

(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.

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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 development 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:

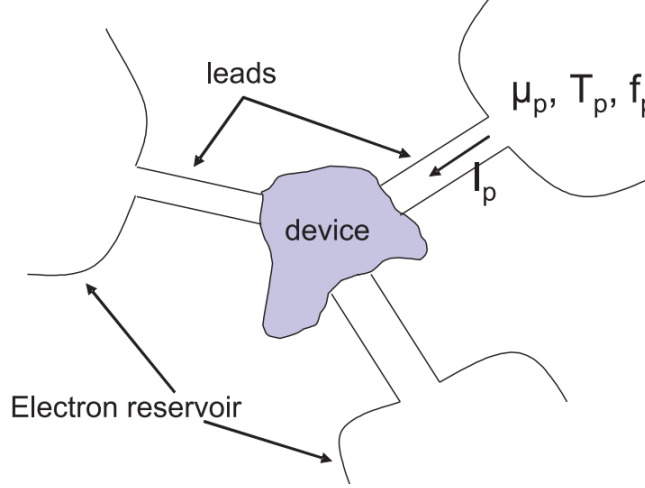


Figure 1: Setup for the Landauer-Büttiker formalism

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

$$I_p = \frac{-e}{h} \sum_q \int T_{qp}(E) (f_p(E) - f_q(E)) dE \quad (2.0.1)$$

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

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

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:

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

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".

3.1 Spin-degenerate system

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

$$H = \sum_{n,m} (t_{nm}^x |n+1, m\rangle \langle n, m| + t_{nm}^y |n, m+1\rangle \langle n, m| + h.c.) + \sum_{n,m} \epsilon_{nm} |n, m\rangle \langle n, m| \quad (3.1.1)$$

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

$$t_{nm}^x = t_{nm}^y = -t = -\frac{\hbar^2}{2m^*a^2} \quad (3.1.2)$$

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.

$$t_{nm}^x = -te^{i2\pi(m-1)\Phi/\Phi_0} \quad (3.1.3)$$

$$t_{nm}^y = -t \quad (3.1.4)$$

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:

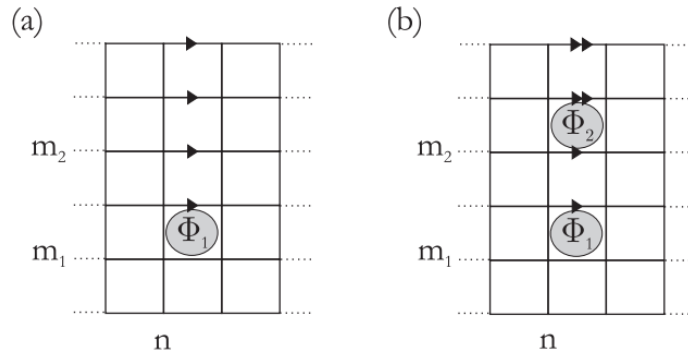


Figure 2: Not uniform magnetic field

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.

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.

Therefore, the result is something like:

$$t_{nm}^x = -te^{i2\pi \sum_{m' < m} \Phi_{nm'}/\Phi_0} \quad (3.1.5)$$

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:

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

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:

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

Here P is the mechanical momentum operator, σ 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:

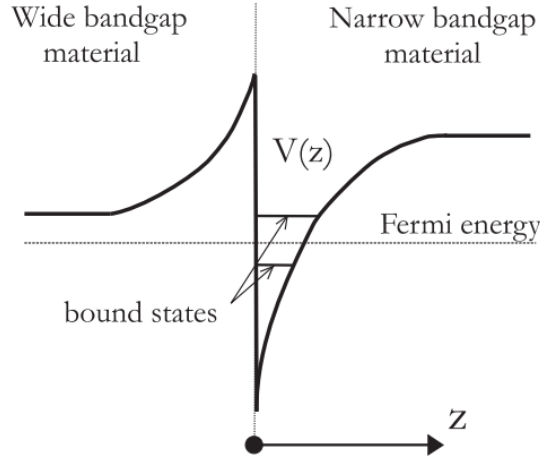


Figure 3: Conduction band at the interface of a semiconductor heterostructure. Band bending creates a potential well $V(z)$ confining the electrons to the XY plane. The asymmetry of this well leads to Rashba spin-orbit coupling.

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 brief 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:

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

or, in the position-spin representation:

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

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 distinguish 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":

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

and G^{\pm} satisfies:

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

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:

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

4.2 4.2 Transmission coefficients and the Green's function

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

$$T_{pq} = \text{Tr} \left[\Gamma_p G_{pq} \Gamma_q G_{pq}^\dagger \right] \quad (4.2.1)$$

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

$$\Gamma_p \equiv i(\sum_p - \sum_p^\dagger) \quad (4.2.2)$$

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

I am not sure about this peculiar thing.

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 numerically expensive. Hence a recursive method is more preferable.

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

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

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

4.3.1 4.3.1 Semiinfinite leads: Self-energy description

We have the following Hamiltonian from Landauer-Büttiker formalism,

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

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:

$$\mathcal{H}_{cd} = H_{cd} + \sum_i \Sigma^i \quad (4.3.3)$$

where Σ^i is called the retarded self-energy of lead i :

$$\Sigma^i = V_{dl}^i g_l^i V_{ld}^i \quad (4.3.4)$$

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 function: analytical solution when the magnetic field is absent; numerical methods when there is a magnetic field.

4.3.2 Recursive technique: Standard method

5 Anchor

References

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

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