# Quantum electronic transport: Landauer formula from the Keldysh approach

Notes used in the lectures of the graduate course "Quantum transport theory and non-equilibrium Green's functions" at the Universidade Federal Fluminense (Niterói, Brazil) in 2015/1. This material adapted from Ref. 1.

These notes present a derivation of the Landauer formula[2,3] using non-equilibrium Green's functions. Here we address the specific problem of ballistic transport model of non-interaction electrons flowing through a quantum dot.

## I. MODEL HAMILTONIAN

We separate the system in two parts, namely the leads (L) and the conductor (C), as exhibited in Figure 1. The model Hamiltonian reads

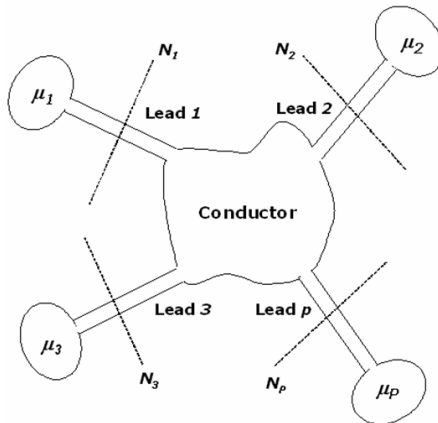$$\mathcal{H} = \mathcal{H}_{\mathrm{L}} + \mathcal{H}_{\mathrm{C}} + \mathcal{H}_{\mathrm{LC}}. \tag{1}$$



FIG. 1: Schematic view of the conductor attached to the leads $p = 1, ..., N$. Each lead is attached to the reservoir $\mu_p$ and contains $N_p$ channels.

The lead Hamiltonian reads

$$\mathcal{H}_{\mathrm{L}} = \sum_{kas} \varepsilon_{kas} c^{\dagger}_{kas} c_{kas}, \tag{2}$$

where the lead channels are labeled by $a = (p, n)$, where $n = 1, \cdots, N_p$ specifies a channel in the lead $p = 1, \cdots, N$. The threshold energy to open the transversal propagation mode $p$ in the lead $n$ is $\varepsilon_{as}$. We assume free motion in the direction along the leads. Hence, $\varepsilon_{kas} = \varepsilon_{as} + \hbar^2 k^2 / 2m^*$, where $m^*$ is the electron effective mass and $k$ is its transversal wave number. The electron spin is $s = \uparrow, \downarrow$ and the $c^\dagger_{kas}(c_{kas})$ are the usual fermionic creation (annihilation) operators, with $\{c^\dagger_{kas}, c_{k'a's'}\} = \delta_{aa'}\delta_{ss'}\delta_{kk'}$. Electrons at the lead $p$ are in thermal equilibrium with the reservoir (at temperature $T$) at which the lead is connected to and characterized by a chemical potential $\mu_p$. Alternatively, leads can also be modeled by semi-infinite tight-binding chains mimicking a continuum[4,12] or by a realistic representation of an actual atomic structure. The later construction is at the heart of molecular electronics, where one models leads as semi-infinite periodic atomic lattices[13–17]. In any case, the decomposition in Eq. (1) only becomes useful when the dynamics in the leads is "simple", in the sense that one can define asymptotic propagating modes by which the electrons are transmitted by the leads between conductor and reservoirs. In actual quantum dots the leads are associated to quantum point contacts, which are certainly very different from semi-infinite leads. However, it can be shown that if they are long enough to make the evanescent modes become negligible, our model is fully justified (see, for instance, Appendix C of Ref. 18).

The conductor Hamiltonian reads

$$\mathcal{H}_C = \sum_{\mu\nu} [H_C]_{\mu\nu} \, d^\dagger_{\mu s} d_{\nu s}, \tag{3}$$

where $d^\dagger_{\mu s}(d_{\mu s})$ creates (annihilates) an electron at the $\mu$-th state of an arbitrary basis that spans the conductor eigenstates. Since we consider $\mathcal{H}_C$ as bilinear, electron-electron interactions are only taken into account at the mean-field level (such as Hartree-Fock). We shall see bellow that the bilinear form of $\mathcal{H}_C$ simplifies enormously the calculation of the conductance. Unfortunately, it does not describe charge fluctuation processes and electronic correlations, excluding Coulomb blockade and Kondo physics. In view of these limitations, it is natural to inquire whether our model is realistic. The answer, obtained by studying the onset of strong electronic correlations[19–21], is affirmative provided the conductor is well coupled to several open modes in each lead. Roughly, this implies the linear conductance to be larger than $2e^2/h$. Our Hamiltonian $\mathcal{H}_C$ also excludes inelastic processes. This is a limitation of our model and not of the NEGF formalism, as reviewed in Ref. 22.

We have chosen not to use a diagonal representation for $\mathcal{H}_C$. This allows for a simple

translation of our results into the scattering matrix language (Section IV A) and, hence, into the Landauer formula. In a tight-binding picture this choice is rather natural: the basis states are sites and the off-diagonal matrix elements $[H_{\rm C}]_{\mu\nu}$ are given by effective hopping terms that depend on the geometry of the conductor[5] and on the material. More elaborate approaches, such as the Density Function Theory (DFT)[23] used in molecular electronics, need a further assumption[13–16]: the Kohn-Sham orbitals have to be identified with single-particle orbitals of Eq. (3)[24]. Albeit this seems to be a sensible compromise, such assumption inherits all characteristics of the Kohn-Sham equations, like the problems to describe the low-lying excitations (spectral properties) of the conductor.

At this stage our model contains leads in thermal equilibrium with their corresponding reservoirs and an isolated conductor. Let us now introduce the leads-conductor coupling term

$$\mathcal{H}_{\rm LC} = \sum_{ka,\mu,s} \left[ V_{ka,\mu} c_{kas}^{\dagger} d_{\mu s} + {\rm H.c.} \right] . \tag{4}$$

While in quantum dots the coupling matrix elements $V$ are frequently taken as free model parameters, in molecular electronics the $V$'s are determined by the overlap between conductor and leads (electrodes) waves functions[14,25]. In the latter case, to assess the conductance one needs a treatment that accurately computes the tails of the conductor wave functions deep inside the spatial region of the leads.

If there is a difference in the chemical potentials $\mu_p$ of the reservoirs, the system is driven out of equilibrium and a current will flow. When the stationary regime is reached, a self-consistent electrostatic potential $U(\mathbf{r})$ is built. The potential $U(\mathbf{r})$ is accounted for in $\mathcal{H}_{\rm C}$. It depends on the applied bias, as well as on the system geometry and material properties. Whereas close to equilibrium the separation between conductor and leads is rather arbitrary, as the applied bias increases the leads should correspond to regions where there is a negligible voltage drop, that is, where $U(\mathbf{r}) - U_{\rm eq}(\mathbf{r})$ becomes constant. Here $U_{\rm eq}(\mathbf{r})$ is the electrostatic potential in the absence of external bias.

In what follows, we will show how to compute the conductance by formally writing a perturbation series in powers of the coupling matrix elements, the interaction terms of our model, and using the non-equilibrium Green's functions (NEGF) technique.

## II. THE CURRENT

Let us begin by deriving the current formula for our model. To simplify our discussion, let us assume that no external magnetic field is present. Hence, within the mean field approximation the spin plays no role. The current in lead $p$ reads

$$I_p(t) = -2e \left\langle \frac{d}{dt} \mathcal{N}_p(t) \right\rangle \tag{5}$$

where $e$ is the electron charge, the factor 2 comes from the two spin projections, and $\langle \cdots \rangle$ stands for thermal averaging. The electron number operator reads

$$\mathcal{N}_p(t) = \sum_{n=1}^{N_p} \sum_k c_{kpn}^\dagger(t) c_{kpn}(t) \tag{6}$$

notice that $a$ was replaced by $(n,p)$ and the spin index is omitted. The equation-of-motion

$$\frac{d}{dt} \mathcal{N}_p(t) = \frac{i}{\hbar} [\mathcal{H}, \mathcal{N}_p(t)] \tag{7}$$

leads immediately to

$$I_p(t) = \frac{2ie}{\hbar} \sum_{nk,\mu} \left[ V_{kpn,\mu} \left\langle c_{kpn}^\dagger(t) d_\mu(t) \right\rangle - \mathrm{H.c.} \right] . \tag{8}$$

Introducing the Keldysh Green's functions[10,11]

$$G_{\mu,kpn}^<(t,t') \equiv \frac{i}{\hbar} \left\langle c_{kpn}^\dagger(t') d_\mu(t) \right\rangle, \qquad \text{and} \qquad G_{kpn,\mu}^<(t,t') \equiv \frac{i}{\hbar} \left\langle d_\mu^\dagger(t') c_{kpn}(t) \right\rangle \tag{9}$$

one writes

$$I_p(t) = 4e \, \mathrm{Re} \left\{ \sum_{nk,\mu} V_{kpn,\mu} G_{\mu,kpn}^<(t,t) \right\} . \tag{10}$$

We shall discuss here only stationary transport processes, where neither $\mathcal{H}$ nor $\mu_p$ depend explicitly on time. Hence, all Green's functions have a single time argument, namely, $G(t,t') \to G(t-t')$.

The standard many-body equilibrium perturbation theory[10,11] relies on adiabatically switching on and off the interaction term and taking expectation values of time-ordered processes, where the initial and final states are at equilibrium and non-interacting at $t \to -\infty$ and $t \to +\infty$, respectively. This is meaningful because, in equilibrium, the initial and final states are the same. In contrast for non-equilibrium situations, in general, the system does not return to its initial thermodynamic equilibrium state as the interactions are switched

off, and an alternative treatment is required. One of the most successful approaches to handle such situations is the Keldysh formulation[26]. The perturbation series is constructed by considering the following path in time: One formally makes the system evolve from a well-defined equilibrium state at $t \to -\infty$ to the time of interest $t = t'$, and then make it evolve from $t = t'$ back in time to its initial state at $t = -\infty$. The advantage of this scheme is that, by construction, one can calculate all physical quantities of interest by computing expectation values with respect a well-known state, in which the system was previously prepared in the past.

In order to implement this scheme, one must construct the non-equilibrium Green's functions in a complex-time contour, as illustrated in Fig. 2. Remarkably, the perturbation expansion of the non-equilibrium Green's functions has exactly the same structure as the corresponding equilibrium expansion (at zero temperature)[26]. As a consequence, the equilibrium and non-equilibrium theories are formally identical. For instance, the contour-ordered Green's function obeys the same Dyson equation as the equilibrium functions[10,26]. However, the complex-time integrations involved in the computation of non-equilibrium Green's functions are harder to deal with than the ordinary time integrations in the equilibrium formalism. This difficulty is circumvented by replacing contour integrals by real time integrals, following the so-called Langreth rules, which are presented in Appendix **??**.

The Keldysh formalism method allows us to obtain a closed expression for $G^<$ in Eq. (10). The derivation is standard[10,27,28]. One proceeds in two steps. First solve the equation-of-motion for the time-ordered Green's function, and then use the Langreth theorem to arrive at the final expression.

The main steps are sketched as follows. Let us define the contact time-ordered Green's function as

$$G_{\mu,kpn}(t - t') = -\frac{i}{\hbar} \left\langle T\Big(d_\mu(t)c_{kpn}^\dagger(t')\Big) \right\rangle, \tag{11}$$

which has the equation-of-motion

$$\left(-i\hbar\frac{\partial}{\partial t'} - \varepsilon_{kpn}\right) G_{\mu,kpn}(t - t') = \sum_\nu G_{\mu\nu}(t - t')V_{\nu,kpn}, \tag{12}$$

where

$$G_{\mu\nu}(t - t') \equiv -\frac{i}{\hbar} \left\langle T\Big(d_\mu(t)d_\nu^\dagger(t')\Big) \right\rangle$$

is the conductor Green's function.

Recalling that the Green's function for the (free) electrons in the leads follows

$$\left(-i\hbar\frac{\partial}{\partial t'} - \varepsilon_{kpn}\right) g_{kpn}(t - t') = \delta(t - t'),$$ (13)

with $g$ diagonal, we write

$$G_{\mu,kpn}(t - t') = \sum_\nu \int dt_1\, G_{\mu\nu}(t - t_1)\, V_{\nu,kpn}\, g_{kpn}(t_1 - t')\,.$$ (14)

Analytic continuation to the Keldysh contour and the Langreth rules allow us to write

$$G^<_{\mu,kpn}(t - t') = \sum_\nu \int_{-\infty}^{+\infty} dt_1 V_{\nu,kpn}\left\{G^r_{\mu\nu}(t - t_1)g^<_{kpn}(t_1 - t') + G^<_{\mu\nu}(t - t_1)g^a_{kpn}(t_1 - t')\right\}$$ (15)

and

$$G^{a(r)}_{\mu,kpn}(t - t') = \sum_\nu \int_{-\infty}^{+\infty} dt_1 V_{\nu,kpn} G^{a(r)}_{\mu\nu}(t - t_1)g^{a(r)}_{kpn}(t_1 - t'),$$ (16)

with $g^<$ and $g^{a(r)}$ given by[10]

$$g^<_{kpn}(t - t') = \frac{i}{\hbar}f_p(\varepsilon_{kpn})e^{-i\varepsilon_{kpn}(t-t')/\hbar},$$ (17)

$$g^r_{kpn}(t - t') = -\frac{i}{\hbar}\theta(t - t')e^{-i\varepsilon_{kpn}(t-t')/\hbar},$$ (18)

$$g^a_{kpn}(t - t') = \frac{i}{\hbar}\theta(t' - t)e^{-i\varepsilon_{kpn}(t-t')/\hbar},$$ (19)

where $f_p(\varepsilon) = [e^{\beta(\varepsilon-\mu_p)} + 1]^{-1}$ is the Fermi function for the $p$th lead with chemical potential $\mu_p$. For later convenience, we also write $\mu_p = \mu_{\text{eq}} - eU_p$, where $U_p$ is the voltage applied on the $p$th contact.

---

**Home work 1:** Obtain the Langreth rules necessary to arrive at Eq. (15) and (16). *Suggestion:* Consult Refs. 10,39.

---

Collecting all results and substituting in Eq. (10), we write the current as

$$I_p(t) = \frac{4e}{\hbar}\text{Im}\left\{\sum_{\mu\nu}\sum_{kn}\int_{-\infty}^{\infty} dt'\, V_{\nu,kpn}V_{kpn,\mu}e^{-i\varepsilon_{kpn}(t-t')/\hbar}\right.$$

$$\left. \times \left[f_p(\varepsilon_{kpn})G^r_{\mu\nu}(t - t') + G^<_{\mu\nu}(t - t')\theta(t - t')\right]\right\}.$$ (20)

Now the current depends only on the conductor Green's functions.

## III. CONDUCTOR GREEN'S FUNCTION

We now turn to the calculation of the conductor Green's functions, namely the retarded $G^r_{\mu\nu}$ and the lesser $G^<_{\mu\nu}$ ones. Let us start by writing the equation-of-motion for the time-ordered Green's function

$$\sum_{\nu'} \left( i\hbar \frac{\partial}{\partial t} \delta_{\mu\nu'} - [H_{\mathrm{C}}]_{\mu\nu'} \right) G_{\nu'\nu}(t-t') = \delta_{\mu\nu} \delta(t-t') + \sum_{kpn} V_{\mu,kpn} G_{kpn,\nu}(t-t') . \qquad (21)$$

We can proceed as we did for the contact Green's function $G_{\mu,kpn}$, that is, transform the above equation-of-motion into an integral equation in real time, make the analytical continuation to the Keldysh contour and use the Langreth rules.

Fortunately, there is a simpler way to obtain the retarded and advanced Green's functions, since they are directly related to the time-ordered one by Fourier transform, namely, $G^{r(a)}(\varepsilon) = \int_{-\infty}^{\infty} dt \exp(i\varepsilon^{(\pm)}t/\hbar)G(t)$, with $\varepsilon^\pm = \varepsilon \pm i0^\pm$, as standard. After Fourier transforming Eq. (21), one obtains $G^{r(a)}$ in the energy representation, namely,

$$\sum_{\nu'} \left( \varepsilon^\pm \delta_{\mu\nu'} - [H_{\mathrm{C}}]_{\mu\nu'} \right) G^{r(a)}_{\nu'\nu}(\varepsilon) = \delta_{\mu\nu} + \sum_{kpn} V_{\mu,kpn} G^{r(a)}_{kpn,\nu}(\varepsilon) . \qquad (22)$$

The contact Green's function $G^{r(a)}_{kpn,\nu}(\varepsilon)$ is obtained from the Fourier transform of Eq. (16) and reads

$$G^{r(a)}_{kpn,\mu}(\varepsilon) = g^{r(a)}_{kpn}(\varepsilon) \sum_{\nu} V_{kpn,\nu} G^{r(a)}_{\nu,\mu}(\varepsilon) . \qquad (23)$$

Inserting $G^{r(a)}_{kpn,\mu}$ into Eq. (22), we arrive at a closed set of equations, that allows us to write

$$\sum_{\nu'} \left[ \varepsilon \delta_{\mu\nu'} - [H_{\mathrm{C}}]_{\mu\nu'} - \Sigma^{r(a)}_{\mu\nu'}(\varepsilon) \right] G^{r(a)}_{\nu'\nu}(\varepsilon) = \delta_{\mu\nu} , \qquad (24)$$

where we have introduced the self-energy

$$\Sigma_{\mu\nu}(\varepsilon) \equiv \sum_{kpn} V_{\mu,kpn}\, g_{kpn}(\varepsilon)\, V^*_{\nu,kpn} , \qquad (25)$$

which gives $\Sigma^{r(a)}$ (or $\Sigma^<$) by identifying $g_{kpn}$ with $g^{r(a)}_{kpn}$ (or $g^<_{kpn}$). Let us replace the sums in $k$ by integrals over energy. For that purpose we define $V_{\mu,pn}(\varepsilon_{kpn}) \equiv V_{\mu,kpn}$ and use the identity[29] $(\varepsilon^\pm - \epsilon)^{-1} = \mp i\pi \delta(\varepsilon - \epsilon) + \mathrm{PV}(\varepsilon - \epsilon)^{-1}$, to write

$$\Sigma^{r(a)}_{\mu\nu}(\varepsilon) = \pm i\pi \sum_{pn} \rho_{pn}(\varepsilon) V_{\mu,pn}(\varepsilon)\, V^*_{\nu,pn}(\varepsilon) + \mathrm{PV} \sum_{pn} \int_{\varepsilon_{pn}}^{\infty} d\epsilon\, \rho_{pn}(\epsilon) V_{\mu,pn}(\epsilon) \frac{1}{\varepsilon - \epsilon} V^*_{\nu,pn}(\epsilon) .$$

Here $\varepsilon_{pn}$ is the threshold energy to open the $n$th propagating mode in the $p$ lead, $\rho_{pn}(\varepsilon)$ is the density of states in this mode, and PV stands for the principal value integral. We model the leads by long rectangular waveguides, where the coupling matrix elements $V_{\mu,np}(\varepsilon)$ are very smooth function of $\varepsilon$. Hence, except for $\varepsilon$ near threshold energies $\varepsilon_{pn}$, the principal value integral gives a negligible contribution to $\Sigma_{\mu\nu}^{r(a)}(\varepsilon)$. The self-energy becomes energy independent and reads

$$\Sigma_{\mu\nu}^{r(a)} \approx \pm \frac{i}{2} \Gamma_{\mu\nu} \ , \tag{26}$$

with $\Gamma_{\mu\nu} \equiv \sum_p [\Gamma_p]_{\mu\nu}$ and

$$[\Gamma_p]_{\mu\nu} = 2\pi \sum_n \rho_{pn} V_{\mu,pn} V_{\nu,pn}^* \ . \tag{27}$$

This useful approximation (*wide-band approximation*) is justified in several situations of physical interest. For instance, considering energy independent coupling matrix elements $V_{\mu,pn}$ is usually an excellent approximation to describe electronic transport in quantum dots at low temperatures, since (as we will see) the conductance is dominated by states close to the Fermi level. Such an approximation is also frequently used to describe asymmetric tunneling barriers and resonant-tunneling systems under high bias. The key observation is that the real part of the self-energy will only renormalize the positions of the poles, while the imaginary part describes the decay processes or the leakage out of the conductor (see discussion in Ref. 29). In distinction, when the atomic structure of the contacts is important, the self-energy $\Sigma^{r(a)}$ depends on $\varepsilon$. In such cases one has to compute the self-energy $\Sigma_{\mu\nu}^{r(a)}(\varepsilon)$, either by decimation technique[30] or by other means[17].

The final result for $G_{\mu\nu}^{r(a)}$ is best cast in a matrix form

$$\mathbf{G}^{r(a)}(\varepsilon) = \left( \varepsilon \mathbf{I} - \mathbf{H}_{\mathrm{C}} \pm \frac{i}{2} \mathbf{\Gamma} \right)^{-1} \tag{28}$$

where $\mathbf{I}$ is the identity matrix.

We now switch to the calculation of $G^<$. In general, this can be a rather difficult task. Sometimes, it is possible to avoid this step. For instance, for the Anderson model with the resonance coupled to single transmission mode leads, Meir and Wingreen[27] envisaged a nice trick that uses current conservation to eliminate $G^<$ from Eq. (20). For the multi-resonance case this scheme requires proportional couplings, *i.e.*, $[\Gamma_p]_{\mu\nu} = \lambda [\Gamma_q]_{\mu\nu}$, where $\lambda$ is a constant. Here $p$ and $q$ label different leads. Unless the system (conductor with leads) has a spatial point-symmetry that makes it invariant under permutations of $p$ with $q$, the proportional coupling is hardly a good approximation for the multi-resonance case.

For a bilinear model Hamiltonian, as the one considered here, the calculation of $G^<$ becomes rather simple: Since we already have an exact expression for $\Sigma_{\mu\nu}(\varepsilon)$, $G^<$ follows directly from the Dyson equation[10]

$$\mathbf{G}^<(\varepsilon) = \mathbf{G}^r(\varepsilon)\mathbf{\Sigma}^<(\varepsilon)\mathbf{G}^a(\varepsilon) \tag{29}$$

where $\mathbf{\Sigma}^<$ is obtained from Eq. (25), namely

$$\Sigma^<_{\mu\nu}(\varepsilon) = \sum_{p=1}^{N} \sum_{kn} V_{\mu,kpn}\, g^<_{kpn}(\varepsilon)\, V^*_{\nu,kpn} \equiv \sum_{p=1}^{N} \left[\Sigma^<_p(\varepsilon)\right]_{\mu\nu} . \tag{30}$$

Following the same steps used to obtain Eq. (26) we write

$$\mathbf{\Sigma}^<_q(\varepsilon) = if_q(\varepsilon)\mathbf{\Gamma}_q. \tag{31}$$

---

**Home work 2:** Obtain Eq. (29). *Suggestion:* Reproduce the derivation presented in Ref. 10, namely find the Dyson equation for $G$ and then apply the Langreth rules.

---

Collecting the above results, we obtain

$$\mathbf{G}^<(\varepsilon) = i \sum_{q=1}^{N} f_q(\varepsilon)\mathbf{G}^r(\varepsilon)\mathbf{\Gamma}_q\mathbf{G}^a(\varepsilon) . \tag{32}$$

The Green's function $\mathbf{G}^<(\varepsilon)$ can be related to the electronic density, namely, $n(\mathbf{r}) = -i\hbar \int d\varepsilon/(2\pi)G^<(\varepsilon, \mathbf{r})$. This important relation provides a natural path to calculate the electrostatic potential $U(\mathbf{r})$ using, for instance, the density functional theory. It is also straightforward to calculate $U(\mathbf{r})$ self-consistently, as reviewed by Ref. [14].

With these elements, we are now ready to return to Eq. (20) and compute the current.

## IV. THE CONDUCTANCE

Let us start transforming the sum over $k$ in Eq. (20) into an integration over energy, like we have done for the self-energy $\Sigma$. We then integrate over $t$ to write

$$I_p = -\frac{2e}{\hbar} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \mathrm{ImTr}\Big\{\mathbf{\Gamma}_p\left[\mathbf{G}^<(\varepsilon) + f_p(\varepsilon)\mathbf{G}^r(\varepsilon)\right]\Big\}. \tag{33}$$

In equilibrium, the chemical potentials at the contact coincide, that is $\mu_q = \mu_{\mathrm{eq}}$ for all $q = 1, \cdots, N$. The fluctuation-dissipation theorem gives $\mathbf{G}^< = -if_{\mathrm{eq}}(\varepsilon)\mathrm{Im}\mathbf{G}^r$, where $f_{\mathrm{eq}}(\varepsilon) = [e^{\beta(\varepsilon-\mu_{\mathrm{eq}})} + 1]^{-1}$. Hence, as expected, the current is $I_p = 0$.

Inserting $\mathbf{G}^r$ from Eq. (28), and $\mathbf{G}^<$ from Eq. (32), into Eq. (20) we write the current as

$$I_p = \frac{2e}{h} \sum_{q=1}^{N} \int_{-\infty}^{\infty} d\varepsilon \Big( f_q(\varepsilon) - f_p(\varepsilon) \Big) \mathrm{Tr}\Big[ \mathbf{\Gamma}_p \mathbf{G}^r(\varepsilon) \mathbf{\Gamma}_q \mathbf{G}^a(\varepsilon) \Big], \qquad (34)$$

which is the central result of this review. To the best of our knowledge, an equation similar to Eq. (34) was first obtained by Caroli and collaborators[31] using NEGF to study the current in a metal-insulator-metal junction. In the context of mesoscopic transport, Eq. (34) was first derived by Pastawski[32]. The derivation we present here closely follows the seminal paper by Meir and Wingreen[27], who discuss the limitations of Eq. (34) and show how to go beyond it in the case of strongly interacting systems.

Let us define the total transmission from terminal $q$ to terminal $p$ at energy $\varepsilon$ as

$$T_{pq}(\varepsilon) = \mathrm{Tr}\Big[ \mathbf{\Gamma}_p \mathbf{G}^r(\varepsilon) \mathbf{\Gamma}_q \mathbf{G}^a(\varepsilon) \Big] \qquad (35)$$

to write the surrent as

$$I_p = \frac{2e}{h} \int_{-\infty}^{\infty} d\varepsilon \sum_{q=1}^{N} \Big[ T_{pq}(\varepsilon) f_q(\varepsilon) - T_{qp}(\varepsilon) f_p(\varepsilon) \Big]. \qquad (36)$$

This result holds for both linear and non-linear elastic transport, since the transmission coefficients $T_{pq}$ depend on the self-consistent electrostatic potential $U(\mathbf{r})$ that encodes information about the applied bias.

Equation (36) is remarkable in many ways. One might ask about the role of the exclusion principle, since the current depends on $\sum_q T_{qp} f_p$ instead of $\sum_q T_{qp} f_p (1 - f_q)$, as standard in a rate equations approach. (In practice, this difference can be noticed when an external magnetic field is present.) The answer is that the transport is fully coherent and any state transmitting electrons from $p$ to $q$ has asymptotic components at both leads. However, electrons flowing from $p$ to $q$ are only in thermal equilibrium with a single reservoir, namely, to one to which the lead $p$ is attached. For more details on this discussion, as well on the role of a magnetic field on the lead states, inelastic and non-coherent transport we recommend the very insightful textbook by Datta[5].

Before addressing the linear regime, let us rewrite the current as

$$I_p = -\frac{2e}{h} \int_{-\infty}^{\infty} d\varepsilon \sum_{q=1}^{N} f_q(\varepsilon) A_{pq}(\varepsilon) \quad \text{with} \quad A_{pq}(\varepsilon) = \mathrm{Tr}\Big[ \mathbf{\Gamma}_p \mathbf{G}^r(\varepsilon) (\mathbf{\Gamma} \delta_{pq} - \mathbf{\Gamma}_q) \mathbf{G}^a(\varepsilon) \Big]. \qquad (37)$$

This is a very convenient expression to use for a multi-lead device[33]. Let us use it to discuss the linear conductance regime. As long as the bias is small, i.e. the chemical potential

differences $\delta\mu$'s do not cause an appreciable change in the Green's functions $G^{r(a)}(\varepsilon)$, one can safely linearize the Fermi function in Eq. (37) around the equilibrium chemical potential $\mu_{\text{eq}}$ and replace Green's function $G^{r(a)}(\varepsilon)$ by the equilibium ones $G_0^{r(a)}(\varepsilon)$. One then finally arrives at the Landauer-Büttiker conductance $G_{pq}$,

$$I_p^{\text{linear}} = \sum_{q=1}^{N} G_{pq} U_q \qquad \text{with} \qquad G_{pq} = \frac{2e^2}{h} \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{\partial f_{\text{eq}}}{\partial \varepsilon} \right) A_{pq}^{\text{eq}}(\varepsilon), \qquad (38)$$

where $U_p$ is the voltage at the contact $p$, and $I_p^{\text{linear}}$ is the linear component of $I_p$. The superscript in $A_{pq}^{\text{eq}}(\varepsilon)$ indicates that $A_{pq}(\varepsilon)$ is calculated using $G_0^{r(a)}(\varepsilon)$. Notice that Eqs. (37) and (38) imply that $\sum_p G_{pq} = 0$ and $\sum_q G_{pq} = 0$. In physical terms, the first sum follows from current conservation, while the second one tells us that the current remains invariant if we change all voltages $\{U_q\}$ by the same amount[33].

Currently, most experiments deal with two-contact devices. In this case, there is no real need to introduce the coefficients $A_{pq}$, since we can write the linear conductance directly as

$$G = \frac{dI}{dU}\bigg|_{U\to 0} = \frac{2e^2}{h} \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) g(\varepsilon), \qquad (39)$$

where

$$g(\varepsilon) = T_{12}(\varepsilon) = \text{Tr}\Big[\mathbf{\Gamma}_1 \mathbf{G}_0^r(\varepsilon) \mathbf{\Gamma}_2 \mathbf{G}_0^a(\varepsilon)\Big] \qquad (40)$$

is the so-called dimensionless conductance.

## A. Connection to the scattering matrix

It remains to discuss the connection between the conduction as given by Eq. (38) and the $S$-matrix, which is the standard way to cast the Landauer formula. This is in principle possible for the linear conductance, since the $S$-matrix encodes all single particle information about equilibrium scattering processes through the conductor. More specifically the scattering matrix elements $S_{ab}(\varepsilon)$ give the probability amplitude of scattering electrons from the incoming channel $b$ to the outgoing channel $a$ at energy $\varepsilon$. Recall that the channel indices label both the propagating mode and the lead, $c = (p, n)$.

Before we proceed, it is important to stress that the Landauer formula can be obtained directly from a linear response theory, without resorting to the full machinery of NEGF. This was first done by Fisher and Lee[34] in 1981. The importance of this paper is hardly

overstated, since it appeared at a time when the validity of the Landauer picture was not fully established. It is not our aim to review the vast literature on the Landauer conductance formula, but we would like to highlight some references that can help the interested reader. A brief historical account and the key ideas behind Eq. (42), as well as some of its applications in connection to experiments are given in Refs. [3,5]. A seminal paper addressing multi-probe experiments and the role of contacts and reservoirs is Ref. [35]. A nice detailed derivation of Eq. (42) using the Kubo linear response formalism is presented in Ref. [36]. The Landauer formula can also be obtained in a compact and elegant way in second quantization, by assuming that the difference in the chemical potentials does not change the conductor Hamiltonian[37].

For the sake of simplicity, we consider a two-lead configuration. The $S$-matrix contains reflection and transmission scattering amplitudes. If there are $N_1$ propagating modes at lead 1 and $N_2$ at lead 2, the $S$-matrix is conveniently written in a block form

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \tag{41}$$

of dimension $(N_1 + N_2)$. Here $r$ $(r')$ gives the reflection amplitudes for scattering states going from lead 1 back to 1 (2 back to 2) and $t$ $(t')$ the transmission amplitudes from 1 to 2 (2 to 1). In the absence of external magnetic fields, time-reversal symmetry is preserved, the $S$-matrix is symmetric, and $t' = t^\dagger$.

The dimensionless conductance is expressed according to the Landauer conductance formula as

$$g = \mathrm{Tr}\left(t\, t^\dagger\right). \tag{42}$$

The generalization for a multi-lead geometry is straightforward and can be found in Ref. [18].

Let us go back to our goal, namely connect Eqs. (40) and (42). For that purpose we rewrite the leads Hamiltonian as

$$\mathcal{H}_{\mathrm{L}} = \sum_{p,n} \int_{\varepsilon_{pn}}^{\infty} d\varepsilon\, \varepsilon\, c_{\varepsilon pn}^\dagger c_{\varepsilon pn} \tag{43}$$

where $\{c_{\varepsilon pn}^\dagger, c_{\varepsilon' p' n'}\} = \delta(\varepsilon - \varepsilon')\delta_{pp'}\delta_{nn'}$. Accordingly, the coupling Hamiltonian becomes

$$\mathcal{H}_{\mathrm{LC}} = \sum_{pn,\mu} \int_{\varepsilon_{pn}}^{\infty} d\varepsilon \left[ W_{\varepsilon pn,\mu} c_{\varepsilon pn}^\dagger d_{\mu s} + \mathrm{H.c.} \right]. \tag{44}$$

Notice that the coupling elements $W$'s have a different dimension than the previously introduced $V$'s. The merit of introducing the operators $c_{\varepsilon pn}^\dagger$ and $c_{\varepsilon pn}$ is that they are related

to asymptotic states $|\chi_{\varepsilon pn}\rangle$, normalized as $\langle \chi_{\varepsilon pn} | \chi_{\varepsilon' p' n'} \rangle = \delta(\varepsilon - \varepsilon') \delta_{pp'} \delta_{nn'}$, standard in resonance scattering theory[18]. In addition, formulating the scattering problem in terms of asymptotic states $|\chi_{\varepsilon pn}\rangle$ automatically guarantees flux conservation[36,38].

The derivation of the resonance $S$-matrix can be found in several textbooks[18,40]. Neglecting direct tunneling between states at different leads[41], one writes

$$\mathbf{S}(\varepsilon) = \mathbf{I} - i2\pi \mathbf{W} \mathbf{G}_0^r(\varepsilon) \mathbf{W}^\dagger, \tag{45}$$

where $[G_0^r]^{-1} = \varepsilon - \mathcal{H}_C + i\pi W^\dagger W$. By direct inspection of the decay width matrix in $G^r$ one identifies

$$\Gamma_{\mu\nu} = 2\pi \sum_c W_{\mu c}^* W_{\nu c} = 2\pi \sum_c V_{\mu c}^* \rho_c V_{\nu c}, \tag{46}$$

where the sum runs over all open channels in the leads. The $V$'s are defined in Eq. (4).

We now compare Eqs. (41) and (45) to extract the transmission matrix $t$. Using $(G^r)^\dagger = G^a$ and the cyclic property of the trace, we write

$$\mathrm{Tr}\left(t\, t^\dagger\right) = (4\pi)^2 \mathrm{Tr}\left(W_1 G_0^r W_2^\dagger W_2 G_0^a W_1^\dagger\right) = \mathrm{Tr}\left[\Gamma_1 G_0^r \Gamma_2 G_0^a\right], \tag{47}$$

which is the desired result. From the point of view of scattering theory, Eq. (47) is quite trivial to obtian if one starts from Eq. (45).

## V. CONCLUSION

The presented material covers the essential steps to obtain the linear conductance of a conductor using non-equilibrium Green's functions. We focused our discussion on technical aspects. The literature on applications and physical consequences of the Landauer formula is vast. Some of this material is nicely discussed by Refs. [3–5,42].

We stress that the mean-field approximation (bilinear form of Eq. (3) is an essential element for our derivation. It allows one to close the equations-of-motion and hence to obtain all Green's functions necessary to calculate the conductance. Therefore the fascinating physics related to Coulomb blockade and electronic correlations is entirely left out of this paper. The NEGF approach can certainly deal with these issues, but the approximation schemes involved are different than those discussed here[27].

We considered Eq. (34) in linear response to obtain the Landauer conductance. By supplying a self-consistent scheme to determine how an applied bias modifies the electrostatic

potential in the conductor Hamiltonian $\mathcal{H}_C$, non-linear quantum elastic transport processes can be addressed. So far theory and experiments do not show quantitative agreement. This is a very active line of research in mesoscopic physics and in molecular electronics.

The purpose of these notes is to provide a quick introduction to NEGF in transport, gathering some of the basic literature and working out a soluble model from scratch to the end. We hope it will be useful for beginners and also serve as a quick reference for partitioners.

## Appendix A: Equations-of-motion

The method of equations-of-motion (EOM) is one of the standard approaches to generate a perturbation series for the double-time Green's functions appearing in Section II. The method became popular after Zubarev's pioneer work[43]. In this Appendix we review its main elements and present Zubarev's notation, which is still often used.

Let consider two operators $A(t)$ and $B(t')$ in the Heisenberg picture and define the Green's function

$$G^{r(a)}(t, t') \equiv \langle\langle A(t); B(t')\rangle\rangle^{r(a)} = \mp \frac{i}{\hbar}\theta(\pm(t - t'))\langle[A(t); B(t')]_\eta\rangle \tag{A1}$$

$$G(t, t') \equiv \langle\langle A(t); B(t')\rangle\rangle = -\frac{i}{\hbar}\langle T[A(t); B(t')]_\eta\rangle \tag{A2}$$

where superscripts $r$ and $a$ denote retarded and advanced Green's functions, respectively. Here, $[A(t); B(t')]_\eta \equiv A(t)B(t') - \eta B(t')A(t)$ gives a commutator ($\eta = 1$) for bosonic operators and an anticommutator ($\eta = -1$) for fermionic ones. $\langle\cdots\rangle$ indicates an average over the grand canonical ensemble

$$\langle\cdots\rangle = \frac{1}{Z}\text{Tr}\left[e^{-\beta(H-\mu N)}\cdots\right], \tag{A3}$$

where $Z = \text{Tr}[e^{-\beta(H-\mu N)}]$ the partition function, $N$ is the number operator, $\mu$ the chemical potential, and $\beta = 1/kT$.

Differentiating the time-ordered Green's function with respect to $t$ leads to

$$i\hbar\frac{d}{dt}\langle\langle A(t); B(t')\rangle\rangle = \delta(t - t')\langle[A(t), B(t')]_\eta\rangle + \langle\langle[A(t), H]; B(t')\rangle\rangle. \tag{A4}$$

The explicit computation of $[A(t), H]$ for the considered model Hamiltonian generates Green's functions other then $\langle\langle A(t); B(t')\rangle\rangle$ in Eq. (A4). Every one of these "new" Green's

functions has its own corresponding equation-of-motion. As a result, one ends up with a set of coupled equations. Unfortunately, in general this set is infinite and one needs to recur to approximation schemes to solve for $\langle\langle A(t); B(t')\rangle\rangle$. Note that $\langle\langle A(t); B(t')\rangle\rangle^{r(a)}$ are also solutions of Eq. (A4), but with different boundary conditions.

The problem simplifies for stationary processes. The system is invariant under time translation and the Green's functions depend only on time differences $t - t'$. It is convenient to Fourier transform the Green's functions and introduce

$$\langle\langle A; B\rangle\rangle_\varepsilon = \int_{-\infty}^{\infty} d(t - t')\langle\langle A(t - t'); B(0)\rangle\rangle e^{i\varepsilon(t-t')/\hbar} . \tag{A5}$$

The integral in Eq. (A5) converges if $\text{Im}(\varepsilon) > 0$ $(\text{Im}(\varepsilon) < 0))$ for retarded (advanced) Green's functions, that means that it is analytic in the upper (lower) complex plane.

The Fourier transform of Eq. (A4) renders

$$\varepsilon\langle\langle A; B\rangle\rangle_\varepsilon = \langle[A, B]_\eta\rangle_\varepsilon + \langle\langle[A, H]; B\rangle\rangle_\varepsilon, \tag{A6}$$

which is algebraic, putting in evidence the advantage of working with the energy representation for stationary processes.

To keep the presentation of Section II general, we have used the time-representation to generate the Green's functions equations-of-motion. The Fourier transform was taken only as the last step. By proceeding that way, it was helpful to have always ready the EOMs for the operators $d_\mu$ and $c_{knp}$, namely

$$i\hbar\dot{d}_\mu = \sum_\nu [H_C]_{\mu\nu} d_\nu + \sum_{knp} V_{\mu,knp} c_{knp} \tag{A7}$$

$$i\hbar\dot{c}_{knp} = \varepsilon_{knp} c_{knp} + \sum_\mu V^*_{\mu,knp} d_\mu . \tag{A8}$$

[1]  A. Hernández, V. M. Apel, F. A. Pinheiro, and C. H. Lewenkopf, Physica A **385**, 148 (2007).

[2]  R. Landauer, IBM J. Res. Develop. **1**, 223 (1957).

[3]  Y. Imry and R. Landauer, Rev. Mod. Phys. **71**, S306 (1999).

[4]  D. K. Ferry and S. M. Goodnick, *Transport in Nanostructures* (Cambridge University Press, Cambridge, 2001).

[5]  S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1996).

[6]  M. Grobis, I. G. Rau, R. M. Potok, and D. Goldhaber-Gordon, *cond-mat/0611480*.

[7]  M. Sigrist, T. Ihn, K. Ensslin, D. Loss, M. Reinwald, and W. Wegscheider Phys. Rev. Lett. **96**, 036804 (2006).

[8]  S. K. Watson, R. M. Potok, C. M. Marcus, and V. Umansky, Phys. Rev. Lett. **91**, 258301 (2003); M. Switkes, C.M. Marcus, K. Campman, and A. C. Gossard, Science **283**, 1905 (1999).

[9]  A. Löfgren et al., Phys. Rev. Lett. **92**, 046803 (2004); R. Leturcq, D. Sanchez, G. Gtz, T. Ihn, K. Ensslin, D. C. Driscoll, and A. C. Gossard Phys. Rev. Lett. **96**, 126801 (2006); D. M. Zumbuhl, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Phys. Rev. Lett. **96**, 206802 (2006).

[10]  H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, New York, 1996).

[11]  H. Bruus and K. Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics*, (Oxford University Press, 2004).

[12]  T. Ando, Phys. Rev. B **44**, 8017 (1991).

[13]  J. Taylor, H. Guo, and J. Wang, Phys. Rev. B **63**, 245407 (2001).

[14]  Y. Xue, S. Datta, and M. A. Ratner, Chem. Phys. **281**, 151 (2002).

[15]  F. Evers, F, Weigend, and M. Koentopp, Phys. Rev. B **69**, 235411 (2004).

[16]  J. B. Neaton, K. H. Khoo, C. D. Spataru, and S. G. Louie, Comp. Phys. Comm. **169**, 1 (2005).

[17]  P. A. Khomyakov, G. Brocks, V. Karpan, M. Zwierzycki, and P. J. Kelly, Phys. Rev. B **72**, 035450 (2005).

[18]  P. A. Mello and N. Kumar, *Quantum Transport in Mesoscopic Systems* (Oxford University Press, 2004).

[19]  K. Flensberg, Phys. Rev. B **48**, 11156 (1993).

[20]  K. A. Matveev, Phys. Rev. B **51**, 1743 (1995); A. Furusaky and K. A. Matveev, Phys. Rev. Lett. **75**, 709 (1995).

[21]  P. W. Brouwer, A. Lamacraft, and K. Flensberg, Phys. Rev. Lett. 94, 136801 (2005); Phys. Rev. B **72**, 075316 (2005).

[22]  R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, J. App. Phys. **81**, 7845 (1997).

[23]  K. Capelle, *cond-mat/0211443*.

[24]  DFT accounts for correlation effects beyond the mean-field. However, in its standard implementations, it is still not suitable to address Coulomb blockade and Kondo physics. This is why the bilinear form of Eq. (3) is often naively described as a mean-field approximation, which in the

case of DFT is inacurate.

[25] C. B. Duke, *Tunneling in Solids*, Suppl. 10, Solid State Physics, Ed. by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic Press, New York, 1969) p. 294.

[26] J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986).

[27] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).

[28] A.-P. Jauho, N. S. Wingreen, and Y. Meir, Phys. Rev. B **50**, 5528 (1994).

[29] R. D. Mattuck, *A Guide to Feynman Diagrams in the Many-Body Problem* (Dover, New York, 1992).

[30] M. P. López Sancho, J. M. López Sancho, and J. Rubio, J. Phys. F **15**, 851 (1985); C. E. T. Gonçalves Dias and B. Koiller, Solid State Commun. **40**, 215 (1981).

[31] C. Caroli, R. Combescot, P. Nozieres ,and D. Saint-James, J. Phys. C **4**, 916 (1971).

[32] H. M. Pastawski, Phys. Rev. B **44**, 6329 (1991); Phys. Rev. B **46**, 4053 (1992).

[33] M. Büttiker, J. Phys. Condens. Matter **5**, 9361 (1993).

[34] D. S. Fisher and P. A. Lee, Phys. Rev. B **23**, 6851 (1981).

[35] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).

[36] A. D. Stone and A. Szafer, IBM J. Res. Dev. **32**, 384 (1988).

[37] Ya. M. Blanter and M. Büttiker, Phys. Rep. **336**, 1 (2000).

[38] H. U. Baranger and A. D. Stone, Phys. Rev. B **40**, 8169 (1989).

[39] G. Stefanucci and R. van Leewen, *Nonequilibrium Many-Body Theory of Quantum Systems* (Cambridge, 2013).

[40] C. Mahaux and H. A. Weidenmuller, *Shell-model Approach to Nuclear Reactions* (North holland, Amsterdam, 1969).

[41] This is quite reasonable approximation, provided the typical length of the conductor $L$ is sufficiently long. The same hypothesis is use in molecular electronics[14].

[42] I. L. Aleiner, P.W. Brouwer, and L.I. Glazman, Phys. Rep. **358**, 309 (2002).

[43] D. N. Zubarev, Sov. Phys. Uspekhi **3**, 320 (1960).

[44] D. C. Langreth, on *Linear and Non-Linear Transport in Solids*, ed. by J. T. Devreese and E. Van Dofen (Plenum, New York, 1076).

FIG. 2: Schematic view of the conductor attached to the leads $p = 1, ..., N$. Each lead is attached to the reservoir $\mu_p$ and contains $N_p$ channels.

FIG. 3: Keldysh contour to calculate contour-ordered Green's functions.