# (Tentative) Calculating Green Function

Taper

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**Abstract**

This is a note for reading the paper [1], and for understanding the code produced from that file.

## Contents



# 1 Chapter 1 - Introductions

This chapter is really a nice introduction to the current fields of mesoscopic physics. The writing is clear and it traces the develpment of this field. It gives me a lucid and holistic historical account of both the important discoveries and motives behind them. I should find those marked regions on pdf inside this part very useful.

# 2 Chapter 2 - 2 Landauer-Büttiker formalism

This chapter introduces the Landauer-Büttiker formalism for calculating the transport properties. The typical setup is illustrated below:

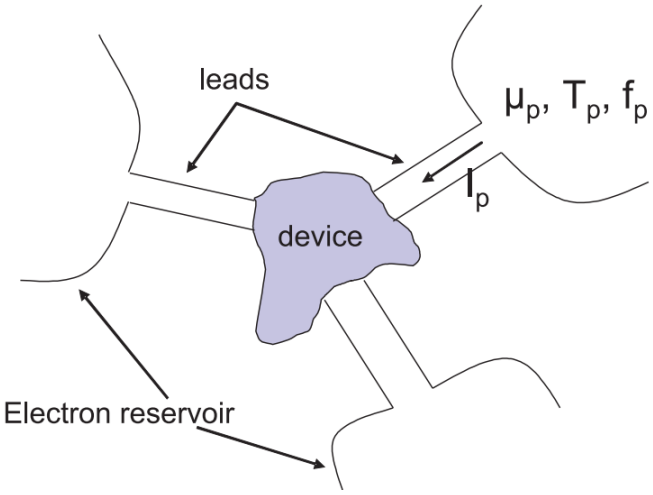


Figure 1: Setup for the Landauer-Büttiker formalism

In that formalism, the currents following through the leads have the following expression:

$$I_p = \frac{-e}{h} \sum_q \int T_{qp}(E) \left(f_p(E) - f_q(E)\right) \mathrm{d}E \tag{2.0.1}$$

where $T_{pq}$ is the transmission coefficients for electrons to go from lead $q$ to lead $p$. This formula can be simplified/linearized into:

$$I_p = \frac{e^2}{h} \sum_q T_{pq}(E_F)(V_p - V_q) \tag{2.0.2}$$

An obvious advantage of Landauer-Büttiker formalism is that it makes the dependence of $I_p$ on experimental setup explicit in the formula.

This chapter continue to discuss some time reversal symmetry (TR) properties of this formula, centring/centering around the coefficient $T_{pq}$. But I am perplexed by that he, while discussing TR, mentions the magnetic field $B$ and formulae like:

$$T_{12}(+B) = T_{12}(-B) \tag{2.0.3}$$

# 3 Chapter 3 - Tight-binding model

Here in this chapter the author presents the fundamental Hamiltonian of the system under consideration.

The process to obtain the Hamiltonian is discretization the Hamiltonian in continuous case, quite the reverse of the first few chapters of A. Zee's QFT in a Nutshell. It should be noted that "a site may represent a region containing many atoms", although "this region should be small compared to physically relevant quantities such as the Fermi wavelength".

Given the formula mentioned in previous chapter, the Hamiltonian presented here seemed seemingly extraneous. Read the introduction here in chapter 4 to understand the underlying logic.

## 3.1 3.1 Spin-degenerate system

Here the general Hamiltonian, using tight-binding model, is mentioned:

$$H = \sum_{n,m} \left( t^x_{nm} \left| n+1, m \right\rangle \left\langle n, m \right| + t^y_{nm} \left| n, m+1 \right\rangle \left\langle n, m \right| + h.c. \right) + \sum_{n,m} \epsilon_{nm} \left| n, m \right\rangle \left\langle n, m \right| \tag{3.1.1}$$

The important thing is to determine the coefficient $t$. In the absence of magnetic field, $t$ is give by:

$$t^x_{nm} = t^y_{nm} = -t = -\frac{\hbar^2}{2m^* a^2} \tag{3.1.2}$$

When magnetic field is present, we effect a so called Peierls substitution to get $t$. The result is, using Landau gauge in one dimensional under a homogeneous magnetic field.

$$t^x_{nm} = -te^{i2\pi(m-1)\Phi/\Phi_0} \tag{3.1.3}$$

$$t^y_{nm} = -t \tag{3.1.4}$$

The author points to a paper, saying that it contains a "lucid discussion on the physics" of Peierls substitution. This might be something worth reading.

When the magnetic field is inhomogeneous, it is generally difficult to choose a gauge to calculate analytically. The author uses a very intuitive discretization process to approach this problem. The process is best illustrated by just the following picture:

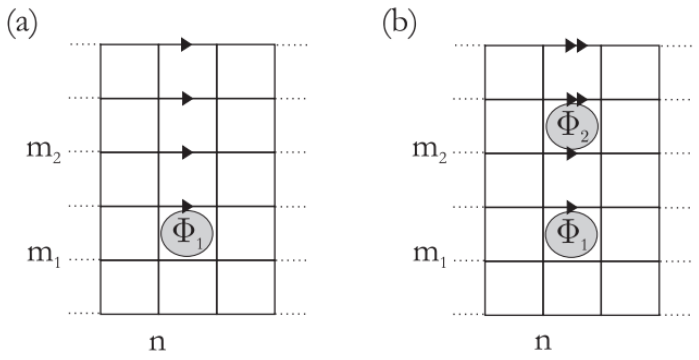


Figure 2: Not uniform magnetic field

Therefore, the result is something like:

$$t^x_{nm} = -te^{i2\pi \sum_{m'<m} \Phi_{nm'}/\Phi_0} \tag{3.1.5}$$

## 3.2 3.2 Including spin degrees of freedom

When the spin is taken into consideration, the formulation should be modified accordingly.

If Zeeman/exchange splitting is considered, then:

$$H_S = -\frac{1}{2} g^* \mu_B \sum_{nm} |n,m\rangle \langle n,m| \otimes (B^{eff}_{nm} \cdot \sigma) \tag{3.2.1}$$

Not that the magnetic field strength here is only "effective".

If Spin-orbit coupling is taken into consideration, [1] the following Hamiltonian should be considered:

$$H_{SO} = \lambda P \cdot (\bigtriangledown V \times \sigma) \tag{3.2.2}$$

Here $P$ is the mechanical momentum operator, $\sigma$ is the three pauli spin matrix $(\sigma_x, \sigma_y, \sigma_z)$.

The tight-binding version of this is too complicated to be presented here, it is on page 16, equation (3.20).

One additional consideration is the Rashba spin-orbit coupling. This is the peculiar result of electrons trapped in a two dimensional surface. In the $Z$ direction, with $Z$ perpendicular to the 2 dimensional plane, the potential looks like something below, called a triangular potential:

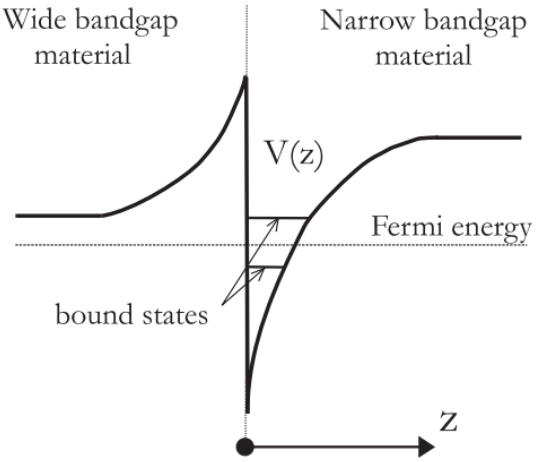


Figure 3: Conduction band at the interface of a semiconductor heterostructure. Band bending creates a potential well $V(z)$ confining the electrons to the XY plane. The asymmetry of this well leads to Rashba spin-orbit coupling.

[1] In my opinion, this is essentially all about Spin-Magnetic field coupling, not just Spin-Orbital coupling.

It is pretty obvious, by equation 3.2.2, that this potential is going into our Hamiltonian. The result in tight-binding model is yet another complicated Hamiltonian, not to be presented here, numbered equation (3.23) on page 18.

# 4 Chapter 4 - Green's function formalism

In this section we finally circled back to the Landauer-Büttiker formalism. Here a breif summary of chapter 3 and 4 is opportune. The purpose of chapter 3 and 4 as a whole, is to calculate the transmission coefficient $T_{qp}$ in equation 2.0.1. Here, chapter 3 establish the Hamiltonian, and chapter 4 uses the Green function to calculate transmission coefficient out of the Hamiltonian.

## 4.1 4.1 Green's functions: The basics

The author takes the definition of Green's function as inverse of Hamiltonian, more specifically:

$$[E - \hat{H}]\hat{G}(E) = 1 \tag{4.1.1}$$

or, in the position-spin representation:

$$[E - H(\vec{x})]G(\vec{x}, \vec{x'}, E) = \delta(\vec{x} - \vec{x'}) \tag{4.1.2}$$

where $\vec{x} = (\vec{r}, \sigma)$, containing in addition to the usual spatial part, the spin part.

The physical meaning is also explained, although I learnt this better in A. Zee's QFT in a Nutshell. However, he notes that to disguish between the source and sink, i.e. to tell whether the Green's function calculated represents a wavefunction resulted from a unit excitation (the sink), or a source for such an excitation, we should incorporate boundary conditions. This is done by adding "an infinitesimal imaginary variable into the energy", "leading to the following definitions":

$$G^{\pm}(\vec{x}, \vec{x'}, E) \equiv \lim_{\eta \to 0^+} G(\vec{x}, \vec{x'}, E \pm i\eta) \tag{4.1.3}$$

and $G^{\pm}$ satisfies:

$$[E \pm i\eta - H(\vec{x})]G^{\pm}(\vec{x}, \vec{x'}, E) = \sigma(\vec{x} - \vec{x'}) \tag{4.1.4}$$

The functions $G^+$ and $G^-$ are called respectively the **retarded and advanced Green's function**. The author mentions that, "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".

Though seemingly extraneous, the operator definition for above Green functions is also mentioned:

$$\hat{G}^{\pm}(E) \equiv \lim_{\eta \to 0^+} \frac{1}{E \pm i\eta - \hat{H}} \tag{4.1.5}$$

## 4.2 4.2 Transmission coefficients and the Green's function

Here it is mentioned than the transmission coefficient is related Green's funciton in the following way:

$$T_{pq} = \mathrm{Tr}\left[\Gamma_p G_{pq} \Gamma_q G_{pq}^\dagger\right] \tag{4.2.1}$$

Here $G_{pq}$ is, to borrow the language of matrix mechanics, a submatrix of the Green's function. $\Gamma_p$ is a abbreviation for the following counting:

I am not sure about this peculiar thing.

$$\Gamma_p \equiv i(\textstyle\sum_p - \sum_p^\dagger) \tag{4.2.2}$$

Here $\sum_p$ is named "self-energy of the lead", something I don't quite understand.

## 4.3 4.3 Lattice Green's function method

In this section, the author builds up a recursive method to calculate the Green's function. The difficulty in calculating Green's function is that the Hamiltonian matrix might be infinite, hence impossible to invert numerically, or the inversion is numercially expensive. Hence a recursive method is more preferable.

We define a notation for one particular submatrix of Green's funciton. $G_{nn'}$ is such that:

$$\langle m, \sigma | G_{nn'}(E) | m', \sigma' \rangle \equiv \langle nm\sigma | G(E) | n'm'\sigma' \rangle = G_{nm\sigma, n'm'\sigma'}(E) \tag{4.3.1}$$

where $(m, n)$ labels columns in the tight-binding lattice, and $\sigma$ is the spin index.

### 4.3.1 4.3.1 Semiinfinite leads: Self-energy description

We have the following Hamiltonian from Landauer-Büttiker formalism,

$$H = H_{cd} + \sum_i (H_l^i + V_{ld}^i + V_{dl}^i) \tag{4.3.2}$$

where $H_{cd}$ is the Hamiltonian for the central device, and $H_{li}$ the Hamiltonian for lead $i$. The coupling between lead and device is described by $V_{ld}^i$ (and its hermitian conjugate $V_{dl}^i$ ).

Here is a improvement on that. It is shown that the central device, including the influence of leads on it, is described by a *finite-dimensional* Hamiltonian:

$$\mathcal{H}_{cd} = H_{cd} + \sum_i \sum^i \tag{4.3.3}$$

where $\sum^i$ is called the retarted self-energy of lead $i$:

$$\sum^i = V_{dl}^i g_l^i V_{ld}^i \tag{4.3.4}$$

Here $g_l^i$ is the Green's function of the isolated semi-infinite lead: $g_l^i = [E + i\eta - H_l^i]^{-1}$.

At this point, the problem of computation is finally solve because we are using nearest neighbour model here. Hence the dimension of some matrix is significantly cut down. Also, author mentions that several methods are available to calculate this Green's funciton: analytical solution when the magnetic field is absent; numerical methods when there is a magnetic field.

Actually, I don't see why the dimension of matrix is infinite in the above 4.3.2, while here the matrix suddenly become fininte.

### 4.3.2 4.3.2 Recursive technique: Standard method

Recursive method is based on the Dyson's equation:

$$\hat{G} = \hat{g} + \hat{g}\hat{V}\hat{G} \tag{4.3.5}$$

(Note that this is an equation of operators!)

Here $g$ is the Green's function of two disconnected subsystems, $G$ is the Green's funciton of the connected system, comprising two previously disconnected subsystems; $V$ describes the hopping between the subsystems. One may already see the spirit of recursive method, by that $G$ appears on both side of the equation.

It should be noted that, strictly speaking, in Dyson's equation there should be two part: the self-energy part and everything else (categorized as external potential). But I am not confident about this.

After this, the author illustrates one simple example of using Dyson's equation to calculate $G$. This process is essentially the same as the standard recursive technique. Therefore I will only mention the standard technique below.

The standard technique is best illustrated with the following diagram:

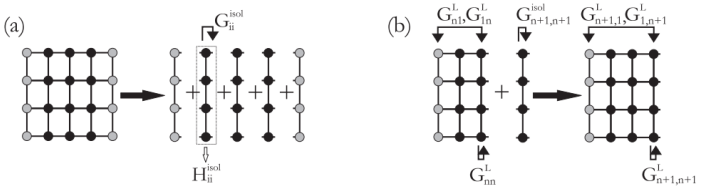


Figure 4: Standard recursive technique

And these equations:

$$G^L_{n+1,n+1} = \left(1 - G^{isol}_{n+1,n+1} V_{n+1,n} G^L_{n,n} V_{n,n+1}\right)^{-1} G^{isol}_{n+1,n+1} \tag{4.3.6}$$

$$G^L_{n+1,1} = G^L_{n+1,n+1} V_{n+1,n} G^L_{n,1} \tag{4.3.7}$$

$$G^L_{1,n+1} = G^L_{1n} V_{n,n+1} G^L_{n+1,n+1} \tag{4.3.8}$$

### 4.3.3 4.3.3 Recursive technique: An extension

The author utilizes a simple bisection method to calculate, best illustrated by the diagram:

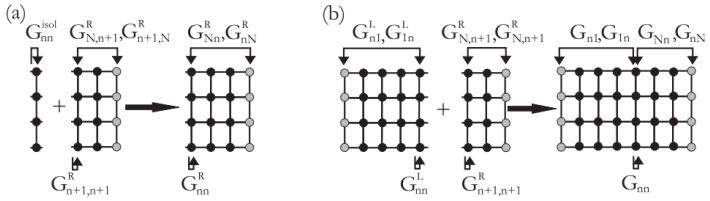


Figure 5: Extended recursive technique

There is, obviously, one final step that requires different formula than the previous steps:

$$G_{n1} = \left(1 - G^L_{nn} V_{n,n+1} G^R_{n+1,n+1} V_{n+1,n}\right)^{-1} \cdot G^L_{n1} \tag{4.3.9}$$

$$G_{1n} = G^L_{1n} + G^L_{1n} V_{n,n+1} G^R_{n+1,n+1} V_{n+1,n} G_{nn} \tag{4.3.10}$$

$$G_{nn} = \left(1 - G^L_{nn} V_{n,n+1} G^R_{n+1,n+1} V_{n+1,n}\right)^{-1} \cdot G^L_{nn} \tag{4.3.11}$$

$$G_{Nn} = G^R_{N,n+1} V_{n+1,n} G_{nn} \tag{4.3.12}$$

$$G_{nN} = G_{nn} V_{n,n+1} G^R_{n+1,N} \tag{4.3.13}$$

# 5 Anchor

# References

[1] Electronic Transport in Mesoscopic Systems, by von Georgo Metalidis. (Link found via Google)

# 6 License