(3.1.4))

Hence from Eq.(3.4.2) we obtain

$$s_{qp} = -\delta_{qp} + \mathrm{i}\hbar\sqrt{v_q v_p}\,G^{\mathrm{R}}_{qp} \tag{3.4.3}$$

This is the desired relation expressing the S-matrix in terms of the Green's function.

Multi-moded leads

The details are slightly more complicated if we take multiple modes in the leads into account. Instead of Eq.(3.4.2) we now have

$$G^{\mathrm{R}}_{qp}(y_q;y_p) = \sum_{m\in p}\sum_{n\in q}\left[\delta_{nm}A_m^- + s'_{nm}A_m^+\right]\chi_n(y_q) \tag{3.4.4}$$

From Eq.(3.3.14) we know that

$$A_m^+ = A_m^- = -\frac{\mathrm{i}}{\hbar v_m}\chi_m(y_p)$$

Also, $s'_{nm} = s_{nm}\sqrt{v_m/v_n}$ (see Eq.(3.1.4))

Hence from Eq.(3.4.4)

$$G^{\mathrm{R}}_{qp}(y_q;y_p) = \sum_{m\in p}\sum_{n\in q} -\frac{\mathrm{i}}{\hbar\sqrt{v_n v_m}}\chi_n(y_q)\left[\delta_{nm} + s_{nm}\right]\chi_m(y_p) \tag{3.4.5}$$

In order to obtain an expression for an individual S-matrix element, we multiply Eq.(3.4.5) by $\chi_m(y_p)\chi_n(y_q)$, integrate over y_p and y_q and make use of the orthogonality relation (see Eq.(3.3.11)):

$$s_{nm} = -\delta_{nm} + \mathrm{i}\hbar\sqrt{v_n v_m}\int\!\!\int \chi_n(y_q)\left[G^{\mathrm{R}}_{qp}(y_q;y_p)\right]\chi_m(y_p)\mathrm{d}y_q\mathrm{d}y_p \tag{3.4.6}$$

Magnetic field in the leads

In general there is a non-zero magnetic field present in the leads which complicates the discussion considerably. Although we can calculate transverse mode wavefunctions even when a magnetic field is present (see Section 1.6) these wavefunctions do not satisfy the orthogonality relation stated in Eq.(3.3.11) (see Exercise E.2.6 at the end of Chapter 2). Consequently the derivation of a Fisher–Lee relation gets more complicated (see for example Eq.(88) of H. U. Baranger and A. D. Stone (1989), *Phys. Rev. B*, **40**, 8169). To simplify our discussion, we will assume that any magnetic field is present only inside the conductor and not in the leads. In an actual calculation we can include a length of the lead as part of the conductor and reduce the vector potential to zero over this length. If the vector potential were to have a transverse component (along y) then this would introduce a spurious magnetic field due to the non-zero $\partial A_y/\partial x$. But as we explained in Section 2.6, the vector potential must be chosen to be purely longitudinal (along x) in every lead, in order to permit us to define scattering states. Thus it can be reduced to zero without introducing spurious effects. This approach has been used by several authors to give sensible results both at low and high magnetic fields (see for example, H. U. Baranger and A. D. Stone (1991), *Phys. Rev. B*, **44**, 10637 and M. J. McLennan *et al.* (1991), *Phys. Rev. B*, **43**, 13846, 14333). However, this is not a necessary assumption. Several authors have reported numerical calculations taking a non-zero magnetic field in the leads into account (see for example, H. Tamura and T. Ando (1991), *Phys. Rev. B*, **44**, 1792, M. Leng and C. S. Lent (1993), *Phys. Rev. Lett.*, **71**, 137 and Y. Wang *et al.* (1994), *Phys. Rev. B*, **49**, 1928).

3.5 Tight-binding model (or the method of finite differences)

Next we address the question of how we can calculate the Green's function (and hence the S-matrix via the Fisher–Lee relation), for an arbitrarily shaped conductor. Basically we need to solve the differential equation for the Green's function (see Eqs.(3.3.8a), (3.3.2)):

$$\left[E - H_{\mathrm{op}}(\mathbf{r}) + \mathrm{i}\eta\right]G^{\mathrm{R}}(\mathbf{r};\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \tag{3.5.1}$$

$$H_{\mathrm{op}}(\mathbf{r}) = \frac{(\mathrm{i}\hbar\nabla + e\mathbf{A})^2}{2m} + U(\mathbf{r}) \tag{3.5.2}$$

for arbitrary $U(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$. We will restrict the discussion to two