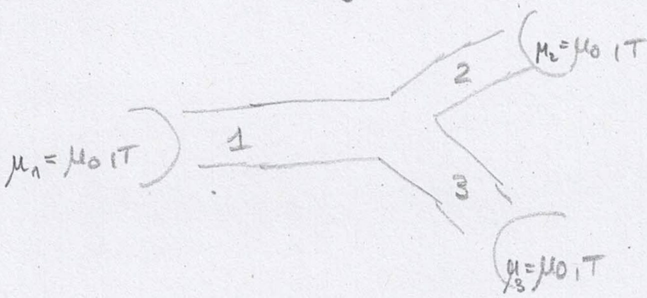
4.4 Multiterminal devices : The beam splitter

The results for the conductance of a mesoscopic device can be extended to a multi-terminal situation.

Here we simply look at the mesoscopic beam splitter



In this case the system is in global equilibrium with respect to three reservoirs.

The conceptual difficulty is that the (infinitesimal) bias drop ~~was~~ applied pairwaise

$$eV_{12} = \mu_1 - \mu_2$$

$$eV_{13} = \mu_1 - \mu_3$$

$$eV_{23} = \mu_2 - \mu_3$$

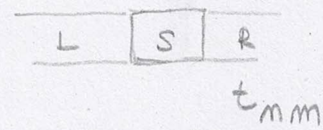
where $\mu_1 = \mu_0 - eV_1$, $\mu_2 = \mu_0 - eV_2$, $\mu_3 = \mu_0 - eV_3$.

↳ to generalize from the two-terminal from a three-terminal (and in general a multiterminal) device, we must keep track of the (small) voltage differences. I.e., we look directly at <u>currents</u> rather than at conductances.

Two-terminal current

Let us consider our two terminal formula for G

$$G = \frac{2e^2}{h} \int_0^\infty dE \; \mathrm{Tr}\{t^\dagger t\} \left(\frac{-\partial f}{\partial E} \right)$$



where $\mathrm{Tr}\{t^\dagger t\} = \sum_{mn} |t_{mn}|^2 \equiv T_{RL}$

describes the tunneling probability $L \to R$

Also $\mathrm{Tr}\{t^\dagger t\} = \mathrm{Tr}\{t'^\dagger t'\} = \sum_{mn} |t'_{mn}|^2 \equiv T_{LR}$

describes the tunneling probability $R \to L$.

↳ From the definition of G in linear response,

$$I = GV, \qquad V = V_L - V_R ,$$

it follows for the current at lead L

$$I_L(V_L, V_R) = \frac{2e^2}{h} G (V_L - V_R)$$

and hence

$$\boxed{I_L(V_L, V_R) = \frac{2e^2}{h} \int_0^\infty dE \left(\frac{-\partial f}{\partial E} \right) \left(T_{RL} V_L - T_{LR} V_R \right)} \qquad (4.58)$$

Three-terminal current

This result is valid for a generic multiterminal device. One finds

$$\boxed{I_\alpha = \frac{2e^2}{h} \sum_{\alpha' \neq \alpha} \int dE \left(-\frac{\partial f}{\partial E}\right)\left(T_{\alpha'\alpha} V_\alpha - T_{\alpha\alpha'} V_{\alpha'}\right)} \qquad (4.59)$$

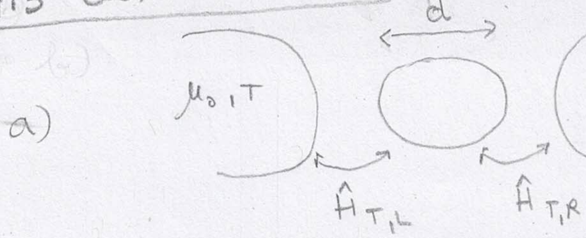
known as the <u>Landauer-Büttiker formula</u>

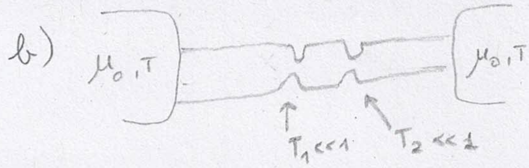
Here the total transmission probabilities from $\alpha \to \alpha'$

$$T_{\alpha\alpha'} = \sum_{mn} |t_{mn\,\alpha'\alpha}|^2$$

were introduced.

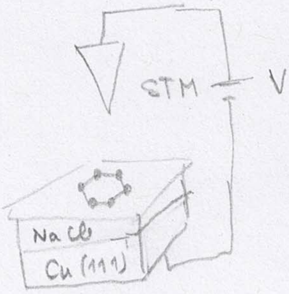
4.5 QUANTUM DOTS



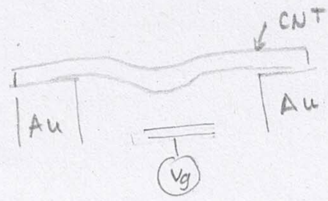


Tunneling barriers form at the interface between the reservoirs and the central systems, or inside the meso/nano system

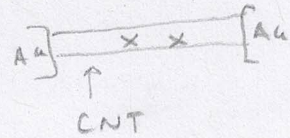
e.g.



STM junctions



suspended CNT with electrostatically defined barriers (through V_g) or bad coupling to metal leads



CNT with two kinks

Physical situation: weak tunneling

In the case of weak tunneling at the barrier, the electrons reside a long time $\sim \hbar \Gamma^{-1} = \hbar(\Gamma_1 + \Gamma_2)^{-1}$ in the dot before they can escape.

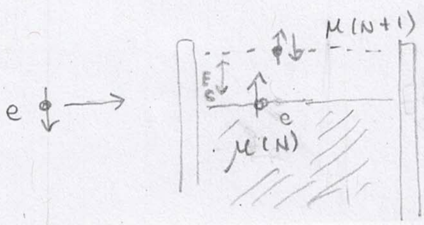
Consequences:

i) sharp resonances $\Rightarrow$ cf. Eq. (4.57)

with broadening $\Gamma_{1,2} \sim T_{1,2} \left(\frac{d\varphi}{dE}\right)^{-1}$

ii) electron-electron interactions may become relevant

$$\boxed{E_C \gtrsim \Gamma, \quad E_C = \mu_{ee}(N+1) - \mu_{ee}(N)}$$



E_C: charging energy = addition energy due to electrostatic charging effects

4.5 Charging energy

The charging energy E_c becomes larger the smaller the dimensions of the confined region

$$E_c = \mu^{ch}_{el}(N+1) - \mu^{ch}_{el}(N)$$

where $\mu_{el}(N) = E^{el}_{N+1} - E^{el}_{N}$

is the electrostatic cost to add an extra charge to a system of N charged particles. For a classical capacitor:

$$\begin{cases} E^{el}_N = \dfrac{(Ne)^2}{2C} \\ C \text{ capacitance} \end{cases} \Rightarrow \mu^{ch}(N) = \frac{e^2}{2C}(2N+1) \,, \quad \boxed{E_c = \frac{e^2}{C}} \tag{4.60}$$

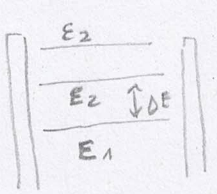
$\Rightarrow$ for small conductors E_c can exceed all other relevant scales at low temperatures

e.g. 2D conductor $C = \epsilon_r \frac{A}{d}$ $\Rightarrow$ cf. Exercise

e.g. suspended CNT quantum dots with $L_d \sim 400$ nm is $E_c \sim$ meV

Quantum dots & metallic islands

A further scale that has to be considered is the (single particle) level spacing ΔE.



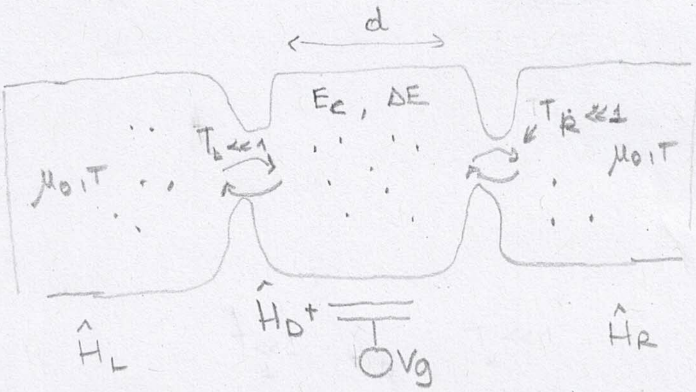
$\Rightarrow$ Total addition energy: $\boxed{\mu(N+1) - \mu(N) \equiv E_{add} \cong E_c + \Delta E}$ (4.61)

i) $E_c \gg \Delta E$ metallic island

ii) $E_c \sim \Delta E$ quantum dot

Conductance of (multiple) quantum dot systems

Bruus & Flensberg Ch. 10.4



i) A gate voltage V_g is used to tune the electron density in the dot

↳ three-terminal device $\quad \hat{H}_D(V_g) = \hat{H}_D - \alpha \hat{N} e V_g \qquad (4.62)$

↑ level arm α

ii) Linear response ⇒ global equilibrium with respect to $\hat{H}_{tot}$

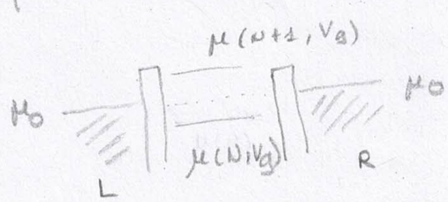
↑ attention what about μ_{dot} ?

iii) Weak tunneling $\quad T_L, T_R \ll 1$

$$\hookrightarrow \quad \hat{\mathcal{H}}_{tot} = \hat{H}_L + \hat{H}_R + \underbrace{\hat{H}_D - \alpha \hat{N} e V_g}_{\hat{H}_D(V_g)} + \underbrace{\hat{H}_{TL} + \hat{H}_{TR}}_{\hat{H}_T} \qquad (4.63)$$

i.e. we consider the system as composed by three distinct parts connected through tunneling Hamiltonians, the central part can be interacting

↳ schematically



iv) Conductance

$$G = - \lim_{\omega \to 0} \frac{\operatorname{Im} \tilde{\chi}_{II}(\omega)}{\omega}$$

with $\quad \hat{I}_\alpha = \frac{d}{dt} \hat{N}_\alpha \quad , \alpha = L, R \qquad$ current at lead / reservoir α

Total Hamiltonian

$$\hat{H}_{tot} = \hat{H}_D - \alpha \hat{N} e V_g + \hat{H}_L + \hat{H}_R + \hat{H}_{TL} + \hat{H}_{TR}$$

where the dot Hamiltonian is

$$\hat{H}_D = \sum_{\sigma} \sum_{i,j} \varepsilon_{ij} \hat{d}^{\dagger}_{i\sigma} d_{j\sigma} + \hat{V}_{ee} \quad , \quad (4.64), \qquad \{|\lambda\rangle = |i\sigma\rangle\}$$

single particle basis

E.g. i = site, energy level

and the reservoirs (leads) are an ensemble of non interacting electrons. E.g. for homogeneous e-gas

$$\hat{H}_\alpha = \sum_{\vec{k}\sigma} \varepsilon_{k} \hat{c}^{\dagger}_{\alpha\vec{k}\sigma} \hat{c}_{\alpha\vec{k}\sigma} \qquad \alpha = L, R \quad , \quad (4.65)$$

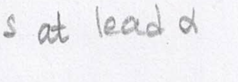
Finally, the tunneling Hamiltonians are

$$\boxed{\hat{H}_{T\alpha} = \sum_{\vec{k}\sigma i} \left[t_{\alpha\vec{k}\sigma i} \, \hat{c}^{\dagger}_{\alpha\vec{k}\sigma} \hat{d}_{i\sigma} + t^{*}_{\alpha\vec{k}\sigma i} \, \hat{d}^{\dagger}_{i\sigma} \hat{c}_{\alpha\vec{k}\sigma} \right]} \quad (4.66)$$

Here $t_{\alpha\vec{k}\sigma i}$ are transmission amplitudes at lead α

Example: single level quantum dot

If the dot possesses only one relevant level

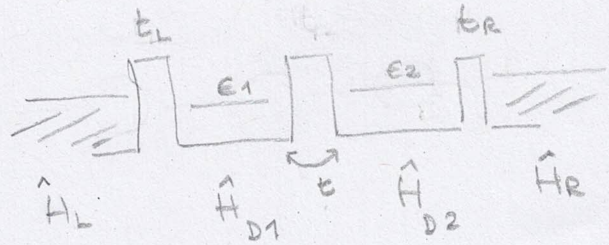


$$\hat{H}_D = \sum_{\sigma} (\varepsilon_d - \alpha e V_g) \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma} + U \hat{n}_{\uparrow} \hat{n}_{\downarrow} \qquad (4.67)$$

which is known also as the single impurity Anderson model (SIAM)

U = Hubbard interaction plays the role of E_c

Example : quantum dots in series



$$\hat{H}_S^0 = \sum_\sigma \left(\varepsilon_{1\sigma} \hat{d}^+_{1\sigma} \hat{d}_{1\sigma} + \varepsilon_{2\sigma} \hat{d}^+_{2\sigma} \hat{d}_{2\sigma} + t \hat{d}^+_{1\sigma} \hat{d}_{2\sigma} + t^* \hat{d}^+_{2\sigma} \hat{d}_{1\sigma} \right) \quad (4.68)$$

and

$$\hat{H}_S = \hat{H}_S^0 + \hat{V}_{ee}$$

where $\hat{V}_{ee} = \frac{1}{2} \sum_{i=1,2} U \hat{n}_{i\sigma} \hat{n}_{i\bar{\sigma}} + \frac{1}{2} \sum_\sigma V_{12} \hat{n}_{1\sigma} \hat{n}_{2\sigma'}$

The tunneling is local. Hence

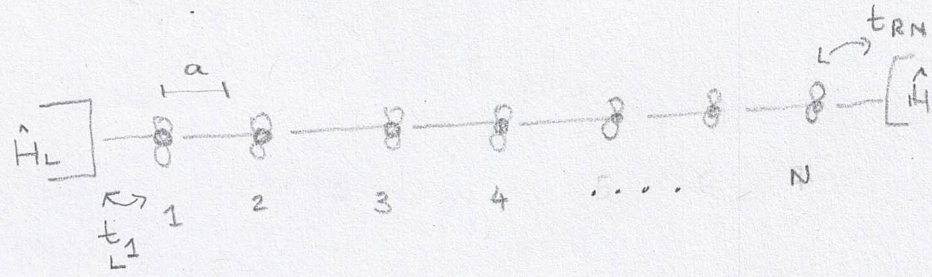
$$\begin{cases} \hat{H}_{TL} = \sum_{\vec{k}\sigma} \left(t_L^* \hat{d}^+_{1\sigma} \hat{c}_{Lk\sigma} + t_L \hat{c}^+_{Lk\sigma} \hat{d}_{1\sigma} \right) & (4.69) \\ \hat{H}_{TR} = \sum_{\vec{k}\sigma} \left(t_R^* \hat{d}^+_{2\sigma} \hat{c}_{Rk\sigma} + t_R \hat{c}^+_{Rk\sigma} \hat{d}_{2\sigma} \right) & (4.69b) \end{cases}$$

where for simplicity k-independent t-amplitudes are considered

Note: Such devices are very popular for quantum information processing

Note: The transmission amplitudes are in general proportional to overlaps of wave functions of the reservoirs / leads with those of the quantum dot at some energy E

Example : finite quantum wire



The former example can be imagined as limiting cases of tight-binding models e.g. for semiconducting or metallic nanowires where the charge carriers are conduction electrons coming from localized ions on a given quasi-one dimensional lattice

e.g. gold nanowires in break junctions, carbon nanotubes, graphene nanoribbons

$$\hat{H}^0_S = \sum_{i=1}^{N}\sum_{\sigma} \varepsilon_{i\sigma} \hat{d}^+_{i\sigma} \hat{d}_{i\sigma} - \sum_{i,j} \left(t_{ij} \hat{d}^+_{i\sigma} \hat{d}_{j\sigma} + h.c. \right)$$ i = atomic position

$$\hat{V}_{ee} = \frac{1}{2} \sum_{\substack{ijke \\ \sigma\sigma'}} v_{ijke} \, \hat{d}^+_{i\sigma} \hat{d}^+_{j\sigma'} \hat{d}_{e\sigma'} \hat{d}_{k\sigma}$$

Special case : local interaction + n.n. hopping t + $\varepsilon_i = \varepsilon$

$$\hat{V}_{ee} = \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$\hat{H}^0_S = \sum_{i=1}^{N} \sum_{\sigma} \varepsilon \hat{d}^+_{i\sigma} \hat{d}_{i\sigma} - t \sum_{i=1}^{N-1} \left(\hat{d}^+_{i\sigma} \hat{d}_{i+1\sigma} + \hat{d}^+_{i+1\sigma} \hat{d}_i \right)$$

↳ Hubbard model

Tunneling Current operator

To evaluate the conductance we need the current correlator

$$\chi_{II}(t) = -\frac{i}{\hbar}\,\theta(t)\,\langle[\hat I(t),\hat I(0)]\rangle_0$$

$\langle\cdots\rangle_0$ with respect to $\hat H_{tot}$

with the current at lead α being

$$\hat I_\alpha(t) = e\frac{d}{dt}\hat N_\alpha(t) = -\frac{ie}{\hbar}[\hat H_{tot},\hat N_\alpha(t)]$$

For a tunneling device described by (4.63)

$$[\hat{\mathcal H}_{tot},\hat N_\alpha(t)] = [\hat{\mathcal H}_{T\alpha},\hat N_\alpha]$$

since $\hat H_{T\alpha}$ does not conserve particles in lead α

with

$$\begin{cases}\hat{\mathcal H}_{T\alpha} = \sum\limits_{i\vec k\sigma}\left(t_{\alpha\vec k\sigma i}\,\hat c^\dagger_{\alpha\vec k\sigma}\,\hat d_{i\sigma} + h.c.\right)\\[2ex] \hat N_\alpha = \sum\limits_{\vec k\sigma}\hat c^\dagger_{\alpha\vec k\sigma}\,\hat c_{\alpha\vec k\sigma}\end{cases}$$

Ex. quantum wire $i = \begin{cases} 1 & \text{if } \alpha = L\\ N & \text{if } \alpha = R\end{cases}$

it holds.

$$[\hat{\mathcal H}_{T\alpha},\hat N_\alpha] = \sum_{i\vec k\sigma}\left(t_{\alpha\vec k\sigma i}\,\hat c^\dagger_{\alpha\vec k\sigma}\,\hat d_{i\sigma} - t^*_{\vec k\sigma i\alpha}\,d^\dagger_{i\sigma}\,\hat c_{\alpha\vec k\sigma}\right)$$

and hence

$$\boxed{\hat I_L = -\frac{ie}{\hbar}[\hat{\mathcal H}_{TL},\hat N_L] \equiv -\frac{ie}{\hbar}\left(\hat L_\alpha - \hat L^\dagger\right)} \quad (4.70)$$

with $\hat L = \sum\limits_{i\vec k\sigma} t_{L\vec k\sigma i}\,\hat c^\dagger_{\alpha\vec k\sigma}\,\hat d_{i\sigma}$ (4.71), notice that $\hat L,\hat L$ also enter in $\hat H_{TL}$

Similarly, we can define

$$\hat{I}_R = -\frac{ie}{\hbar}[\hat{H}_{TR}, \hat{N}_R] \equiv -\frac{ie}{\hbar}(\hat{R} - \hat{R}^+) \qquad (4.70b)$$

Further, because we look at the steady state current, $I = \langle I_L \rangle = I_L = -I_R$

in case of time independent voltages ⇒ we can calculate the current in any of the leads, or even we can define

$$\hat{I} \equiv \gamma \hat{I}_L - (1-\gamma)\hat{I}_R \quad (4.70c)$$ where we use that $\langle \hat{I}_R \rangle = -\langle \hat{I}_L \rangle$

Note: This transformation turns out to be very useful for some simple systems. In linear response, where both reservoirs are in equilibrium with equal μ_0, T, it enables one to work with an effective single reservoir for which the evaluation of $\langle \ldots \rangle_0$ becomes easier. The simple case is the single impurity Anderson model or, more generally, the case of tunneling systems with proportional coupling:

$$\Gamma_L = c\,\Gamma_R, \qquad (4.71)$$

where Γ_L and Γ_R are rate matrices $[t^{-1}]$ at the left/right reservoirs to be defined later.

Conductance of tunneling structures (Kubo)

According to Kubo formula

$$G = -\lim_{\omega \to 0} \frac{\mathrm{Im}\, \tilde{\chi}_{II}(\omega)}{\omega}$$

where $\chi_{II}(t) = -\frac{i}{\hbar}\,\theta(t)\,\langle [\hat{I}(t), \hat{I}(0)] \rangle_0$ e.g. $\hat{I} = \hat{I}_L$

and

$$\begin{cases} \hat{I}_L(t) = -\frac{ie}{\hbar}\left[\hat{L}(t) - \hat{L}^{+}(t)\right] \\ \hat{L} = \sum_{ik\sigma} t^{*}_{\alpha k\sigma i}\, \hat{c}^{+}_{\alpha k\sigma}\, d_{i\sigma} \end{cases}$$

$\Rightarrow$ We are faced with the evaluation of four correlators

$$\langle [\hat{I}_L(t), \hat{I}_L(0)] \rangle_0 = \frac{e^2}{\hbar^2}\Big\{ \langle [\hat{L}^{+}(t), \hat{L}(0)] \rangle_0 + \langle [\hat{L}(t), \hat{L}^{+}(0)] \rangle_0$$

$$- \langle [\hat{L}(t), \hat{L}(0)] \rangle_0 - \langle [\hat{L}^{+}(t), \hat{L}^{+}(0)] \rangle_0 \Big\} \quad (4.72)$$

Because $\hat{L}$ contains two fermionic operators, each of the correlators contains expectation values of the form

$$\langle c_i^{p} d_j^{\bar{p}} c_k^{p'} d_e^{\bar{p}'} \rangle_0$$

with $p = \pm$, $\bar{p} = -p$

and $c^{+} = c^{+}$, $c^{-} = c$

For an interacting system, the evaluation of such correlator becomes quite intricate since Wick's theorem does not apply.

↳ it can be easier to evaluate $\langle \hat{I}_L(t) \rangle$ beyond linear response, directly (as seen next)

Things simplify in two special cases:

i) noninteracting systems ⇒ $\Gamma \gg E_c$

ii) interacting systems with proportional coupling $\Gamma_R = c\Gamma_L$

In the following we focus on these cases. For case i) one recovers the famous formula by Fisher and Lee (*)

$$\boxed{G = \frac{2e^2}{h} \int dE \, \mathrm{Tr}\left\{ \tfrac{1}{\hbar^2} \Gamma^L \tilde{G}^R \Gamma^R \tilde{G}^A \right\} \left(-\frac{\partial f}{\partial E} \right)} \qquad (4.73)$$

which expresses the conductance in terms of the retarded and advanced Green's functions $\tilde{G}^{R,A}$ of the central (noninteracting) system

Note: from the Landauer formula it follows also the relation to the S-matrix approach

$$\mathrm{Tr}\{t^\dagger t\} = \sum_n T_n(E) = \mathrm{Tr}\left\{ \tfrac{1}{\hbar^2} \Gamma^L \tilde{G}^R \Gamma^R \tilde{G}^A \right\}$$

(*) $[G(t)] = [\hbar^{-1}] = [E^{-1} t^{-1}]$, $[\tilde{G}(\omega)] = [E^{-1}]$

For case ii) one finds

$$\boxed{G = \frac{2e^2}{h} \int dE \left(-\frac{\partial f}{\partial E}\right) \mathrm{Tr}\left\{\frac{\Gamma^L(E)\,\Gamma^R(E)}{\Gamma^L(E)+\Gamma^R(E)}\, A(E)\right\}} \quad (4.74)$$

where $\boxed{A(E) = -2\,\mathrm{Im}\,\tilde{G}^R(E)}$ (4.75)

is the spectral function of the interacting central system

Note: If we want to go beyond linear response and at the same time be able to include electron-electron interactions, other methods must be used. These are:

i) The reduced density matrix approach (RDM)

ii) The non equilibrium Green's function method (NEGF)

iii) Path integral approaches (PI)

They all give formally exact expressions for the current. Depending on the physical problem, one can be more advantageous than another one.

Note: NEGF: Using the NEGF method, Meir and Wingreen [1] have shown that Eqs. (4.73) and Eqs. (4.74) are easily obtained from the more general current formulas:

i) noninteracting case ($I = I_L$)

$$\boxed{I = \frac{e}{h} \int dE \; \mathrm{Tr}\left\{\hbar^2 \Gamma^L \tilde{G}^R \Gamma^R \tilde{G}^A\right\}\left(f_L(E) - f_R(E)\right)} \qquad (4.73b)$$

where $\tilde{G}^R$, $\tilde{G}^A$ are now to be calculated at finite bias and

$$f_\alpha = \frac{1}{e^{\beta(E-\mu_\alpha)}+1}, \quad \mu_\alpha = \mu_0 + eV_\alpha, \quad V_L - V_R = V$$

ii) proportional coupling

$$\boxed{I = \frac{e}{h} \int dE \; \mathrm{Tr}\left\{\hbar \frac{\Gamma^L(E)\Gamma^R(E)}{\Gamma^L(E) + \Gamma^R(E)} A(E)\right\}\left(f_L(E) - f_R(E)\right)} \qquad (4.74b)$$

where $A(E)$ is to be calculated at finite bias

If i) or ii) do not apply, the current formulae become more complicated and involve explicit calculation of other Green's functions (lesser Green's function $\tilde{G}^<$) in the NEGF approach. According to ref. 1 one obtains the exact result

$$\boxed{I = \frac{ie}{h} \int dE \; \mathrm{Tr}\left\{\hbar \Gamma^L(E)\tilde{G}^<(E) + f_L(E)\hbar\Gamma^L(E)\left[\tilde{G}^R(E) - \tilde{G}^A(E)\right]\right\}} \qquad (4.75)$$

(1) Meir and Wingreen, PRL 68, 2512 (1992)

Note Despite exact, the evaluation of the current I requires to get

$\tilde{G}^<$, $\tilde{G}^{R,A}$. This becomes in practice untractable in

the presence of interactions (i.e. $E_c \gtrsim \Gamma$).

For that, one usually prefers to use the RDM or PJ

formalisms $\rightsquigarrow$ direct calculation of $I_L(t) = \mathrm{Tr}\{\hat{\rho}^{(t)}_{tot} \hat{I}_L\}$.

Before doing this, we analyze the conductance of

a single level QD for which i) holds if $U=0$ and ii)

can be applied as well.

This will enable us to introduce novel concepts

e.g. the self energy, and see how interactions

can affect a simple single-particle description.