Transport through quantum dot(s)

A project submitted to the Department of Physics Ramakrishna Mission Vivekanananda Educational and Research Institute, Belur Math in partial fulfilment of the requirements for the degree M.Sc in Physics

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Certificate

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Chapter 1

Keldysh Formalism

We start with a brief review of equilibrium quantum field theory before developing the non-equilibrium approach.

1.1 Second Quantisation formalism

Second quantisation is simply a different formulation of quantum mechanics which makes it easier to handle many body systems.

1.1.1 Identical Particles

Quantum Mechanics can be used to determine whether a group of particles are indistinguishable or not. Interchange of particles produces another solution for the Schrodinger equation. Quantum mechanically it is impossible to keep track of the wavefunctions because they may overlap, thus identical particles must always be considered as a group. An n-particle wavefunction of identical particles can by symmetric or anti-symmetric. Particles which have symmetric wavefunctions are called bosons and can be shown to have integral spin while those with anti-symmetric wavefunctions can be shown to have half-integral spins and are called fermions.

1.1.2 Number representation

Since, identical particles should be treated as a group, the actual particle state is does not matter rather the number of particles in a state does. So, we switch to the representation, where the number of particles in a particular state n_s gives the state, $|\{n_s\}\rangle$. We define annihilation and creation operators, $a^\dagger$ and a, operators which add

or remove particles from a particular state. We define the bosonic operators as:

$$a_i^\dagger \left|n_1, n_2, ..., n_i = n, ..., n_N\right\rangle = \sqrt{N+1)} \left|n_1, n_2, ..., n_i = n+1, ..., n_N\right\rangle$$
$$a \left|n_1, n_2, ..., n_i = n, ..., n_N\right\rangle = \sqrt{N} \left|n_1, n_2, ..., n_i = n-1, ..., n_N\right\rangle$$

These satisfy the relation $[a^\dagger, a]_- = 1$. Similarly, the fermionic operators would be defined as

$$a_i^\dagger \left|n_1, n_2, ..., n_i = 0, ..., n_N\right\rangle = \left|n_1, n_2, ..., n_i = 1, ..., n_N\right\rangle$$
$$a \left|n_1, n_2, ..., n_i = 1, ..., n_N\right\rangle = \left|n_1, n_2, ..., n_i = 0, ..., n_N\right\rangle$$

These satisfy the relation $[a^\dagger, a]_+ = 1$ and $a^2 = \left(a^\dagger\right)^2 = 0$, since removing or adding two operators to a fermionic state is not possible from the exclusion principle. We now look at a way to represent operators in this basis. For a one-body operator, in it's diagonal basis it has the form $\hat{O} = \Sigma_{i=0}^N \hat{o_i}$. Suppose we assume a one-body operator is diagonal in the $|\lambda\rangle$ basis. Then $\langle\lambda_1', ..., \lambda_N'|\hat{O}|\lambda_1, ..., \lambda_N\rangle = \left(\Sigma_{i=0}^N \hat{o_{\lambda_i}}\right) \langle\lambda_1', ..., \lambda_N'|\lambda_1, ..., \lambda_N\rangle = \langle\lambda_1', ..., \lambda_N'| \left(\Sigma_{\lambda=0}^\infty \hat{o_\lambda} n_\lambda\right) |\lambda_1, ..., \lambda_N\rangle$. The second quantised representation in the diagonal basis is thus $\hat{O} = \Sigma_{\lambda=0}^\infty \hat{o_\lambda} n_\lambda = \Sigma_{\lambda=0}^\infty \hat{o_\lambda} a_\lambda^\dagger a_\lambda$. In any arbitrary basis, we thus get the relation $\hat{O} = \Sigma_{\lambda\mu\nu} \langle\mu|\hat{O}|\nu\rangle \, a_\mu^\dagger a_\nu$. This is the second quantised representation for a one particle operator. Physically, this represents the situation that the operator takes a particle in state ν and scatters it to μ. Similarly, a two particle operator can be written as $\hat{O} = \Sigma_{\mu\mu'\nu\nu'} \langle\mu, \mu'|\hat{O}|\nu\nu'\rangle \, a_\mu^\dagger a_{\mu'}^\dagger a_\nu a_{\nu'}$

1.2 The interaction "picture"

Apart from the well known Schrodinger and Heisenberg representations, one can also work in the interaction representation where both the wavefunction and operators have time dependency but the time evolution of the wavefunction is only governed by the interacting part of the Hamiltonian (hence the name!).

$$\hat{O} = e^{iH_0 t} O e^{-iH_0 t} \qquad \text{(Interaction picture)}$$
$$\hat{\phi} = e^{iH_0 t} e^{-iHt} \phi$$

We denote the operator $e^{iH_0 t} e^{-iHt}$ by U and calculate it's time dependence:

$$\begin{aligned} \frac{\partial}{\partial t} U(t) &= i e^{iH_0 t} (H_0 - H) e^{-iHt} \\ &= i \hat{V}(t) U(t) \end{aligned} \tag{1.1}$$

We integrate both sides with respect to time

$$U(t) = 1 - i \int_0^t dt_1 \hat{V}(t_1) U(t_1) \tag{1.2}$$

Repeatedly iterating gives us:

$$\begin{aligned} U(t) &= \sum_{n=0}^{\infty}(-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 ..... \int_0^{t_{n-1}} dt_n \hat{V}(t_1)\hat{V}(t_2).....\hat{V}(t_n) \\ &= 1 + \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \int_0^t dt_2 ..... \int_0^t dt_n T\{\hat{V}(t_1)\hat{V}(t_2).....\hat{V}(t_n)\} \\ &= T\exp[-i\int_0^t dt_1 \hat{V}(t_1)] \end{aligned} \tag{1.3}$$

where T is the time ordering operator i.e. it sends operators with earlier time argument to the right.[1]For two operators, the operator is defined as $T\{\hat{V}(t_1)\hat{V}(t_2)\} = \Theta(t_1 - t_2)\hat{V}(t_1)\hat{V}(t_2) + \Theta(t_2 - t_1)\hat{V}(t_2)\hat{V}(t_1)$. Here Θ is the Heaviside step function[2]. We next define the S-matrix (Scattering matrix) by

$$\begin{aligned} \hat{\psi}(t) &= S(t,t')\psi(t') \\ &= S(t,t')U(t')\psi(0) \end{aligned}$$

Thus,

$$S(t,t') = U(t)U^{\dagger}(t') \tag{1.4}$$

1.3 Green's function at T = 0 K

Green's functions are required for dealing with systems where the Hamiltonian is not exactly solvable. We start with a Hamiltonian, $H = H_0 + V$ where H_0 can be solved exactly. The term V represents the remaining part of H and usually has small effects. Many-body problems usually proceed by starting with a system completely describable by H_0 and then introducing V and calculating it's effects. Analogous to classical physics they are named as such because they satisfy the wave equation with a Dirac delta in homogeneity. We define the Green's function as

$$G(r,t,r',t') = -i\left\langle\right| T\{\phi(t)\phi^{\dagger}(t')\} \left|\right\rangle \tag{1.5}$$

Here, T represents the time ordering operator and $|\rangle$ represents the normalised ground state of the system, an eigenstate of the full Hamiltonian H. However since the theory is based on knowing the ground state of the full Hamiltonian $|\rangle$ we have to rely on the Gell-Mann Low theorem which links the ground state of the full Hamiltonian to that of the unperturbed Hamiltonian by

$$|\rangle = S(0,-\infty)\,|\rangle_0 \tag{1.6}$$

[1]The necessity of the time ordering operator comes from the possible non-commutativity of the field operators at different times.We obviously want the earlier operator to act first.

[2]

The physical justification for the above is that we start with the unperturbed system as $t \to -\infty$ and adiabatically bring it $t = 0$ and switch on the interaction. Another commonly made assumption is that the final state at $t \to \infty$ is related to the ground state of the unperturbed Hamiltonian by only a phase factor.[3] This is not true for systems which are not in equilibrium. There we cannot assume the system comes from or goes to a state free of interactions. Thus we must look for another way of handling the asymptotic limit, which brings us to the next section.

1.4 Green's function at non-equilibrium

We can instead define the green's function on a contour C, which starts and ends at $t = t_0$ goes along the real axis and passes through t and t' only once. The contour ordered Green's function is defined as

$$G(r, t, r', t') = -i\langle T_c\{\phi(t)\phi^\dagger(t')\}\rangle \tag{1.7}$$

where T_c is the contour-ordering operator defined on the contour C. Since the times t and t' can lie on any of the two branches of the contour, equation (1.7) can be broken into four different green's functions. If we take the upper branch of the contour as C_1 and the lower as C_2 the definitions are:

- If t,$t' \in C_1$ then $G(t, t') = G_c(t, t') = -i\langle T\{\phi(t)\phi^\dagger(t')\}\rangle$
- If $t \in C_1$,$t' \in C_2$ then $G(t, t') = G^<(t, t') = -i\langle\phi(t)\phi^\dagger(t')\rangle$
- If $t \in C_2$,$t' \in C_1$ then $G(t, t') = G^>(t, t') = -i\langle\phi^\dagger(t')\phi(t)\rangle$
- If t,$t' \in C_2$ then $G(t, t') = G_{\tilde{c}}(t, t') = -i\langle\tilde{T}\{\phi(t)\phi^\dagger(t')\}\rangle$

$\tilde{T}$ represents the anti-time ordering operator. The four green's functions are linked by the relation $G_c + G_{\tilde{c}} = G^< + G^>$. For our convenience we further define the advanced and retarded green's functions:

- $G^r(t, t') = i\theta(t' - t)\langle\{\phi(t)\phi^\dagger(t')\}\rangle = \theta(t' - t)[G^<(t, t') - G^>(t, t')]$
- $G^a(t, t') = -i\theta(t - t')\langle\{\phi(t)\phi^\dagger(t')\}\rangle = \theta(t - t')[G^>(t, t') - G^<(t, t')]$

Thus the equilibrium and non-equilibrium theories are structurally equivalent and only differ in the replacement of real integrals by contour ones.

1.4.1 Analytic continuation

For computation purposes, we need to express the contour integral in terms of real integrals. We can do this using the simple rules given by Langreth in [4]. Suppose

[3] See Appendix A for rigorous arguments for the above

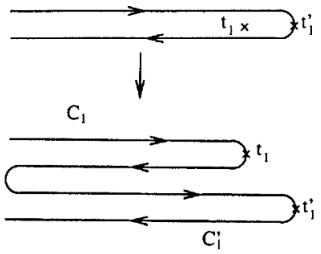


Figure 1.1: Deformation of the contour. Image from [14]

we have a term of the form $C(t',t) = \int_C d\tau A(t',\tau)B(\tau,t)$. Let t' be in the upper half of the contour and t_2 be in the lower half of the contour. We want expressions for the analytic continuations of $C(t',t)$, $C^<(t',t)$ and $C^>(t',t)$. To obtain the expressions we first deform the contours as shown in Figure 1.1. Now we split the integral into $C(t',t) = \int_{C_1} d\tau A(t',\tau)B(\tau,t) + \int_{C_2} d\tau A(t',\tau)B(\tau,t)$. We consider the first integral $\int_{C_1} d\tau A(t',\tau)B(\tau,t)$. The integration variable τ is always in the first contour thus, we can write $B(\tau,t)$ as $B^<(\tau,t)$. We split the integral into the two branches of C_1. (Note that we assume both contours C_1 and C_2 start and end at $t_0 \to \infty$.) This gives us $\int_{C_1} d\tau A(t',\tau)B^<(\tau,t) = \int_{-\infty}^{t'} d\tau A(t',\tau)B^<(\tau,t) + \int_{t'}^{-\infty} d\tau A(t',\tau)B^<(\tau,t)$. Using a similar logic as the previous one we can replace $A(t',\tau)$ with $A^>(t',\tau)$ and $A^<(t',\tau)$ in the two integrals respectively. This finally gives us $\int_{C_1} d\tau A(t',\tau)B(\tau,t) = \int_{\in fty}^{-\infty} d\tau A^r(t',\tau)B^<(\tau,t)$. Using a similar argument for the second term we obtain the relation $C^< = \int_{-\infty}^{\infty}[A^rB^< + A^<B^a]$. We can use analogous arguments for $C^>(t',t)$. Similarly, we can extend the argument easily to products of three terms and so on.

The results are summarised in table 1.1 as given in [14].

1.4.2 Fluctuation-Dissipation theorem

The spectral function defined as

$$A(k,\omega) = i[G^>(k,\omega) - G^<(k,\omega)] \tag{1.8}$$

is useful for computing the density of states

$$\rho(\omega) = \int \frac{d^3k}{(2\pi)^3} A(k,\omega) \tag{1.9}$$

and has the property

$$\int \frac{d\omega}{2\pi} A(k,\omega) = 1 \tag{1.10}$$

Contour	Real axis
$\mathrm{C} = \int_C AB$	$C^< = \int_t [A^r B^< + A^< B^a]$ $C^r = \int_t A^r B^r$
$\mathrm{D} = \int_C ABC$	$D^< = \int_t [A^r B^r C^< + A^r B^< C^a + A^< B^a C^a]$ $D^r = \int_t A^r B^r C^r$
$C(\tau, \tau') = A(\tau, \tau')B(\tau, \tau')$	$C^<(t,t') = A^<(t,t')B^<(t,t')$ $C^r(t,t') = A^<(t,t')B^r(t,t') + A^r(t,t')B^<(t,t') + A^r(t,t')B^r(t,t')$
$D(\tau, \tau') = A(\tau, \tau')B(\tau', \tau)$	$D^<(t,t') = A^<(t,t')B^>(t',t)$ $D^r(t,t') = A^<(t,t')B^a(t',t) + A^r(t,t')B^<(t',t)$

Table 1.1: Langreth rules

A very simple manipulation will allow us to write the Green's function in terms of the spectral function. We start with the definition of $G^<$ in Fourier basis.

$$G^<(\omega) = i \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \psi^\dagger(0)\psi(t) \rangle \tag{1.11}$$

We can insert a complete basis of states in between to get

$$\begin{aligned} G^<(\omega) &= i \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{n,m} \langle n|\rho\psi^\dagger(0)|m\rangle \langle m|e^{iHt}\psi(0)e^{-iHt}|n\rangle \\ &= \frac{i}{Z} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{n,m} e^{-\beta(E_n - \mu n_n)} e^{i(E_m - E_n)t} \langle n|\psi^\dagger(0)|m\rangle \langle m|\psi(0)|n\rangle \\ &= \frac{i}{Z} \sum_{n,m} 2\pi\delta(\omega + E_m - E_n) e^{-\beta(E_n - \mu n_n)} \langle n|\psi^\dagger(0)|m\rangle \langle m|\psi(0)|n\rangle \end{aligned} \tag{1.12}$$

Similarly we will get

$$G^>(\omega) = \frac{i}{Z} \sum_{n,m} 2\pi\delta(\omega + E_n - E_m) e^{-\beta(E_m - \mu n_m)} \langle n|\psi(0)|m\rangle \langle m|\psi^\dagger(0)|n\rangle \tag{1.13}$$

Combining the two we get

$$G^>(\omega) = -e^{\beta(\omega-\mu)} G^<(\omega) \tag{1.14}$$

We can now use the definition of the spectral function in equation 1.8 to get the relation

$$G^<(\omega) = \frac{iA(\omega)}{e^{\beta(\omega-\mu)} + 1} \tag{1.15}$$

This is known as the fluctuation-dissipation theorem because it links the part which describes the fluctuation of the system ($G^<$) to the dissipative part A. The proportionality factor in (1.15) is simply the Fermi function.

Chapter 2

Mesoscopic Transport

A transport problem concerns the flow of current through a particular substance. Work on electron transport in mesoscopic systems only began in the 1980's. There are many important length scales at play in mesoscopic systems and at low temperatures ($50\text{mk} - 4\text{K}$), the mesoscopic regime is usually characterised by the following relation between length scales [2]

$$a_0 \ll \lambda_F \lesssim l_0 < \mathcal{L} < l_\phi \lesssim l_{in} \tag{2.1}$$

where

- a_0 is the Bohr radius
- λ_F is the Fermi wavelength
- l_0 is the elastic mean free path
- $\mathcal{L}$ is the sample size
- l_ϕ is the coherence length
- l_{in} is the energy relaxation length

There are two main viewpoints to the transport problem [7].

1. The current is a response to an externally applied electrical field
2. Carrier flow causes a buildup on the boundaries which generates an inhomogenous electric field across the sample. The field is a consequence of the current flow.

The first viewpoint leads to the familiar transport theories of Drude or Boltzmann to be found in any textbook of solid state physics. [8] [9]. The second viewpoint is known as the Landauer approach and is the focus of this chapter.

2.1 Landauer Formula

Lanaduer in [6] formulated an expression for the current through a disordered region of non-interacting electrons. He based this on the approach he pioneered in [5], that scatterers could induce local fields which act on the current carriers. His approach consisted of the following approximations which we present here:

Approximation 1 We consider the battery to simply act as a reservoir of electrons. The energy required to extract an electron from the reservoir and bring it into the system is measured by the electrochemical potential of the reservoir. The potential bias across the system is thus the difference in electrochemical potentials per unit charge.

$$V = \frac{\mu_L - \mu_R}{e}$$

Our problem is reduced to the sample sandwiched between large materials connected to an open reservoir.

Approximation 2: We next assume that the system has a steady-state solution and we wait long enough to perform our calculation at the steady state. The steady state condition for the current holds at all instants of time

$$\langle \hat{I} \rangle_t = \langle \hat{I} \rangle = \text{constant}$$

Approximation 3: Our second approximation of steady state simply relegates the role of the reservoirs to that of preparing and sending wave-packets without changing the current in time. We can now replace our first approximation with that of a closed system having scattering boundary conditions at infinity.

Approximation 4: We consider a mean field approximation for the whole Hamiltonian.

$$\hat{H} = \hat{H}^{mf} + \hat{V} \tag{2.2}$$

where $\hat{H}^{mf}$ is the part of the Hamiltonian experiencing the mean field of other electrons and $\hat{V}$ is the interaction beyond the electrons. Thus, we are now left with a one-particle problem.

Approximation 5 We assume that the channels through which the scattering occurs are independent, that is the off-diagonal elements of the density matrix are zero. This assumes that the system interacts with the environments quickly enough to dissipate all correlations. Finally, we neglect all possible differences between electrons injected into the system from the terminal. We assume, that the electrons injected from the left (right) reservoir come from a local equilibrium distribution

$$f_{L(R)} = \frac{1}{e^{\frac{E-\mu_{L(R)}}{k_B T}} + 1} \tag{2.3}$$

We will now derive expressions for the total current through the system and it's conductance. Firstly, we consider the general case of when the right and left leads are differently populated. Following approximation 5, the density matrix of the system can be written as an incoherent sum of left and right moving electrons.

$$\rho = \sum_L |\psi_L\rangle \, f_L \, \langle\psi_R| + \sum_R |\psi_R\rangle \, f_R \, \langle\psi_R| \tag{2.4}$$

The current is then calculated as

$$\begin{aligned} I = tr(\rho\hat{I}) &= tr((\sum_L |\psi_L\rangle \, f_L \, \langle\psi_L| + \sum_R |\psi_R\rangle \, f_R \, \langle\psi_R|)\hat{I}) \\ &= tr(\rho\hat{I}) = tr((\sum_L |\psi_L\rangle \, f_L \, \langle\psi_L| + \sum_R |\psi_R\rangle \, f_R \, \langle\psi_R|)\hat{I}) \end{aligned}$$

Now we evaluate the expression

$$\begin{aligned} &= \sum_i \{\sum_L \langle\Psi_{ik_i}|\psi_L\rangle \, f_L \, \langle\psi_L|\hat{I}|\Psi_{ik_i}\rangle + \sum_R \langle\Psi_{ik_i}|\psi_R\rangle \, f_R \, \langle\psi_R|\hat{I}|\Psi_{ik_i}\rangle\} \\ &= \sum_L \langle\psi_L|\hat{I}|\psi_L\rangle \, f_L + \sum_R \langle\psi_R|\hat{I}|\psi_R\rangle \, f_R \\ &= I_L f_L + I_R f_R \end{aligned}$$

Deep into the left lead, the wavefunction is the original left moving wavepacket plus a linear combination of all reflected wavepackets.

$$\Psi_{ik_i} = \psi_{ik_i} + \sum_{f=1}^{N_L^C} \mathcal{R}_{if}\psi_{fk_f} \tag{2.5}$$

Deep into the right lead, the wavefunction is simply the sum of all transmitted wavepackets

$$\Psi_{ik_i} = \sum_{f=1}^{N_R^C} \mathcal{T}_{if}\psi_{fk_f} \tag{2.6}$$

Evaluating the current deep in the leads we get

$$I_L(E_i) = I_i(E_i)\left(1 - \sum_{f=1}^{N_L^C} R_{if}\right) \tag{2.7}$$

$$I_R(E_i) = I_i(E_i)\sum_{f=1}^{N_R^C} T_{if} \tag{2.8}$$

where $I_i(E_i) = \frac{v_i}{L_x}$ and $\sum_{f=1}^{N_L^C} R_{if} + \sum_{f=1}^{N_R^C} T_{if} = 1$ Now to get the total current we need to integrate over all energy using the density of states.

$$I_L = 2e \int dE \sum_{f=1}^{N_L^C} \sum_{f=1}^{N_R^C} D_i(E_i) I_i(E_i) T_{if} = \frac{e}{\pi\hbar} \int dE \mathcal{T}_{LR}(E) \tag{2.9}$$

$$I_R = -2e \int dE \sum_{f=1}^{N_L^C} \sum_{f=1}^{N_R^C} D_i(E_i) I_i(E_i) T_{if} = -\frac{e}{\pi\hbar} \int dE \mathcal{T}_{RL}(E) \tag{2.10}$$

Thus, the current is

$$I = \frac{e}{\pi\hbar} \int_{-\infty}^{\infty} dE [f_L(E) - f_R(E)] \mathcal{T}(E) \tag{2.11}$$

where $\mathcal{T}(E) = \mathcal{T}_{RL}(E) = \mathcal{T}_{LR}(E)$ due to steady state. To calculate the conductance between two probes, we take the zero bias limit of (2.11). When $\mu_L - \mu_R \to 0$ we have $f_L = f_R + \frac{df_R}{dE}(\mu_L - \mu_R) + ...$ At zero temperature, the derivative of the Fermi function is a Dirac delta. Thus, we have

$$\begin{aligned} I &= \frac{2e}{\hbar} \int_{-\infty}^{\infty} dE \delta(E - \mu_R)(\mu_L - \mu_R) \mathcal{T}(E) \\ &= \frac{2e^2}{\hbar} V \mathcal{T}(\mu_R) \end{aligned}$$

Finally using $G = \frac{I}{V}$, we get:

$$G_{\text{2-probe}} = \frac{2e^2}{h} \sum_{i=1}^{N_c^R} \sum_{i=1}^{N_c^L} \mathcal{T}_{if} \tag{2.12}$$

Thus the conductance can be simply written in terms of the transmission of non-interacting electrons. The observation of the quantised conductance in electron gas in 1988 [3] brought the largely ignored Landauer formula into prominence and it was generalised by the work of Meir and Wingreen. We can now use some results from single particle scattering theory[7][11] to recast (2.11) into a form which will help us compare our results with the Meir-Wingreen formula. The transmission coefficients can be linked to S-matrix elements using the T-matrix.[7][10][11]

$$\mathcal{T}_{LR}(E) = \sum_{i=1}^{N_C^L} \sum_{f=1}^{N_C^R} T_{if} = Tr(\tau^\dagger \tau) \tag{2.13}$$

The S-matrix elements are linked to the Green's function giving us the relations

$$\mathcal{T}_{LR} = Tr\{\hat{\Gamma}_R \hat{G}^a \hat{\Gamma}_L \hat{G}^r\} \tag{2.14}$$

$$\mathcal{T}_{RL} = Tr\{\hat{\Gamma}_L \hat{G}^a \hat{\Gamma}_R \hat{G}^r\} \tag{2.15}$$

The Gamma operators are related to the self-energy

$$\hat{\Gamma}_R = -2Im\{\Sigma_R^+(z)\} = -2Im\{V^*G(z)V\} \tag{2.16}$$
$$\hat{\Gamma}_L = -2Im\{\Sigma_L^+(z)\} = -2Im\{V^*G(z)V\} \tag{2.17}$$

The final result is

$$I = \frac{e}{\pi\hbar}\int_{\infty}^{\infty} dE[f_L(E) - f_R(E)]\mathrm{Tr}\{\hat{\Gamma}_R\hat{G}^a\hat{\Gamma}_L\hat{G}^r\} \tag{2.18}$$

2.2 Meir-Wingreen formula

A similar result for interacting electrons was developed by Meir and Wingreen in [12] by using the same assumptions but instead restricting the mean field assumptions upto the lead only. The description of the resulting non-equilibrium situation inside the conductor requires the use of the Keldysh formalism described in Chapter 1.

Approximation We take the 'partition approach' that is we assume that at $t \to -\infty$ the leads and the central region are separated and they are at thermal equilibrium respectively.

The Hamiltonian can be written down as the sum of three terms: the non-interacting region of the leads($H_{\text{leads}} = \sum_{k;\alpha\in L,R}\epsilon_{k\alpha}c_{k\alpha}^\dagger c_{k\alpha}$), the coupling between the central region ($H_{\text{con}} = \sum_{n,k;b\in L,R}V_{n,kb}c_{kb}^\dagger d_n$) and the electrodes and the interacting central region, $H_{\text{cent}} = \sum_n\left(\{d_n^\dagger\}\{d_n\}\right)$. The full Hamiltonian is thus

$$\hat{H} = \sum_{k;\alpha\in L,R}\epsilon_{k\alpha}c_{k\alpha}^\dagger c_{k\alpha} + \sum_{n,k;b\in L,R}V_{n,kb}c_{kb}^\dagger d_n + V_{n,kb}^* d_n^\dagger c_{kb} + \sum_n\left(\{d_n^\dagger\}\{d_n\}\right) \tag{2.19}$$

The current that flows from the left electrode can be defined by the expectation value of the rate of change of the number of electrons that flows into the central region, given by the number operator ($N_L = \sum_{k;\alpha\in L}c_{k\alpha}^\dagger c_{k\alpha}$).

$$\begin{aligned}
I_L &= -e\left\langle\frac{dN_L}{dt}\right\rangle \\
&= -ie\left\langle[\hat{H}, N_L]\right\rangle && \text{From the Heisenberg equation,} \\
&= -ie\left\langle[\hat{V}_{LC} + \hat{V}_{LC}^\dagger, N_L]\right\rangle && \text{Since the other terms commute,} \\
&= -ie\left\langle[\hat{V}_{LC}, N_L]\right\rangle + \left\langle[\hat{V}_{LC}^\dagger, N_L]\right\rangle \\
&= -ie\left\langle\sum_{n,k;\alpha\in L}\sum_{j;\beta\in L}V_{n,k\alpha}[c_{k\alpha}^\dagger d_n, c_{j\beta}^\dagger c_{j\beta}]\right\rangle + \left\langle\sum_{n,k;\alpha\in L}\sum_{j;\beta\in L}V_{n,k\alpha}^*[d_n^\dagger c_{k\alpha}, c_{j\beta}^\dagger c_{j\beta}]\right\rangle
\end{aligned}$$

$$
\begin{aligned}
&= -ie\left\langle \sum_{n,k;\alpha\in L}\sum_{j;\beta\in L} V_{n,k\alpha}[c^\dagger_{k\alpha}, c^\dagger_{j\beta}c_{j\beta}]d_n \right\rangle + \left\langle \sum_{n,k;\alpha\in L}\sum_{j;\beta\in L} V^*_{n,k\alpha} d^\dagger_n [c_{k\alpha}, c^\dagger_{j\beta}c_{j\beta}] \right\rangle \\
&= -ie\left\langle \sum_{n,k;\alpha\in L}\sum_{j;\beta\in L} -V_{n,k\alpha}c^\dagger_{j\beta}\{c^\dagger_{k\alpha}, c_{j\beta}\}d_n \right\rangle + \left\langle \sum_{n,k;\alpha\in L}\sum_{j;\beta\in L} V^*_{n,k\alpha} d^\dagger_n \{c_{k\alpha}, c^\dagger_{j\beta}\}c_{j\beta} \right\rangle \\
&= ie\left\langle \sum_{n,j;\beta\in L} V_{n,j\beta}c^\dagger_{j\beta}d_n - V^*_{n,j\beta}d^\dagger_n c_{j\beta} \right\rangle \qquad \text{using the anti commutation relations,} \\
&= ie\sum_{n,j;\beta\in L} V_{n,j\beta}\left\langle c^\dagger_{j\beta}d_n \right\rangle - V^*_{n,j\beta}\left\langle d^\dagger_n c_{j\beta}\right\rangle \qquad (2.20)
\end{aligned}
$$

The operator terms in the above expression look like the lesser Green's functions defined in . We thus define them as such

$$G^<_{n,k\alpha}(t-t') = i\left\langle c^\dagger_{k\alpha}(t')d_n(t)\right\rangle \qquad (2.21)$$

$$G^<_{k\alpha,n}(t-t') = i\left\langle d^\dagger_n(t')c_{k\alpha}(t)\right\rangle \qquad (2.22)$$

The current is thus defined in terms of the lesser Green's function.

$$I = e\sum_{n,k;\alpha\in L} V_{n,k\alpha}G^<_{n,k\alpha}(t-t') - V^*_{n,k\alpha}G^<_{k\alpha,n}(t-t') \qquad (2.23)$$

To calculate the lesser Green's function, we use the equation of motion of full's green's function defined in . We thus get,

$$i\frac{dG_{n,k\alpha}}{dt} = \left\langle T\left\{\frac{dc^\dagger_{k\alpha}}{dt}d_n\right\}\right\rangle \qquad (2.24)$$

Using the Heisenberg Equations of motion, we obtain,

$$
\begin{aligned}
i\frac{dG_{n,k\alpha}}{dt} &= \left\langle T\left\{-i[c^\dagger_{k\alpha}, \hat{H}]d_n\right\}\right\rangle \\
&= -i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{leads}]d_n\right\}\right\rangle - i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{con}]d_n\right\}\right\rangle - i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{cen}]d_n\right\}\right\rangle \\
&= -i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{leads}]d_n\right\}\right\rangle - i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{con}]d_n\right\}\right\rangle
\end{aligned}
$$

We replace and simplify the first term

$$
\begin{aligned}
i\frac{dG_{n,k\alpha}}{dt} &= -i\left\langle T\left\{\sum_{j;\beta\in L}\epsilon_{j\beta}[c^\dagger_{k\alpha}, c^\dagger_{j\beta}c_{j\beta}]d_n\right\}\right\rangle - i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{con}]d_n\right\}\right\rangle \\
&= -i\left\langle T\left\{\epsilon_{k\alpha}c^\dagger_{k\alpha}d_n\right\}\right\rangle - i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{con}]d_n\right\}\right\rangle \\
&= -\epsilon_{k\alpha}G_{n,k\alpha} - i\left\langle T\left\{[c^\dagger_{k\alpha}, \hat{H}_{con}]d_n\right\}\right\rangle
\end{aligned}
$$

We can similarly simplify the last term and by defining one final Green's function

$$G_{n,m}(t-t') = i\left\langle T\left\{d_m^\dagger d_n\right\}\right\rangle \tag{2.25}$$

we obtain

$$\left(-\epsilon_{k\alpha} - i\frac{d}{dt}\right) G_{n,k\alpha} = \sum_m G_{n,m}(t-t')V^*_{m,k\alpha} \tag{2.26}$$

The coefficient of $G_{n,k\alpha}$ is simply the inverse of the green's function associated with the lead $g_{k\alpha}$. Thus we get the equation:

$$G_{n,k\alpha}g^{-1}_{k\alpha} = \sum_m G_{n,m}(t-t')V^*_{m,k\alpha}$$

which simplifies to,

$$G_{n,k\alpha} = \sum_m \int dt_1 G_{n,m}(t-t_1)V^*_{m,k\alpha}g_{k\alpha}(t_1-t')$$

Applying the Langreth rules of section 1.4, we get,

$$G_{n,k\alpha} = \sum_m \int dt_1 V^*_{m,k\alpha}[G^r_{n,m}(t-t_1)g^<_{k\alpha}(t_1-t') + G^<_{n,m}(t-t_1)g^a_{k\alpha}(t_1-t')]$$

Taking the Fourier transform, we thus finally obtain the lesser green's function

$$G^<_{n,k\alpha}(\omega) = \sum_m V^*_{m,k\alpha}[G^r_{nm}(\omega)g^<_{k\alpha} + G^<_{nm}(\omega)g^a_{k\alpha}] \tag{2.27}$$

The fluctuation-dissipation theorem gives us an expression for $g^<_{k\alpha}$ as

$$g^<_{k\alpha}(\omega) = 2\pi i f_L(\omega)\delta(\omega-\epsilon_{k\alpha}) \tag{2.28}$$
$$g^>_{k\alpha}(\omega) = -2\pi i[1-f_L(\omega)]\delta(\omega-\epsilon_{k\alpha}) \tag{2.29}$$

We first take the Fourier transform of (2.23) to get

$$I = e\sum_{n,k;\alpha\in L}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}V_{n,k\alpha}G^<_{n,k\alpha}(\omega) - V^*_{n,k\alpha}G^<_{k\alpha,n}(\omega) \tag{2.30}$$

We now plug in (2.27) and simplify using (2.28) to get

$$\begin{aligned} I &= e\sum_{n.k;\alpha\in L}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}V_{n,k\alpha}G^<_{n,k\alpha}(\omega) + V^*_{n,k\alpha}(G^<_{n,k\alpha}(\omega))^* \\ &= 2e\sum_{n,k;\alpha\in L}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}Re\{V_{n,k\alpha}G^<_{n,k\alpha}(\omega)\} \\ &= 2e\sum_{m,n,k;\alpha\in L}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}Re\{V_{n,k\alpha}V^*_{m,k\alpha}[G^r_{nm}(\omega)g^<_{k\alpha} + G^<_{nm}(\omega)g^a_{k\alpha}]\} \end{aligned} \tag{2.31}$$

We define a level-width function by:

$$\Gamma_L(\epsilon)_{mn} = 2\pi \sum_\alpha \rho_\alpha(\epsilon) V_{n,k\alpha} V^*_{m,k\alpha} \tag{2.32}$$

We transform the momentum summation in (2.31) into an energy integration with the density of states a $\rho_\alpha(\epsilon)$ and use (2.32) and (2.28) to get:

$$\begin{aligned}
I_L &= 2e \sum_{m,n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} d\epsilon \rho_\alpha(\epsilon) Re\{V_{n,\alpha}(\epsilon) V^*_{m,\alpha}(\epsilon)[G^r_{nm}(\omega)) g^<(\omega) + G^<_{nm}(\omega) g^a(\omega)]\} \\
&= 2e \sum_{m,n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} d\epsilon Re\{\Gamma_L(\epsilon)_{mn}[G^r_{nm}(\omega)) g^<(\omega) + G^<_{nm}(\omega) g^a(\omega)]\} \\
&= 2e \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} d\epsilon Re\{Tr\left(\frac{\Gamma_L(\epsilon)}{2\pi}[G^r(\omega)) g^<(\omega) + G^<(\omega) g^a(\omega)]\right)\} \\
&= e \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} d\epsilon Tr\left(\frac{\Gamma_L(\epsilon)}{2\pi}[G^r(\omega) g^<(\omega) + G^<(\omega) g^a(\omega) - G^<(\omega)) g^r(\omega) - G^a(\omega) g^<(\omega)]\right) \\
&= ie \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} Tr\left(\Gamma_L(\epsilon)[f_L(\epsilon)(G^r(\epsilon) - G^a(\epsilon)) + G^<(\epsilon)]\right)
\end{aligned} \tag{2.33}$$

A similar expression can be found for I_R and using $I = \frac{1}{2}(I_L - I_R)$ we get

$$\begin{aligned}
I &= \frac{ie}{2} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} Tr\left(\Gamma_L(\epsilon)[f_L(\epsilon)(G^r(\epsilon) - G^a(\epsilon)) + G^<(\epsilon)] - \Gamma_R(\epsilon)[f_R(\epsilon)(G^r(\epsilon) - G^a(\epsilon)) + G^<(\epsilon)]\right) \\
&= \frac{ie}{2} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} Tr\left((\Gamma_L(\epsilon) f_L(\epsilon) - \Gamma_R(\epsilon) f_R(\epsilon))(G^r(\epsilon) - G^a(\epsilon)) + (\Gamma_L(\epsilon) - \Gamma_R(\epsilon)) G^<(\epsilon)\right)
\end{aligned} \tag{2.34}$$

(2.34) is the Meir-Wingreen formula. Further simplification can be achieved if we take $\Gamma_L = \lambda \Gamma_R$. Since, $I_L = -I_R$, we can write $I = \frac{I_L}{1+\lambda} - \frac{\lambda I_R}{1+\lambda}$. Thus, we get:

$$\begin{aligned}
I &= ie \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} Tr\left(\frac{\lambda\Gamma_R(\epsilon)[f_L(\epsilon)(G^r(\epsilon) - G^a(\epsilon)) + G^<(\epsilon)]}{1+\lambda} - \frac{\lambda\Gamma_R(\epsilon)[f_R(\epsilon)(G^r(\epsilon) - G^a(\epsilon)) + G^<(\epsilon)]}{1+\lambda}\right) \\
&= ie \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} Tr\left(\frac{\lambda\Gamma_R(\epsilon)(f_L(\epsilon) - f_R(\epsilon))(G^r(\epsilon) - G^a(\epsilon))}{1+\lambda}\right) \\
&= ie \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} (f_L(\epsilon) - f_R(\epsilon)) Tr\left(\frac{\lambda\Gamma_R(\epsilon)}{1+\lambda}(G^r(\epsilon) - G^a(\epsilon))\right) \\
&= ie \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} (f_L(\epsilon) - f_R(\epsilon)) Tr\left(\frac{\Gamma_L(\epsilon)\Gamma_R(\epsilon)}{\Gamma_L(\epsilon) + \Gamma_R(\epsilon)}(G^r(\epsilon) - G^a(\epsilon))\right)
\end{aligned} \tag{2.35}$$

Non-interacting central region

To check our formula, we consider a non-interacting central region. If it is correct, we should get back the original Landauer formula. The Hamiltonian then takes the form:

$$\hat{H} = \sum_{k;\alpha\in L,R} \epsilon_{k\alpha} c^\dagger_{k\alpha} c_{k\alpha} + \sum_{n,k;b\in L,R} V_{n,kb} c^\dagger_{kb} d_n + V^*_{n,kb} d^\dagger_n c_{kb} + \sum_n \epsilon_n d^\dagger_n d_n \tag{2.36}$$

The Dyson and Keldysh equations thus give us:

$$G^< = G^a(E)\Sigma^<(E)G^r(E) \tag{2.37}$$

Using the lesser self energy equation we get

$$\Sigma^<(E) = i[f_l(E)\Gamma_L(E) + f_R(E)\Gamma_R(E)] \tag{2.38}$$

Substituting these into (2.34) gives us the result of (2.18).

$$I = \frac{e}{\pi\hbar}\int_\infty^\infty dE[f_L(E) - f_R(E)]\mathrm{Tr}\{\hat{\Gamma}_R\hat{G}^a\hat{\Gamma}_L\hat{G}^r\}$$

2.3 The rate equation

(2.34) is an exact solution for the system but it is still a nontrivial matter to use it practically. This, is because we still need to calculate the Green's function for the full interacting Hamiltonian. Some properties of a given system may however still be studied by using approximate results. We look at one such approximation derived using the master equation approach.

We consider a Hamiltonian, $H = H_{sys} + H_{res} + H_{Int}$ where the terms in order are the Hamiltonian for a system, for a reservoir and for the coupling between them. The total density matrix thus follows the von-Neumann equation $\frac{d\rho_{tot}}{dt} = -i[H, \rho_{tot}]$. Our goal is to find the master equation for the density matrix of the subsystem by tracing out the degrees of freedom of the reservoir $\rho_S(t) = tr_{res}(\rho_{tot})$. If we now switch to the interaction picture, we get the following equation of motion

$$\frac{d\rho_I}{dt} = -i[H_{int}, \rho_I] \tag{2.39}$$

We can integrate it to get

$$\rho_I(t) = \rho_I(0) - i\int_0^t dt'[H_{int}, \rho_I] \tag{2.40}$$

Henceforth, we'll drop the label I and assume that all operators are in the interaction picture unless specified. For our initial condition, we assume that the interaction has

been turned on at $t = 0$ thus at $t = 0$, $\rho(0) = \rho_{sys}(0) \otimes \rho^0_{res}$. Here, ρ^0_{res} represents the density matrix of the reservoir at equilibrium. If we now substitute (2.40) into (2.39) and take the trace over the leads on both sides we get:

$$\frac{d\rho_{sys}}{dt} = -\int_0^t dt' tr_{res}[H_{int}(t), [H_{int}(t'), \rho(t')]] \tag{2.41}$$

We take that the initial condition implies that the term, $tr_{res}[H_{int}, \rho] = 0$. [1] We can continue the process to get an expansion in higher order terms of ρ, but we'll stop at the second order and make a critical assumption. We assume that the reservoir has many more degrees of freedom than the system and the effect of any interaction by the system on the reservoir dissipates quickly and does not react back on the system i.e. R remains in thermal equilibrium.[16] This permits us to write the terms in (2.41) as $tr_{res}[H_{int}(t), [H_{int}(t'), \rho(t')] = \rho_{sys}(t') \otimes tr_{res}[H_{int}(t), [H_{int}(t'), \rho_{res}(t')]$. A much stronger form of the above assumption is often taken in the literature, $\rho(t) = \rho_{sys}(t) \otimes \rho^0_{res}$.But this is not necessary and may also be superfluous.[17][18] This is known as the weak-interaction approximation or Born approximation, in line with it's use in scattering theory. We get:

$$\frac{d\rho_{sys}}{dt} = -\int_0^t dt' tr_{res}[H_{int}(t), [H_{int}(t'), \rho_{sys}(t') \otimes \rho^0_{res}]] \tag{2.42}$$

The second critical assumption we make is known as the Markov assumption following it's use in probability theory. Analogously thus we posit that the behaviour of the system depends only on it's state at the present time and not on it's history of evolution. This is equivalent to replacing $\rho_{sys}(t') = \rho_{sys}(t)$ in (2.42). The physical basis of this assumption is that the thermal time scale is much smaller than the time scale of the system dynamics.[2]This allows to replace the lower limit of the integrand to $-\infty$ to get the final equation:

$$\frac{d\rho_{sys}}{dt} = -\int_0^\infty dt' tr_{res}[H_{int}(t), [H_{int}(t - t'), \rho_{sys}(t) \otimes \rho^0_{res}]] \tag{2.43}$$

This is the Wagness-Bloch-Redfield master equation.

[1] This is true for the system we will consider, since the interaction Hamiltonian will contain only a single reservoir electron operator, each term will cause a change in the electron number of the state and the resulting trace will be zero.

[2] See [16] and [17] for an in-depth discussion of the Markov approximation.

Chapter 3

Applications

3.1 Single quantum dot

Having gone through two equivalent ways of looking at our electrode-nanonjunction-electrode we will now try to apply our results in to a concrete system: a single quantum dot coupled to leads with different chemical potentials and temperatures. The Hamiltonian of the system $H = H_{lead} + H_{dot(s)} + H_{int}$. We will model the single quantum dot system using an Anderson-type model

$$H_{\text{int}} = \sum_{\sigma} \epsilon_0 d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow \tag{3.1}$$

This was done using the Meir-Wingreen formula in [12] and [13] [1]. Here we will look at the results using the rate equation method.

3.1.1 Rate equation formalism

We will now simplify the (2.43) to a simpler form by assuming a the above Hamiltonian. Next,we use the relations $\rho_{dot,I}(t) = e^{(iH_{dot}t)}\rho(t)e^{(-iH_{dot}t)}$ and $H_{hyb,I} = e^{-i(H_{leads}+H_{dot})t}H_{hyb}e^{i(H_{leads}+H_{dot})t}$ and replace them in (2.43) to get

$$\dot{\rho}(t) = -i[H_{dot}, \rho_{dot}(t)] - \int_0^\infty dt' tr_{leads}([H_{hyb}, [e^{i(H_{leads}+H_{dot})t'}H_{hyb}e^{-i(H_{leads}+H_{dot})t'}, \rho_{dot}\otimes\rho^0_{leads}]]) \tag{3.2}$$

By introducing dot states $|n\rangle$ and lead states $||i\rangle\rangle$ we can bring the equation to a form which resembles the rate equation.

We now assume the density matrix is diagonal in the dot state basis. This is possible because the off-diagonal elements of the density matrix represent the coherence between different sub-states of the system. In general, if two states are related by an observable

[1] Relevant derivations are also worked out in [7] and [14]

which strongly couples with the environment (such as charge) then the off-diagonal elements rapidly decay.[2]. Taking the diagonal matrix element of the equation, we get

$$\dot{\rho}^{dot}_{mm} = \sum_i \int_0^\infty dt' \, \langle\langle i| | \langle m| \left[H_{hyb}, [e^{i(H_{leads}+H_{dot})t'} H_{hyb} e^{-i(H_{leads}+H_{dot})t'}, \rho_{dot} \otimes \rho^0_{leads}]\right] |m\rangle \, ||i\rangle\rangle \tag{3.3}$$

In the second term after opening the commutator bracket, we can simply term by term. We show here the first term

$$\begin{aligned}
&= \sum_i \int_0^\infty dt' \, \langle\langle i| | \langle m| H_{hyb} e^{i(H_{leads}+H_{dot})t'} H_{hyb} e^{-i(H_{leads}+H_{dot})t'} \rho_{dot} \otimes \rho^0_{leads} |m\rangle \, ||i\rangle\rangle \\
&= \sum_p \sum_{ij} \int_0^\infty dt' \, \langle\langle i| | \langle m| H_{hyb} e^{i(H_{leads}+H_{dot})t'} |p\rangle \, ||j\rangle\rangle \, \langle\langle j| | \langle p| H_{hyb} e^{-i(H_{leads}+H_{dot})t'} \rho_{dot} \otimes \rho^0_{leads} |m\rangle \, ||i\rangle\rangle \\
&= \sum_{pq} \sum_{ij} \int_0^\infty dt' e^{i(E_p+\epsilon_j)t'} \, \langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, \langle\langle j| | \langle p| H_{hyb} e^{-i(H_{leads}+H_{dot})t'} |q\rangle \, \langle q| \rho_{dot} \otimes \rho^0_{leads} |m\rangle \, ||i\rangle\rangle \\
&= \sum_{pq} \sum_{ij} \int_0^\infty dt' e^{i(E_p+\epsilon_j-E_q-\epsilon_m)t'} \, \langle\langle i| | \rho^0_{leads} \, ||i\rangle\rangle \, \langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, \langle q| \rho_{dot} |m\rangle \, \langle\langle j| | \langle p| H_{hyb} |q\rangle \, ||i\rangle\rangle \\
&= \pi \sum_{pq} \sum_{ij} \langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, \langle q| \rho_{dot} |m\rangle \, \langle\langle i| | \rho^0_{leads} \, ||i\rangle\rangle \, \langle\langle j| | \langle p| H_{hyb} |q\rangle \, ||i\rangle\rangle \, \delta(E_p + \epsilon_j - E_q - \epsilon_m)
\end{aligned}$$

Simplifying each of the four terms one by one gives us

$$\begin{aligned}
\dot{\rho}^{dot}_{mm} = -\pi \sum_{pq} \sum_{ij} \{ &\langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, \langle q| \rho_{dot} |m\rangle \, W_i \, \langle\langle j| | \langle p| H_{hyb} |q\rangle \, ||i\rangle\rangle \, \delta(E_p+\epsilon_j-E_q-\epsilon_i) \\
&- \langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, \langle p| \rho_{dot} |q\rangle \, W_j \, \langle\langle j| | \langle q| H_{hyb} |m\rangle \, ||i\rangle\rangle \, \delta(E_q + \epsilon_j - E_m - \epsilon_i) \\
&- \langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, \langle p| \rho_{dot} |q\rangle \, W_j \, \langle\langle j| | \langle q| H_{hyb} |m\rangle \, ||i\rangle\rangle \, \delta(E_m + \epsilon_i - E_p - \epsilon_j) \\
&+ \langle\langle i| | \langle p| H_{hyb} |q\rangle \, ||j\rangle\rangle \, \langle m| \rho_{dot} |p\rangle \, W_i \, \langle\langle j| | \langle q| H_{hyb} |m\rangle \, ||i\rangle\rangle \, \delta(E_m + \epsilon_i - E_q - \epsilon_j) \}
\end{aligned} \tag{3.4}$$

Since the off-diagonal elements of the density matrix are 0, the only terms that remain in the sum are for $q = m$ or $p = m$. So the 2nd and 3rd terms cancel out leaving us with

$$\dot{P}_m = -\pi \sum_{ij} \sum_p |\{\langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle|^2 (W_i P_m - W_j P_p) \delta(E_p + \epsilon_j - E_m - \epsilon_i) \tag{3.5}$$

Defining the transition rate as $R_{n\to m} \equiv \pi \sum_{ij} W_j |\{\langle\langle i| | \langle m| H_{hyb} |p\rangle \, ||j\rangle\rangle \, |\delta(E_p + \epsilon_j - E_m - \epsilon_i)$ gives us

$$\dot{p}_m = \sum_n R_{n\to m} P_n - \sum_n R_{m\to n} P_m \tag{3.6}$$

[2]See [17] and the subsequently cited Zurek paper

This is the rate equation. We can now link the first term in the transition rate to the Fermi function using the definition

$$tr_{\text{leads}}(c_{kb}^{\dagger} e^{iH_{leads}t'} c_{kb} e^{-iH_{leads}t'}) = -iG_{kb}^{<}(-t') \tag{3.7}$$

The fluctuation dissipation theorem links the lesser green's function to the spectral function

$$G_{\alpha k\sigma}^{<} = if(\omega - \mu_\alpha) A_{\alpha k\sigma}(\omega - \mu_\alpha) \tag{3.8}$$

This finally leads us to the form

$$\frac{dp_m}{dt} = \sum_n W_{n\to m} p_n - \sum_n W_{m\to n} p_m \tag{3.9}$$

where,

$$W_{n\to m} = \sum_{x=L,R} f(e_m - e_n - \mu_x) \left[\sum_{\sigma,i,j=A,B} \Gamma_{xij\sigma} \langle m|d_{i\sigma}^{\dagger}|n\rangle \langle n|d_{j\sigma}|m\rangle \right] \tag{3.10}$$

Weak coupling regime

In the weak coupling regime, $\Gamma << k_B T$ we take Γ to be constant and solve the rate equation. For a single quantum dot, connected to two electrodes at different potential and temperature we get the following variation for the current versus temperature difference.

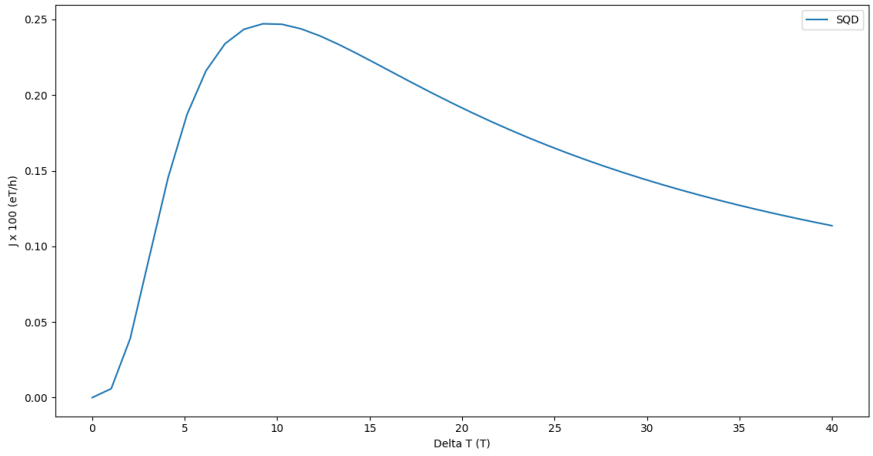


Figure 3.1: A single interacting quantum dot, with parameters $\Gamma = T/20$, $U = 30T$, $\epsilon = 10T$, $\mu_L = 28T$ and $\mu_R = 22T$.

The maxima of the current occurs due to the fact that the the current flows in different directions through the two energy levels. The direction of the current through a

particular channel solely depends on the value of the Fermi function at that energy. This is the minimum setup required for the non-monotic dependence of current on the temperature difference.

3.2 The double quantum dot system

Once again for a system of double quantum dots we will look at the setup of two quantum dots connected parallely to reservoirs at different potential and temperature.

3.2.1 Non-interacting dots

For non-interacting dots the Hamiltonian is given by

$$H_{\text{dot}} = \sum_{i=A,B} \epsilon_i d_i^\dagger d_i \tag{3.11}$$

We compare the results with the single quantum dot of the previous chapter in figure 3.2. The nature of the graphs are identical with a scaling behaviour. This behaviour can be attributed to the spin degeneracy of the levels in the single quantum dot.

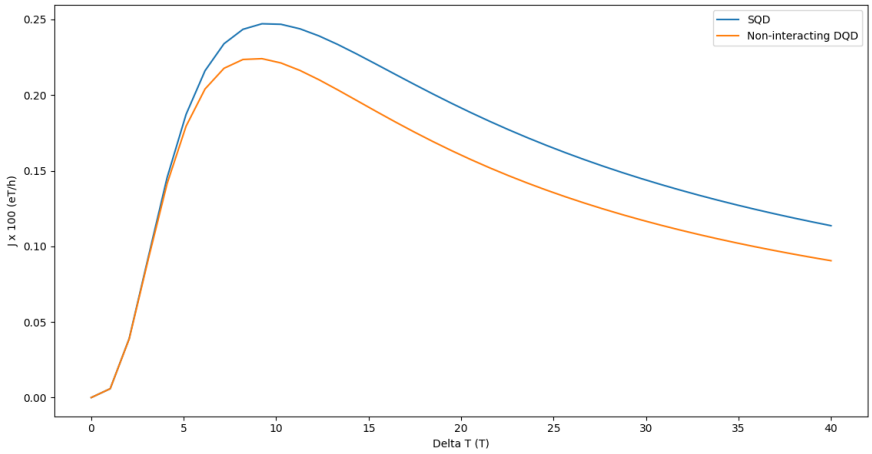
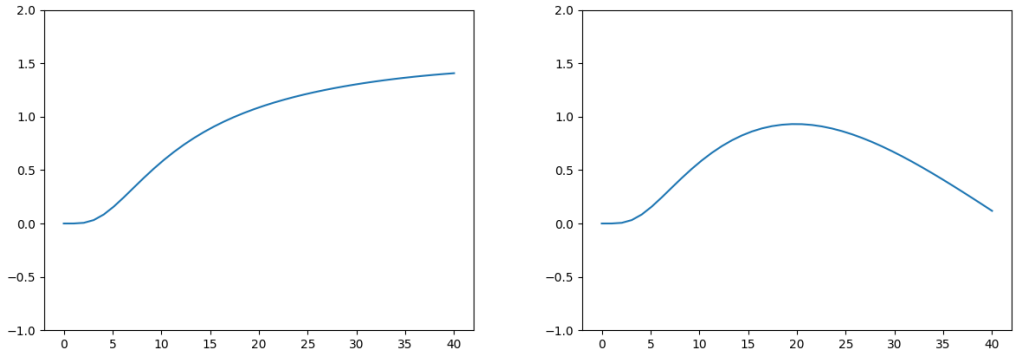


Figure 3.2: Comparison of the current flowing through a single interacting quantum dot versus a double non-interacting quantum dot connected in parallel, with parameters $\Gamma = T/20$, $\epsilon = 10T$, $\mu_L = 28T$ and $\mu_R = 22T$. The energy levels differ by $30T$



(a) (b)

Figure 3.3: J vs ΔT for two different interaction strengths $U_0 = U_1 = U = 100T$ and $300T$ respectively. Other parameter values: $\Gamma = T/10$, $\epsilon_A = 10T$, $\epsilon_B = 40T$, $\mu_L = 20T$, $\mu_R = 30T$.

3.2.2 Interacting dots

For interacting dots connected in parallel, we take the central Hamiltonian to be

$$H_{\text{dot}} = \sum_{\substack{\sigma \\ i=A,B}} \epsilon_i d^\dagger_{i\sigma} d_{i\sigma} + U_0 \sum_{i=A,B} \hat{n}_{i\downarrow}\hat{n}_{i\uparrow} + U_1 \hat{n}_A \hat{n}_B \tag{3.12}$$

The results of solving the rate equation for two different interaction strengths are given in 3.3. Similar to the single quantum dot, we once again have a maxima before the current falls off. Competing channels and their respective alignment are at play here again. The non-monotic dependence of the current on temperature can be exploited for energy harvesting using the quantum dots. This aspect is explored in [19].

Chapter 4

Summary and further work

In this project we have explored the various ways of calculating the current flowing through a nanosystem connected to two reservoirs with a potential and temperature difference. We started by studying a fully non-interacting result called the Landauer formula and then exploring the work of Meir and Wingreen who considered only the central region to be interacting. To make the final solution computationally tractable we look at a first order approximation of the current derived using a master equation formalism. Finally, we calculated the current for a couple of simple examples. The rate equation method we finally used has a drawback of only working in the weak coupling limit $\Gamma << k_B T$. A lot of interesting phenomena using quantum dots such as Kondo-like behaviour cannot be studied in this regime. Thus, other approaches such as NRG or Slave boson methods have been employed which can capture the relevant physics. [20][21][22][23][24] These methods are however more computationally intensive. In the future I hope to learn and employ these methods.

Appendix A

Quantum Mechanics of transport

We define the quantum mechanical current operator and discuss some quantum mechanics following [7] and [25]. The current density operator is defined as

$$\hat{j} = \frac{1}{2}\sum_i \delta(\hat{r} - \hat{r}_i)\hat{v}_i + \hat{v}_i\delta(\hat{r} - \hat{r}_i) \tag{A.1}$$

The corresponding current operator is then defined as

$$\hat{I} = \int_S dS \cdot \hat{j}(\hat{r}, t) \tag{A.2}$$

The spectrum of the current operator consists of discrete eigenvectors corresponding to confined currents as well as continuum values.The eigenstates of I are not square-integrable but we can construct states with a small interval δI of current

$$|\psi_{\delta I}\rangle = \frac{1}{\sqrt{\delta I}}\int_I^{I+\delta I} dI\,|\psi_I\rangle \tag{A.3}$$

and these are square-integrable and belong to the Hilbert space. They are also orthonormal

$$\langle\psi_{\delta I'}|\psi_{\delta I}\rangle = \delta_{I'I} \tag{A.4}$$

For a many particle system in general, the value of current is not enough to specify the complete system and we usually need other observables. Thus, current measurement only allows us to know the states statistically and we have to resort to using the density matrix formalism.

Appendix B

The Gell-Mann Low theorem

We provide here a proof of the Gell-Mann Low [26] theorem following [15]:

Theorem Consider a system described by a Hamiltonian $H = H_0 + e^{-\epsilon|t|}H_I$, where $H_I = \lambda V$ for some coupling constant λ. If the following terms exists to all orders in the perturbation theory then it is an eigenstate of the full Hamiltonian H.

$$\lim_{\epsilon\to 0} \frac{S_\epsilon(0,-\infty)\,|\phi_0\rangle}{\langle\phi_0|S_\epsilon(0,-\infty)|\psi_0\rangle} \equiv \frac{|\psi_0\rangle}{\langle\phi_0|\psi_0\rangle} \tag{B.1}$$

Here $|\phi_0\rangle$ is the ground state of H_0.

Proof In the interaction picture we have

$$|\psi_I(t)\rangle = S_\epsilon(t,t_0)\,|\psi_I(t_0)\rangle$$

The time development operator has the same expansion as given in (1.3).

$$S_\epsilon(t,t_0) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 .... \int_{t_0}^{t} dt_n e^{-\epsilon(|t_1|+....+|t_n|)} T\{\hat{H}_I(t_1)\hat{H}_I(t_2)....\hat{H}_I(t_n)\} \tag{B.2}$$

Now as $t_0 \to -\infty$, H approaches H_0. In this limit we can write

$$|\psi_I(t_0)\rangle = e^{\frac{iH_0t_0}{\hbar}}\,|\psi_S(t_0)\rangle = e^{\frac{iE_0t_0}{\hbar}} e^{-\frac{iE_0t_0}{\hbar}}\,|\phi_0\rangle = |\phi_0\rangle$$

We thus obtain the relation

$$|\psi_I(t_0)\rangle = S_\epsilon(0,-\infty)\,|\phi_0\rangle \tag{B.3}$$

To take the limit $\epsilon \to 0$ we start with the expression

$$\begin{aligned}(\hat{H}_0 - E_0)\,|\psi_0(\epsilon)\rangle &= (\hat{H}_0 - E_0)S_\epsilon(0,-\infty)\,|\phi_0\rangle \\ &= (\hat{H}_0 S_\epsilon(0,-\infty) - S_\epsilon(0,-\infty)\hat{H}_0)\,|\phi_0\rangle \\ &= [H_0, S_\epsilon(0,-\infty)]\,|\phi_0\rangle\end{aligned} \tag{B.4}$$

To evaluate the commutator bracket we consider the expansion in (B.2) and directly insert it into the commutator bracket. For the nth term of the series we have

$$[\hat{H}_0, \hat{H}_I(t_i)\hat{H}_I(t_j).....\hat{H}_I(t_k)] = \\ [\hat{H}_0, \hat{H}_I(t_i)]\hat{H}_I(t_j).....\hat{H}_I(t_k) + \hat{H}_I(t_i)[\hat{H}_0, \hat{H}_I(t_j).....\hat{H}_I(t_k)]$$

Expanding all the commutators gives us:

$$[\hat{H}_0, \hat{H}_I(t_i)\hat{H}_I(t_j).....\hat{H}_I(t_k)] = [\hat{H}_0, \hat{H}_I(t_i)]\hat{H}_I(t_j).....\hat{H}_I(t_k) \\ + \hat{H}_I(t_i)[\hat{H}_0, \hat{H}_I(t_j)].....\hat{H}_I(t_k)] + ... + \hat{H}_I(t_i)\hat{H}_I(t_j).....[\hat{H}_0, \hat{H}_I(t_k)] \quad \text{(B.5)}$$

Here i,j,k represent a possible time ordering of n time indices. Now the equation of motion in the interaction picture gives

$$-i\hbar\frac{\partial \hat{H_I}(t)}{\partial t} = [H_0, H_I(t)]$$

Thus the commutators in (B.5) each yield a derivative simplifying the expression to:

$$[\hat{H}_0, \hat{H}_I(t_i)\hat{H}_I(t_j).....\hat{H}_I(t_k)] = -i\hbar\left(\sum_{l=1}^{n}\frac{\partial}{\partial t_l}\right)\hat{H}_I(t_i)\hat{H}_I(t_j).....\hat{H}_I(t_k) \quad \text{(B.6)}$$

Now from the definition of the time ordering operator and using the identity

$$\left(\sum_{l=1}^{n}\frac{\partial}{\partial t_l}\right)\theta(t_p - t_q)\theta(t_q - t_r).....\theta(t_u - t_v) = 0$$

we have

$$-i\hbar T\{\left(\sum_{l=1}^{n}\frac{\partial}{\partial t_l}\right)\hat{H}_I(t_i)\hat{H}_I(t_j).....\hat{H}_I(t_k)\} = -i\hbar\left(\sum_{l=1}^{n}\frac{\partial}{\partial t_l}\right)T\{\hat{H}_I(t_i)\hat{H}_I(t_j).....\hat{H}_I(t_k)\}$$

This gives us the expression

$$(\hat{H}_0 - E_0)\,|\psi_0(\epsilon)\rangle = \sum_{n=0}^{\infty}\frac{(-i)^{n+1}\hbar}{n!}\int_{-\infty}^{0}dt_1....\int_{-\infty}^{0}dt_n e^{-\epsilon(|t_1|+....+|t_n|)} \\ \left(\sum_{l=1}^{n}\frac{\partial}{\partial t_l}\right)T\{\hat{H}_I(t_1)\hat{H}_I(t_2)....\hat{H}_I(t_n)\}\,|\phi_0\rangle \quad \text{(B.7)}$$

Now all the derivatives make the same contribution in the integral as the dummy variables can simply be switched, thus we can write the sum of derivatives as n times a single derivative.

$$(\hat{H}_0 - E_0)\,|\psi_0(\epsilon)\rangle = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}\hbar}{n!} \int_{-\infty}^{0} dt_1 .... \int_{-\infty}^{0} dt_n e^{-\epsilon(|t_1|+....+|t_n|)} \left(n\frac{\partial}{\partial t_1}\right) T\{\hat{H}_I(t_1)\hat{H}_I(t_2)....\hat{H}_I(t_n)\}\,|\phi_0\rangle \quad \text{(B.8)}$$

We next carry out integration by parts over t_1. This yields the result

$$(\hat{H}_0 - E_0)\,|\psi_0(\epsilon)\rangle = \sum_{n=0}^{\infty} \frac{(-i)^{n+1}\hbar}{(n-1)!} \int_{-\infty}^{0} dt_2 .... \int_{-\infty}^{0} dt_n e^{-\epsilon(|t_1|+....+|t_n|)} T\{\hat{H}_I(t_1)\hat{H}_I(t_2)....\hat{H}_I(t_n)\}|_{-\infty}^{0} + \int_{-\infty}^{0} dt_1 \epsilon e^{-\epsilon(|t_1|+....+|t_n|)} T\{\hat{H}_I(t_1)\hat{H}_I(t_2)....\hat{H}_I(t_n)\}\,|\phi_0\rangle \quad \text{(B.9)}$$

The first term is merely the integrand evaluated at $t_1 = 0$ and $t_1 = -\infty$. The lower limit contributes 0 to the integrand while the upper limit has the term $\hat{H_I}(0)$. 0 being the latest time is always on the left and thus can be taken outside the time-ordering operator. The remaining terms are simply the $(n-1)^{(th}$ of the series and simply summing over leads to $S_\epsilon(0, -\infty)$ again. Thus giving us

$$(\hat{H}_0 - E_0)\,|\psi_0(\epsilon)\rangle = -H_I\,|\psi_0\rangle + \epsilon \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{(n-1)!} \int_{-\infty}^{0} dt_1 .... \int_{-\infty}^{0} dt_n e^{-\epsilon(|t_1|+....+|t_n|)} T\{\hat{H}_I(t_1)\hat{H}_I(t_2)....\hat{H}_I(t_n)\}\,|\phi_0\rangle \quad \text{(B.10)}$$

Now since $H_I = \lambda V$ we can factor the λ out to get the coefficient in front as

$$\frac{(-i)^{n-1}\lambda^n}{(n-1)!} = i\lambda\frac{\partial}{\partial\lambda}\frac{(-i)^n\lambda^n}{(n)!} \quad \text{(B.11)}$$

Thus giving us the series for $S_\epsilon(0, -\infty)$ again. This finally gives us

$$(\hat{H} - E_0)\,|\psi_0(\epsilon)\rangle = i\lambda\frac{\partial}{\partial\lambda}\,|\psi_0(\epsilon)\rangle \quad \text{(B.12)}$$

This can be rewritten as

$$\left(\hat{H} - E_0 - i\epsilon\lambda\frac{\partial}{\partial\lambda}\right)|\psi_0(\epsilon)\rangle = 0$$

Now we have the identity:

$$\left(\frac{\partial}{\partial\lambda}\right)\frac{|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} = \frac{\frac{\partial}{\partial\lambda}|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} - |\psi_0(\epsilon)\rangle\frac{\partial}{\partial\lambda}\ln\langle\phi_0|\psi_0(\epsilon)\rangle$$
$$\implies \frac{\frac{\partial}{\partial\lambda}|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} = \left(\frac{\partial}{\partial\lambda}\right)\frac{|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} + \frac{|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle}\frac{\partial}{\partial\lambda}\ln\langle\phi_0|\psi_0(\epsilon)\rangle$$

Inserting this into the previous equation we get

$$\left(\hat{H} - E_0 - i\epsilon\lambda\frac{\partial}{\partial\lambda}\right)\frac{|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} = \frac{i\epsilon\lambda|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle}\frac{\partial}{\partial\lambda}\ln\langle\phi_0|\psi_0(\epsilon)\rangle \tag{B.13}$$

Now if we multiply (B.12) by $\frac{\langle\phi_0|}{\phi_0|\psi_0(\epsilon)}$, we get

$$\frac{\langle\psi_0|\hat{H}_I|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} = i\epsilon\lambda\frac{\partial}{\partial\lambda}\ln\langle\phi_0|\psi_0(\epsilon)\rangle \equiv E - E_0 \tag{B.14}$$

If we combine equations 13 and 14, we thus finally get

$$\left(\hat{H} - E\right)\frac{|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} = i\epsilon\lambda\frac{\partial}{\partial\lambda}\frac{|\psi_0(\epsilon)\rangle}{\langle\phi_0|\psi_0(\epsilon)\rangle} \tag{B.15}$$

We now take the limit $\epsilon \to 0$. The right hand side goes to 0 and we are left with:

$$\hat{H}\frac{|\psi_0\rangle}{\langle\phi_0|\psi_0\rangle} = E\frac{|\psi_0\rangle}{\langle\phi_0|\psi_0\rangle} \tag{B.16}$$

This proves that the state obtained adiabatically from the non-interacting ground state is an eigenstate of the full hamiltonian but this does not prove that it is a ground state (although it usually is.) ■

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