

# One particle NEGF

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## 1 Goals

The aim of this text is to provide some intuitive explanations of one particle Green's functions in a compact form together with derivations of the expressions for the current and the density matrix.

## 2 Green's functions

Discrete Schrödinger equation:

$$H|n\rangle = E|n\rangle \quad (1)$$

We divide the Hamiltonian and wavefunction of the system into contact ( $H_{1,2}$ ,  $|\psi_{1,2}\rangle$ ) and device ( $H_d$ ,  $|\psi_d\rangle$ ) subspaces:

$$\begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_d & \tau_2^\dagger \\ 0 & \tau_2 & H_2 \end{pmatrix} \begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} \quad (2)$$

where  $\tau_{1,2}$  describes the interaction between device and contacts. In general we have  $N$  contacts ( $H_{1,\dots,N}$ ) connecting ( $\tau_{1,\dots,N}$ ) the device  $H_d$  to the reservoirs. Here we will assume that the contacts are independent, i.e., there are no cross terms ( $\tau$ ) between the different contacts.

We define the Green's function<sup>1</sup>:

$$(E - H)G(E) = I \quad (3)$$

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<sup>1</sup>Others may use the opposite sign.

## 2.1 Why do we want to calculate the Green's function?

The Green's function gives the response of a system to a constant perturbation  $|v\rangle$  in the Schrödinger equation:

$$H|\psi\rangle = E|\psi\rangle + |v\rangle \quad (4)$$

The response to this perturbation is:

$$(E - H)|\psi\rangle = -|v\rangle \quad \rightarrow \quad (5)$$

$$|\psi\rangle = -G(E)\bar{v} \quad (6)$$

Why do we need the response to this type of perturbation? Well, it turns out that it's usually easier (see next section) to calculate the Green's function than solve the whole eigenvalue problem<sup>2</sup> and most (all for the one-particle system, I think?) properties of the system can be calculated from the Green's function, e.g., below we will use the Green's function to calculate the wavefunction of the contact ( $|\psi_2\rangle$ ) when we know the wavefunction on the device ( $|\psi_d\rangle$ ). From Eq. 2:

$$H_2|\psi_2\rangle + \tau_2|\psi_d\rangle = E|\psi_2\rangle \quad \rightarrow \quad (7)$$

$$(E - H_2)|\psi_2\rangle = \tau_2|\psi_d\rangle \quad \rightarrow \quad (8)$$

$$|\psi_2\rangle = g_2(E)\tau_2|\psi_d\rangle \quad (9)$$

where  $g_2$  is the Green's function of the isolated contact 2 ( $(E - H_2)g_2 = I$ ). It is important to note that since we have an infinite system, we obtain two types of solutions for the Green's functions<sup>3</sup>, the retarded and the advanced<sup>4</sup> solutions corresponding to outgoing and incoming waves in the contacts.

*Notation:* We will denote the retarded Green's function with  $G$  and the advanced with  $G^\dagger$  (and maybe  $G^R$  and  $G^A$  occasionally). Here, CAPITAL  $G$  denotes the full Green's function and its sub-matrices  $G_1$ ,  $G_d$ ,  $G_{1d}$  etc.

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<sup>2</sup>Especially for infinite systems.

<sup>3</sup> When the energy coincides with energy band of the contacts there are two solutions corresponding to outgoing or incoming waves in the contacts.

<sup>4</sup>In practice these two solutions are usually obtained by adding an imaginary part to the energy. By taking the limit to zero of the imaginary part one of the two solutions is obtained. If the limit  $\rightarrow 0^+$  is taken the retarded solution is found,  $\rightarrow 0^-$  gives the advanced. This can be seen from the Fourier transform of the time dependent Green's function.

Lowercase is used for the Green's functions of the isolated subsystems, e.g.,  $(E - H_2) g_2 = I$ .

Note that by using the retarded Green's function of the isolated contact ( $g_2$ ) in Eq. 9 we obtain the solution corresponding to a outgoing wave in the contact. Using the advanced Green's function ( $g_2^\dagger$ ) would give the solution corresponding to an incoming wave.

## 2.2 Self-Energy

The reason for calculating the Green's function is that it is easier than solving the Schrödinger equation. Also, the Green's function of the device ( $G_d$ ) can be calculated separately without calculating the whole Green's function ( $G$ ). From the definition of the Green's function we obtain:

$$\begin{pmatrix} E - H_1 & -\tau_1 & 0 \\ -\tau_1^\dagger & E - H_d & -\tau_2^\dagger \\ 0 & -\tau_2 & E - H_2 \end{pmatrix} \begin{pmatrix} G_1 & G_{1d} & G_{12} \\ G_{d1} & G_d & G_{d2} \\ G_{21} & G_{2d} & G_2 \end{pmatrix} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \quad (10)$$

Selecting the three equations in the second column:

$$(E - H_1) G_{1d} - \tau_1 G_d = 0 \quad (11)$$

$$-\tau_1^\dagger G_{1d} + (E - H_d) G_d - \tau_2^\dagger G_{2d} = I \quad (12)$$

$$(E - H_2) G_{2d} - \tau_2 G_d = 0 \quad (13)$$

We can solve Eqs. 11 and 13 for  $G_{1d}$  and  $G_{2d}$ :

$$G_{1d} = g_1 \tau_1 G_d \quad (14)$$

$$G_{2d} = g_2 \tau_2 G_d \quad (15)$$

substitution into Eq. 12 gives:

$$-\tau_1^\dagger g_1 \tau_1 G_d + (E - H_d) G_d - \tau_2^\dagger g_2 \tau_2 G_d = I \quad (16)$$

from which  $G_d$  is simple to find:

$$G_d = (E - H_d - \Sigma_1 - \Sigma_2)^{-1} \quad (17)$$

where  $\Sigma_1 = \tau_1^\dagger g_1 \tau_1$  and  $\Sigma_2 = \tau_2^\dagger g_2 \tau_2$  are the so called self-energies.

Loosely one can say that the effect of the contacts on the device is to add the self-energies to the device Hamiltonian since when we calculate the

Green's function on the device we just calculate the Green's function for the effective Hamiltonian  $H_{\text{effective}} = H_d + \Sigma_1 + \Sigma_2$ . However, we should keep in mind that we can only do this when we calculate the Green's function. The eigen-values and -vectors of this effective Hamiltonian are not quantities we can interpret easily.

### 2.3 The spectral function

Another important use of the Green's function is the spectral function:

$$A = i(G - G^\dagger) \quad (18)$$

which gives *all* solutions to the Schrödinger equation!

To see this we first note that for any perturbation  $|v\rangle$  we get two solutions ( $|\psi^R\rangle$  and  $|\psi^A\rangle$ ) to the perturbed Schrödinger equation:

$$(E - H)|\psi\rangle = -|v\rangle \quad (19)$$

from the advanced and retarded Green's functions:

$$|\psi\rangle^R = -G|v\rangle \quad (20)$$

$$|\psi\rangle^A = -G^\dagger|v\rangle \quad (21)$$

The difference of these solutions ( $|\psi^R\rangle - |\psi^A\rangle = (G - G^\dagger)|v\rangle = -iA|v\rangle$ ) is a solution to the Schrödinger equation:

$$(E - H)(|\psi^R\rangle - |\psi^A\rangle) = (E - H)(G - G^\dagger)|v\rangle = (I - I)|v\rangle = 0 \quad (22)$$

which means that  $|\psi\rangle = A|v\rangle$  is a solution to the Schrödinger equation for any vector  $|v\rangle$ !

To show that the spectral function actually gives *all* solutions to the Schrödinger equation is a little bit more complicated and we need the expansion of the Green's function in the eigenbasis:

$$G = \frac{1}{E - H} = \int_k \frac{|k\rangle\langle k|}{E + i\delta - \epsilon_k} \quad (23)$$

where the  $\delta$  is the small imaginary part (see footnote 3),  $|k\rangle$ 's are all eigenvectors<sup>5</sup> to  $H$  with the corresponding eigenvalues  $\epsilon_k$ . Expanding the spectral function

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<sup>5</sup>Normalized!

in the eigenbasis gives:

$$A = i \left( \frac{1}{E + i\delta - H} - \frac{1}{E - i\delta - H} \right) = \quad (24)$$

$$= i \int dk |k\rangle\langle k| \left( \frac{1}{E + i\delta - \epsilon_k} - \frac{1}{E - i\delta - \epsilon_k} \right) = \quad (25)$$

$$= \int dk |k\rangle\langle k| \frac{2\delta}{(E - \epsilon_k)^2 + \delta^2} = \quad (26)$$

where  $\delta$  is our infidecimal imaginary part of the energy. Letting  $\delta$  go to zero gives:

$$A = 2\pi \int dk \delta(E - \epsilon_k) |k\rangle\langle k| = \quad (27)$$

$$= 2\pi \text{DOS}(E) |k(E)\rangle\langle k(E)| \quad (28)$$

(here  $\delta(E - \epsilon_n)$  is the delta function) which can be seen since  $\frac{2\delta}{(E - \epsilon_n)^2 + \delta^2}$  goes to zero everywhere but at  $E = \epsilon_n$ , integrating over  $E$  (with a test function) gives the  $2\pi\delta(E - \epsilon_n)$  factor.  $\text{DOS}(E)$  is the density of states. Eq. 28 shows that the spectral function gives us all solutions to the Schrödinger equation.

### 3 Response to an incoming wave

In the nonequilibrium case reservoirs with different chemical potentials will inject electrons and occupy the states corresponding to incoming waves in the contacts. Therefore, we want to find the solutions corresponding to these incoming waves.

Consider contact 1 isolated from the other contacts and the device. At a certain energy we have solutions corresponding to an incoming wave that is totally reflected at the end of the contact. We will denote these solutions with  $|\psi_{1,n}\rangle$  where 1 is the contact number and  $n$  is a quantum number (we may have several modes in the contacts). We can find all these solutions from the spectral function  $a_1$  of the isolated contact (as described above).

Connecting the contacts to the device we can calculate the wavefunction on the whole system caused by the incoming wave in contact 1. To do this we note that a wavefunction should be of the form  $|\psi_{1,n}\rangle + |\psi^R\rangle$  where  $|\psi_{1,n}\rangle$  is the totally reflected wave and  $|\psi^R\rangle$  is the retarded response of the whole

system. Putting in the anzats  $|\psi_{1,n}\rangle + |\psi^R\rangle$  into the Schrödinger equation gives:

$$\begin{pmatrix} H_1 + \tau_1 + \\ H_d + \tau_1^\dagger + \tau_2^\dagger + \\ H_2 + \tau_2 \end{pmatrix} (|\psi_{1,n}\rangle + |\psi^R\rangle) = E (|\psi_{1,n}\rangle + |\psi^R\rangle) \quad (29)$$

$$\begin{pmatrix} E|\psi_{1,n}\rangle + \\ \tau_1^\dagger|\psi_{1,n}\rangle + \\ 0 \end{pmatrix} + \begin{pmatrix} H_1 + \tau_1 + \\ H_d + \tau_1^\dagger + \tau_2^\dagger + \\ H_2 + \tau_2 \end{pmatrix} |\psi^R\rangle = E (|\psi_{1,n}\rangle + |\psi^R\rangle) \quad (30)$$

$$H|\psi^R\rangle = E|\psi^R\rangle - \tau_1^\dagger|\psi_{1,n}\rangle \quad (31)$$

(note the change in notation ???) and we see that  $|\psi^R\rangle$  is nothing else the response of the whole system to a perturbation of  $-\tau_1^\dagger|\psi_{1,n}\rangle$ , c.f., Eq. 9:

$$|\psi^R\rangle = G\tau_1^\dagger|\psi_{1,n}\rangle \quad (32)$$

Note that we have chosen the retarded response which means that the only part of the wave that is traveling towards the device is the incoming wave (part of  $|\psi_{1,n}\rangle$ ). We will make full use of this fact below.

It will be useful to have the expressions for the device wavefunction  $|\psi_d\rangle$  and contact wavefunction ( $|\psi_{1,2}\rangle$ ). The device part is straightforward:

$$|\psi_d\rangle = G_d\tau_1^\dagger|\psi_{1,n}\rangle \quad (33)$$

and from Eq. 9 or Eq. 15:

$$|\psi_2\rangle = g_2\tau_2|\psi_d\rangle = g_2\tau_2G_d\tau_1^\dagger|\psi_{1,n}\rangle \quad (34)$$

Note, to calculate the wavefunction in the contact containing the incoming wave (contact 1) we need to add the incoming wave, giving a slightly more complicated expression:

$$|\psi_1\rangle = (1 + g_1\tau_1G_d\tau_1^\dagger)|\psi_{1,n}\rangle \quad (35)$$

Knowing the wavefunctions corresponding to incoming waves in different contacts enables us to fill up the different solutions according to the electron reservoirs filling the contacts.

## 4 Charge density matrix

In the non equilibrium case we are often interested in two quantities: the current and the charge density matrix. Lets start with the charge density (which allows us to use a self-consistent scheme to describe charging).

The charge density matrix is defined as:

$$\rho = \sum_k f(k, \mu) |\psi_k\rangle \langle \psi_k| \quad (36)$$

where the sum runs over all states with the occupation number  $f(k, \mu)$  (pure density matrix) (note the similarity with the spectral function  $A$ , in equilibrium you find the density matrix from  $A$  and not as described below). In our case, the occupation number is determined by the reservoirs filling the incoming waves in the contacts such that:

$$f(k, \mu_1) = \frac{1}{1 + e^{(E_k - \mu_1)/k_B T}} \quad (37)$$

is the Fermi-Dirac function with the chemical potential ( $\mu_1$ ) and temperature ( $T$ ) of the reservoir responsible for injecting the electrons into the contacts.

The wavefunction on the device given by an incoming wave in contact 1 (see Eq. 33) is:

$$|\psi_d\rangle = G_d \tau_1^\dagger |\psi_{1,n}\rangle \quad (38)$$

Adding up all states from contact 1 gives:

$$\rho_d[\text{from contact 1}] = \int_{E=-\infty}^{\infty} dE \text{DOS}(E) f(E, \mu_1) |\psi_d\rangle \langle \psi_d| = \quad (39)$$

$$= \int_{E=-\infty}^{\infty} dE f(E, \mu_1) \sum_k \text{DOS}(E) G_d \tau_1^\dagger |\psi_{1,k}\rangle \langle \psi_{1,k}| \tau_1 G_d^\dagger = \quad (40)$$

$$= \int_{E=-\infty}^{\infty} dE f(E, \mu_1) G_d \tau_1^\dagger \left( \sum_k \text{DOS}(E) |\psi_{1,k}\rangle \langle \psi_{1,k}| \right) \tau_1 G_d^\dagger = \quad (41)$$

$$= [\text{Eq. 28}] = \int_{E=-\infty}^{\infty} dE f(E, \mu_1) G_d \tau_1^\dagger \frac{a_1}{2\pi} \tau_1 G_d^\dagger \quad (42)$$

introducing the new quantity  $\Gamma_1 = \tau_1^\dagger a_1 \tau_1 = i (\Sigma_1 - \Sigma_1^\dagger)$  we obtain the simple formula:

$$\rho[\text{from contact 1}] = \frac{1}{2\pi} \int_{E=-\infty}^{\infty} dE f(E, \mu_1) G_d \Gamma_1 G_d^\dagger \quad (43)$$

The total charge density thus becomes a sum over all contacts:

$$\rho = \frac{2 \text{ (for spin)}}{2\pi} \int_{E=-\infty}^{\infty} dE \sum_i f(E, \mu_i) G_d \Gamma_i G_d^\dagger \quad (44)$$

## 5 Probability Current

Having different chemical potentials in the reservoirs filling the contacts gives rise to a current. In the next section we will calculate this current in a similar way as the charge density was calculated. But to do this we need an expression for the current from the wavefunction.

In the continuum case we can calculate the current from the velocity operator. However, for a discrete Hamiltonian it is not so clear what the velocity operator is. Therefore, we derive an expression for the current from the continuity equation (using two contacts). In steady-state, the probability to find an electron on the device ( $\sum_i |\psi_i|^2$  where the sum runs over the device subspace) is conserved:

$$0 = \frac{\partial \sum_i |\psi_i|^2}{\partial t} = \quad (45)$$

$$= \sum_i \frac{\partial \langle \psi | i \rangle \langle i | \psi \rangle}{\partial t} = \quad (46)$$

$$= \sum_i \left( \frac{\partial \langle \psi | i \rangle}{\partial t} \langle i | \psi \rangle + \langle \psi | i \rangle \frac{\partial \langle i | \psi \rangle}{\partial t} \right) \quad (47)$$

$$= \frac{i}{\hbar} \sum_i (\langle \psi | H | i \rangle \langle i | \psi \rangle - \langle \psi | i \rangle \langle i | H | \psi \rangle) \quad (48)$$

$$= \frac{i}{\hbar} (\langle \psi | H | \psi_d \rangle - \langle \psi_d | H | \psi \rangle) \quad (49)$$

$$= \frac{i}{\hbar} (\langle \psi | H_d + \tau_1 + \tau_2 | \psi_d \rangle - \langle \psi_d | H_d + \tau_1^\dagger + \tau_2^\dagger | \psi \rangle) = \quad (50)$$

$$= \frac{i}{\hbar} (\langle \psi_1 | \tau_1 | \psi_d \rangle - \langle \psi_d | \tau_1^\dagger | \psi_1 \rangle + \langle \psi_2 | \tau_2 | \psi_d \rangle - \langle \psi_d | \tau_2^\dagger | \psi_2 \rangle) \quad (51)$$



We interpret the term in the first (square) bracket as the incoming probability current into the device from contact 1 and the second bracket from contact 2. Generalising to an arbitrary contact  $i$  gives us the electric current as the charge (-e) times the probability current:

$$I_i = -\frac{ie}{\hbar} \left( \langle \psi_i | \tau_i | \psi_d \rangle - \langle \psi_d | \tau_i^\dagger | \psi_i \rangle \right) \quad (52)$$

where  $I_i$  is defined as positive for a current from the contacts into the device. We can now put in the expressions for the wavefunctions in the same way as for the density matrix.

## 6 Electrical Current

To calculate the total current through the device we only need to put in the wavefunction of the device and the contacts ( $|\psi_d\rangle$ ,  $|\psi_1\rangle$ ,  $|\psi_2\rangle$ ) from Eqs. 33, 35 and 9 and add all the contributions together. Thus the current into the device from an incoming wave of one energy ( $E$ ) in contact 1 ( $|\psi_{1,n}\rangle$ ) through the coupling defined by  $\tau_2$  is:

$$i_{2 \text{ from } 1} = -\frac{ie}{\hbar} \left( \langle \psi_2 | \tau_2 | \psi_d \rangle - \langle \psi_d | \tau_2^\dagger | \psi_2 \rangle \right) = \quad (53)$$

$$= -\frac{ie}{\hbar} \left( \langle \psi_{1,n} | \tau_1 G_d^\dagger \tau_2^\dagger g_2^\dagger \tau_2 G_d \tau_1^\dagger | \psi_{1,n} \rangle - \quad (54)$$

$$\langle \psi_{1,n} | \tau_1 G_d^\dagger \tau_2^\dagger g_2 \tau_2 G_d \tau_1^\dagger | \psi_{1,n} \rangle \right) = \quad (55)$$

$$= -\frac{ie}{\hbar} \langle \psi_{1,n} | \tau_1 G_d^\dagger \tau_2^\dagger (g_2^\dagger - g_2) \tau_2 G_d \tau_1^\dagger | \psi_{1,n} \rangle = \quad (56)$$

$$= \frac{e}{\hbar} \langle \psi_{1,n} | \tau_1 G_d^\dagger \Gamma_2 G_d \tau_1^\dagger | \psi_{1,n} \rangle \quad (57)$$

Adding over the modes  $n$  and noting that the levels are filled from the reservoir connected to contact 1 gives:

$$I_{2 \text{ from } 1} = 2 \text{ (for spin)} \frac{e}{\hbar} \int_{E=-\infty}^{\infty} dE \sum_n \text{DOS}(E) \langle \psi_{1,n} | \tau_1 G_d^\dagger \Gamma_2 G_d \tau_1^\dagger | \psi_{1,n} \rangle \quad (58)$$

$$= \frac{2e}{\hbar} \int_{E=-\infty}^{\infty} dE \sum_{m,n} \text{DOS} \langle \psi_{1,n} | \tau_1 | m \rangle \langle m | G_d^\dagger \Gamma_2 G_d \tau_1^\dagger | \psi_{1,n} \rangle = \quad (59)$$

$$= \frac{2e}{\hbar} \int_{E=-\infty}^{\infty} \sum_m \langle m | G_d^\dagger \Gamma_2 G_d \tau_1^\dagger \left( \sum_n \text{DOS}(E) |\psi_{1,n}\rangle \langle \psi_{1,n}| \right) \tau_1 | m \rangle \quad (60)$$

$$= \frac{2e}{\hbar} \int_{E=-\infty}^{\infty} \sum_m \langle m | G_d^\dagger \Gamma_2 G_d \tau_1^\dagger \frac{a_1}{2\pi} \tau_1 | m \rangle = \quad (61)$$

$$= \frac{e}{\pi \hbar} \int_{E=-\infty}^{\infty} \text{Tr} \left( G_d^\dagger \Gamma_2 G_d \Gamma_1 \right) \quad (62)$$

which is the formula for the current through the device when connected to two contacts.

In the same way as above:

$$I_{1 \text{ from } 1} = \frac{e}{\pi \hbar} \int_{E=-\infty}^{\infty} \text{Tr} \left( G_d^\dagger \Gamma_1 G_d \Gamma_1 - A_d \Gamma_1 \right) \quad (63)$$