PART II

QUANTUM TRANSPORT

(in interacting nanostructures)

Chapter 3   Basic concepts of quantum transport

3.1   Mesoscopic conductors

Electronic transport in mesoscopic systems is a field of condensed matter physics emerged in the late 1970s. It deals with systems containing several thousand of atoms, and thus bridging between the macroscopic classical world and the microscopic quantum realm. This is encoded in the word itself mesoscopic (van Kampen, 1976)

$$\mu\acute{\epsilon}\sigma o \varsigma \ : \quad \text{in the middle}$$

$$\sigma\kappa o\pi\acute{\epsilon}\omega : \quad \text{to look at, to observe}$$

$$(\varphi\acute{u}\sigma\iota\varsigma : \quad \text{nature})$$

If   L is the system size, it holds:

$$1 \, mm \gg L \gg a_o \qquad (3.1)$$

where $a_o \sim 0.5\text{Å}$ is the Bohr radius. This is a vast field. We shall focus in the following on coherent nanostructures, which have become object of intense investigation from the middle 1990s. They include semiconducting heterostructures, molecular junctions or carbon-based nanostructures. In order to fix better the ideas let me introduce 3 characteristic length scales:

1 - de Broglie wavelength λ

2 - mean free path L_m
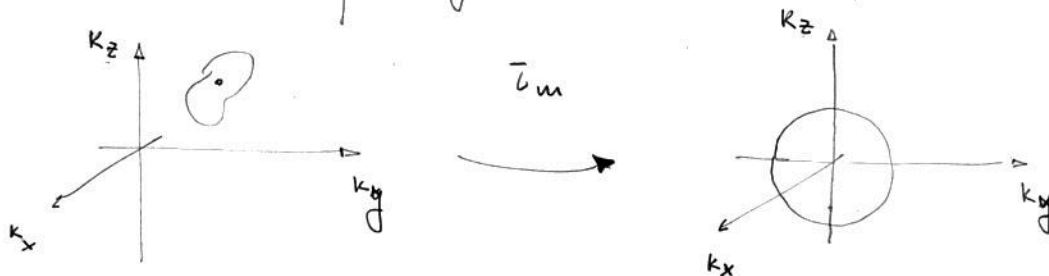
3 - phase - relaxation length L_φ

1 - de Broglie wavelength λ:

$$\lambda = \frac{h}{mv} \qquad (3.2)$$

This length is a measure of the wave particle duality. On length scales much larger than λ a system behaves classically. For a 2DEG the typical λ taken for electrons at $v = v_F$ is $\lambda_f \tilde{=} 35\,nm$.

2 - mean free path L_m.

An electron in a perfect crystal moves as in vacuum but with an effective mass. Nevertheless there are impurities, phonons, other electrons which disturb this simple picture. L_m is usually defined as $L_m = v_f \tau_m$ where τ_m is the average time an electron takes to change its momentum. In other words, given an initial distribution peaked at $\vec{u}$, the time it takes to equilibrate. (Notice that e-e does not contribute to the τ_m since it conserves - globally - the electronic momentum).

Again in a 2DEG typically $L_m = 30\,\mu m$ and $\tau_m \tilde{=} 100\,ps$

3 - phase-relaxation length $L\varphi$. Electrons (and all quantum system in general) acquire a phase in time associated to their energy. This is also what ensures the (phase coherent) space propagation of a wave packet:

$$\psi(x, t_o) = \int dk\, e^{-\alpha^2(k-k_o)^2} e^{ikx} e^{-i\omega_k t_o} \qquad (3.3)$$

assuming for example a linear dispersion relation $\omega = ck$

$$\psi(x,t_0) = \int_{-\infty}^{+\infty} dk\, e^{-\alpha^2(k-k_0)^2} e^{ik(x-ct)} = e^{-(x-ct)^2/4\alpha^2} \underbrace{e^{ik_0(x-ct)}}_{e^{i\varphi(t)}}$$

In case of dephasing processes, inelastic processes change the energy of the propagating particle $\Rightarrow$ its phase. A typical experiment to measure dephasing length is an Aharonov-Bohm ring.

path 1

path 2
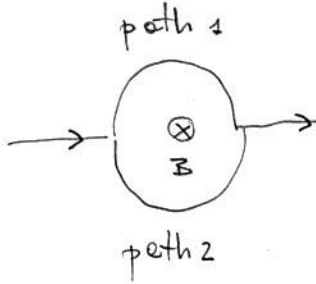
The conductance through the system show oscillations as a function of the magnetic field. The amplitude of the oscillations is reduced by dephasing processes.
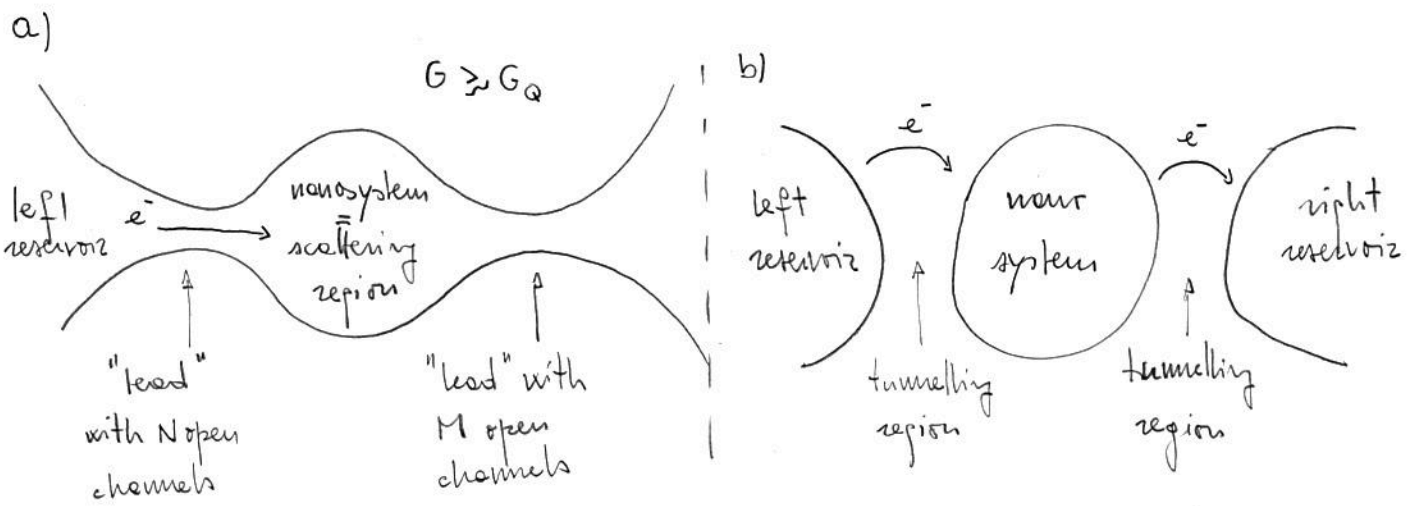
Using the characteristic lengths we can classify:

$$
\begin{array}{ll}
L \gg L_m & \text{diffusive} \\
L \gg L_\varphi & \text{incoherent} \\
L \gg \lambda & \text{(semiclassical}
\end{array}
\left.\right\} \text{conventional transport}
$$

$$
\begin{array}{ll}
L \ll L_m & \text{ballistic} \\
L \ll L_\varphi & \text{coherent} \\
L \ll \lambda & \text{quantum mechanical}
\end{array}
\left.\right\} \rightarrow \text{Mesoscopic transport}
$$

What we have in mind is an electrical circuit of which the nanostructure is part. The nanostructure is connected to "electron reservoirs" or "contacts" kept at different electrochemical potentials which allow transfer of charge or other degrees of freedom e.g. spin, energy associated to the carriers. We deal with open quantum systems, where the contacts are seen as thermalized subsystems.

A generic nanodevice is considered typically in two different ways, depending on "how good" the coupling to the reservoir is:

a)

$$G \gg G_Q$$

left reservoir e^- → nanosystem $\equiv$ scattering region

"lead" with N open channels

"lead" with M open channels

b)

left reservoir e^- nano system e^- right reservoir

tunnelling region

tunnelling region

A measure of how strong the contacts are, is provided by the ratio G/G_Q between the conductance G of the nanostructure:

$$G = \lim_{V \to 0} \frac{dI}{dV} \qquad (3.4)$$

and the conductance quantum $G_Q = \frac{2e^2}{h}$. If $G \gg G_Q$ many electrons traverse a nanostructure simultaneously. This occurs via several transport channels represented by the ideal leads. Often a description of the central region as "scattering region" is performed. The scattering formalism of Landauer and Büttiker is then a powerful tool to describe these systems in particular in absence of e-e interaction.
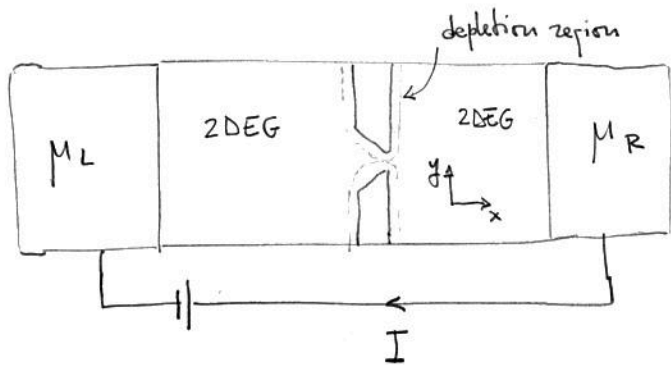
3.2 A QUANTUM POINT CONTACT

Nanostructures can be designed and manufactured with several methods. One possibility is to pattern them on the top of a GaAs/AlGaAs based heterostructure or of other sources of 2DEGs. (e.g. a graphene layer) by standard lithographic techniques. To this extend one exploits the fact that a 2DEG forms at the interface between

GaAs and AlGaAs. To laterally confine the electrons one defines
a metallic pattern on top of the heterostructure. Applying a negative
gate voltage depletes the electrons under the pattern, thereby confining
the electrons to the ungated region.

metal gate

50 nm   n-AlGaAs
20 nm   AlGaAs

GaAs
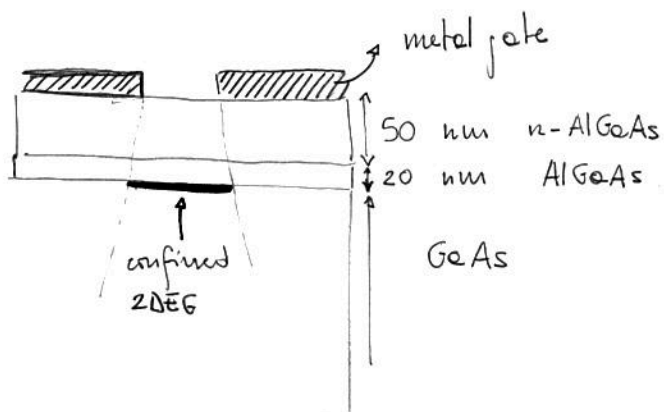
confined
2DEG

a) Cross section of a
laterally confined 2DEG

depletion region

M_L 2DEG   2DEG M_R

y
x

I

b) Top view of a quantum
point contact. (QPC)

Alternatively one starts from "natural" nanostructures as eg. molecules,
self assembled QD, self assembled nanowires, carbon nanotubes and integrates
them in electrical circuits via different techniques.

From a theoretical point of view a QPC is described by electrons
in a 2 dimensional confinement with an additional x dependent con-
finement in the y direction. Because the confinement is largest
at the bottle neck, this induces an effective barrier for the
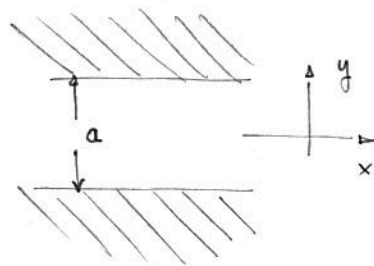electrons to travel along the longitudinal direction. (x)

In general one can look at the QPC as an electron wave guide:
of variable cross section. We assume an __adiabatic__ wave guide i.e.
with dimensions varying so smoothly that a factorizing ansatz still holds:

i)   Confinement constant in x

$$\psi_n(x,y) = \Phi_n(y) e^{ikx}$$

$$E = E_n + \frac{\hbar^2 k_x^2}{2m^*}$$

$$E_n = \frac{\pi^2 \hbar^2}{8m^*} \frac{n^2}{a^2}$$

ii)   Adiabatic confinement

$$\psi_n(x,y) = \varphi_n(x) \Phi_n(y;x)$$

$$E_n = E_n(x) = \frac{\pi \hbar^2}{2m^*} \frac{n^2}{a(x)^2}$$

$\psi(x)$ satisfies the equation $\left(-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + E_n(x) \right) \varphi_n(x) = E \varphi_n(x)$

We have discrete energy levels ("subbands" or "modes") due to the confinement.
The term $E_n(x)$ plays the role of a potential barrier for the longitudinal
motion. Moreover the barrier becomes larger upon increasing n. If we
assume as first approximation an impenetrable barrier ⇒ we can
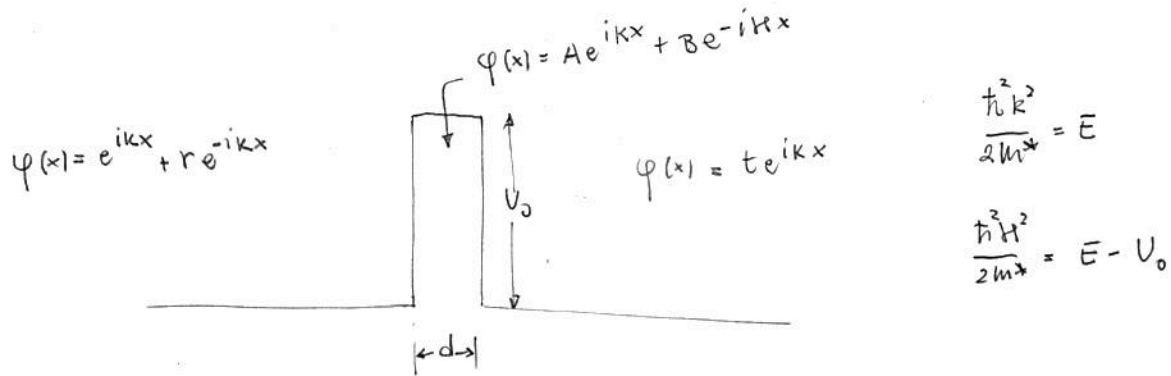count the number of open channels: $E_n(x) < E_F$ $\forall x$.
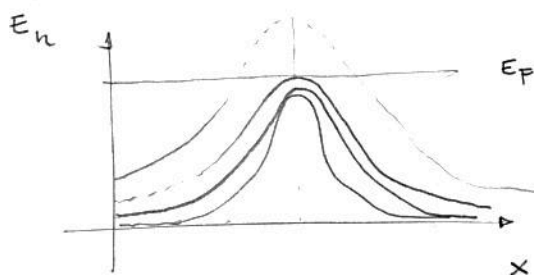
3 channels open.
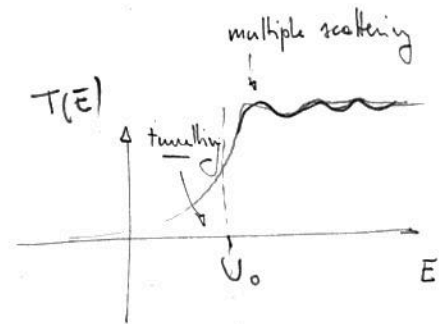
In general, though, the barrier is not impenetrable and one

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obtains an energy dependent transmission coefficient $T_n(E)$.
$T_n(E)$ is obtained by solving the scattering problem.

Eg. The transmission through a rectangular barrier reads:

$$\varphi(x) = A e^{iKx} + B e^{-iKx}$$

$$\varphi(x) = e^{ikx} + r e^{-ikx}$$

$$\varphi(x) = t e^{ikx}$$

V_0

$$\frac{\hbar^2 k^2}{2m^*} = E$$

$$\frac{\hbar^2 H^2}{2m^*} = E - V_0$$

$|\leftarrow d \rightarrow|$

by imposing $\varphi(x)$ to be C^1 on $\mathbb{R}$

$$T(E) \equiv t^2 = \cfrac{1}{1 + \left(\cfrac{\sin Hd\, (k^2 - H^2)}{2kH} \right)^2}$$

$T(E)$

multiple scattering

tunneling

V_0 E

One striking result first observed when measuring the conductance $G = \lim\limits_{V \to 0} \frac{dI}{dV}$ of a QPC vs. gate voltage V_G (B.J. van Wees et al. PRB 43 12431 (1991) is that at low temperatures it changes in steps of $\frac{2e^2}{h} = G_Q$, i.e. it is QUANTIZED. Each step reflects a new transverse subband entering the transport window $\mu_L - \mu_R$. In order to evaluate the current we first observe that since there are no sinks nor sources I is equal in every cross section We take conveniently one far from the bottle neck. As a second assumption we take the unpenetrable barrier potential $\Rightarrow T_n = 0, 1$ for closed, open channels respectabely. It follows for the current

$$I = 2e \sum_n \frac{1}{L} \sum_{k_x} \left[\underbrace{\frac{1}{\hbar} \frac{\partial \varepsilon_k}{\partial k_x}}_{v_n} f_L(\varepsilon_n) T_n(\varepsilon_n) + \frac{1}{\hbar} \frac{\partial \varepsilon_n}{\partial(-k_x)} f_R(\varepsilon_n) T(\varepsilon_n) \right] \quad (3.4)$$

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where
$$f_{L,R}(\varepsilon) = \frac{1}{1 + e^{\beta(E - \mu_{L,R})}} \qquad (3.5)$$

Thus, with $\frac{1}{L}\sum_{k_x} \rightarrow \frac{1}{2\pi}\int dk_x = \frac{1}{2\pi}\int d\varepsilon \frac{\partial k_x}{\partial \varepsilon}$ and impenetrable barriers

$$I = \frac{2e}{h} N_{open} \int d\varepsilon \left[f_L(\varepsilon) - f_R(\varepsilon) \right] = \frac{2e}{h} N_{open} (\mu_L - \mu_R)$$

$$\Rightarrow \qquad G = \left. \frac{dI}{dV} \right|_{V=0} = \frac{2e^2}{h} N_{open}$$

3.3 Tunneling structures

In the following we shall discuss quantum transport for systems in the low conductance regime $G \lesssim G_Q$ which can be conveniently described by a Hamiltonian of the form (cf. 2.7)

$$\hat{H} = \hat{H}_{res} + \hat{H}_S + \hat{H}_T \qquad (3.6)$$

where the tunnelling Hamiltonian $\hat{H}_T$ provides the coupling of the system to the contacts and is considered as a perturbation. One can think to various realization of the Hamiltonian (3.6). e.g. in STM set-ups where the system of interest is e.g. an adatom or a molecule on a thin insulating substrate. I

STM tip

insulating layer

metallic substrate (in general conducting)

V_b

$d\hat{z}$
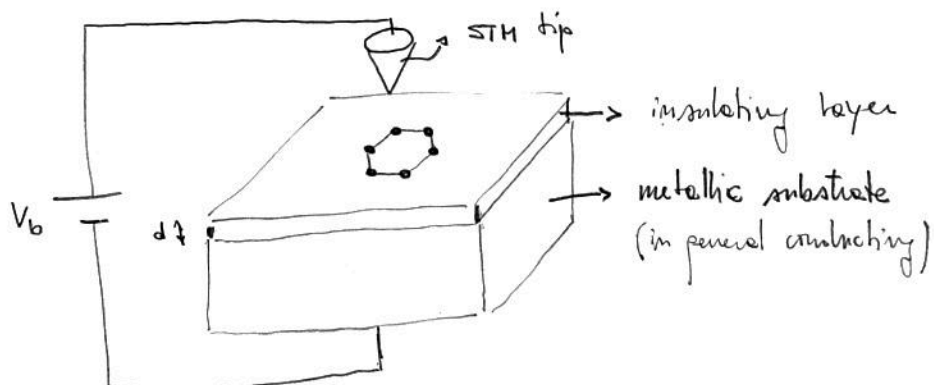
The entire structure is immersed in ultra high vacuum. The vacuum region between the tip and the molecule and the insulating region (of thickness d) between the molecule and the conducting substrate provides tunnelling barriers. In the example sketched, we consider a planar molecule (benzene), whose molecular orbitals decay exponentially along the z direction on a length scale a_z. We can think the electrons in a potential (scalar field) $V(\vec{r})$. If we restrict to the "relevant" condition in which the tip is standing above the molecule and we plot $V(x_{tip}, y_{tip}, z)$, we can visualize the relevant parameters for the device
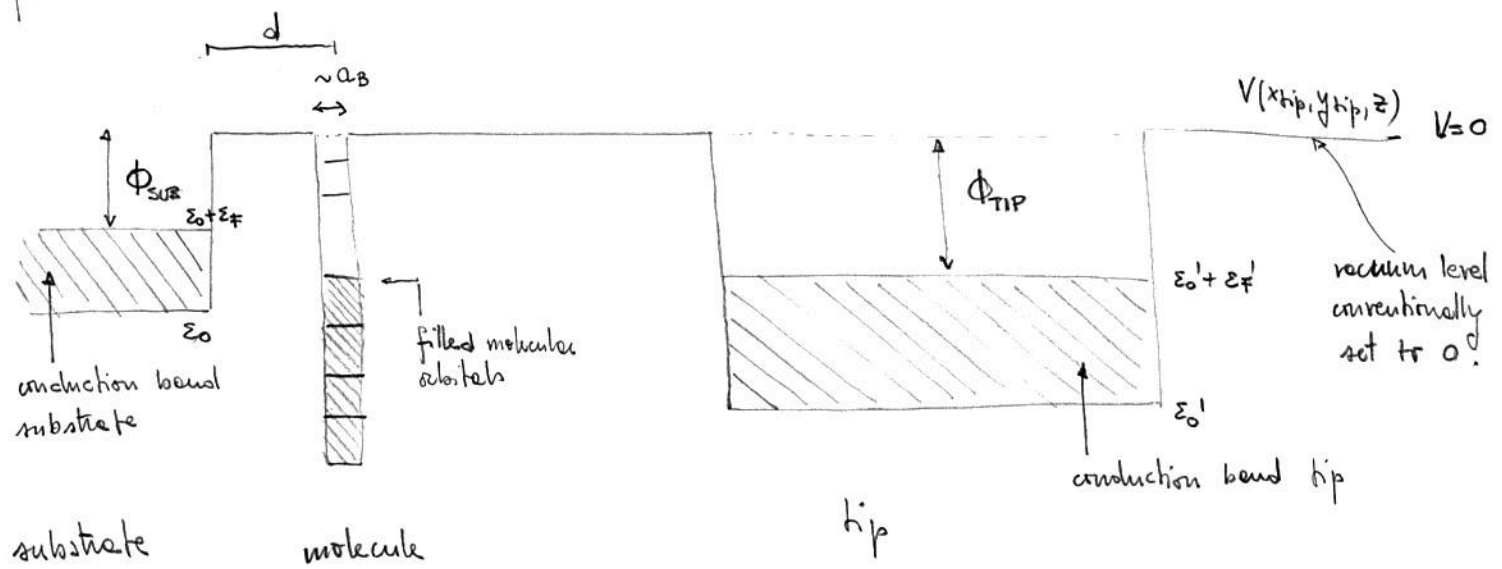
One other possibility is provided by a quantum dot electrostatically defined in a 2DEG or obtained by contacting a carbon nanotube or a molecule to metal with large contact resistance. (e.g. gold)
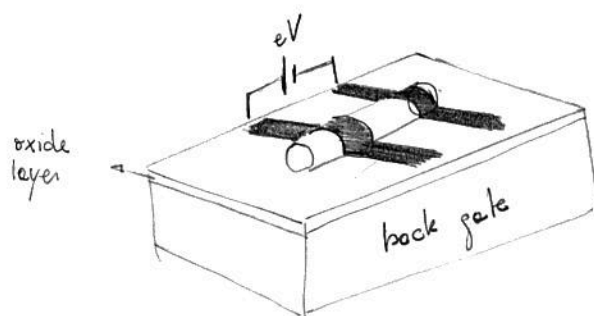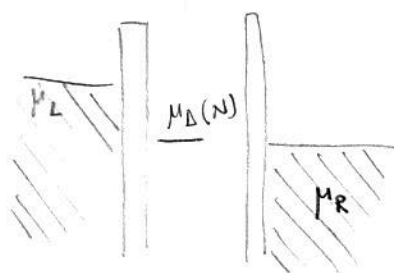
The Hamiltonian (3.6) has the same form of (2.7) where the correspondence between the open system and the tunnelling structure is given by

$$H_B \longrightarrow H_{res}$$
$$H_{S-B} = V \longrightarrow H_T \qquad (3.7)$$

In the following we shall evaluate the current-voltage characteristics of such nanostructures based on the density-matrix formalism, using the expression:

$$I_L = \text{Tr}\left\{\hat{\rho}_{tot}\, \hat{I}_L\right\} = \text{Tr}_{sys}\left\{\text{Tr}_{res}\left\{\hat{\rho}_{tot}\, \hat{I}_L\right\}\right\} \qquad (3.8)$$

where $\hat{I}_L$ is the current operator through the left reservoir (playing the role of "source" if the applied bias $V > 0$). An expression for the current operator can be readily obtained from:

$$I_L = -\frac{d}{dt}\langle e\hat{N}_L \rangle = -\frac{d}{dt}\,\text{Tr}\left\{e\hat{N}_L\, \hat{\rho}_{tot}(t)\right\} = -\text{Tr}\left\{e\hat{N}_L\left(-\frac{i}{\hbar}[\hat{H},\hat{\rho}(t)]\right)\right\} =$$

$$= +\frac{i}{\hbar}\,\text{Tr}\left\{e\hat{N}_L\, \hat{H}\, \hat{\rho}(t)\right\} - \frac{i}{\hbar}\,\text{Tr}\left\{e\hat{N}_L\, \hat{\rho}(t)\, \hat{H}\right\} \qquad = \quad \text{cyclic property of the trace}$$

$$= \text{Tr}\left\{\frac{i}{\hbar}e[\hat{N}_L,\hat{H}]\,\rho(t)\right\} \qquad \longrightarrow$$

$$\boxed{\hat{I}_L = e\frac{i}{\hbar}[\hat{N}_L,\hat{H}] \qquad (3.9)} \quad \Longrightarrow \quad \boxed{\hat{I}_L = e\frac{i}{\hbar}[\hat{N}_L,\hat{H}_T] \qquad (3.9b)}$$

where $\hat{N}_L$ is the number operator of the left contact. Thus, in this approach, the quantity to be determined is the total density operator $\hat{\rho}_{tot}$ and, in turn, the reduced density matrix $\hat{\rho}_{red} = \text{Tr}_{res}\left\{\hat{\rho}_{tot}\right\}$ (3.10)

For example, let us consider as an example the Anderson impurity model

$$\hat{H} = \overbrace{\sum_{k\sigma\alpha} \varepsilon_k c^\dagger_{\alpha k\sigma} c_{\alpha k\sigma}}^{\hat{H}_{res}} + \overbrace{\sum_\sigma \varepsilon_d d^\dagger_\sigma d_\sigma}^{\hat{H}_S} + \overbrace{t_\alpha \sum_{\alpha k\sigma} \left(c^\dagger_{\alpha k\sigma} d_\sigma + d^\dagger_\sigma c_{\alpha k\sigma} \right)}^{\hat{H}_T} \qquad (3.11)$$

where $\alpha = L, R$ $\sigma = \uparrow, \downarrow$ and k is the momentum of the electron in the lead. It follows that

$$\hat{I}_L = e\frac{i}{\hbar} \left[\sum_{Lk\sigma} c^\dagger_{Lk\sigma} c_{Lk\sigma} , \hat{H} \right] = \hat{N}_L \text{ commutes with } \hat{H}_S \text{ and } \hat{H}_{res}$$

$$= e\frac{i}{\hbar} \sum_{k\sigma} \left[c^\dagger_{Lk\sigma} c_{Lk\sigma} , \hat{H}_T \right] = e\frac{i}{\hbar} \sum_{k\sigma}\sum_{\alpha q\tau} \left[c^\dagger_{Lk\sigma} c_{Lk\sigma} , t_\alpha\left(c^\dagger_{\alpha q\tau} d_\tau + d^\dagger_\tau c_{\alpha q\tau} \right) \right]$$

$$= e\frac{i}{\hbar} \sum_{k\sigma}\sum_{\alpha q\tau} t_\alpha \left(\left[c^\dagger_{Lk\sigma} c_{Lk\sigma} , c^\dagger_{\alpha q\tau} \right] d_\tau + d^\dagger_\tau \left[c^\dagger_{Lk\sigma} c_{Lk\sigma} , c_{\alpha q\tau} \right] \right)$$

$$= e\frac{i}{\hbar} \sum_{k\sigma}\sum_{\alpha q\tau} t_\alpha \left(c^\dagger_{Lk\sigma} d_\tau - d^\dagger_\tau c_{Lk\sigma} \right) \delta_{\alpha L} \delta_{qk} \delta_{\sigma\tau} =$$

$$= e\frac{i}{\hbar} \sum_{k\sigma} t_L \left(c^\dagger_{Lk\sigma} d_\sigma - d^\dagger_\sigma c_{Lk\sigma} \right) \qquad (3.12)$$

The current operator is a mixed system and reservoir operator. This is a common feature in this approach. Since then the expectation values of operators is independent of the representation one can write:

$$I_L(t) = \text{Tr}\left\{ \hat{I}_{L,I}(t)\, \tilde{\rho}_I(t) \right\} \qquad (3.13)$$

Notice that, in principle, the time evolution of the entire density operator $\hat{\rho}_I(t)$ is needed to evaluate (3.13).

An alternative way of calculating the current through the system is to relate it to the variation of charge ON THE SYSTEM. In this approach, though we have access at first side only to the sum of the current to the different leads:

$$I_L + I_R = \frac{d}{dt} Tr\{\hat{N}_s \rho(t)\} = \frac{d}{dt} Tr_{sys}\{\hat{N}_s \, Tr_{res}\{\hat{\rho}(t)\}\} =$$

$$= Tr_{sys}\{\hat{N}_s \, \dot{\rho}_{red}(t)\} \qquad (3.14)$$

This expression of the current depends now on the equation of motion for the reduced density matrix. If we analyze the simple case in which $\dot{\rho}_{red}(t) = \mathcal{L} \rho_{red}(t)$. (e.g. second order Markov approximation) it is easy to separate $\mathcal{L}$ into a right and a left contribution $\mathcal{L} = \mathcal{L}_L + \mathcal{L}_R$ and thus obtain:

$$I_\alpha = Tr_{sys}\{\hat{N}_s \mathcal{L}_\alpha \rho_{red}(t)\}. \qquad (3.15)$$

In practice 3.15 can always be transformed into
$$Tr_{sys}\{I_\alpha \rho_{red}(t)\}$$

Notice that, if we calculate the current using $\frac{d}{dt}\langle N_\alpha \rangle$ or $\frac{d}{dt}\langle N_s \rangle$ we need, at first sight, different information about the evolution of the density operator. Let us return to this purpose to the Nakajima Zwanzig approach. This time we will keep the Interaction picture.

$$\rho_I(t) = P \rho_I(t) + Q \rho_I(t) \qquad \text{where} \quad P\rho = Tr_{res}\{\rho\} \otimes \rho_{res}.$$

If now we write $H_T = \sum_i Q_i F_i$ and F_i does not conserve the particle number on the lead $\Rightarrow Tr_{res}\{F_i \rho_{res}\} = 0$ the same for $Tr_{res}\{N_\alpha F_i \rho_{res}\}$
It follows that:

$$I_\alpha = \text{Tr}\left\{\hat{I}_{\alpha I}\,\hat{\rho}_I\right\} = \text{Tr}\left\{\hat{I}_{\alpha,I}\left(P\hat{\rho}_I + Q\hat{\rho}_I\right)\right\} =$$

$$= \text{Tr}\left\{e\frac{i}{\hbar}\left[\hat{N}_\alpha,\hat{H}_{T,I}\right]P\hat{\rho}_I + e\frac{i}{\hbar}\left[\hat{N}_\alpha,\hat{H}_{T,I}\right]Q\hat{\rho}_I\right\} \qquad (3.16)$$

But $P\hat{\rho}_I = \left(\text{Tr}_{res}\{\hat{\rho}_I\}\right)\otimes \rho_{res}$ conserves the reservoir particle number

while $\hat{H}_{T,I}$ doesn't $\Rightarrow \text{Tr}_{res}\left\{e\frac{i}{\hbar}\left[\hat{N}_\alpha,\hat{H}_{T,I}\right]P\hat{\rho}_I\right\}=0$ and the

first term in (3.16) vanishes. We are left with

$$I_\alpha = \text{Tr}\left\{\hat{I}_{\alpha,I}\,Q\hat{\rho}_I\right\}$$

$$(3.17)$$

In summary, if the current is calculated as $-\frac{d}{dt}\langle N_L\rangle$ we obtain
that only the non factorized component of the density operator contributes
to the calculation of the average. In the other case

$$I_L + I_R = e\frac{d}{dt}\text{Tr}\left\{\hat{N}_s\,\rho_I(t)\right\} = e\frac{d}{dt}\text{Tr}_{sys}\left\{\hat{N}_s\,\text{Tr}_{res}\{\rho_I(t)\}\right\} =$$

$$= e\frac{d}{dt}\text{Tr}\left\{\hat{N}_s\,P\rho_I\right\} = \boxed{e\text{Tr}\left\{\hat{N}_s\,P\dot{\rho}_I\right\}.} \qquad (3.18)$$

and only the time evolution of the factorized component of ρ_I is
apparently needed. The connection between the two approaches is obtained
by remembering that (for factorized initial conditions) $\qquad$ (2.60),(2.61)

$$Q\rho_I(t) = \int_0^t ds\ G(t,s)\,Q\mathcal{L}(s)\,P\rho_I(s)$$

$$P\dot{\rho}_I = P\mathcal{L}\int_0^t ds\ G(t,s)\,Q\mathcal{L}(s)\,P\rho(s) = P\mathcal{L}\,Q\rho_I$$