QUANTUM TRANSPORT
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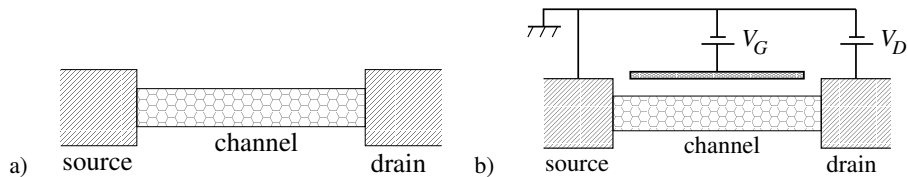
CHAPTER 1

INTRODUCTION

Figure 1.1   a) The basic system and b) the corresponding potentials applied.

The lecture closely follows the excellent book of Supriyo Datta [1]. Fig. 1.1 shows the basic system to deal with in this course. Both "source" and "drain" represent infinite leads, where the "channel" is some nanoscale system that is connected to it. The difference between source and drain is solely the voltage. Voltages are defined relative to the source by definition.

The quantities frequently used during the course are

e unit of charge $1.602{\times}10^{-19}$ C

h Planck constant $6.626{\times}10^{-34}$ Js, $\hbar = h/2\pi$

m electron mass $9.11{\times}10^{-31}$ kg

$G_0 = q^2/h$ conductance quantum $38.7{\times}10^{-6}$ S = $[25.8{\times}10^3 \ \Omega]^{-1}$

energies in eV, 1 eV = 1.602×10^{-19} J, binding energy of the electron in the hydrogen atom $E_0 = \frac{e^2}{8\pi\varepsilon_0 a_0} = 13.6$ eV

ε_0 vacuum permittivity 8.854×10^{-12} F/m

a_0 Bohr radius $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529\times10^{-11}$ m
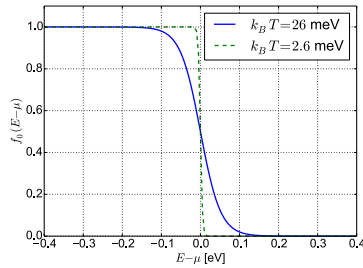
1.1 What makes electrons flow ?

Figure 1.2   Fermi distribution for different temperatures ($T = 298$ K and $T = 29.8$ K).

Source and drain can be seen as continous electron reservoirs that are filled up to the corresponding Fermi energy μ_S and μ_D respectively. Taking finite temperature T into account, the levels are occupied according to the Fermi function (fig. 1.2)

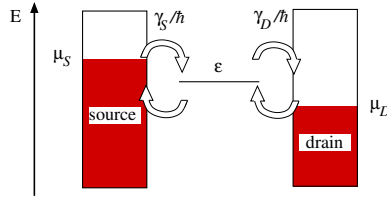$$f(E - \mu) = \frac{1}{1 + \exp[(E - \mu)/k_B T]} \ .$$
(1.1)

Figure 1.3   Source and drain under bias with a conducting level.

This corresponds to the situation depicted in fig. 1.3, where the single level at energy ε is coupled to the electrodes. The coupling can be quantified by the coupling strength $\gamma_S/\hbar$, which gives the probability for electron flow per unit time.

Denoting the number of electrons in the channel with energy ε by N, we can express the current from the source as

$$I_S = \frac{e\gamma_S}{\hbar}(f_S - N)$$
(1.2)

and similarly from the drain as

$$I_D = \frac{e\gamma_D}{\hbar}(f_D - N) \ .$$
(1.3)

Here γ_S, γ_D denote the couplings between the channel and source and drain, respectively. We have suppressed the depndence of $I_{S,D}, f_{S,D}$ and N on the states energy for brevity. At steady state conditions we have $I_S + I_D = 0$ so that we can extract the nuber of electrons in the channel

$$N = \frac{\gamma_S f_S + \gamma_D f_D}{\gamma_S + \gamma_D} \tag{1.4}$$

and get the current

$$I(\varepsilon) = \frac{e}{\hbar} \frac{\gamma_S \gamma_D}{\gamma_S + \gamma_D} [f_S(\varepsilon) - f_D(\varepsilon)] \,. \tag{1.5}$$
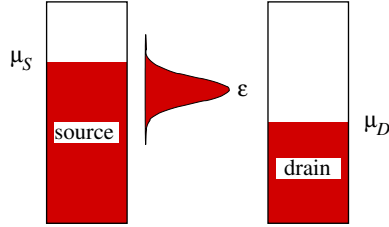
1.2 Quantum of conductance

Figure 1.4   Same as fig. 1.3, but with broadened level.

Current for $\gamma_S = \gamma_D$ and $f_S(\varepsilon) = 1$ and $f_D(\varepsilon) = 0$

$$I(\varepsilon) = \frac{e}{2\hbar} \gamma_S \tag{1.6}$$

This suggests that by increasing the coupling $\gamma_s (= \gamma_D)$ we could increase the current up to infinity. This is wrong, due to the coupling the energy level gets broadened (Lorentzian)

$$D_\varepsilon(E) = \frac{\gamma/2\pi}{(E - \varepsilon)^2 + (\gamma/2)^2} \,, \quad \int dE D_\varepsilon(E) = 1 \,, \quad D_\varepsilon(E) \underset{\gamma \to 0}{\to} \delta(E - \varepsilon) \tag{1.7}$$

It turns out that $\gamma = \gamma_S + \gamma_D$ which is reasonable as the larger the couplings, the broader the level. How to deal with a broadened level ? Instead of a regarding a single level (eq. (1.5))

$$I = \frac{e}{\hbar} \frac{\gamma_S \gamma_D}{\gamma_S + \gamma_D} [f_S(\varepsilon) - f_D(\varepsilon)]$$

we have to integrate over a distribution of levels that all contribute to the current

$$I = \frac{e}{\hbar} \frac{\gamma_S \gamma_D}{\gamma_S + \gamma_D} \int_{-\infty}^{\infty} dE \, D_\varepsilon(E)[f_S(E) - f_D(E)] \tag{1.8}$$

At low temperatures we have

$$f_S(E) - f_D(E) = \begin{cases} 1 & \text{for } \mu_S > E > \mu_D \\ 0 & \text{otherwise} \end{cases} \tag{1.9}$$

and therefore

$$I = \frac{e}{\hbar} \frac{\gamma_S \gamma_D}{\gamma_S + \gamma_D} \int_{\mu_D}^{\mu_S} dE \, D_\varepsilon(E) \tag{1.10}$$

For small bias $\mu_S - \mu_D$ and strong coupling, $D_\varepsilon(E)$ will be approximately constant within $[\mu_D, \mu_S]$, so that we might write

$$I = \frac{e}{\hbar}\frac{\gamma_S\gamma_D}{\gamma_S + \gamma_D}(\mu_S - \mu_D)\frac{(\gamma_S + \gamma_D)/2\pi}{(E - \varepsilon)^2 + [(\gamma_S + \gamma_D)/2]^2} \tag{1.11}$$

The maximal value is reached when $E = \varepsilon$ and we note that $\mu_S - \mu_D = eV_D$, hence

$$I = \frac{e^2}{h}V_D\frac{4\gamma_S\gamma_D}{(\gamma_S + \gamma_D)^2} \ . \tag{1.12}$$

The maximum is reached at $\gamma_S = \gamma_D$ which leads the conductivity to be

$$G_0 \equiv \frac{I}{V_D} = \frac{e^2}{h} \ , \tag{1.13}$$

the *quantum of conductance*. Note, that this result is independent of the coupling.
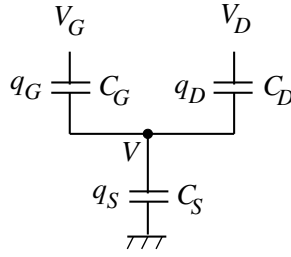
1.3 Potential profile

Figure 1.5   Capacitor model for the electrostatic potentials.

Up to now we have assumed that the channels' energy is uneffected by the voltages applied and the charge going through. In order to get the electrostatic potential from the voltages applied, we can construct a capacitor model as depicted in fig. 1.5. Considering the charge balance ($q_S = q_D + q_G$) and using $q = CV$, we get for the voltage at the channel V

$$C_SV = C_D(V_D - V) + C_G(V_G - V) \tag{1.14}$$

corresponding to the electrostatic potential

$$U_{\text{static}} = -eV = -\frac{C_D}{C}eV_D - \frac{C_G}{C}eV_G \tag{1.15}$$

where $C = C_S + C_D + C_G$. This energy corresponds to a solution of the Poisson equation without charges

$$\nabla \cdot (\varepsilon_r\nabla V) = 0 \tag{1.16}$$

and the boundary conditions given by the voltages V_D, V_G applied. We get another contribution from the change of the charge due to the electrons filled into the channel $\Delta\rho = -eN$, corresponding to the Poisson equation

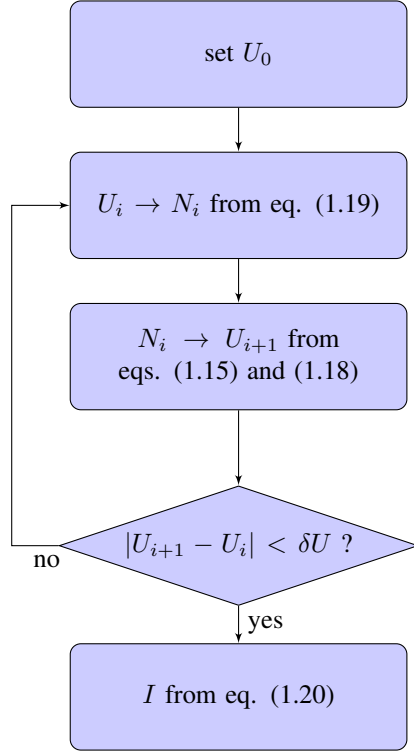$$\nabla \cdot (\varepsilon_r\nabla V) = -\frac{\Delta\rho}{\varepsilon_0} \tag{1.17}$$

Figure 1.6 Flow chart of the iterative scheme.

leading to the total potential in the channel

$$U = U_{\text{static}} + \frac{e^2}{C}N \tag{1.18}$$

where e^2/C is the energy needed to charge the channel by a full electron. The number of electrons corresponding to the potential U can then be obtained by the expression (1.4) for a broadened level

$$N = \int_{-\infty}^{\infty} dE \ D_\varepsilon(E - U)\frac{\gamma_S f_S(E) + \gamma_D f_D(E)}{\gamma_S + \gamma_D} \tag{1.19}$$

and the current from eq. (1.8). The self-constent strategy can be depicted by the scheme depicted in fig. 1.6.

After convergence the current can be obtained from (c. f. eq. (1.8))

$$I = \frac{e}{\hbar}\frac{\gamma_S\gamma_D}{\gamma_S + \gamma_D} \int_{-\infty}^{\infty} dE \ D_\varepsilon(E - U)[f_S(E) - f_D(E)] \tag{1.20}$$

Such iterative procedures can be aided in convergence by mixing where the new potential U_{new} is build as a mixture from the old U_{old} and the calculated U_{calc} from the actual N_{new}, i.e.

$$U_{\text{new}} = U_{\text{old}} + \alpha(U_{\text{calc}} - U_{\text{old}}) \tag{1.21}$$

and $0 < \alpha < 1$.

1.4 Generalized formulation

The number of electrons in the broadened channel is given by [eqs. (1.4) and (1.19)]

$$N = \int_{-\infty}^{\infty} dE \, n(E) \tag{1.22}$$

where

$$n(E) = D_\varepsilon(E) \left(\frac{\gamma_S}{\gamma_S + \gamma_D} f_S(E) + \frac{\gamma_D}{\gamma_S + \gamma_D} f_D(E) \right) \tag{1.23}$$

This equation can be written as

$$n(E) = \frac{1}{2\pi} \left[A_S(E) f_S(E) + A_D(E) f_D(E) \right] \tag{1.24}$$

where we have introduced the spectral functions

$$A_S(E) = G(E) \, \gamma_S \, G^+(E) \, , \quad A_D(E) = G(E) \, \gamma_D \, G^+(E) \tag{1.25}$$

that are defined over the Greens function

$$G(E) = [E - \varepsilon + i\gamma_S/2 + i\gamma_D/2]^{-1} \, . \tag{1.26}$$

In order to proof eq. (1.24) we write the spectral functions explicitely

$$A_S(E) \quad = \quad \frac{\gamma_S}{(E - \varepsilon)^2 + [(\gamma_S + \gamma_D)/2]^2} \tag{1.27}$$

$$A_D(E) \quad = \quad \frac{\gamma_D}{(E - \varepsilon)^2 + [(\gamma_S + \gamma_D)/2]^2} \tag{1.28}$$

from which it is easy to see, that

$$A_S(E) f_S(E) + A_D(E) f_D(E) =$$
$$\frac{\gamma_S + \gamma_D}{(E - \varepsilon)^2 + [(\gamma_S + \gamma_D)/2]^2} \left[\frac{\gamma_S}{\gamma_S + \gamma_D} f_S(E) + \frac{\gamma_D}{\gamma_S + \gamma_D} f_S(E) \right] \, . \tag{1.29}$$

Similarly, we can generalize the expression of the current in eq. (1.8) to

$$I = \frac{q}{h} \int_{-\infty}^{\infty} dE \, \bar{T}(E) \left[f_S(E) - f_D(E) \right] \tag{1.30}$$

where we have introduced the transmission function

$$\bar{T}(E) = \gamma_S \, G(E) \, \gamma_D \, G^+(E) \, . \tag{1.31}$$

1.5 Multi-level conductors

Eqs. (1.24) and (1.31) are very general results as we will see later in this course. These quantities have been formulated for a channel with a single conducting level up to now. Real channels have many conductiong levels, not just one as we assumed up to now. Then we will have the transitions

$$\varepsilon \to [H] \qquad \text{Hamiltonian matrix}$$
$$\gamma \to [\Gamma(E)] \qquad \text{Broadening matrix}$$
$$2\pi D(E) \to [A(E)] \qquad \text{Spectral function}$$
$$2\pi n(E) \to [G^n(E)] \qquad \text{Correlation function}$$
$$N \to [\rho] \qquad \text{Density matrix}$$

where we note that the broadening matrix $\Gamma(E)$ will be described via the "self-energy" matrix $\Sigma(E)$ with

$$\Gamma = i\left[\Sigma(E) - \Sigma^+(E)\right] \tag{1.32}$$

and we have used $G^n(E)$ to denote what is usually written as $-iG^<(E)$ in the literature.

CHAPTER 2

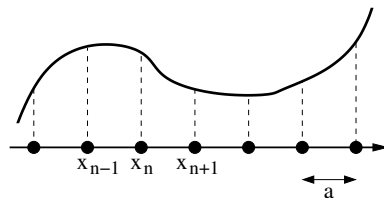# SCHRÖDINGER EQUATION

2.1 Finite difference method

Figure 2.1   A function with finite support $\dots, x_{n-1}, x_n, x_{n+1}, \dots$

The one dimensional Schrödinger equation is defined via the Hamiltonian

$$\hat{H} = -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + U(x) \ . \tag{2.1}$$

Transform the *differential* equation into a finite difference equation (see fig. 2.1)

$$\left.\left(\frac{\partial^2 \psi}{\partial x^2}\right)\right|_{x=x_n} \to \frac{1}{a^2}[\psi(x_{n-1}) - 2\psi(x_n) + \psi(x_{n+1})] \tag{2.2}$$

where $a = x_{n+1} - x_n$. Similarly we discretize the potential

$$U(x)\psi(x)|_{x=x_n} \to U(x_n)\psi(x_n) \tag{2.3}$$

The means that we transform

the differential operator $\hat{H}$ into   a matrix $[H]$
the wave function $\psi(x,t)$ into   a vector $\{\psi(t)\}$

and the Schrödinger equation is converted

from   partial differential eq.   into   a matrix equation
from $i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$ into $i\hbar\frac{d}{dt}\{\psi(t)\} = [H]\{\psi(t)\}$

The Hamiltonian matrix is then

$$H_{n,m} = [U_n + 2t_0]\delta_{n,m} - t_0\delta_{n,m-1} - t_0\delta_{n,m+1} \tag{2.4}$$

where $t_0 = \hbar/(2ma^2)$ and $U_n = U(x_n)$. Explicitely

$$[H] = \begin{array}{c c c c c c c}
 & x_1 & x_2 & \ldots & x_{n-1} & x_n & x_{n+1} \\
x_1 & U_1 + 2t_0 & -t_0 & & 0 & 0 & 0 \\
x_2 & -t_0 & U_2 + 2t_0 & & 0 & 0 & 0 \\
\ldots & & & \ldots & & \ldots & \\
x_{n-1} & 0 & 0 & & U_{n-1} + 2t_0 & -t_0 & 0 \\
x_n & 0 & 0 & & -t_0 & U_n + 2t_0 & -t_0 \\
x_{n+1} & 0 & 0 & & 0 & t_0 & U_{n+1} + 2t_0
\end{array} \tag{2.5}$$

and

$$\{\psi\} = \{\psi(x_1)\ \psi(x_2)\ \ldots\} \equiv \{\psi_1\ \psi_2\ \ldots\}. \tag{2.6}$$

2.2 Example: Particle in the box

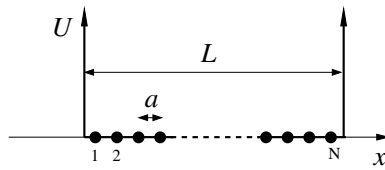**Figure 2.2**   The box potential.

One of the simplest problems is the "particle in the box", i.e. solving the Schrödinger equation for the potential depicted in fig. 2.2. The eigenstates are

$$\phi_\alpha(x) \propto \sin(k_\alpha x) \quad \text{with} \quad k_\alpha = \alpha\frac{\pi}{L}, \ \alpha = 1, 2, \ldots . \tag{2.7}$$

and their energy is
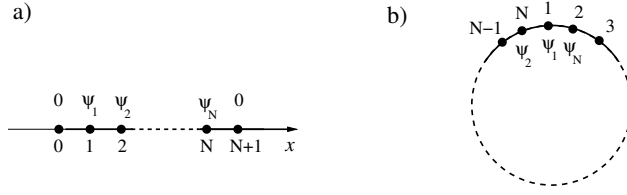
$$E_\alpha = \frac{\hbar^2 k_\alpha^2}{2m} . \tag{2.8}$$

We could solve this on a discrete lattice of $N = 100$ points, writing the 100×100 matrix

$$
[H] = \begin{array}{c c c c c c}
 & 1 & 2 & \ldots & N-1 & N \\
1 & 2t_0 & -t_0 & & 0 & 0 \\
2 & -t_0 & 2t_0 & & 0 & 0 \\
\ldots & & & \ldots & & \ldots \\
N-1 & 0 & 0 & & 2t_0 & -t_0 \\
N & 0 & 0 & & -t_0 & 2t_0
\end{array} \tag{2.9}
$$

where $t_0 = \hbar^2/(2ma^2)$. The discretisation

$$
-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \to t_0 \left[\psi(x_{n-1}) - 2t_0 \psi(x_n) + t_0 \psi(x_{n+1}) \right] \tag{2.10}
$$

can be expected to be accurate onle when ψ varies slowly on a length scale a. For the basis functions $\phi_\alpha \propto \sin(k_\alpha x) \propto e^{ik_\alpha x} - e^{-ik_\alpha x}$ we get in the dicretized version of the kinetic energy operator

$$
t_0 \left[\phi_\alpha(x_{n-1}) - 2t_0 \phi_\alpha(x_n) + t_0 \phi_\alpha(x_{n+1}) \right] = 2t_0 \left[1 - \cos(k_\alpha a) \right] \phi_\alpha(x_n) \tag{2.11}
$$

i. e. the numeric version has the same Eigenfunctions as the analytic one, but for different energies. For $k_\alpha a \ll 1$ we can expand the $\cos$ function and get the analytic result (c.f. fig.

Figure 2.3   Energies from eqs. (2.8) and (2.11).

2.3)

$$
E_\alpha \approx 2t_0 \left[1 - 1 + (k_\alpha a)^2/2 \right] = \frac{\hbar^2 k_\alpha^2 a^2}{2ma^2} \ . \tag{2.12}
$$

2.3 Boundary conditions

Strictly speaking, the statement that $\phi_\alpha \propto \sin(k_\alpha x)$ are also the eigenfunctions of the discrete version is not completely correct as we have ignored the boundary, where we get the kinetic energy operator as

$$
t_0[-2\psi(x_1) + \psi(x_2)] \ \text{and} \ t_0[\psi(x_{N-1}) - 2\psi(x_N)] \tag{2.13}
$$

as $\psi(x_0) = \psi(x_{N+1}) = 0$. This corresponds to Zero boundary conditions, see fig. 2.4. We could also apply periodic boundary conditions that wold correspond mathematically to

a)

b)

Figure 2.4 a) Zero and b) periodic boundary conditions.

the Hamiltonian

$$[H] = \begin{array}{c c} & \begin{array}{ccccc} 1 & 2 & \ldots & N-1 & N \end{array} \\ \begin{array}{c} 1 \\ 2 \\ \ldots \\ N-1 \\ N \end{array} & \left(\begin{array}{ccccc} 2t_0 & -t_0 & & 0 & -t_0 \\ -t_0 & 2t_0 & & 0 & 0 \\ & & \ldots & & \ldots \\ 0 & 0 & & 2t_0 & -t_0 \\ -t_0 & 0 & & -t_0 & 2t_0 \end{array} \right) \end{array} \qquad (2.14)$$

where the only change are the elements $H_{1,N}$ and $H_{N,1}$. Therefore we can expect this change to be small if N is large. We have now the peridicty condition

$$\psi(x_{n+1}) = \psi(L + x_1) \equiv \psi(x_1) \qquad (2.15)$$

which is fullfilled by the Eigenfunctions

$$\phi_\alpha(x) \propto \sin(k_\alpha x) \text{ and } \cos(k_\alpha x) \qquad (2.16)$$

where

$$k_\alpha = \alpha \frac{2\pi}{L}, \ \alpha = 1, 2, \ldots . \qquad (2.17)$$

Note that we now get two wave functions with just half of the k_α values that are doubly spaced in k. For each k_α we can either use the two orthogonal real Eigenfunctions (corresponding to standing waves)

$$\sin(k_\alpha x) \text{ and } \cos(k_\alpha x) \qquad (2.18)$$

or their orthogonal complex combinations

$$e^{ikx} \text{ and } e^{-ikx} \qquad (2.19)$$

(corresponding to moving waves).

Number of eigenvalues: $(N \times N)$ Hamiltonian has N eigenvalues. On a discrete lattice with spacing a

$$\sin(k_\alpha x) = \sin\left(\left[k_\alpha + \frac{2\pi}{a}\right] x\right) \qquad (2.20)$$

$$\Rightarrow 0 < k_\alpha a \leq 2\pi$$

	zero bc	periodic bc
condition	$\phi(0) = \phi(L) = 0$	$\phi(x + L) = \phi(x)$
solutions	$\sin(k_\alpha x); k_\alpha = \alpha \frac{\pi}{L}; \alpha = 1, 2, \ldots$	$\sin(k_\alpha x), \cos(k_\alpha x); k_\alpha = \alpha \frac{2\pi}{L}; \alpha = 0, 1, \ldots$
descrete lattice	$0 < k_\alpha a \leq 2\pi$	$-\pi < k_\alpha a \leq +\pi$

CHAPTER 3

BASIS FUNCTIONS

3.1 General description

A wave function can be expressed in terms of basis functions

$$\phi(\mathbf{r}) = \sum_{m=1}^{\infty} \phi_m u_m(\mathbf{r}) \approx \sum_{m=1}^{M} \phi_m u_m(\mathbf{r}) \tag{3.1}$$

which can be expressed as a vector

$$\phi(\mathbf{r}) \rightarrow \{\phi_1 \ \phi_2 \ \ldots \ \phi_M\}^T \tag{3.2}$$

where 'T' denotes transpose. When we use the special basis $\{u(\mathbf{r})\}$ of step functions in space, we get the real space representation

$$\phi(\mathbf{r}) \rightarrow (\phi(\mathbf{r}_1) \ \phi(\mathbf{r}_2) \ \ldots \ \phi(\mathbf{r}_M))^T = \mathbf{u}\phi \ . \tag{3.3}$$

Substituting eq. (3.1) into the Schrödinger equation

$$E\phi(\mathbf{r}) = \hat{H}\phi(\mathbf{r}) \tag{3.4}$$

leads to

$$E \sum_m \phi_m u_m(\mathbf{r}) = \sum_m \phi_m \hat{H} u_m(\mathbf{r}) \ . \tag{3.5}$$

Multiplication of both sides with $u_n^*(\mathbf{r})$ from the left and integration over space gives

$$E \sum_m S_{nm} \phi_m = \sum_m H_{nm} \phi_m \qquad (3.6)$$

which can be written in matrix notation

$$E [S] \{\phi\} = [H] \{\phi\} \qquad (3.7)$$

with

$$S_{nm} = \int d\mathbf{r} \; u_n^*(\mathbf{r}) u_m(\mathbf{r}) = \langle\, n \,|\, m \,\rangle \qquad (3.8)$$

$$H_{nm} = \int d\mathbf{r} \; u_n^*(\mathbf{r}) \; \hat{H} \; u_m(\mathbf{r}) = \langle\, n \,|\hat{H}|\, m \,\rangle \qquad (3.9)$$

Equation (3.10) can be solved as

$$E [S] \{\phi\} = [S]^{-1} [H] \{\phi\} \qquad (3.10)$$

and leads to a set of eigenvalues E_α and eigenvectors $\{\phi_\alpha\}$. The functions in real space are then reconstructed by

$$\phi_\alpha(\mathbf{r}) = \frac{1}{\sqrt{Z_\alpha}} \sum_m \underbrace{\{\phi_\alpha\}_m}_{\phi_{m\alpha}} u_m(\mathbf{r}) \qquad (3.11)$$

where Z_α is the normalization constant

$$1 \equiv \int d\mathbf{r} \; \phi_\alpha^*(\mathbf{r}) \phi_\alpha(\mathbf{r}) \;\; \rightarrow \;\; Z_\alpha = \sum_n \sum_m \phi_{n\alpha}^* \phi_{m\alpha} S_{nm} \; . \qquad (3.12)$$

3.2 Specific example: H$_2^+$
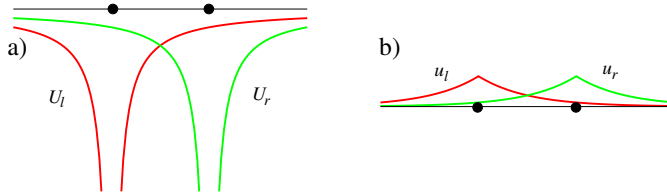
Figure 3.1 a) Potentials and b) basis functions for H$_2^+$.

The H$_2^+$ SEQ is

$$E\phi(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U_l(\mathbf{r}) + U_r(\mathbf{r}) \right] \phi(\mathbf{r}) \qquad (3.13)$$

and we write the approximative solution as

$$\phi(\mathbf{r}) = \phi_l u_l(\mathbf{r}) + \phi_r u_r(\mathbf{r}) \qquad (3.14)$$

where u_l, u_r are hydrogen 1s wavefunctions at left and right nuclei, respectively. I. e.

$$E_H u_{l/r}(\mathbf{r}) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U_{l/r}(\mathbf{r}) \right] u_{l/r}(\mathbf{r}) \text{ with } E_H = \text{-13.6 eV .} \tag{3.15}$$

At large separations R we get two degenerate solutions

$$(\phi_l \ \phi_r) = (1 \ 0) \text{ and } (\phi_l \ \phi_r) = (0 \ 1) \text{ with } E \approx E_H \tag{3.16}$$

We can now express the matrices

$$S = \begin{bmatrix} 1 & s \\ s & 1 \end{bmatrix} \tag{3.17}$$

with the overlap

$$s = \int d\mathbf{r} \ u_l^*(\mathbf{r}) u_r(\mathbf{r}) \ \geq 0 \tag{3.18}$$

and

$$H = \begin{bmatrix} E_H + a & E_H s + b \\ E_H s + b & E_H + a \end{bmatrix} \tag{3.19}$$

with

$$a = \int d\mathbf{r} \ u_l^* U_r u_l = \int d\mathbf{r} \ u_r^* U_l u_r \ \leq 0 \tag{3.20}$$
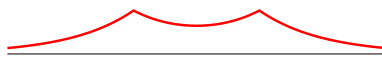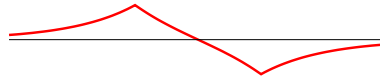
$$b = \int d\mathbf{r} \ u_l^* U_r u_r = \int d\mathbf{r} \ u_l^* U_l u_r$$

$$= \int d\mathbf{r} \ u_r^* U_l u_l = \int d\mathbf{r} \ u_r^* U_r u_l \ \leq 0 \tag{3.21}$$

where $|a| > |b|$.

The SEQ becomes

$$E \begin{pmatrix} \phi_l \\ \phi_r \end{pmatrix} = \begin{bmatrix} 1 & s \\ s & 1 \end{bmatrix}^{-1} \begin{bmatrix} E_H + a & E_H s + b \\ E_H s + b & E_H + a \end{bmatrix} \begin{pmatrix} \phi_l \\ \phi_r \end{pmatrix} \tag{3.22}$$

and a straightforward calculation gives the two solutions corresponding to binding (B) and anti-binding (A) states

$E_B = E_H + \frac{a+b}{1+s}$
$(\phi_l \ \phi_r) = (1 \ 1)$

$\phi_B(\mathbf{r}) = \frac{1}{\sqrt{Z_B}}(u_l(\mathbf{r}) + u_r(\mathbf{r}))$

$E_B = E_H + \frac{a-b}{1-s}$
$(\phi_l \ \phi_r) = (1 \ -1)$

$\phi_A(\mathbf{r}) = \frac{1}{\sqrt{Z_A}}(u_l(\mathbf{r}) - u_r(\mathbf{r}))$

How accurate are the solutions with just two basis functions ?

We could also use other basis functions of hydrogen: 2s, $2p_x$, $2p_y$, $2p_y$, 3s, ... and would end up with a matrix that can be expressed schematically as

$$\begin{bmatrix} E_{1s} & M \\ M & E_{2s} \end{bmatrix} \tag{3.23}$$

where M is significant only if $M \sim |E_{1s} - E_{2s}|$ where $|E_{1s} - E_{2s}| \approx 10$ eV for hydrogen. The 1s basis can be expected to give a good description for not to small R.

3.3 Basis functions as conceptual tool

The Hilbertspace can be seen as vector space, a state vector can be written as

$$\psi = \phi_1 u_1 + \phi_2 u_2 + \phi_3 u_3 + \ldots \tag{3.24}$$

or in Dirac notation

$$|\Phi\rangle = \sum_m \phi_m |u_m\rangle \tag{3.25}$$

where ϕ_m are just usual numbers. The scalar product can be discretized on a 3D lattice

$$\langle f | g \rangle = \int d\mathbf{r} \, f^*(\mathbf{r})g(\mathbf{r}) \approx a^3 \sum_m f^*(\mathbf{r}_m)g(\mathbf{r}_m) \; . \tag{3.26}$$

An othogonal basis fullfills

$$\langle m | n \rangle = \int d\mathbf{r} \, u_m^*(\mathbf{r})u_n(\mathbf{r}) = \delta_{mn} \; . \tag{3.27}$$

We often have to deal with non-orthogonal basis functions like in the H_2^+ example above, where i.e.

$$\int d\mathbf{r} \, u_l^*(\mathbf{r})u_r(\mathbf{r}) = e^{-R}\left[1 + R + (R^2/3)\right] \neq 0 \tag{3.28}$$

with the nuclear separation R. In general

$$S_{mn} = \langle m | n \rangle \tag{3.29}$$

and we can create an orthogonal basis

$$\tilde{u}_i(\mathbf{r}) = \sum_n [S^{-1/2}]_{ni}(\mathbf{r}) \tag{3.30}$$

as

$$\begin{aligned} \int d\mathbf{r} \, \tilde{u}_i^*(\mathbf{r})\tilde{u}_j(\mathbf{r}) &= \sum_n \sum_m [S^{-1/2}]_{in} S_{nm} [S^{-1/2}]_{mj} \\ &= [S^{-1/2}SS^{-1/2}] = [I]_{nm} = \delta_{mn} \; . \end{aligned} \tag{3.31}$$

Operators are represented as

$$\langle n |\hat{A}| m \rangle = \int d\mathbf{r} \, u_m^*(\mathbf{r})\hat{A}u_n(\mathbf{r}) = [A]_{mn} \tag{3.32}$$

CHAPTER 4

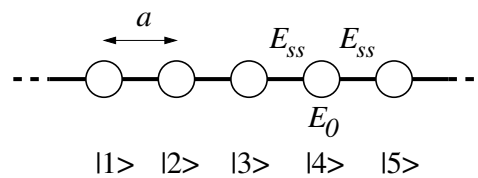# BAND STRUCTURE

4.1 1D solid

Figure 4.1 1D infinite chain model.

We start with a simple model for a one dimensional (1D) solid composed of N atoms. The atoms shall be separated by a and we consider only one single orbital per atom. Considering only overlaps by nearest neighbors, we end up with the $(N \times N)$ Hamiltonian matrix

$$
[H] =
\begin{array}{c}
 \\
|1\rangle \\
|2\rangle \\
\cdots \\
|N-1\rangle \\
|N\rangle
\end{array}
\begin{array}{cccccc}
|1\rangle & |2\rangle & \cdots & |N-1\rangle & |N\rangle \\
E_0 & E_{ss} & & 0 & E_{ss} \\
E_{ss} & E_0 & & 0 & 0 \\
& & \cdots & & \cdots \\
0 & 0 & & E_0 & E_{ss} \\
E_{ss} & 0 & & E_{ss} & E_0
\end{array}
\tag{4.1}
$$

where E_0 is the energy of the state for an isolated atom and E_{ss} is the off diagonal element. Note, that we have applied the periodic boundary condition, which is at first sight not realistic for and infnite chain. We will see soon that this description gives the correct limit for $N \to \infty$.

Note also, that the Hamiltonian (4.1) is formallly the same as the finite difference Hamiltonian (2.14) that we have discussed already. The Schrödinger equation

$$E\psi_n = E_0\psi_n + E_{ss}\psi_{n+1} + E_{ss}\psi_{n-1} \tag{4.2}$$

can be solved analytically by the Ansatz

$$\psi_n = \psi_0\, e^{ikna} \ . \tag{4.3}$$

Cancelling the common factor $\psi_0 e^{ikna}$ leads to

$$E = E_0 + E_{ss}e^{ika} + E_{ss}e^{-ika} = E_0 + 2E_{ss}\cos(ka) \ . \tag{4.4}$$

We get N eigenvalues (see also fig. 4.2)

$$E_\alpha = E_0 + 2E_{ss}\cos(k_\alpha a) \quad \text{where} \quad k_\alpha a = \alpha\frac{2\pi}{N} \quad \text{and} \quad \alpha = 0, 1, \dots, N-1 \ . \tag{4.5}$$

For $N \to \infty$ the energy depending on k forms a "band" for which the energetics is called
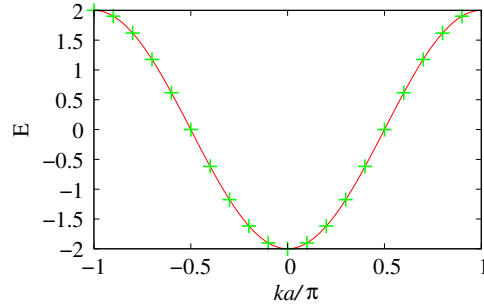

Figure 4.2   Energy E versus ka/π for $E_0 = 0$ and $E_{ss} = -1$. The crosses denote the eigenvalues of the matrix (4.1) for $N = 20$.

the "band structure" of the chain.

We have used $E_{ss} < 0$ in the example of fig. 4.2, a choice that is very reasonable for the overlap of two s wave functions (remember that both a and b integrals in eqs. (3.20) and (3.21) of the H_2^+ model). This does not have to be the case for instance for the overlap of p orbitals where $E_{pp} > 0$ is well possible.

4.2   Lattice with a basis

We now consider a 1D solid, which has to states in the unit cell. This could either describe a situation where we have two atoms that are nearer to each other (e.g. through Peirls distortion), or two basis functions on the same atom. The hamiltonian can now be written
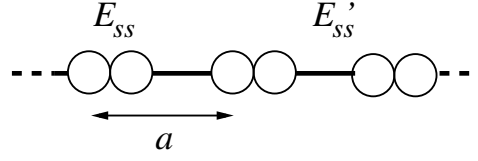
Figure 4.3   A one dimensional solid with two atoms in the unit cell.

as

$$[H] = \begin{array}{c c c c c c} & |1A\rangle & |1B\rangle & |2A\rangle & |2B\rangle & \dots \\ |1A\rangle & E_0 & E_{ss} & 0 & 0 & \dots \\ |1B\rangle & E_{ss} & E_0 & E'_{ss} & 0 & \dots \\ |2A\rangle & 0 & E'_{ss} & E_0 & E_{ss} & \dots \\ |2B\rangle & 0 & 0 & E_{ss} & E_0 & \dots \\ & \dots & \dots & \dots & \dots & \dots \end{array} \qquad (4.6)$$

where we have two distinct off-diagonal elements E_{ss} and E'_{ss}. Note, that the Hamiltonian corresponds to the assymmetric situation that state $|n, A\rangle$ exclusively couples to state $|n-1, B\rangle$ on the "left" and $|n, B\rangle$ exclusively couples to state $|n+1, A\rangle$ on the "right".

We could combine the elements of the matrix into (2×2) blocks and write

$$[H] = \begin{array}{c c c c c} & |1\rangle & |2\rangle & |3\rangle & \dots \\ |1\rangle & H_{11} & H_{12} & 0 & \dots \\ |2\rangle & H_{21} & H_{22} & H_{23} & \dots \\ |3\rangle & 0 & H_{32} & H_{33} & \dots \\ & \dots & \dots & \dots & \dots \end{array} \qquad (4.7)$$

where

$$H_{nn} = \begin{bmatrix} E_0 & E_{ss} \\ E_{ss} & E_0 \end{bmatrix} \quad H_{n,n+1} = \begin{bmatrix} 0 & 0 \\ E'_{ss} & 0 \end{bmatrix} \quad H_{n,n-1} = \begin{bmatrix} 0 & E'_{ss} \\ 0 & 0 \end{bmatrix} . \qquad (4.8)$$

The matrix (4.7) is now of the form as eq. (4.1) and we can write the SEQ $E\{\psi\} = [H]\{\psi\}$ as

$$E\phi_n = H_{nn}\phi_n + H_{n,n-1}\phi_{n-1} + H_{n,n+1}\phi_{n+1} \qquad (4.9)$$

where ϕ_n is a (2×1) vector and the element H_{mn} a (2×1) matrix. the equation (4.9) can be solved by the Ansatz

$$\phi_n = \phi_0 e^{ikna} \qquad (4.10)$$

leading to

$$\begin{aligned} E\{\phi_0\} &= [H_{nn}]\{\phi_0\} + [H_{n,n-1}]e^{-ika}\{\phi_0\} + [H_{n,n+1}]e^{ika}\{\phi_0\} \\ &= \begin{bmatrix} E_0 & E_{ss} + E'_{ss}e^{ika} \\ E_{ss} + E'_{ss}e^{-ika} & E_0 \end{bmatrix} \{\phi_0\} . \end{aligned} \qquad (4.11)$$

Solving this eigenvalue equation is straightforward and gives

$$E = E_0 \pm \left[E_{ss}^2 + E'^2_{ss} + 2E_{ss}E'_{ss}\cos(ka) \right]^{1/2} \qquad (4.12)$$

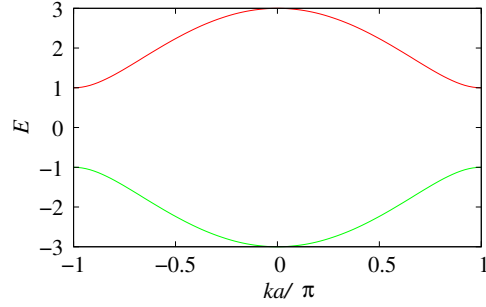giving two energies as shown in fig. 4.4.

Figure 4.4   Energies in the two state model for $E_0 = 0$, $E_{ss} = -1$, and $E'_{ss} = -2$.
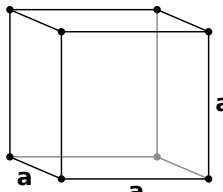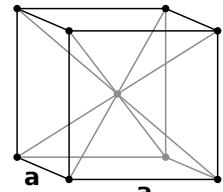
4.3 Size quantization

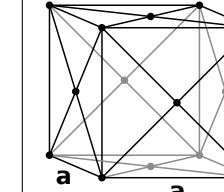| name	simple cubic	body centered cubic (BCC)	face centered cubic (FCC)
reciprocal	simple cubic	FCC	BCC
examples	NaCl	Fe	Cu, Ag, Au

Figure 4.5   The three most important cubic lattice structures.

Similar to the 1D structures discussed above, where the energy levels $E(k)$ are labeled in terms of the momentum k, in 3D the energy is a function the momentum $\mathbf{k}$. The periodicity is now in all three dimensions and many metals have cubic structures as shown in fig. 4.5. The band structure is can be rather complicated, but can be approximated by a quasi free particle model with effective mass m_c (see fig. 4.6)

$$E(\mathbf{k}) = E_c + \frac{\hbar^2 k^2}{2m_c} \; . \tag{4.13}$$

Confinement in some direction, e. g. the z direction, leads to the emergence of "subbands" where the energy is

$$E_\alpha(\mathbf{k}) = E_c + \frac{\hbar^2(k_x^2 + k_y^2)}{2m_c} + \alpha^2 \varepsilon_z \;\; \text{with} \;\; \varepsilon_z = \frac{\hbar^2 \pi^2}{2m_c L_z^2}, \; \alpha = 1, 2, \ldots \; . \tag{4.14}$$

Similarly for a quantum wire (1D)

$$E_\alpha(\mathbf{k}) = E_c + \frac{\hbar^2(k_x^2)}{2m_c} + \alpha^2 \varepsilon_z + \beta^2 \varepsilon_y \; . \tag{4.15}$$

Special points:

Γ : $\mathbf{k} = 0$

L : $\mathbf{k} = \hat{\mathbf{e}}_x \cdot 2\pi/a$

X : $\mathbf{k} = (\hat{\mathbf{e}}_x + \hat{\mathbf{e}}_y + \hat{\mathbf{e}}_z) \cdot 2\pi/a$
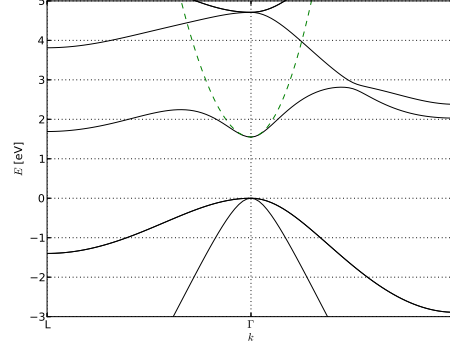
Figure 4.6 Band structure model for common semiconductors (for GaAs after Datta [1]). The broken line is the energy according to an effective mass model with $E_c = 1.55$ eV and $m_c = 0.12\,m$ (m is the electron mass).

4.4 Density of states

We saw in the introduction, that the conduction crucially depends on the density of available states $D(E)$ in the channel. We therfore ask the question, how the confinement influences the density of states (DOS). Periodic boundary conditions L_x, L_y, L_z restricts the momenta to

$$k_x = \frac{2\pi}{L_x}\nu_x \ , \ \ k_y = \frac{2\pi}{L_y}\nu_y \ , \ \ k_z = \frac{2\pi}{L_z}\nu_z \tag{4.16}$$

where ν_x, ν_y, ν_z are integers. We as how many states are there up to a given k and assume that the number of states are sufficiently dense such that we can replace the summations by integrals

$$\sum_{k_x} \to \int \frac{dk_x}{2\pi/L_x} \ , \ \ \sum_{k_y} \to \int \frac{dk_y}{2\pi/L_y} \ , \ \ \sum_{k_z} \to \int \frac{dk_z}{2\pi/L_z} \tag{4.17}$$

The we get for 1D to 3D

$$N(k) = \frac{L}{2\pi}\int_{-k}^{k} dk = \frac{L}{2\pi}2k = \frac{kL}{\pi} \quad \text{for 1D} \tag{4.18}$$

$$N(k) = \frac{L_x L_y}{(2\pi)^2}\int_0^{2\pi} d\varphi \int_0^{k} dK\, K = \frac{L_x L_y}{(2\pi)^2}\pi k^2 = \frac{k^2 L_x Ly}{4\pi} \quad \text{for 2D} \tag{4.19}$$

$$N(k) = \frac{L_x L_y L_z}{(2\pi)^3}\frac{4\pi}{3}k^3 = \frac{k^3 L_x L_y L_z}{6\pi^2} \quad \text{for 3D} \tag{4.20}$$

Using the dispersion relation (4.13) we get $N(E)$ and from there the density of states
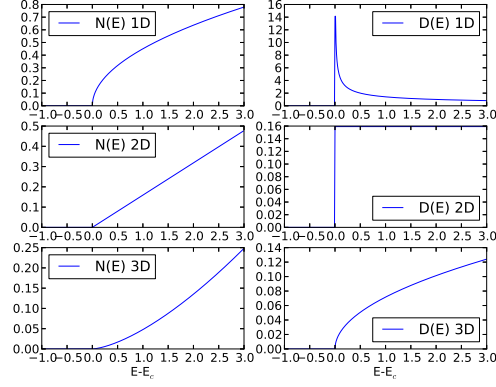
$$D(E) = \frac{d}{dE}N(E) \tag{4.21}$$

Figure 4.7 $N(E)$ and $D(E)$ from 1D to 3D in atomic units ($\hbar = m_c = 1$) and $L = S = V = 1$.

which are explicit

$$N(E) = L\frac{\sqrt{2m_c(E - E_c)}}{\pi\hbar} \qquad D(E) = \frac{L}{2\pi}\sqrt{\frac{2m_c}{E - E_c}} \qquad \text{1D}$$

$$N(E) = \underbrace{S}_{L_x L_y}\frac{2m_c}{\hbar^2}(E - E_c) \qquad D(E) = \frac{S}{4\pi}\frac{2m_c}{\hbar^2} \qquad \text{2D}$$

$$N(E) = \underbrace{V}_{L_x L_y L_z}\frac{1}{6\pi^2}\left[\frac{2m_c}{\hbar^2}(E - E_c)\right]^{3/2} \qquad D(E) = \frac{V}{4\pi^2}\left[\frac{2m_c}{\hbar^2}\right]^{3/2}\sqrt{E - E_c} \qquad \text{3D}$$

and shown in fig. 4.7.

CHAPTER 5

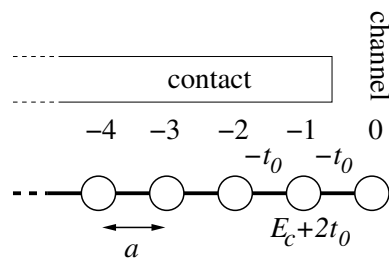# LEVEL BROADENING

5.1 1D example

Figure 5.1   1D semi infinite chain model.

We consider semi-infinite 1D wire in the model depicted in fig. 5.1. We treat the first point labled "0" as our channel. Decoupled from the contact

$$E\psi = (E_c + 2t_0)\psi$$

and coupled

$$E\psi = (E_c + 2t_0)\psi - t_0\Phi_{-1} \tag{5.1}$$

The contact wave functions Φ_n satisfy the infinite series of eqts

$$E\Phi_n = -t_0\Phi_{n-1} + (E_c + 2t_0)\Phi_n - t_0\Phi_{-n1} \tag{5.2}$$

The solutions are plane waves, we can write

$$\Phi_n = Be^{ikna} + Ce^{-ikna} \tag{5.3}$$

with the energy

$$E = E_c + 2t_0(1 - \cos ka) \tag{5.4}$$

Using our solution (5.3)

$$\psi \equiv \Phi_0 = B + C \tag{5.5}$$

and for the neighboring

$$\Phi_{-1} = Be^{-ika} + Ce^{ika} = \psi e^{ika} + B[e^{-ika} - e^{ika}] \tag{5.6}$$

such that we can express the SEQ of the contact as

$$E\psi = \underbrace{(E_c + 2t_0)}_{H}\psi \underbrace{-t_0 e^{ika}}_{\Sigma}\psi + \underbrace{2it_0 B \sin ka}_{S} \tag{5.7}$$

We arrived at the form

$$E\psi = [H + \Sigma]\psi + S \tag{5.8}$$

with the self energy

$$\Sigma = -t_0 e^{ika} \tag{5.9}$$

and the source term

$$S = 2it_0 B \sin ka . \tag{5.10}$$

5.2 General formulation

In order to generalize these findings, we first consider the wave functions of the contact. The contact is thought to be described in a large basis of dimension R. Its electrons satisfy the Schrödinger eq.

$$[E[I]_R - [H]_R]\{\Phi\}_R = \{0\} \tag{5.11}$$

If we connect the channel to the contact, we have to modify the equation

$$[E[I]_R - [H]_R + i[\eta]_R]\{\Phi\}_R = \{S\}_R \tag{5.12}$$

where $[\eta]_R = 0^+[I]_R$ describes the extraction of electrons[1] and $\{S\}_R$ is responsible for the reinjection of electrons (the results obtained will be in dependent of $\{S\}_R$). The transition from (5.11) to (5.12) represents a fundamental change of viewpoint: Rather than having

---

[1] A positive $[\eta]_R$ corresponds to electron extraction. To show this, we consider the time dependent Schrödinger eq.

$$i\hbar\partial_t\phi = H\phi \tag{5.13}$$

with the solutions

$$\phi(t) = \phi_0 e^{-i(E/\hbar)t} . \tag{5.14}$$

Adding a negative complex energy contribution $E \to E - i|\eta|$ leads to a wave-funtion that decays with increasing time

$$\phi(t) = \phi_0 e^{-iEt/\hbar} e^{-|\eta|t/\hbar} . \tag{5.15}$$

discrete eigenenergies E_α, we regard E as continous variable now due to the possibility of excitation from external sources that maintain the constant electrochemical potential.

We now need to couple the channel described by its Hamiltonian H to the contacts via the matrix τ

$$\begin{bmatrix} EI_R - H_R + i\eta_R & -\tau^+ \\ -\tau & EI - H \end{bmatrix} \begin{Bmatrix} \Phi_R + \chi_R \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix} \qquad (5.16)$$

where we have also introduced the scatterd wave $\{\chi\}_R$ in the contact due to the coupling to the channel. Except of E all quantities are vectors or matrices of the sizes:

$$H_R, I_R, \eta_R \quad : \quad (R \times R) \qquad (5.17)$$
$$H, I \quad : \quad (d \times d) \qquad (5.18)$$
$$\tau : (d \times R) \quad , \quad \tau^+ : (R \times d) \qquad (5.19)$$
$$\{\Phi_R\}, \{\chi_R\}, \{S_R\} \quad : \quad (R \times 1) \qquad (5.20)$$
$$\{\psi\} \quad : \quad (d \times 1) \qquad (5.21)$$

where $R \gg d$ (d is the dimension of the channel). The injection from the external sources remains unchanged such that we may use eq. (5.12) to write two coupled equations for the contact and the channel

$$[EI_R - H_R + i\eta]\{\chi_R\} - [\tau^+]\{\psi\} = \{0\} \qquad (5.22)$$
$$[EI - H]\{\psi\} - [\tau]\{\chi_R\} = [\tau]\{\Phi_R\} . \qquad (5.23)$$

We are mainly interested in the channel wavefunction $\{\psi\}$ and use eq. (5.22) to express $\{\chi_R\}$ in terms of this quantity

$$\{\chi_R\} = G_R \tau^+ \{\psi\} \qquad (5.24)$$

where we have used the contact Green's function

$$G_R \equiv [EI_R - H_R + i\eta]^{-1} . \qquad (5.25)$$

This allows us to write the equation involving $\{\psi\}$ only as

$$[EI - H - \Sigma]\{\psi\} = \{S\} \qquad (5.26)$$

with the self energy and the source

$$\Sigma \equiv \tau\, G_R\, \tau^+ \; ; \; \{S\} \equiv \tau\{\Phi_R\}. \qquad (5.27)$$

Evaluation of Σ ans S in real space

Generally, $[G_R(E)]$ is of large size $(R \times R)$ and Φ_R of size $(R \times 1)$. The coupling $[\tau]$ is $(d \times R)$. The channel dimension $d \ll R$, and the contact dimension R might go to infinity.

In real space, there is only coupling by the surface of the contact, i.e. $[\tau]$ is of size $(d \times r)$ where r is finite and $r \ll R$. The self energy can be expected as

$$\begin{array}{cccc} [\Sigma] = & [\tau] & [g_R] & [\tau^+] \\ (d \times d) & (d \times r) & (r \times r) & (r \times d) \end{array} \qquad (5.28)$$

and

$$
\{S\} = \quad [\tau] \quad \{\Phi_R\}
$$
$$
(d \times 1) \quad (d \times r) \quad (r \times 1)
$$

(5.29)

For the example presented in sec. 5.1 one can show

$$
\tau = -t_0 \quad \{\Phi_R\} = -2iB \sin ka
$$

(5.30)

and

$$
g_R = -\frac{e^{ika}}{t_0} \ .
$$

(5.31)

Evaluation in eigenstates of the contact

Expressed in eigenstates of the contact, the Green's function reads

$$
[G_R(E)] =
\begin{bmatrix}
\frac{1}{E-\epsilon_1+i0^+} & 0 & \cdots \\
0 & \frac{1}{E-\epsilon_2+i0^+} & \cdots \\
\cdots & \cdots & \cdots
\end{bmatrix}
$$

(5.32)

but $[\tau]$ is of size $(R \times R)$ now and can not be reduced. The explicit forms are

$$
\Sigma_{ij}(E) = \sum_n \frac{[\tau]_{in}[\tau^+]_{nj}}{E - \epsilon_n + i0^+}
$$

(5.33)

$$
S_i(E) = \sum_n [\tau]_{in} \{\Phi_R\}_n \ .
$$

(5.34)

The corresponding summations can often be transfered to integrals and evaluated analytically.

5.3   Local density of states

For finite sytems we have a descrete set of eigenstates with energies ϵ_α leading to the density of states

$$
D(E) = \sum_\alpha \delta(E - \epsilon_\alpha)
$$

(5.35)

If we are interested in the density of states in the channel we can weigth the states by the wave function at channel positions d

$$
D(d; E) = \sum_\alpha |\phi_\alpha(d)|^2 \delta(E - \epsilon_\alpha) \ .
$$

(5.36)

Generally we have

$$
D(\mathbf{r}; E) = \sum_\alpha |\phi_\alpha(\mathbf{r})|^2 \delta(E - \epsilon_\alpha)
$$

(5.37)

which is the diagonal element of the more general spectral function

$$
A(\mathbf{r}, \mathbf{r}'; E) = 2\pi \sum_\alpha \phi_\alpha(\mathbf{r}) \delta(E - \epsilon_\alpha) \phi_\alpha^*(\mathbf{r}')
$$

(5.38)

similar as the electron density

$$n(\mathbf{r}) = \sum_\alpha |\phi_\alpha(\mathbf{r})|^2 f_0(\epsilon_\alpha - \mu) \tag{5.39}$$

is the diagonal element of the density matrix

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_\alpha \phi_\alpha(\mathbf{r}) f_0(\epsilon_\alpha - \mu) \phi_\alpha^*(\mathbf{r}') \ . \tag{5.40}$$

We can use the eigenstates $\{\phi_\alpha\}$ to write (5.40) as a matrix

$$[\rho]_{\alpha\beta} = \sum_\gamma \int d\mathbf{r} \int d\mathbf{r}' \ \phi_\alpha^*(\mathbf{r}) \phi_\gamma(\mathbf{r}) \rho(\mathbf{r}, \mathbf{r}') \phi_\gamma^*(\mathbf{r}') \phi_\beta(\mathbf{r}') \tag{5.41}$$

$$= \begin{bmatrix} f_0(\epsilon_1 - \mu) & 0 & \dots \\ 0 & f_0(\epsilon_2 - \mu) & \dots \\ \dots & \dots & \dots \end{bmatrix} \tag{5.42}$$

or formally

$$[\rho] = f_0([H] - \mu[I]) \ . \tag{5.43}$$

Similarly we may write the spectral function as

$$[A(E)] = 2\pi \delta(E[I] - [H]) \ . \tag{5.44}$$

Summing over the diagonal of the density matrix gives the number of electrons

$$N = \text{Trace}[\rho] = \sum_\alpha f_0(\epsilon_\alpha - \mu) \tag{5.45}$$

and similarly we get the DOS

$$D(E) = \frac{1}{2\pi} \text{Trace}[A(E)] = \sum_\alpha \delta(E - \epsilon_\alpha) \ . \tag{5.46}$$

In order to show the connection to the Green's function, we use the identity

$$2\pi\delta(E - \epsilon_\alpha) = \left[\frac{2\eta}{(E - \epsilon_\alpha)^2 + \eta^2} \right]_{\eta \to 0^+} \tag{5.47}$$

$$= i \left[\frac{1}{E - \epsilon_\alpha + i\eta} - \frac{1}{E - \epsilon_\alpha - i\eta} \right]_{\eta \to 0^+} \tag{5.48}$$

to write

$$2\pi\delta(E[I] - [H]) = i \left(\left[(E + i0^+)[I] - [H] \right]^{-1} - \left[(E - i0^+)[I] - [H] \right]^{-1} \right) \tag{5.49}$$

or equivalently

$$[A(E)] = i([G(E)] - [G^+(E)]) \tag{5.50}$$

with

$$G(E) = \left[(E + i0^+)[I] - [H] \right]^{-1} \tag{5.51}$$

$$G^+(E) = \left[(E - i0^+)[I] - [H] \right]^{-1} \ . \tag{5.52}$$

The density matrix might be expressed in terms of the spectral function as

$$[\rho] = f_0([H] - \mu[I]) \quad = \quad \int_{-\infty}^{\infty} dE \, f_0(E - \mu) \, \delta(E[I] - [H]) \tag{5.53}$$

$$= \quad \int_{-\infty}^{\infty} dE \, f_0(E - \mu) \, [A(E)] \tag{5.54}$$

and the number of electrons

$$N = \int_{-\infty}^{\infty} dE \, f_0(E - \mu) \, D(E) \,. \tag{5.55}$$

5.4 Channel Green's function

The total Hamiltonian of the channel (H) and the contact (H_R) is

$$\bar{H} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix} \tag{5.56}$$

where $[H_R]$ is huge, that's why we call it a reservoir. Similarly we can write the spectral and the Green's functions as

$$\bar{A} = \begin{bmatrix} A & A_{dR} \\ A_{Rd} & A_R \end{bmatrix} \quad \bar{G} = \begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_R \end{bmatrix} . \tag{5.57}$$

The Green's function can be evaluated as

$$\bar{G} = \begin{bmatrix} (E + 0^+)I - H & -\tau \\ -\tau^+ & (E + 0^+)I_R - H_R \end{bmatrix}^{-1} . \tag{5.58}$$

We are searching the inverse of a known matrix of the form

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} \tag{5.59}$$

where we are particularly interseted in the entry a (the channels Green's function). Eq. (5.60) is

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \cdot \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \tag{5.60}$$

where the two equations containing a are

$$Aa + Bc = I \tag{5.61}$$

and

$$Ca + Dc = 0 \quad \Rightarrow \quad c = -D^{-1}Ca \tag{5.62}$$

such that we can express c through a and combine (5.61) and (5.62) to

$$[A - BD^{-1}C]a = I \quad \Rightarrow \quad a = [A - BD^{-1}C]^{-1} \,. \tag{5.63}$$

For the Green's function of the channel we get therefore

$$G = \left[(E + i0^+)I - H - \tau G_R \tau^+ \right]^{-1} \tag{5.64}$$

with the contact Green's function

$$G_R = \left[(E + i0^+)I_R - H_R \right]^{-1} . \tag{5.65}$$

5.5 Lifetime

We can express the Green's function in an eigenstate basis

$$[G(E)] = \begin{bmatrix} \frac{1}{E-\epsilon_1+i0^+} & 0 & \cdots \\ 0 & \frac{1}{E-\epsilon_2+i0^+} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \tag{5.66}$$

and Fourier transform (FT) to the time domain

$$[\tilde{G}^r(t)] = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \, e^{-iEt/\hbar}[G(E)] \tag{5.67}$$

where r stands for the "retarted" Green's function. The integral can be evalueated by a contour integration in the complex plane and the solution is also diagonal

$$[\tilde{G}^r(t)] = -\frac{i}{\hbar}\theta(t)e^{-0^+t} \begin{bmatrix} e^{-i\epsilon_1 t/\hbar} & 0 & \cdots \\ 0 & e^{-i\epsilon_2 t/\hbar} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}, \tag{5.68}$$

where $\theta(t)$ denotes the step function that is zero for negative and one for positive t. The proof is simple for the inverse FT as

$$[G(E)]_{ii} = \int_{-\infty}^{\infty} dt \, e^{iEt/\hbar}[\tilde{G}^r(t)]_{ii} \tag{5.69}$$

$$= -\frac{i}{\hbar} \int_0^{\infty} dt \, e^{i(E-\epsilon_i)t/\hbar} e^{-0^+t} \tag{5.70}$$

$$= \frac{1}{E-\epsilon_i+i0^+} \, . \tag{5.71}$$

Fourier transform of G^+ with

$$[G(E)] = \begin{bmatrix} \frac{1}{E-\epsilon_1-i0^+} & 0 & \cdots \\ 0 & \frac{1}{E-\epsilon_2-i0^+} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \tag{5.72}$$

leads to the "advanced" Green's function

$$[\tilde{G}^a(t)] = \frac{i}{\hbar}\theta(-t)e^{0^+t} \begin{bmatrix} e^{-i\epsilon_1 t/\hbar} & 0 & \cdots \\ 0 & e^{-i\epsilon_2 t/\hbar} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} . \tag{5.73}$$

Both $\tilde{G}^r(t)$ and $\tilde{G}^a(t)$ fullfill the time dependent SEQ with a $\delta(t)$ source term

$$\begin{aligned} \left(i\hbar\frac{\partial}{\partial t} - [H]\right)\tilde{G}^r(t) = [I]\delta(t) \qquad \text{causal} \\ \left(i\hbar\frac{\partial}{\partial t} - [H]\right)\tilde{G}^a(t) = [I]\delta(t) \qquad \text{non causal} \end{aligned} \tag{5.74}$$

and can be interpreted as the answer of the system on a perturbation at $t = 0$. The two solutions are connected by

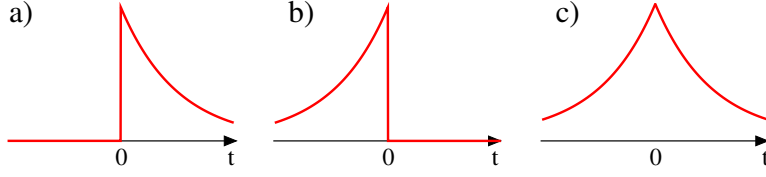$$[\tilde{G}^a(t)] = [\tilde{G}^r(-t)]^* \, . \tag{5.75}$$

Figure 5.2 Time dependence of a) $|\tilde{G}^r(t)|$, b) $|\tilde{G}^a(t)|$ and c) $|\tilde{A}(t)|$.

The causal and non causal nature of $\tilde{G}^r(t)$ and $\tilde{G}^a(t)$ is depicted in fig. 5.2. The FT of the spectral function

$$[\tilde{A}(t)] = i[\tilde{G}^r(t) - \tilde{G}^a(t)] \tag{5.76}$$

fullfills

$$\left(i\hbar\frac{\partial}{\partial t} - [H]\right)\tilde{A}(t) = 0 \tag{5.77}$$

and its time dependence is depicted in fig. 5.2 c).

Meaning of the self-energy Σ

For this derivation, we ignore the energy dependence of Σ and write down the equation for $\tilde{G}^r(t)$ for a single state ϵ

$$\left(i\hbar\frac{\partial}{\partial t} - \epsilon - \Sigma\right)\tilde{G}^r(t) = \delta(t) \tag{5.78}$$

with the solution after eq. (5.68)

$$\tilde{G}^r(t) = -\frac{i}{\hbar}\theta(t)e^{-i(\epsilon+\Sigma)t/\hbar} \tag{5.79}$$

$$= -\frac{i}{\hbar}\theta(t)e^{-i\epsilon't/\hbar}e^{-\gamma t/(2\hbar)} \tag{5.80}$$

where

$$\epsilon' = \epsilon + \text{Re}\Sigma \quad \text{and} \quad \gamma = -2\text{Im}\Sigma \tag{5.81}$$

The probability after excitation is

$$|\tilde{G}^r(t)|^2 = \frac{1}{\hbar^2}\theta(t)e^{-\gamma t/\hbar} \tag{5.82}$$

and the corresponding lifetime

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} = -\frac{2\text{Im}\Sigma}{\hbar} \tag{5.83}$$

The time dependent Green's function corresponding to (5.79) is

$$G(E) = \frac{1}{E - \epsilon' + i\gamma/2} \tag{5.84}$$

such that we can reconstruct the density of states by

$$\frac{A(E)}{2\pi} = D(E) = \frac{i}{2\pi}\left[\frac{1}{E - \epsilon' + i\gamma/2} - \frac{1}{E - \epsilon' - i\gamma/2}\right] = \frac{\gamma/(2\pi)}{(E - \epsilon')^2 + (\gamma/2)^2}. \tag{5.85}$$

Note, that we exactly arrived at the DOS that we have assumed for a broadened state in eq. (1.7).

In our example of section 5.1 we had

$$\Sigma = -t_0 e^{ika} = -t_0 \cos ka - it_0 \sin ka \tag{5.86}$$

resulting in a lifetime (5.83)

$$\frac{1}{\tau} = \frac{2t_0 \sin ka}{\hbar} \ . \tag{5.87}$$

The velocity associated with k is

$$v = \frac{1}{\hbar}\frac{dE}{dk} = \frac{1}{\hbar}\frac{d}{dk}[2t_0(1 - \cos ka)] = \frac{2at_0}{\hbar} \sin ka \tag{5.88}$$

such that the lifetime can be expressed in the physically understandable form

$$\tau = \frac{a}{v} \ , \tag{5.89}$$

i.e. the time that is needed to travel through the unit cell. More generally, we can write

$$[H + \Sigma(E)] = [H + \Sigma_H(E)] - i\frac{[\Gamma(E)]}{2} \tag{5.90}$$

with the hermitian part of the self energy

$$\Sigma_H(E) = \frac{1}{2}[\Sigma(E) + \Sigma^+(E)] \tag{5.91}$$

and the broadening matrix

$$\Gamma(E) = i[\Sigma(E) - \Sigma^+(E)] \ . \tag{5.92}$$

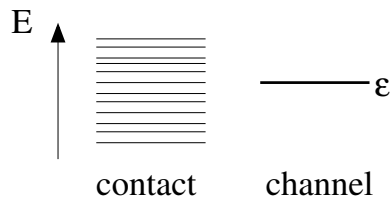## 5.6 What constitutes a reservoir ?

Figure 5.3   A single channel state coupled to the contact with dense states.

We consider a single channel state coupled to the contact with dense states as depicted in fig. 5.3. The total Hamiltonian for this configuration can be written

$$[H] = \begin{bmatrix} \epsilon & \tau_1 & \tau_2 & \dots \\ \tau_1^* & \epsilon_1 & 0 & \dots \\ \tau_2^* & 0 & \epsilon_2 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \tag{5.93}$$

where the channel state ϵ is coupled to all contact states ϵ_i through τ_i. The self energy resulting from the coupling to the contact (the reservoir) is

$$\Sigma(E) = \sum_r \frac{|\tau_r|^2}{E - \epsilon_r + i0^+} \ . \tag{5.94}$$

The broadening is

$$\gamma(E) = i[\Sigma(E) - \Sigma^+(E)] = \sum_r \frac{|\tau_r|^2 0^+}{(E - \epsilon_r)^2 + (0^+)^2} \tag{5.95}$$

which can be approximated by an integral when the ϵ_r are closely spaced

$$\gamma(E) = \int d\epsilon_r \ D_R(\epsilon_r) \frac{|\tau_r|^2 0^+}{(E - \epsilon_r)^2 + (0^+)^2} \tag{5.96}$$

where $D_R(E)$ is the density of states in the contact. The Lorentzian in eq. (5.96) is highly peaked around E such that we can pull $D_R(E)$ and τ out of the integral to get

$$\gamma(E) = D_R(E)|\tau(E)|^2 \int d\epsilon_r \ \frac{0^+}{(E - \epsilon_r)^2 + (0^+)^2} = 2\pi D_R(E)|\tau(E)|^2 \ . \tag{5.97}$$

Therfore two properties are needed for a good coupling between the channel and the contact:

1. a strong coupling $|\tau(E)|^2$ and

2. a set of available states $D_R(E)$.

CHAPTER 6

COHERENT TRANSPORT

6.1 Overview

We want to get an overview of the results first and derive them in the following sections.

As we have seen in sec. 1.1, the flow of current requires to apply different potentials at source and drain. This is expressed via two different electrochemical potentials resulting in the Fermi functions

$$f_1(E) \equiv f_0(E - \mu_1) \quad = \quad \frac{1}{\exp[(E - \mu_1)/k_B T] + 1} \tag{6.1}$$

$$f_2(E) \equiv f_0(E - \mu_2) \quad = \quad \frac{1}{\exp[(E - \mu_2)/k_B T] + 1} \,. \tag{6.2}$$

We are now able to generalize the single state model of sec. 1.1

$$\epsilon \to [H] \qquad \text{Hamiltonian matrix}$$

$$\gamma_{1,2} \to [\Gamma_{1,2}] \quad \text{broadening matrix} \quad [\Gamma_{1,2}] = i[\Sigma_{1,2} - \Sigma_{1,2}^+]$$

We saw, that the coupling broadens the level(s) and transfers the descrete eigenvalues to a continous E. The density matrix can be expressed as [c.f. eq. (5.54)]

$$[\rho] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} \, [G^n(E)] \tag{6.3}$$

where the correlation function in equilibrium is

$$[G^n(E)]_{\text{eq}} = [A(E)]f_0(E - \mu) \ . \tag{6.4}$$

Note, that the correlation function is often written as $G^<(E)$ in the literature.

Non-eqilibrium density matrix

When a voltage is applied, we will see in sec. 6.2 that the correlation function can be expressed as

$$[G^n] = [A_1]f_1 + [A_2]f_2 \tag{6.5}$$

(we skipped the dependence of E for clarity) such that there are two spectral functions in equilibrium with their contacts. The spectral functions can be written as

$$[A_1] = G\Gamma_1 G^+ \quad [A_2] = G\Gamma_2 G^+ \tag{6.6}$$

with the coupled channel Green's function

$$[G(E)] = [EI - H - \Sigma_1 - \Sigma_2]^{-1} \ . \tag{6.7}$$

The total spectral function is the sum of the two

$$[A] = i[G - G^+] = [A_1] + [A_2] \ . \tag{6.8}$$

Current

In section 6.3 we will show that the current I_i at terminal $i = 1, 2$ can be written as

$$I_i = -\frac{e}{h} \int_{-\infty}^{\infty} dE \ \tilde{I}_i(E) \tag{6.9}$$

with the dimensionless current per unit energy

$$\tilde{I}_i = \text{Trace}[\Gamma_i A]f_i - \text{Trace}[\Gamma_i G^n] \ . \tag{6.10}$$

One level model

It is instructive to compare how these expressions appear in the one level model from sec. 1.1. In explicit, we have

From eq. (6.7)	$G(E) = [E - \epsilon + i\Gamma/2]^{-1}$
From eq. (6.6)	$A_i(E) = \frac{\Gamma_i}{(E-\epsilon)^2 + (\Gamma/2)^2}$
From eq. (6.8)	$A(E) = \frac{\Gamma}{(E-\epsilon)^2 + (\Gamma/2)^2}$
From eq. (6.5)	$G^n(E) = A(E)\left(\frac{\Gamma_1}{\Gamma}f_1(E) + \frac{\Gamma_2}{\Gamma}f_2(E)\right)$,

where the last eq. should be compared to (1.23). From eqs. (6.9) and (6.10) we conclude that the current at the two contacts is given by

$$I_1 = \frac{e}{h} \int_{-\infty}^{\infty} dE \, \Gamma_1[A(E)f_1(E) - G^n(E)] \tag{6.11}$$

$$I_2 = \frac{e}{h} \int_{-\infty}^{\infty} dE \, \Gamma_2[A(E)f_2(E) - G^n(E)] \tag{6.12}$$

which compare to eqs. (1.2) and (1.3) that were

$$I_1 = \frac{e\gamma_1}{\hbar}(f_1 - N) \text{ and } I_2 = \frac{e\gamma_1}{\hbar}(f_2 - N) .$$

Transmission

Combining eqts. (6.5), (6.8) and (6.10) we obtain

$$
\begin{aligned}
\tilde{I}_1 = -\tilde{I}_2 &= \text{Trace}[\Gamma_1 A f_1 - \Gamma_1 G^n] \\
&= \text{Trace}[\Gamma_1 A f_1 - \Gamma_1 A_1 f_1 - \Gamma_1 A_2 f_2] \\
&= \text{Trace}[\Gamma_1 A_1 f_1 + \Gamma_1 A_2 f_1 - \Gamma_1 A_1 f_1 - \Gamma_1 A_2 f_2] \\
&= \bar{T}(E) \left(f_1(E) - f_2(E)\right)
\end{aligned}
\tag{6.13}
$$

where the transmission function

$$\bar{T}(E) = \text{Trace}[\Gamma_1 A_2] = \text{Trace}[\Gamma_2 A_1] \tag{6.14}$$

appears.

Transmission from Green's function

The transmission function can be expressed in terms of the channel Green's function using eq. (6.6) as

$$\bar{T}(E) = \text{Trace}[\Gamma_1 G \Gamma_2 G^+] = \text{Trace}[\Gamma_2 G \Gamma_1 G^+] . \tag{6.15}$$
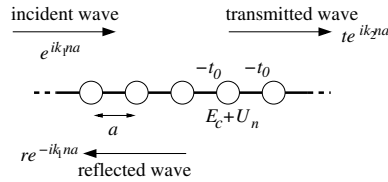

Figure 6.1 Reflection and transmission picture for the 1D chain.

We will illustrate this approach by our standard example of an infinite wire as depicted in fig. 6.1. We want to calculate the transmission coefficient

$$\bar{T}(E) = \frac{v_2}{v_1} |t|^2 \tag{6.16}$$

where the velocity ratio is included as the transmission is the ratio of the transmitted to the incident current ans the current is the velocity times the probability $|\psi|^2$.

We use the approach of section 5.1 to eliminate the semi-infinite contacts

$$[EI - H - \Sigma_1 - \Sigma_2]\{\psi\} = \{S\} \rightarrow \{\psi\} = G\{S\} \tag{6.17}$$

where G is given by eq. (6.7). The Σ_1 and Σ_2 matrices represent the effects of the two contacts. Each one has only one non-zero entry [N points in the channel, see eq. (5.9)]

$$[\Sigma_1]_{1,1} = -t_0 e^{ik_1 a} \quad , \quad [\Sigma_2]_{N,N} = -t_0 e^{ik_2 a} \tag{6.18}$$

corresponding to the points of the channel, where the contacts are connected. The source term is a column vector with only one entry, where the wave is incident (5.10)

$$\{S\}_1 = 2it_0 \sin k_1 a = i\hbar \frac{v_1}{a} \tag{6.19}$$

In general, for the same energy E, the velocities can be different at the two ends of the lattice as there might be different potentials

$$E = E_c + U_1 + 2t_0 \cos k_1 a = E_c + U_N + 2t_0 \cos k_2 a \ . \tag{6.20}$$

From $\{\psi\} = G\{S\}$ we can write

$$t = |\{\psi\}_N| = |[G]_{N,1}\{S\}_1| \tag{6.21}$$

such that the transmission using (6.16) is

$$\bar{T}(E) = \frac{\hbar v_1}{a} \frac{\hbar v_2}{a} |[G]_{N,1}|^2 \ . \tag{6.22}$$

The direct approach from eq. (6.15) would have given the same result as

$$[\Gamma_1]_{1,1} = i\left[[\Sigma_1]_{1,1} - [\Sigma_1^+]_{1,1}\right] = 2t_0 \sin k_1 a = \hbar \frac{v_1}{a} \tag{6.23}$$

and

$$[\Gamma_2]_{N,N} = i\left[[\Sigma_2]_{N,N} - [\Sigma_2^+]_{N,N}\right] = 2t_0 \sin k_2 a = \hbar \frac{v_2}{a} \ . \tag{6.24}$$

6.2 Density matrix

For a channel with one contact, we started with the SEQ

$$\begin{bmatrix} EI_R - H_R + i\eta & -\tau^+ \\ -\tau & EI - H \end{bmatrix} \begin{Bmatrix} \Phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix} \tag{6.25}$$

and showed, that the waves ψ, χ are arising from spill-over of the wave-functions Φ_R in the isolated contact. We obtained

$$\{\chi\} = G_R \tau^+ \{\psi\}$$

where

$$\begin{aligned} [G_R] &= [EI_R - H_R + i\eta]^{-1} \tag{6.26} \\ \{\psi\} &= [G]\{S\} \tag{6.27} \\ [G] &= [EI - H - \Sigma]^{-1} \tag{6.28} \\ \Sigma &= \tau G_R \tau^+ \tag{6.29} \\ \{S\} &= \tau\{\Phi_R\} \ . \tag{6.30} \end{aligned}$$

With only one contact, we have an equilibrium problem and the spectral function is filled according to the Fermi function of the contact with

$$A(E) = i[G(E) - G^+(E)] \ . \tag{6.31}$$

We will derive the same results from a different viewpoint now. The density matrix of the contact

$$\rho_R(\mathbf{r}, \mathbf{r}') = \sum_\alpha \Phi_\alpha(\mathbf{r}) f_0(\epsilon_\alpha - \mu) \Phi_\alpha(\mathbf{r}') \tag{6.32}$$

is in matrix notation

$$[\rho_R] = \sum_\alpha f_0(\epsilon_\alpha - \mu) \{\Phi_\alpha\} \{\Phi_\alpha\}^+ . \tag{6.33}$$

Now, we wish to calculate the density matrix of the channel via the source term corresponding to each eigenstate $\{\Phi_\alpha\}$ through $\{\psi_\alpha\} = G\{S_\alpha\} = G\tau\{\Phi_\alpha\}$

$$\begin{aligned}
[\rho] &= \sum_\alpha f_0(\epsilon_\alpha - \mu) \{\psi_\alpha\}\{\psi_\alpha\}^+ \\
&= \int_{-\infty}^{\infty} dE\, f_0(E - \mu) \sum_\alpha \delta(E - \epsilon_\alpha) \{\psi_\alpha\}\{\psi_\alpha\}^+ \\
&= \int_{-\infty}^{\infty} dE\, f_0(E - \mu) G\tau \left[\sum_\alpha \delta(E - \epsilon_\alpha) \{\Phi_\alpha\}\{\Phi_\alpha\}^+ \right] \tau^+ G^+ \\
&= \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu) G\tau A_R \tau^+ G^+
\end{aligned} \tag{6.34}$$

where we have used the expression for the spectral function of the contact

$$A_R(E) = \sum_\alpha \delta(E - \epsilon_\alpha) \{\Phi_\alpha\}\{\Phi_\alpha\}^+ \tag{6.35}$$

From eq. (6.29)

$$\Gamma = i[\Sigma - \Sigma^+] = i[\tau G\tau^+ - \tau G^+ \tau^+] = \tau A \tau^+ \tag{6.36}$$

such that we can conclude using (6.34)

$$[G^n] = [G\Gamma G^+] f_0(E - \mu) . \tag{6.37}$$

In order to show, that this is the same as eq. (6.4) we need the following identity. If

$$[G] = [EI - H - \Sigma]^{-1} \text{ and } \Gamma = i[\Sigma - \Sigma^+] \tag{6.38}$$

then

$$A \equiv i[G - G^+] = G\Gamma G^+ = G^+ \Gamma G . \tag{6.39}$$

The proof is as follows. As H is hermitian we obtain

$$(G^+)^{-1} - G^{-1} = \Sigma - \Sigma^+ = -i\Gamma \tag{6.40}$$

and therfore by multiplication with G form the left and G^+ from the right, we get

$$-iG\Gamma G^+ = G[(G^+)^{-1} - G^{-1}]G^+ = G - G^+ = -iA \tag{6.41}$$

and similarly

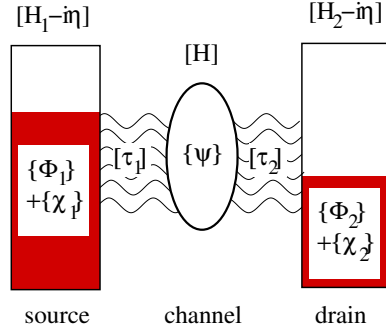$$-iG^+ \Gamma G = G^+[(G^+)^{-1} - G^{-1}]G = G - G^+ = -iA . \tag{6.42}$$

Figure 6.2 The channel with two contacts.

Channel with two contacts

Before connecting the channel, the electrons in source and drain have the wave function $\{\Phi_1\}$ and $\{\Phi_2\}$, respectively, that satisfy

$$[EI - H_1 + i\eta]\{\Phi_1\} = \{S_1\} \quad \text{and} \quad [EI - H_2 + i\eta]\{\Phi_2\} = \{S_2\} \tag{6.43}$$

with the Hamiltonians H_1, H_2 of source and drain. The overall SEQ is (see also fig. 6.2)

$$\begin{bmatrix} EI - H_1 + i\eta & -\tau_1^+ & 0 \\ -\tau_1 & EI - H & -\tau_2 \\ 0 & -\tau_2^+ & EI - H_2 + i\eta \end{bmatrix} \begin{Bmatrix} \Phi_1 + \chi_1 \\ \psi \\ \Phi_2 + \chi_2 \end{Bmatrix} = \begin{Bmatrix} S_1 \\ 0 \\ S_2 \end{Bmatrix} \tag{6.44}$$

Similar as in sec. 5.2 we obtain from the first and third line in eq. (6.44)

$$\{\chi_1\} = G_1\tau_1^+\{\psi\} \quad \text{and} \quad \{\chi_2\} = G_2\tau_2^+\{\psi\} \tag{6.45}$$

where we have used the Green's functions of isolated source and drain

$$G_1(E) = [EI - H_1 + i\eta]^{-1} \quad \text{and} \quad G_2(E) = [EI - H_2 + i\eta]^{-1} . \tag{6.46}$$

From the second equation, we get

$$[EI - H - \Sigma_1 - \Sigma_2]\{\psi\} = \{S\} \tag{6.47}$$

where two self energies

$$\Sigma_1 = \tau_1 G_1\tau_1^+ \quad \text{and} \quad \Sigma_2 = \tau_2 G_2\tau_2^+ \tag{6.48}$$

appear. The corresponding broadening matrices are

$$\Gamma_1 = \tau_1 A_{R,1}\tau_1^+ \quad \text{and} \quad \Gamma_2 = \tau_2 A_{R,2}\tau_2^+ \tag{6.49}$$

with the spectral functions of the isolated contacts

$$A_{R,1} = i[G_1 - G_1^+] \quad \text{and} \quad A_{R,2} = i[G_2 - G_2^+] . \tag{6.50}$$

We explicitely keep the label R for the contact in these functions in order to not confuse with the A_1 and A_2 used in eqs. (6.5) and (6.8).

We use the channel Green's function

$$G(E) = [EI - H - \Sigma_1 - \Sigma_2]^{-1} \tag{6.51}$$

to obtain the density matrix in that we express the channel wave function as

$$\{\psi\} = G\{S\} \quad \rightarrow \quad \{\psi\}\{\psi\}^+ = G\{S\}\{S\}^+G^+ . \tag{6.52}$$

Similar as in sec. 5.2, the source term in eq. (6.47) is

$$\{S\} = \tau_1\{\Phi_1\} + \tau_2\{\Phi_2\} , \tag{6.53}$$

i.e. it has additive contributions from both contacts. The contributions to the density matrix can be expressed as

$$\{S\}\{S\}^+ = \tau_1\{\Phi_1\}\{\Phi_1\}^+\tau_1^+ + \tau_2\{\Phi_2\}\{\Phi_2\}^+\tau_2^+ \tag{6.54}$$

where the cross terms vanish due to the missing overlap of the two contacts. Similar to the derivation for a single contact in eq. (6.34), we can state the general rule for the action the channel's density matrix

$$\{\Phi_R\}\{\Phi_R\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu)[A_R(E)] . \tag{6.55}$$

In the same way, by expressing the channel wave functions as

$$\{\psi\}\{\psi\}^+ = G\tau\{\Phi_R\}\{\Phi_R\}^+\tau^+G^+ \tag{6.56}$$

the rule gets

$$\{\psi\}\{\psi\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu)[G\tau A_R\tau^+G^+] . \tag{6.57}$$

Using the rule for the two contributions to the density matrix shows that we may write

$$\begin{aligned} [\rho] &= \int_{-\infty}^{\infty} \frac{dE}{2\pi} \left([G\tau_1 A_{R,1}\tau_1^+G^+]f_1 + [G\tau_2 A_{R,2}\tau_2^+G^+]f_2\right) \\ &\equiv \int_{-\infty}^{\infty} \frac{dE}{2\pi} [G^n] \end{aligned} \tag{6.58}$$

where f_1 and f_2 might differ describing the non-equilibrium situation. We can use the brodening matrices in eq. (6.49) to express the correlation function

$$[G^n] = [G\Sigma^{\text{in}}G^+] \tag{6.59}$$

with

$$[\Sigma^{\text{in}}] = [\Gamma_1]f_1 + [\Gamma_2]f_2 . \tag{6.60}$$

We can view the correlation function of the channel to consist of two spectral functions

$$A_1 = G\Gamma_1G^+ \quad \text{and} \quad A_2 = G\Gamma_2G^+ \tag{6.61}$$

to write

$$[G^n] = [A_1]f_1 + [A_2]f_2 \tag{6.62}$$

proofing eq. (6.5). In comparison to the equilibrium result

$$[G^n]_{\text{eq}} = [A]f_0(E - \mu) \tag{6.63}$$

one can think of two parts in the channel's spectral function that are in equilibrium with μ_1 and μ_2, respectively. From eq. (6.39) we see

$$A = G\Gamma G^+ = G(\Gamma_1 + \Gamma_2)G^+ = A_1 + A_2 \tag{6.64}$$

proofing eq. (6.8).

6.3 Inflow/outflow

We again consider first only one contact and write the SEQ using eq. (5.16)

$$E \left\{ \begin{matrix} \psi \\ \Phi \end{matrix} \right\} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R - i\eta_R \end{bmatrix} \left\{ \begin{matrix} \psi \\ \Phi \end{matrix} \right\} \tag{6.65}$$

where we have used the abbrevation $\{\Phi\} = \{\Phi_R + \chi\}$ and dropped the constant source term $\{S_R\}$. The corresponding time dependent SEQ (TDSEQ) is

$$i\hbar \frac{d}{dt} \left\{ \begin{matrix} \psi \\ \Phi \end{matrix} \right\} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R - i\eta_R \end{bmatrix} \left\{ \begin{matrix} \psi \\ \Phi \end{matrix} \right\} . \tag{6.66}$$

The flow is the change in the probability density, for which we can write

$$|\psi|^2 = \psi^+ \psi = \text{Trace}[\psi^+ \psi] = \text{Trace}[\psi \psi^+] \tag{6.67}$$

as $\psi^+ \psi$ is just a number and therefore equal to its trace. From the TDSEQ eq. (6.66) we get

$$\frac{d\psi}{dt} = \frac{1}{i\hbar} [H\psi + \tau\Phi] \tag{6.68}$$

$$\frac{d\psi^+}{dt} = -\frac{1}{i\hbar} [\psi^+ H + \Phi^+ \tau^+] \tag{6.69}$$

such that we can write the current as

$$I = \dot{\psi}^+ \psi + \psi^+ \dot{\psi} = \text{Trace}[\psi^+ \tau\Phi - \Phi^+ \tau^+ \psi]/(i\hbar) . \tag{6.70}$$

Noting that $\{\Phi\} = \{\Phi_R + \chi\}$, we can divide the current conceptually into an inflow connected with and $\{\Phi_R\}$ and an outflow connected with the scattered wave $\{\chi\}$

$$I = \underbrace{\text{Trace}[\psi^+ \tau\Phi_R - \Phi_R^+ \tau^+ \psi]/(i\hbar)}_{\text{Inflow}} - \underbrace{\text{Trace}[\chi^+ \tau^+ \psi - \psi^+ \tau\chi]/(i\hbar)}_{\text{Outflow}} . \tag{6.71}$$

Using $\{S\} = [\tau]\{\Phi_R\}$ and $\{\psi\} = [G]\{S\}$ we can write

$$\begin{aligned} \text{Inflow} &= \text{Trace}[S^+ G^+ S - S^+ GS]/(i\hbar) \\ &= \text{Trace}[S^+ AS]/\hbar \end{aligned} \tag{6.72}$$

since $A = i[G - G^+]$. We can now use the replacement rule of eq. (6.55)

$$\{\Phi_R\}\{\Phi_R\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu)[A_R(E)] .$$

and use $\{S\} = [\tau]\{\Phi_R\}$ to obtain

$$\{S\}\{S\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu)[\tau A_R \tau^+] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu)[\Gamma] \tag{6.73}$$

where we have used eq. (6.36) in the last step. The inflow becomes

$$\text{Inflow} = \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu) \text{Trace}[\Gamma A] . \tag{6.74}$$

Similarly, we can use $\{\chi\} = [G_R][\tau^+]\{\psi\}$ to obtain the outflow as

$$\text{Outflow} = \text{Trace}[\psi^+\tau G_R^+\tau^+\psi - \psi^+\tau G_R\tau^+\psi]/(i\hbar)$$
$$= \text{Trace}[\psi^+\tau A_R\tau^+\psi]/\hbar = \text{Trace}[\psi\psi^+\Gamma]/\hbar \qquad (6.75)$$

Using the rule from eq. (6.57)

$$\{\psi\}\{\psi\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E-\mu)[G\tau A_R\tau^+G^+] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} [G^n] \qquad (6.76)$$

we can write the outflow as

$$\text{Outflow} = \frac{1}{\hbar}\int_{-\infty}^{\infty} \frac{dE}{2\pi}\,\text{Trace}[\Gamma G^n] \ . \qquad (6.77)$$

Outflow and inflow are equal in equilibrium as we have defined in eq. (6.4)

$$[G^n]_{\text{eq}} = A f_0(E-\mu) \ .$$
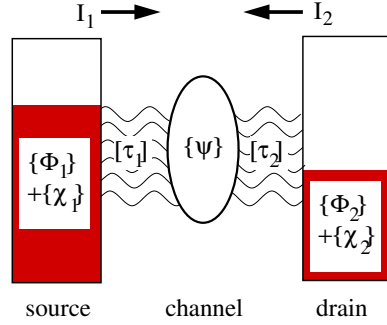
Channel with two contacts

Figure 6.3   The channel with two contacts and the currents I_1 and I_2.

We are now ready to consider the channel connected to two contacts as depicted in fig. 6.3. We consider one of the interfaces, say the one with the source contact and write the current as

$$I_1 = \underbrace{\text{Trace}[\psi^+ \tau_1 \Phi_1 - \Phi_1^+ \tau_1^+ \psi]/(i\hbar)}_{\text{Inflow}} - \underbrace{\text{Trace}[\chi_1^+ \tau_1^+ \psi - \psi^+ \tau_1 \chi_1]/(i\hbar)}_{\text{Outflow}} . \qquad (6.78)$$

We can use again $\{\psi\} = [G]\{S\}$ and the source term from contact 1 $\{S_1\} = \tau_1\{\Phi_1\}$ to express

$$\begin{aligned}
\text{Inflow} &= \text{Trace}[S^+ G^+ S_1 - S_1^+ GS]/(i\hbar) \\
&= \text{Trace}[(S_1^+ + S_2^+)G^+ S_1 - S_1^+ G(S_1 + S_2)]/(i\hbar) . \qquad (6.79)
\end{aligned}$$

The source terms are uncorrelated due to missing spatial overlap of the contacts, i.e.

$$S_1 S_2^+ = S_2 S_1^+ = 0 \qquad (6.80)$$

and therefore

$$\text{Inflow} = \text{Trace}[S_1 S_1^+ G^+ - S_1 S_1^+ G]/(i\hbar) = \text{Trace}[S_1 S_1^+ A]/\hbar \qquad (6.81)$$

We use the replacement rule eq. (6.55)

$$\{\Phi_1\}\{\Phi_1\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E - \mu)[A_{R,1}(E)] .$$

to obtain

$$\{S_1\}\{S_1\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_1 [\tau_1 A_{R,1} \tau_1^+] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_1 [\Gamma_1] \qquad (6.82)$$

with the shorthand $f_1 = f_0(E - \mu_1)$. The inflow becomes

$$\text{Inflow} = \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_1 \text{Trace}[\Gamma_1 A] . \qquad (6.83)$$

Similarly, the outflow becomes [see eq. (6.75)]

$$\text{Outflow} = \text{Trace}[\psi^+ \tau_1 G_1^+ \tau_1^+ \psi - \psi^+ \tau_1 G_1 \tau_1^+ \psi]/(i\hbar) = \text{Trace}[\psi\psi^+ \Gamma_1]/\hbar \qquad (6.84)$$

and by using the rule (6.76)

$$\{\psi\}\{\psi\}^+ \Rightarrow \int_{-\infty}^{\infty} \frac{dE}{2\pi} [G^n]$$

we get

$$\text{Outflow} = \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{dE}{2\pi} \text{Trace}[\Gamma_1 G^n] \ . \tag{6.85}$$

The net current I_i at terminal i is given by the difference between inflow and outflow (multiplied by the electron charge $-e$)

$$I_i = -\frac{e}{\hbar} \int_{-\infty}^{\infty} \frac{dE}{2\pi} \tilde{I}_i(E) \tag{6.86}$$

with

$$\tilde{I}_i(E) = f_i \, \text{Trace}[\Gamma_i A] - \text{Trace}[\Gamma_i G^n] \tag{6.87}$$

proofing eq. (6.10).

6.4 Transmission

In this section, we will give the connection to the transmission formalism often used in the literature. We started in sec. 6.1 by combining the now proved eq. (6.87) with the now proved eqs. $[G^n] = [A_1]f_1 + [A_2]f_2$ (6.5) and $[A] = [A_1] + [A_2]$ (6.8) to write

$$\tilde{I}_1 = \bar{T}_{12}(E) \, [f_1(E) - f_2(E)] \ \text{ with } \ \bar{T}_{12} \equiv \text{Trace}[\Gamma_1 A_2] \tag{6.88}$$

$$\tilde{I}_2 = \bar{T}_{21}(E) \, [f_2(E) - f_1(E)] \ \text{ with } \ \bar{T}_{21} \equiv \text{Trace}[\Gamma_2 A_1] \ . \tag{6.89}$$

We expect the currents to be equal and opposite which would be ensured if

$$\text{Trace}[\Gamma_1 A_2] = \text{Trace}[\Gamma_2 A_1] \tag{6.90}$$

holds. As the first step we can write

$$\text{Trace}[\Gamma_1 A] = \text{Trace}[\Gamma_1 G\Gamma G^+] = \text{Trace}[\Gamma G^+ \Gamma_1 G] = \text{Trace}[\Gamma A_1] \tag{6.91}$$

from which we can conclude by subtracting $\text{Trace}[\Gamma_1 A_1]$ from both sides

$$\text{Trace}[\Gamma_1 A_2] = \text{Trace}[\Gamma_1 A] - \text{Trace}[\Gamma_1 A_1] = \text{Trace}[\Gamma A_1] - \text{Trace}[\Gamma_1 A_1] = \text{Trace}[\Gamma_2 A_1] \tag{6.92}$$

as $\Gamma = \Gamma_1 + \Gamma_2$ and $A = A_1 + A_2$. This allows to write the current as

$$I = \frac{e}{h} \int_{-\infty}^{\infty} dE \ \bar{T}(E) \, [f_1(E) - f_2(E)] \tag{6.93}$$

where

$$\bar{T}(E) \equiv \text{Trace}[\Gamma_1 A_2] = \text{Trace}[\Gamma_2 A_1]$$
$$= \text{Trace}[\Gamma_1 G\Gamma_2 G^+] = \text{Trace}[\Gamma_2 G\Gamma_1 G^+] \ . \tag{6.94}$$

In order to calculate the transmission function $\bar{T}(E)$, one usually solves the scattering problem

$$\bar{T}(E) = \sum_m \sum_n |t_{mn}|^2 = \text{Trace}[tt^+] \tag{6.95}$$

where t is the scattering matrix describing the system.
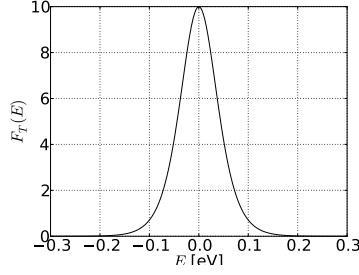
Landauer formula

Figure 6.4   The thermal broadening function for $k_B T = 25$ meV.

For small bias V, we can write the current as

$$I \approx \underbrace{I(V = 0)}_{=0} + \frac{dI}{dV}\Big|_{V=0} V \tag{6.96}$$

where

$$dI = \frac{e}{h} \int_{-\infty}^{\infty} dE \, \delta\bar{T}(E) \underbrace{[f_1 - f_2]_{V=0}}_{=0} + \frac{e}{h} \int_{-\infty}^{\infty} dE \, \bar{T}(E) \, \delta[f_1 - f_2] \, . \tag{6.97}$$

The variation of the difference between the Fermi functions is

$$\delta[f_1 - f_2] = f_0(E - \mu - edV) - f_0(E - \mu) = -\frac{df_0}{dE}\Big|_{E=\mu} edV \tag{6.98}$$

where the termal broadening function

$$F_T(E) = -\frac{df_0}{dE} = [4k_B T \cosh^2(E/(2k_B T))]^{-1} \tag{6.99}$$

appears that is depicted in fig. 6.4. It is highly peaked around $E = 0$ and we can express the low bias current as

$$I = \frac{e^2}{h} V \int_{-\infty}^{\infty} dE \, \bar{T}(E) F_T(E - \mu) \tag{6.100}$$

and the corresponding conductance as

$$G = \frac{e^2}{h} T \tag{6.101}$$

with

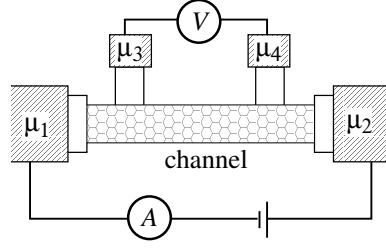$$T = \int_{-\infty}^{\infty} dE \, \bar{T}(E) F_T(E - \mu) \, . \tag{6.102}$$

Figure 6.5 Schematics of a four point measurement.

Büttiker equations

A very efficient method for the measurement of conductance in particular for small resistance is the four point measurement. The basic principle is depicted in fig. 6.5. Büttiker generalized the Landauer expression

$$G = \frac{e^2}{h}T \quad \rightarrow \quad I = \frac{e}{h}T \underbrace{[\mu_1 - \mu_2]}_{=eV} \tag{6.103}$$

by writing the current at the ith contact as

$$I_i = \frac{e}{h}\sum_j T_{ij}\left[\mu_i - \mu_j\right]. \tag{6.104}$$

In principle there are 8 unknown variables, i.e. four currents and four potentials. According to Kirchhoff's law the currents must add to zero $\sum_i I_i = 0$ one can set $\mu_2 = 0$, leaving 6 variables. The Büttiker equations can be expressed in matrix form

$$\begin{Bmatrix} I_1 \\ I_2 \\ I_3 \end{Bmatrix} = \frac{e}{h} \begin{bmatrix} T_{12} + T_{13} + T_{14} & -T_{13} & -T_{14} \\ -T_{31} & T_{31} + T_{32} + T_{34} & -T_{34} \\ -T_{41} & -T_{43} & T_{41} + T_{42} + T_{43} \end{bmatrix} \begin{Bmatrix} \mu_1 \\ \mu_3 \\ \mu_4 \end{Bmatrix}. \tag{6.105}$$

In the absence of magnetic fields, the coefficients are reciprocal $T_{ij} = T_{ji}$, but eq. (6.105) is also valid in Hall effect measurements. In addition to these three equations, knowing $\mu_1, I_3 = I_4 = 0$ allows to calculate I_1, μ_3 and μ_4 and therefore the four point conductance
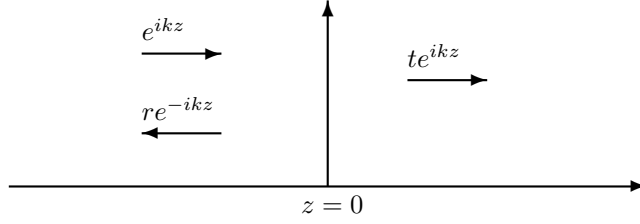
$$G = \frac{eI_1}{\mu_3 - \mu_4}. \tag{6.106}$$

6.5 An analytical example

Sacttering theory

We consider a linear conductor with a repulsive potential $U(z) = U_0\delta(z)$ as depicted in fig. 6.6. The coefficients t and r are obtained by requiring the wave function to be continuous at $z = 0$

$$[\psi]_{z=0^+} - [\psi]_{z=0^-} = 0 \quad \rightarrow \quad t - (1 + r) = 0 \tag{6.107}$$

Figure 6.6   Scattering on a δ-potential.
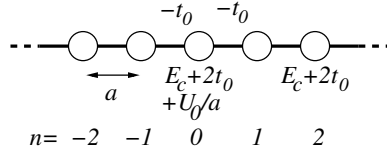
and the derivative to be

$$[\frac{d\psi}{dz}]_{z=0^+} - [\frac{d\psi}{dz}]_{z=0^-} = \frac{2mU_0}{\hbar^2}[\psi]_{z=0} \;\; \rightarrow \;\; ik[t - (1-r)] = \frac{2mU_0}{\hbar^2}\,t \;. \quad (6.108)$$

Combining these two equations yields ($v = \hbar k/m$)

$$t = \frac{i\hbar v}{i\hbar v - U_0} \;\; \rightarrow \;\; T = |t|^2 = \frac{\hbar^2 v^2}{\hbar^2 v^2 + U_0^2} \;. \quad (6.109)$$

Sacttering theory on a discrete lattice

Figure 6.7   Discrete lattice version for scattering on a δ-potential.

The discrete lattice version of the problem is depicted in fig. 6.7. The δ-potential is represented by the potential U_0/a at site 0, i.e. the SEQ is

$$E\psi_0 = [E_c + 2t_0 + U_0/a]\psi_0 - t_0\psi_{+1} - t_0\psi_{-1} \quad (6.110)$$

and we write

$$\psi_0 = 1 + r = t \quad (6.111)$$
$$\psi_{+1} = te^{ika} = \psi_0 e^{ika} \quad (6.112)$$
$$\psi_{-1} = e^{-ika} + re^{ika} = \psi_0 e^{ika} - 2i\sin ka \quad (6.113)$$

such that eq. (6.110) gets

$$[E - E_c - 2t_0 - U_0/a + 2t_0 e^{ika}]\psi_0 = 2it_0\sin ka \;. \quad (6.114)$$

Using the dispersion relation on the lattice (5.4)

$$E = E_c + 2t_0(1 - \cos ka) \quad (6.115)$$

we can simplify this to

$$[-U_0/a + 2it_0 \sin ka]\psi_0 = 2it_0 \sin ka . \tag{6.116}$$

Using the corresponding velocity from eq. (5.88)

$$\hbar v(E) = 2at_0 \sin ka \tag{6.117}$$

the wave function at site 0 can be expressed as

$$\psi_0 = \frac{i\hbar v(E)}{i\hbar v(E) - U_0} \tag{6.118}$$

and therefore the transmission becomes

$$T(E) = |t|^2 = |\psi_0|^2 = \frac{\hbar^2 v(E)^2}{\hbar^2 v(E)^2 + U_0^2} , \tag{6.119}$$

i.e. the same result as eq. (6.109). Note, that the velocities of the continuous and the discrete calculations are not the same, however.
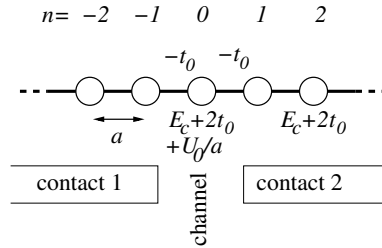
Green's function method

Figure 6.8   Green's function version for scattering on a δ-potential.

Finally, we treat the same problem by the Green's function method. We treat one point as the channel with the Hamiltonian of the isolated system

$$[H] = E_c + 2t_0 + U_0/a \tag{6.120}$$

and the effects of the semi-infinite contacts expressed through the self-energy matrices of size (1×1), see eq. (5.9),

$$[\Sigma_1] = [\Sigma_2] = -t_0 e^{ika} \tag{6.121}$$

where k is related to the energy E through the dispersion relation (5.4) such that

$$[\Gamma_{1,2}(E)] = i[\Sigma_{1,2}(E) - \Sigma_{1,2}(E)^+] = 2t_0 \sin ka = \hbar v/a . \tag{6.122}$$

We can no write down the Green's function

$$G = [EI - H - \Sigma_1 - \Sigma_2]^{-1} = [E - E_c - 2t_0 + 2t_0 e^{ika} - U_0/a]^{-1} , \tag{6.123}$$

which is simplified using the dispersion relation to

$$G = [2it_0 \sin ka - U_0/a]^{-1} = \frac{a}{i\hbar v - U_0} \tag{6.124}$$

such that the transmission becomes

$$T(E) = \text{Trace}[\Gamma_1 G \Gamma_2 G^+] = \frac{\hbar^2 v(E)^2}{\hbar^2 v(E)^2 + U_0^2} \; , \tag{6.125}$$

i.e. the same result as eq. (6.119).

CHAPTER 7

INCOHERENT TRANSPORT

Up to now we have considered a channel that is connected solely to the two contacts. This is not the complete reality as real channels interact with the environment.

7.1 Why does an atom emit light ?

We consider two states (of eg. an atom) with energies $\epsilon_1 < \epsilon_1$ that can be described by the Hamiltonian

$$i\hbar \frac{d}{dt} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \epsilon_1 & U_{12}^s \\ U_{21}^s & \epsilon_2 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} \tag{7.1}$$

where we have added the couplings by the environment U_{12}^s and U_{21}^s explicitly.

We expect that the rate for a transition from state 2 to 1 as

$$S(2 \rightarrow 1) = K_{2\rightarrow 1} f_2 (1 - f_1) \tag{7.2}$$

where $f_2(1 - f_1)$ describes the probability that the system is in state $|2\rangle$ with state $|1\rangle$ empty. The upward transition rate is in the same way

$$S(1 \rightarrow 2) = K_{1\rightarrow 2} f_1 (1 - f_2) . \tag{7.3}$$

The rates have to be equal in equilibrium such that

$$\frac{K_{1\rightarrow 2}}{K_{2\rightarrow 1}} = \frac{f_2(1 - f_1)}{f_1(1 - f_2)} = \frac{(1 - f_1)/f_1}{(1 - f_2)/f_2} . \tag{7.4}$$

The occupation factors f_1, f_2 are given by the Fermi function (1.1)

$$f_n = \frac{1}{1 + \exp[(\epsilon_n - \mu)/k_B T]} \quad \rightarrow \quad (1 - f_n)/f_n = \exp\left(\frac{\epsilon_n - \mu}{k_B T}\right) \tag{7.5}$$

and therefore eq. (7.4) states

$$\left(\frac{K_{1\to 2}}{K_{2\to 1}}\right) = \exp\left(-\frac{\epsilon_2 - \epsilon_1}{k_B T}\right). \tag{7.6}$$

The rates for emission and absorption of photons are

$$K_{1\to 2} = \alpha N_\omega \qquad\qquad \text{photon absorption} \tag{7.7}$$
$$K_{2\to 1} = \alpha(N_\omega + 1) \qquad\qquad \text{photon emission} \tag{7.8}$$

where N_ω is the number of photons present[1]. This number is given by the Bose-Einstein factor

$$N_\omega = \frac{1}{\exp[(\hbar\omega)/k_B T] - 1} \tag{7.9}$$

which leads to the rate ratio

$$\left(\frac{K_{1\to 2}}{K_{2\to 1}}\right) = \exp\left(-\frac{\hbar\omega}{k_B T}\right). \tag{7.10}$$

and as $\hbar\omega = \varepsilon_2 - \varepsilon_1$ eq. (7.10) is consistent with eq. (7.6).

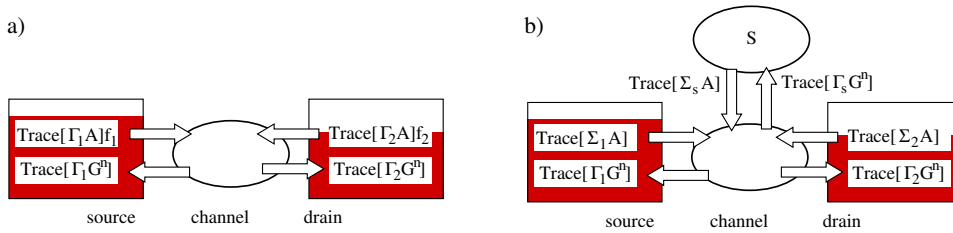## 7.2   The environment as third terminal

Figure 7.1   a) Coherent versus b) incoherent transport.

Up to now, the transport between source and drain involved scattering, but was completely coherent. Incoherent transport has to involve another partner to our channel. We will treat this third partner in a similar way as source and drain (see fig. 7.1) through its

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[1]Absorption and stimulated emission are proportional to the number of photons present. Emission can also be spontaneous.

matrices Γ_s, Σ_s:

coherent	incoherent
$G^n = G\Sigma^{\text{in}}G^+$	
$A = i[G - G^+]$	
$\Gamma = i[\Sigma - \Sigma^+]$	
$\Sigma^{\text{in}} = \Gamma_1 f_1 + \Gamma_2 f_2$	$\Sigma^{\text{in}} = \Sigma_1^{\text{in}} + \Sigma_2^{\text{in}} + \Sigma_s^{\text{in}}$
$G = [EI - H - \Sigma]^{-1}$	$G = [EI - H_0 - U - \Sigma]^{-1}$
$\Sigma = \Sigma_1 + \Sigma_2$	$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_s$

The main differenec is, that the "contact" describing the environment does not have a defined energy distribution according to a Fermi function, but is still described as a self-energy term.

The density matrix can still evaluated from the correlation function

$$[\rho] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} \, G^n(E) \tag{7.11}$$

and the current a terminal i can be written as

$$I_i = \frac{e}{h} \int_{-\infty}^{\infty} dE \, \tilde{I}_i(E) \tag{7.12}$$

with

$$\tilde{I}_i = \text{Trace}[\Sigma_i^{\text{in}} A] - \text{Trace}[\Gamma_i G^n] \, . \tag{7.13}$$

7.3 Inflow and outflow for three levels

We consider three levels, where ϵ is in the middle of two others that are separated by $\hbar\omega$ from it, i.e. $\epsilon_b - \epsilon = \epsilon - \epsilon_a = \hbar\omega$. The rates for absorption K^{ab} and for emission K^{em} are

$$K^{ab} \propto N_\omega \tag{7.14}$$

$$K^{em} \propto N_\omega + 1 \, . \tag{7.15}$$

We assume for the temperature to be low as compared to $\hbar\omega$ such that $N_\omega \ll 1$ and we have to consider emission only. Using N, N_a, N_b for the number of electrons in the states we can write the inflow and outflow into the state of energy ϵ as

$$\text{inflow} = K^{em} N_b (1 - N) = K^{em} N_b - K^{em} N_b N \tag{7.16}$$

$$\text{outflow} = K^{em} N (1 - N_a) \, . \tag{7.17}$$

We count the negative term in the inflow to the outflow[2] and arrive to the form

$$\text{inflow} = K^{em} N_b \tag{7.18}$$

$$\text{outflow} = K^{em} N (1 - N_a + N_b) \, . \tag{7.19}$$

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[2]this is not only a academic assignment, see [1]

Inflow

We have used before in eqs. (6.59), (6.60) that

$$[\Sigma^{\text{in}}] = [\tau A_R \tau^+] f = [\tau G_R^n \tau^+] \tag{7.20}$$

where A_R, G_R^n are spectral and correlation functions of the contact. In case of the contact it is it's correlation function that causes the inscattering into the channel. This is different for the emission process as here it is the channel's correlation function, which causes the inscattering, such that we can write

$$\Sigma_s^{\text{in}}(E) = \int_0^\infty \frac{d(\hbar\omega)}{2\pi} \, D^{em}(\hbar\omega) G^n(E + \hbar\omega) \, . \tag{7.21}$$

where $G^n(E + \hbar\omega)$ replaces N_b in eq. (7.18) and D^{em} is the absorption function replacing the matrices τ, τ^+. The absorption and emission functions in their simplest version can be expressed as

$$D^{em}(\hbar\omega) \equiv (N_\omega + 1) D_0(\hbar\omega) \tag{7.22}$$

$$D^{ab}(\hbar\omega) \equiv N_\omega D_0(\hbar\omega) \tag{7.23}$$

such that we can write the inscattering function including absorption as

$$\Sigma_s^{\text{in}}(E) = \int_0^\infty \frac{d(\hbar\omega)}{2\pi} \, D_0(\hbar\omega) \left[(N_\omega + 1) G^n(E + \hbar\omega) + N_\omega G^n(E - \hbar\omega) \right] \, . \tag{7.24}$$

Outflow

For the outflow term, we again replace N_b by $G^n(E + \hbar\omega)$ and $1 - N_a$ by $G^p(E - \hbar\omega)$ to arrive at

$$\Gamma_s^{\text{in}}(E) = \int_0^\infty \frac{d(\hbar\omega)}{2\pi} \, D^{em}(\hbar\omega) \left[G^p(E - \hbar\omega) + G^n(E + \hbar\omega) \right] \tag{7.25}$$

where we have used the quantity

$$G^p = A - G^n \tag{7.26}$$

that describes the density of empty states (holes) just as G^n describes the electron density. Including absorption, the full expression of the broadening function is

$$\Gamma_s^{\text{in}}(E) = \int_0^\infty \frac{d(\hbar\omega)}{2\pi} \, D_0(\hbar\omega) \quad ((N_\omega + 1)[G^p(E - \hbar\omega) + G^n(E + \hbar\omega)] +$$
$$N_\omega [G^n(E - \hbar\omega) + G^p(E + \hbar\omega)]) \tag{7.27}$$

7.4   Ohm's law

We have seen that the conductance at low bias can be expressed by the Landauer formula eq. (6.101)

$$G = \frac{e^2}{h} T \ \text{ with } \ T = \int_{-\infty}^\infty dE \, \bar{T}(E) F_T(E - \mu) \, .$$

The transition generally is proportional to the number of modes N in the channel, such that we can write

$$G = \frac{2e^2}{h} \bar{T} N \tag{7.28}$$

where $\bar{T}$ denotes the average transmission per mode (two spins per mode). For large conductors the number of modes will be proportional to the conductor's cross section S, i.e. $N \propto S$. In order to arrive at Ohm's law

$$G \propto S/L \tag{7.29}$$

we need to understand why T / L, which is not the case for coherent transport, where T is constant.

We consider the conductor to be split into two sections in series with transition probabilities T_1 and T_2. What is the propability for transmission ? The partical can go straight through with proability $T_1 T_2$, but can also be reflected at the second part and again at the first, and then transmitted in the second attempt resulting in the probability $T_1 R_1 R_2 T_2$ ($R_i = 1 - T_i, i = 1, 2$). The reflections can happen also more than one time. Summing up all the possibilities the transmission becomes

$$T = T_1 T_2 (1 + R_1 R_2 + (R_1 R_2)^2 + (R_1 R_2)^3 + \dots) = \frac{T_1 T_2}{1 - R_1 R_2} \tag{7.30}$$

which can be seen by Taylor expansion of

$$\frac{1}{1 - x} = 1 + x + x^2 + x^3 + \dots . \tag{7.31}$$

Expression of T using transmission functions only gives

$$T = \frac{T_1 T_2}{T_1 + T_2 - T_1 T_2} \tag{7.32}$$

and therefore

$$\frac{1}{T} = \frac{1}{T_1} + \frac{1}{T_2} - 1 . \tag{7.33}$$

Requiring the transmission to be a function of $L = L_1 + L_2$, eq. (7.33) is solved by

$$T(L) = \frac{\Lambda}{\Lambda + L} \tag{7.34}$$

where Λ is a constant of the order of the mean free path, i.e. the length for which the transmission probability is $1/2$. The conductance gets according to (7.28)

$$G = \frac{2e^2}{h} M \frac{\Lambda}{\Lambda + L} \tag{7.35}$$

and the resistance can be written as the sum of two terms

$$\frac{1}{G} = \underbrace{\frac{h}{2e^2 M}}_{\text{interface}} + \underbrace{\frac{h}{2e^2 M} \frac{L}{\Lambda}}_{\text{device}} \tag{7.36}$$

where the first can be interpreted as interface resistance independent of L while the second is the device resistance that depends on L. The device resistance is thus

$$R_{\text{device}} = \frac{1}{G_{\text{device}}} = \frac{h}{2e^2 M} \frac{1 - T}{T} \tag{7.37}$$

and goes to zero for a ballistic conductor ($T = 1$). In this case the resistance corresponding to the quantum of conductance is purely represented as contact resistance.

REFERENCES

1. S. Datta, *Quantum Transport: Atom to Transistor* (Cambridge University Press, Cambridge, England, 2005).