

2.5 Quantum expressions for conductance: Real-space Green function technique

*The iconolaters of Byzantium were subtle folk,
who claimed to represent God to his great glory,
but who, simulating God in images, thereby
dissimulated the problem of his existence.*

— Jean Baudrillard, *The Perfect Crime*

2.5.1 Lattice model for the two-probe measuring geometry

In this Section we give practical meaning to different quantum expressions for conductance introduced thus far (Kubo or Landauer-like) by: starting from the Hamiltonian of a single electron in a random potential \rightarrow finding the Green functions in a real-space representation (i.e., corresponding matrices) for the sample placed between two semi-infinite disorder-free leads \rightarrow showing how to plug in efficiently these Green functions into the relevant conductance formulas.

In most of the problems studied in the thesis a disordered electron sample is modeled microscopically by a tight-binding Hamiltonian (TBH) on a finite hypercubic lattice³⁰ $N \times N_y \times N_z$ (lattice constant is denoted by a)

$$\hat{H} = \sum_{\mathbf{m}} \varepsilon_{\mathbf{m}} |\mathbf{m}\rangle \langle \mathbf{m}| + \sum_{\langle \mathbf{m}, \mathbf{n} \rangle} t_{\mathbf{mn}} |\mathbf{m}\rangle \langle \mathbf{n}|. \quad (2.74)$$

This model is widely used in the localization theory. Here $t_{\mathbf{mn}}$ are nearest-neighbor hopping matrix element between s-orbitals $\langle \mathbf{r} | \mathbf{m} \rangle = \psi(\mathbf{r} - \mathbf{m})$ on adjacent atoms located on sites \mathbf{m} of the lattice. The disorder is simulated by taking either the on-site potential (diagonal elements in the Hamiltonian matrix) $\varepsilon_{\mathbf{m}}$ or the hopping (off-diagonal elements) $t_{\mathbf{mn}}$, or both, to be a random variable characterized by some probability distribution. The on-site energies $\varepsilon_{\mathbf{m}}$

³⁰We simplify notation by using $N \equiv N_x$ for the number of sites along the x -axis.

correspond to the potential energy, while hopping matrix elements $t_{\mathbf{mn}}$ are the kinetic energy (and depend on the effective mass of an electron). The hopping defines the unit of energy. In the Chapters to follow, specific random variable distributions will be employed. Here we are interested only in the generic methods applicable to any Hamiltonian. The TBH is a matrix (in site-representation) of dimension $\sim (L/a)^d$, which is sparse since nearest-neighbor condition means that most of the elements are zero. It can be considered as a model of either a nanoscale conductor,³¹ or a discretized version of a continuous one-particle hamiltonian $\hat{H} = -\hbar^2\nabla^2/2m + U(\mathbf{r})$. In a discretized interpretation the continuous position vector \mathbf{r} is replaced by the position of a point \mathbf{m} on a discrete lattice, and derivatives are approximated by finite differences [43].

The standard theoretical view of our two-probe measurement circuits is shown on Fig. 2.1. The sample is placed between two semi-infinite ideal leads. Each lead is modeled by the same clean TBH \hat{H}_L , with $\varepsilon_{\mathbf{m}} = 0$ and $t_{\mathbf{mn}} = t_L$, which is defined on an infinite Hilbert space of site states $|\mathbf{m}\rangle$. The coupling between the end layer sites in the lead and corresponding sites in the sample are taken into account through TBH, \hat{H}_C , which describes only hopping $t_{\mathbf{mn}} = t_C$ between these sites. The leads are connected at infinity to a particle reservoirs through smooth contacts. Left and right reservoirs (large conductors) are at a constant chemical potential μ_L and μ_R , respectively. Thus they are biased relative to each other by a battery of voltage $V = (\mu_L - \mu_R)/e$. Each reservoir injects the fully thermalized carriers into the lead. The distribution function of electrons to be injected is equilibrium Fermi-Dirac with chemical potential of the reservoir. It is assumed that reservoirs are large enough conductors such that passage of current does not disturb these equilibrium char-

³¹Our lattices will be small, containing typically several thousands of atoms. This is the limitation imposed by the available computer memory and computational complexity [42] of matrix operations. For example, less than 20 atoms are placed along the length of the conductor. This is why we use the term nanoscale (or atomic-scale) conductor.

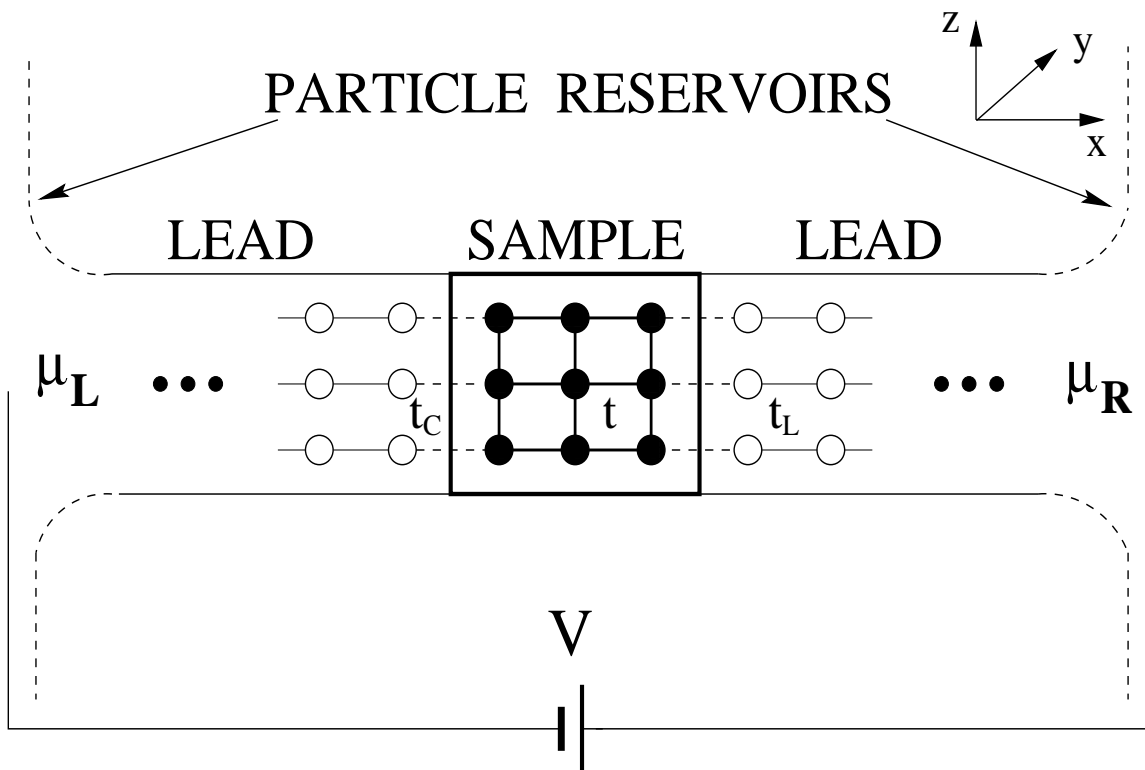


Figure 2.1: A two-dimensional version of our actual 3D model of a two-probe measuring geometry. Each site hosts a single s-orbital which hops to six (or fewer for surface atoms) nearest neighbors. The hopping matrix element is t (within the sample), t_L (within the leads), and t_C (coupling of the sample to the leads). The leads are semi-infinite and connected smoothly at $\pm\infty$ to reservoirs biased by the chemical potential difference $\mu_L - \mu_R = eV$.

acteristics (i.e., chemical potential can be defined and stays the same as in the reservoir decoupled from the conductor). The transport in the central part is phase-coherent. Thus the reservoirs account for the dissipation necessary to establish the steady state. They accept non-equilibrium distribution of electrons from the non-dissipative conductor and provide the thermalization. Even though resistance is related to the dissipation, its value is determined solely by the momentum relaxation processes caused by the scatterers inside the disordered region. However, only the leads at a fixed potential are explicitly taken into account when calculating transport properties. The leads provide the boundary condition for the relevant equations. Since electron leaving the central mesoscopic sample loses the phase-coherence, leads, in a practical way for theoretical calculations, introduce the heuristic construction of the perfect macroscopic reservoirs.

2.5.2 Green function inside the disordered conductor

The direct inversion (2.43) of TBH for the whole system, consisting of semi-infinite leads and the sample,

$$\hat{G}^{r,a}(\mathbf{m}, \mathbf{n}) = (E - \hat{H}(\mathbf{m}, \mathbf{n}) \pm i\eta)^{-1}, \quad (2.75)$$

would lead into a trouble since $\hat{H}(\mathbf{m}, \mathbf{n})$ is an infinite matrix ($\hat{H} = \hat{H}_S + \hat{H}_L + \hat{H}_C$). The site representation of the Green operator $\hat{G}^{r,a}$ is a Green function matrix

$$\hat{G}^{r,a}(\mathbf{m}, \mathbf{n}) = \langle \mathbf{m} | \hat{G}^{r,a} | \mathbf{n} \rangle, \quad (2.76)$$

and the matrix of Hamiltonian in this representation is a band diagonal matrix [104] of the bandwidth $2N_y N_z + 1$. The usual method in the literature to avoid this is to use the periodic boundary conditions [45]. However, this would generate a discrete energy spectrum, instead of continuous one of our open system, and is plagued with problems which we explicitly demonstrate in Sec. 4.2. The correct handling of the leads and openness of the system was initiated by Caroli *et al.* [102], as discussed in general terms in Sec. 2.4.3. Instead of just

truncating the matrix (2.75), which would lead to a conductor with reflecting boundaries instead of open one where electrons can enter and leave the conductor, the leads are taken into account through the exact “self-energy” terms describing the “interaction” of the finite-size conductor with the leads.

If we consider just the sample and one lead³² then Green function for this system can be written in the form of a block matrix [43]

$$\hat{G}^r = \begin{pmatrix} \hat{G}_L^r & \hat{G}_{L-S}^r \\ \hat{G}_{S-L}^r & \hat{G}_S^r \end{pmatrix} = \begin{pmatrix} E + i\eta - \hat{H}_L & \hat{H}_C \\ \hat{H}_C^\dagger & E + i\eta + \hat{H}_S \end{pmatrix}^{-1}, \quad (2.77)$$

where we have shorten the notation by using operator labels without respective matrix indices. The partition above follows from the intrinsic separation of the Hilbert space of states, brought about by the physical separation of lead and the sample in the lattice space. The diagonal blocks are: infinite matrix \hat{G}_L^r , connecting the sites in the left lead; and finite \hat{G}_S^r connecting the states on the lattice sites inside the conductor. The off-diagonal blocks, \hat{G}_{L-S}^r and \hat{G}_{S-L}^r , connect the states in the lead and the sample. The matrix of the coupling Hamiltonian $\hat{H}_C(\mathbf{m}_L, \mathbf{m}_S) = t_C$ is non-zero only for the adjacent sites in the lead \mathbf{m}_L and the sample \mathbf{m}_S . The set of matrix equations for \hat{G}_S^r follows from $\hat{H} \cdot \hat{G}^r = \hat{I}$

$$[E + i\eta - \hat{H}_L] \cdot \hat{G}_{L-S}^r + \hat{H}_C \cdot \hat{G}_S^r = 0, \quad (2.78)$$

$$\hat{H}_C^\dagger \cdot \hat{G}_{L-S}^r + [E + i\eta - \hat{H}_S] \cdot \hat{G}_S^r = \hat{I}. \quad (2.79)$$

The Equation (2.78) can be solved for \hat{G}_{L-S}^r

$$\hat{G}_{L-S}^r = -\hat{g}_L^r \cdot \hat{H}_C \cdot \hat{G}_S^r, \quad (2.80)$$

$$\hat{g}_L^r = (E + i\eta - \hat{H}_L)^{-1}, \quad (2.81)$$

³²To clarify notation, we use the subscript L for a general lead and subscript L for the left lead or reservoir in a two-probe geometry.

where we recognize \hat{g}_L^r as a Green function of a bare semi-infinite lead. This is still an infinite matrix, but can be found exactly as demonstrated in the following Section. Using \hat{G}_{L-S}^r (2.80) in Eq. (2.79) we get

$$\hat{G}_S^r = (E - \hat{H}_S - \hat{H}_C^\dagger \cdot \hat{g}_L^r \cdot \hat{H}_C)^{-1}. \quad (2.82)$$

The final result is a Green function inside a finite-size disordered region which “knows” about the semi-infinite leads, and relevant boundary conditions at infinity they provide, through the “self-energy” function³³

$$\hat{\Sigma}^r(\mathbf{m}_S, \mathbf{n}_S) = t_C^2 \hat{g}_L^r(\mathbf{m}_L, \mathbf{n}_L). \quad (2.83)$$

Since the self-energy provides a well defined imaginary part (which then “helps” the Green function to become retarded or advanced), we drop the small $i\eta$ in Eq. (2.82). The self-energy $\hat{\Sigma}^r(\mathbf{m}_S, \mathbf{n}_S)$ is non-zero only between the sites $(\mathbf{m}_S, \mathbf{n}_S)$ on the edge layer of the sample which are adjacent to the sites $(\mathbf{m}_L, \mathbf{n}_L)$ lying on the edge layer of the lead. This follows from the structure of lead-sample coupling matrix \hat{H}_C . If the sample is attached to many leads (multi-probe geometry) then one should add the self-energy terms generated by each lead, i.e., in our two-probe case

$$\hat{G}_S^r = (E - \hat{H}_S - \hat{\Sigma}^r)^{-1}, \quad (2.84)$$

where $\hat{\Sigma}^r = \hat{\Sigma}_L^r + \hat{\Sigma}_R^r$. Advanced functions are obtained in a standard way: $\hat{G}^a = [\hat{G}^r]^\dagger$, and $\hat{\Sigma}^a = [\hat{\Sigma}^r]^\dagger$. In the following Section we give a derivation of a Green function $\hat{g}_L^r(\mathbf{m}_L, \mathbf{n}_L)$ on the end layer of the lead.

The self-energies “measuring” the coupling of the sample to the leads can be related to the average time an electron spends inside the sample before escaping into the leads. This

³³Analogous terms in Green functions appear when solving the Dyson equation in diagrammatic perturbation theory [1]. Here we use the same name, following Ref. [43], keeping in mind that no approximation is taken for the self-energy (as is usually done when discussing self-energies in perturbation theory by summing only a specific set of diagrams).

can be understood from the following simple arguments. The open system is surrounded by an ideal conducting medium. In that case we cannot talk about eigenstates. Nevertheless, we can formally use an effective Hamiltonian, which is inverted to get the Green function,

$$[\hat{H}_S + \hat{\Sigma}^r]|\alpha_{\text{eff}}\rangle = E_{\alpha}^{\text{eff}}|\alpha_{\text{eff}}\rangle. \quad (2.85)$$

This is not a Hermitian operator, and total probability is not conserved. If we write the formal eigenenergy [43] using the eigenvalue of the corresponding isolated system E_{α} ,

$$E_{\alpha}^{\text{eff}} = E_{\alpha} - \zeta'_{\alpha} - i\frac{\zeta_{\alpha}}{2}, \quad (2.86)$$

then its imaginary part ζ_{α} gives the “lifetime” of an electron in state α before escaping into the leads. The probability to stay in the state $|\alpha\rangle$ decays as $|\exp(-iE_{\alpha}^{\text{eff}}t/\hbar)|^2 = \exp(-2\zeta_{\alpha}t/\hbar)$, and the escape time into the leads is $\tau_{\text{esc}} = \hbar/2\zeta_{\alpha}$. The “loss” of electrons into the leads is also illustrated by the following identity [43]

$$\int \nabla \cdot \mathbf{j}(\mathbf{r}) = \frac{1}{\hbar} \int d\mathbf{r} d\mathbf{r}' \Psi^*(\mathbf{r})\Gamma(\mathbf{r}, \mathbf{r}')\Psi(\mathbf{r}'), \quad (2.87)$$

where $\hat{\Gamma} = -2\text{Im}\hat{\Sigma} = i(\hat{\Sigma}^r - \hat{\Sigma}^a)$, and the evolution of wave functions $\Psi(\mathbf{r})$ is determined by the effective Hamiltonian $\hat{H}_S + \hat{\Sigma}^r$.

Even though the eigenstates are not defined in the standard quantum-mechanical sense, one can still use the local density of states (LDOS) given by the imaginary part of the Green function

$$\rho(\mathbf{m}, E) = -\frac{1}{\pi}\text{Im}\hat{G}_S^r(\mathbf{m}, \mathbf{m}; E). \quad (2.88)$$

It turns out that this LDOS is qualitatively similar to the LDOS of 2D and 3D closed system. We check this explicitly by comparing (2.88) to LDOS of a closed system obtained from exact diagonalization studies, cf. Fig. 3.2. However, in quasi-1D conductors LDOS computed from (2.88) is quite different from LDOS

$$\rho(\mathbf{r}, E) = \sum_{\alpha} |\Psi_{\alpha}(\mathbf{r})|^2 \delta(E - E_{\alpha}), \quad (2.89)$$

defined in terms of exact eigenstates of a closed system [5].

2.5.3 The Green function for an isolated semi-infinite ideal lead

In the previous Section we learned that the Green function matrix $\hat{G}_S^r(\mathbf{m}, \mathbf{n})$ (2.84) at a continuous energy E can be computed numerically by inverting the finite matrix $E - \hat{H}_S - \hat{\Sigma}^r$. This requires to know the matrix elements $\hat{g}^r(\mathbf{m}_B, \mathbf{n}_B)$ of the Green operator for (each) isolated semi-infinite lead between the states $|\mathbf{m}_B\rangle$ located on the sites \mathbf{m}_B at the open boundary of the lead. The lead is modeled by TBH on a rectangular lattice $N_{\text{inf}} \times N_y \times N_z$, where $N_{\text{inf}} \rightarrow \infty$ to make the lead semi-infinite. The exact eigenstates of such lead (which has uniform cross section) are separable into a tensor product $|\mathbf{k}\rangle = |k_x\rangle \otimes |k_y, k_z\rangle$. Here $|k_y, k_z\rangle$ are transverse eigenstates (i.e., eigenstates of each isolated transverse layer)

$$|k_y, k_z\rangle = \sqrt{\frac{2}{N_y + 1}} \sqrt{\frac{2}{N_z + 1}} \sum_{n_y=1}^{N_y} \sum_{n_z=1}^{N_z} \sin(k_y n_y a) \sin(k_z n_z a) |n_y, n_z\rangle, \quad (2.90)$$

where $|n_y, n_z\rangle$ denotes the orbitals of the arbitrary 2D layer. We choose a hard wall boundary conditions in \hat{y} and \hat{z} direction, so the state $\langle \mathbf{m} | k_y, k_z \rangle$ vanishes at the sites $|\mathbf{m}\rangle$ belonging to the transverse boundary surfaces. This makes the transverse states $|k_y, k_z\rangle$ quantized with eigenvalues (dispersion relation)

$$\varepsilon(k_y, k_z) = 2t_L [\cos(k_y a) + \cos(k_z a)], \quad (2.91)$$

defined by discrete $k_y(i) = i\pi/(N_y + 1)a$, and $k_z(j) = j\pi/(N_z + 1)a$. Here i runs from 1 to N_y and j runs from 1 to N_z . The longitudinal eigenstates $|k_x\rangle$ (i.e., on the 1D chains) are

$$\langle n_x | k_x \rangle = \sqrt{\frac{2}{N_{\text{inf}}}} \sin(k_x n_x a), \quad (2.92)$$

with eigenvalues $\varepsilon(k_x) = 2t_L \cos(k_x a)$. These states vanish at the open end on which $n_x = 0$.

The Green function $\hat{g}^r(\mathbf{m}_B, \mathbf{n}_B)$ can be expanded in terms of the exact eigenstates $|\mathbf{k}\rangle$,

$$\begin{aligned} \langle \mathbf{m}_B | \hat{g}^r | \mathbf{n}_B \rangle &= \sum_{\mathbf{k}} \frac{\langle \mathbf{m}_B | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{n}_B \rangle}{E - 2t_L \cos(k_x a) - \varepsilon(k_y, k_z) + i\eta} \\ &= \sum_{k_y, k_z} \langle m_y, m_z | k_y, k_z \rangle \langle k_y, k_z | n_y, n_z \rangle \\ &\quad \times \frac{2}{N_{\text{inf}}} \sum_{k_x} \frac{\sin^2 k_x a}{E - \varepsilon(k_y, k_z) + i\eta - 2t_L \cos(k_x a)}, \end{aligned} \quad (2.93)$$

where only sites at the edge $n_x = 1$ are needed ($|\mathbf{n}_B\rangle \equiv |n_x = 1, n_y, n_z\rangle$). When $N_{\text{inf}} \rightarrow \infty$, k_x is continuous and the sum \sum_{k_x} can be replaced by the integral

$$\begin{aligned} J(k_y, k_z) &= \frac{2}{N_{\text{inf}}} \sum_{k_x} \frac{\sin^2 k_x a}{E - \varepsilon(k_y, k_z) + i\eta - 2t_L \cos(k_x a)} \\ &= \frac{a}{4\pi t_L} \int_0^{\pi/a} dk_x \frac{2 - e^{2ik_x a} - e^{-2ik_x a}}{(E_J + i\eta)/2t_L - \cos(k_x a)}, \end{aligned} \quad (2.94)$$

where we shorten the notation with $E_J = E - \varepsilon(k_y, k_z)$. This integral can be solved by converting it into a complex integral over the unit circle and finding the residues at the poles lying inside the circle

$$J(k_y, k_z) = -\frac{1}{4i\pi t} \oint_{|w|=1} \frac{1 - w^2}{w^2/2 + 1/2 - Yw}. \quad (2.95)$$

Here Y denotes the expression $Y = (E_J + i\eta)/2t_L$. The poles of the integrand are at $w_{1,2} = Y \mp \sqrt{Y^2 - 1}$ and have the following properties: (a) $w_1 w_2 = 1$, for any $|Y|$; (b) $|w_1| < 1$, $|w_2| > 1$, for $|Y| > 1$; and (c) $|Y| \leq 1$, both poles lie on the unit circle. If (c) is satisfied, then $+i\eta$ ($\eta \rightarrow 0^+$) is needed to define the retarded Green function

$$J(k_y, k_z) = -\frac{1}{t_L} \text{Res} \left(\frac{1 - w^2}{(w - w_1)(w - w_2)} \right)_{w=w_1} = \frac{1}{2t_L^2} \left(E_J - i\sqrt{4t_L^2 - E_J^2} \right). \quad (2.96)$$

If $|Y| > 1$, then

$$J(k_y, k_z) = \frac{1}{2t_L^2} \left(E_J - \text{sgn } E_J \sqrt{E_J^2 - 4t_L^2} \right), \quad (2.97)$$

because one pole is always inside the circle, and the small imaginary term $i\eta$ is not required to define the Green function.

We summarize the results of this section by giving the complete expression for the self-energies introduced by each lead L (in a two-probe case left L and right R)

$$\begin{aligned} \hat{\Sigma}_L^r(\mathbf{m}, \mathbf{n}) &= \frac{2}{N_y + 1} \frac{2}{N_z + 1} \sum_{k_y, k_z} \sin(k_y m_y a) \sin(k_z m_z a) \\ &\quad \times \frac{t_C^2}{2t_L^2} \left(E_J - i\sqrt{4t_L^2 - E_J^2} \right) \sin(k_y n_y a) \sin(k_z n_z a), \end{aligned} \quad (2.98)$$

for $|E_J| < 2t_L$, and

$$\begin{aligned} \hat{\Sigma}_L^r(\mathbf{m}, \mathbf{n}) &= \frac{2}{N_y + 1} \frac{2}{N_z + 1} \sum_{k_y, k_z} \sin(k_y m_y a) \sin(k_z m_z a) \\ &\times \frac{t_C^2}{2t_L^2} \left(E_J - \text{sgn } E_J \sqrt{E_J^2 - 4t_L^2} \right) \sin(k_y n_y a) \sin(k_z n_z a), \end{aligned} \quad (2.99)$$

for $|E_J| > 2t_L$. In these expression it is assumed that \mathbf{n} and \mathbf{m} are the sites on the edge layers (first or Nth) of a conductor.

2.5.4 One-dimensional example: single impurity in a clean wire

To illustrate the power of concepts introduced above, we provide a “back of the envelope” calculation for the single impurity, modeled by an on-site potential ε , in a clean infinite 1D chain ($\varepsilon_{\mathbf{m}} = 0$ on all other site). The same problem is solved using \mathbf{T} -matrix in a lengthy calculation elaborated in Ref. [33]. Our derivation assumes that impurity is the “sample” from Fig 2.1 and the rest of the chain are the “leads” with hopping parameter t throughout the system. The Green function of the “sample” is just a number $G^r(E)$ (i.e., 1×1 matrix)

$$G_{\text{in}}^r(E) = [E - \varepsilon - (E - i\sqrt{4t^2 - E^2})]^{-1}, \quad (2.100)$$

for $|E| < 2t$. This gives the local density of states (2.88), which is independent of the lattice site, inside the band

$$\rho_{\text{in}}(E) = -\frac{1}{\pi} \text{Im } G_{\text{in}}^r(E) = \frac{1}{\pi} \frac{\sqrt{4t^2 - E^2}}{\varepsilon^2 + 4t^2 - E^2}. \quad (2.101)$$

For energies outside the band, e.g., $E > 0 > 2t$ the Green function is

$$G_{\text{out}}^r(E) = [E - \varepsilon - (E - \sqrt{E^2 - 4t^2}) + i\eta]^{-1}, \quad (2.102)$$

where a small imaginary part is added to E because the “self-energy” generated by the “leads” is real. The corresponding LDOS is

$$\rho_{\text{out}}(E) = -\frac{1}{\pi} \text{Im } G_{\text{out}}^r(E) = \frac{1}{\pi} \frac{\eta}{(\sqrt{E^2 - 4t^2} - \varepsilon)^2 + \eta^2} \xrightarrow{\eta \rightarrow 0^+} \delta(-\varepsilon + \sqrt{E^2 - 4t^2}), \quad (2.103)$$

where delta function properties lead to the following simplification

$$\delta(-\varepsilon + \sqrt{E^2 - 4t^2}) = \frac{\sqrt{E_p^2 - 4t^2}}{E_p} \delta(E - E_p). \quad (2.104)$$

Thus, the delta function singularity in LDOS appears outside the band of a 1D chain. This is signaling the appearance of a bound state at the energy $E_p = \text{sgn } \varepsilon \sqrt{\varepsilon^2 + 4t^2}$. In a clean chain ($\varepsilon = 0$) LDOS is singular at the band edges (Fig. 2.2). Thus, the introduction of a single impurity is enough to smooth out the band edge singularities in 1D. These proceeds in accordance with the sum rule: LDOS summed over all sites and energies is constant, meaning that weight is transferred from the continuous spectrum at each site \mathbf{n} into the discrete level LDOS, proportional to the overlap of the discrete state with $|\mathbf{n}\rangle$ (Fig. 2.2).

2.5.5 Equivalent quantum conductance formulas for the two-probe geometry

Finally, we employ the Green function for the open finite-size conductor (2.84) in the computation of linear quantum (i.e., zero-temperature) conductance. The Landauer-type formula (2.73) is obtained from the Keldysh technique of Sec. 2.4.3

$$G = \frac{2e^2}{h} \text{Tr} \left(\hat{\Gamma}_L \hat{G}_{1N}^r \hat{\Gamma}_R \hat{G}_{N1}^a \right) = \frac{2e^2}{h} \text{Tr} (\mathbf{t} \mathbf{t}^\dagger), \quad (2.105)$$

$$\mathbf{t} = \sqrt{\hat{\Gamma}_L} \hat{G}_{1N}^r \sqrt{\hat{\Gamma}_R}. \quad (2.106)$$

Here \hat{G}_{1N}^r , and \hat{G}_{N1}^a are matrices whose elements are the Green functions connecting the layer 1 and N of the sample.³⁴ Thus, only the block $N_y N_z \times N_y N_z$ of the whole matrix $\hat{G}^r(\mathbf{n}, \mathbf{m})$ (2.84) is needed to compute the conductance. The Hermitian operator

$$\hat{\Gamma}_L = i(\hat{\Sigma}_L^r - \hat{\Sigma}_L^a) = -2 \text{Im } \hat{\Sigma}_L > 0, \quad (2.107)$$

³⁴We avoid using subscript S here since it is clear from the discussion above that all Green functions which we are going to use are defined inside the sample.

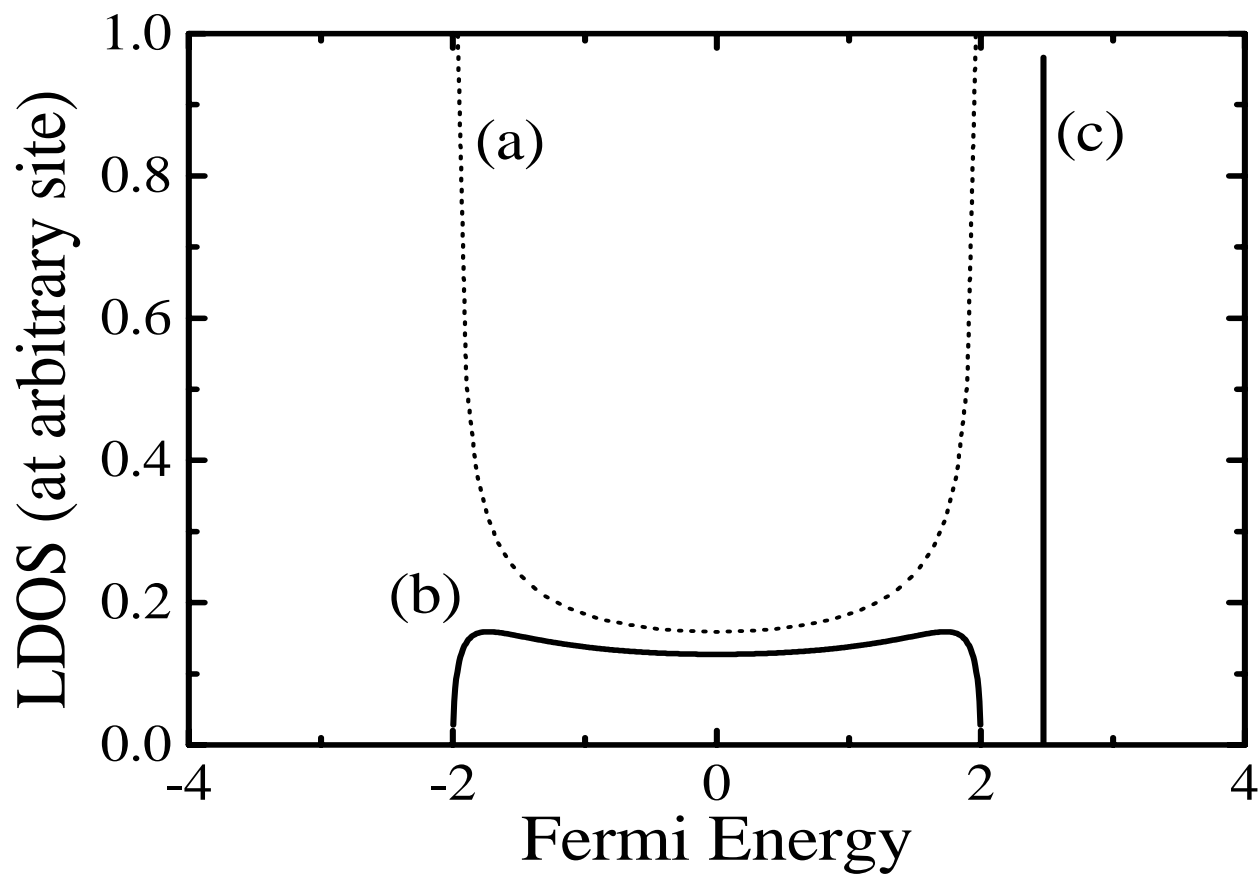


Figure 2.2: Local density of states (LDOS) at an arbitrary site of a 1D chain, described by a tight-binding Hamiltonian, for: (a) energies inside the band of a clean 1D chain, (b) energies inside the band of a 1D chain with one impurity of on-site energy $\varepsilon = 1$, and (c) outside the band of a 1D chain with one impurity of on-site energy $\varepsilon = 1$.

is the counterpart of the spectral function for the Green operator, $\hat{A} = i(\hat{G}^r - \hat{G}^a)$. Therefore, it is related to the imaginary part of the self-energy $\hat{\Sigma}_L$ introduced by the left lead. The operator $\hat{\Gamma}_L$ “measures” the coupling of an open sample to the left lead ($\hat{\Gamma}_R$ is equivalent for the right lead). Although the product of full matrices, connecting the sites of the whole sample, is more complicated than what is shown in Eq. (2.105), the trace is the same. This follows from the fact that $\hat{\Gamma}_L$, like the self-energy $\hat{\Sigma}_L$, has non-zero elements between the orbitals on the sites of layer 1 and N of the conductor. Thus, the expression under the trace in Eq. (2.105) is evaluated only in the Hilbert space spanned by the orbitals located on the edge layers of the sample. This is in the same spirit as the computation of Landauer’s **S**-matrix (cf. Sec. 2.4.2), i.e., without worrying about the “internal state of the conductor”.

The positive definiteness of $\hat{\Gamma}_L$ means that its square root is well defined

$$\sqrt{\hat{\Gamma}_L} = \sum_n \gamma_n^{1/2} \hat{P}_n. \quad (2.108)$$

Here the operator \hat{P}_n is the spectral projector onto eigensubspace corresponding to the eigenvalue γ_n . By “reshuffling” the matrices under the trace (using its cyclical properties) we can get the Hermitian matrix $\mathbf{t}\mathbf{t}^\dagger$. The matrix $\mathbf{t}\mathbf{t}^\dagger$ has the same trace as the initial non-Hermitian matrix $\hat{\Gamma}_L \hat{G}_{1N}^r \hat{\Gamma}_R \hat{G}_{N1}^a$. We recognize in this Hermitian product the transmission matrix \mathbf{t} from the Landauer formula (2.54). The Green function expression for \mathbf{t} will allow us to find the transmission eigenvalues T_n by diagonalizing $\mathbf{t}\mathbf{t}^\dagger$. The corresponding eigenvectors define a way in which atomic orbitals in the definition of TBH contribute to each conducting channel. Therefore, the computation of \hat{G}^r makes it possible to study both conductance and more detailed mesoscopic transmission characteristics of the sample.

An equivalent formula for the quantum conductance follows from the Kubo formalism (cf. Sec. 2.4.1). The Kubo formula for the static quantum conductance³⁵ is given in terms

³⁵After disorder averaging the symmetries of the systems will be restored and all diagonal components of the, in general conductance tensor are approximately equal. Therefore, we denote the conductance as a scalar.

of the Green functions (2.47) as

$$G = \frac{4e^2}{h} \frac{1}{L_x^2} \text{Tr} \left(\hbar \hat{v}_x \text{Im} \hat{G} \hbar \hat{v}_x \text{Im} \hat{G} \right). \quad (2.109)$$

In this formula we will use the site representation of the velocity operator v_x which is obtained from the commutator in Eq. (2.40) with the tight-binding Hamiltonian (2.74)

$$\langle \mathbf{m} | \hat{v}_x | \mathbf{n} \rangle = \frac{i}{\hbar} t_{\mathbf{m}\mathbf{n}} (m_x - n_x). \quad (2.110)$$

The length of rectangular sample in the \hat{x} direction is denoted by $L_x = Na$. The use of the formula (2.109), together with the Green function $\hat{G}^{r,a} = (E - \hat{H} \pm i\eta)^{-1}$ for finite-size system (without attaching the leads), would lead into ambiguity requiring some numerical trick to handle $i\eta$ (as was done historically in the literature [106]). However, if we employ the Green function (2.84), the Kubo formula (2.109) produces a result completely equivalent to the Landauer-type conductance formula (2.105) introduced above. As emphasized before, the Green function (2.84) takes into account leads and corresponding boundary conditions, i.e., the presence of reservoirs. The leads effectively destroy the phase memory of electrons which is the same what realistic modeling of reservoirs (i.e., inelastic processes occurring in them) would do. This type of discussion, brought about by mesoscopic physics [67], can help us also to understand some experiments. For example, a current passed through a carbon nanotube [107] would heat the sample to 20 000 K (and obviously melt it completely) if the dissipation occurred across the sample and not in some “reservoirs”.

What is the most efficient way to use these formulas for conductance? Optimization of computations is essential because of the limited memory and speed of computers. Thus, the formulas should not be employed in a way which requires more operations than required. Careful analysis of all physical properties of the conduction process is the best guidance in achieving efficient algorithms. It also helps to differentiate the real computational complexity [42] of the problem from the apparent one. Since nearest-neighbor TBH of the sample is a band diagonal matrix of bandwidth $2N_y N_z + 1$, one can shorten the time needed to compute the Green function (2.84) by finding the LU decomposition [104] of a band diagonal

matrix. In the Landauer-type formula (2.105) we need only $(N_z N_y)^2$ elements of the whole Green function (2.84). They can be obtained from the LU decomposition³⁶ of the band diagonal matrix $E - \hat{H} - \hat{\Sigma}^r$ by a forward-backward substitution [104]. The trace operation in formula (2.105) is also performed only over matrices of size $N_y N_z \times N_y N_z$. This procedure requires the same computational effort as the recursive Green function method [93, 105] usually found in the literature.³⁷

It might appear at the first sight that the trace in the Kubo formula (2.109) should be performed over the whole Green function matrix (i.e., the space of states inside the conductor). A better answer is obtained once we invoke the results of the discussion on current conservation in Sec. 2.2 and the derivation of this formula from Sec. 2.4.1. Namely, the formula is derived by volume integrating the Kubo NLCT

$$G = \frac{1}{V^2} \int_{\Omega} d\mathbf{r} \mathbf{E}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r}) = \frac{1}{V^2} \int_{\Omega} d\mathbf{r} d\mathbf{r}' \mathbf{E}(\mathbf{r}) \cdot \underline{\sigma}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}'). \quad (2.111)$$

Here we have the freedom to choose any electric field factors $\mathbf{E}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r}')$ because of the DC current conservation.³⁸ The electric field can be taken as homogeneous and non-zero in some region of the conductor. Therefore, the trace operation in formula (2.109) is reduced

³⁶The most advanced numerical linear algebra routines are provided by the LAPACK package (available at <http://www.netlib.org>).

³⁷In the recursive Green function method the self-energy from the left lead $\hat{\Sigma}_L^r$ is iterated through the sample, using the appropriate matrix Dyson equation [105], and finally matched with the self-energy coming from the right lead $\hat{\Sigma}_R^r$. In this procedure matrices of dimension $N_y N_z$ are inverted N times.

³⁸The current conservation³⁸ was essential in arriving at the Kubo formula (2.109). Therefore, the claims, sometimes found in the literature [64], that conductance can be computed by tracing over $\hat{v}_x \hat{G}^a \hat{v}_x \hat{G}^r$ (instead of the expression in Eq. (2.109)) are incorrect because such operator products do not conserve the current inside the disordered region [82] (and its trace is in fact negative in some energy interval).

to the Hilbert space spanned by the states in that part of the conductor. Since velocity operator \hat{v}_x (2.110) has non-zero matrix element only between two adjacent layers, the minimal extension of the field is two layers in the \hat{x} direction. The layers are arbitrary (can be chosen either inside the conductor or on the boundary). That the conductance computed from tracing over any two layers is the same is a consequence of current I being constant on each cross section. Thus, one needs to find $4(N_z N_y)^2$ elements of the Green function (2.84) and trace over the matrices of size $2N_z N_y \times 2N_z N_y$. This is a bit more complicated than tracing in the Landauer-type formula (2.105). It is interesting that to get the proper conductance in this way one should replace L_x in the denominator of Eq. (2.109) with the lattice constant a . So, if one traces “blindly” over the whole conductor the denominator should contain the number of pairs of adjacent layers $(N - 1)a$ instead of $L_x = Na$. In the rest of the thesis we mostly prefer the Landauer-type formula because of the less time consuming evaluation of Green functions and the trace.³⁹

We complete the discussion of conductance formulas with some remarks on the conceptual issues which arise when applying them to finite-size conducting systems. In both Eqs. (2.105) and (2.109) the transport coefficients are computed using the Hamiltonian of an isolated system (although the dissipation occurs in the reservoirs). The connection of the sample to the reservoirs changes the boundary conditions for the eigenstates, transforms the discrete spectrum of the finite sample into a continuous one, and modifies the way electrons loose energy and phase coherence. Nevertheless when the coupling between the system and the reservoirs is strong (*sic* !) it is assumed that it has no influence on the conductance. We study such “counterintuitive” (for the quantum intuition) feature in Sec. 4.2 and Ch.5 by looking at the influence of leads on the conductance of our model. It is shown there that these requires to consider carefully the relationship between relevant energy scales.

³⁹In order to reduce the time needed to compute the trace of four matrices one should multiply them inside the trace in the following way: $\text{Tr}[\mathbf{A} \cdot \mathbf{B} \cdot \mathbf{C} \cdot \mathbf{D}] = \text{Tr}[(\mathbf{A} \cdot \mathbf{B}) \cdot (\mathbf{C} \cdot \mathbf{D})]$.