Electron Transport in Nano-Structure

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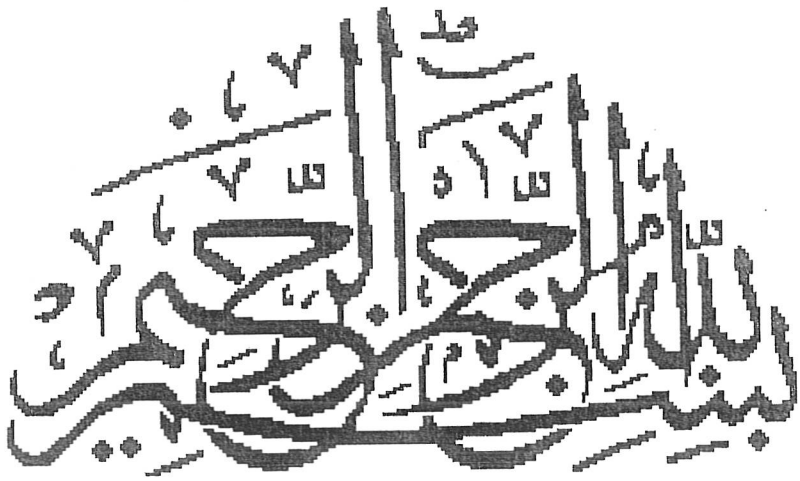

In the name of Allah, Most Gracious, Most Merciful.

This work is submitted as a dissertation
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CERTIFICATE

This is to certify that the work in this dissertation has been carried out by ***Mr. Bilal Tariq*** under my supervision in Condensed matter Physics, Department of Physics, Quaid-i-Azam University, Islamabad, Pakistan.

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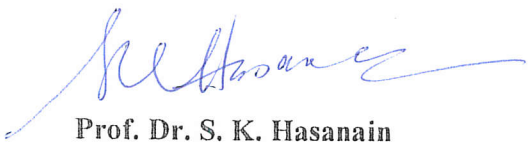

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Dedicated
To
Beloved Parents

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ABSTRACT

The emerging field of nano-electro-mechanical systems (NEMS), in which the modes of a nanomechanical oscillator play the role of an active device, is receiving much attention due to its technological importance. The characteristic component that gives the name to these devices is an oscillator of nanometer size coupled to the electrons on the dot that transfer electrons one-by-one between a source and a drain lead. From a fundamental point of view, it is important to understand the interplay between the electronic transport and the nanomechanical motion of the oscillator quantum mechanically.

In this thesis, we describe a formalism for calculating dc current-voltage characteristics of nanostructures connected between two leads taking into account the interaction inside the device. The method is based on nonequilibrium Green's functions (NEGF) techniques and a Meir-Wingreen type formula for the current through an interacting region. We discuss the quantum transport of electrons through a resonant tunnel junction coupled to a nanomechanical oscillator at zero temperature. By using the Green's-function technique, we calculate the transport properties of electrons through a single dot strongly coupled to a single oscillator. In addition to the main resonant peak of electrons on the dot, we find satellite peaks due to the creation of phonons. These satellite peaks become sharper and more significant with increasing coupling strength between the electrons and the oscillator.

Contents

Chapter 1

Introduction and Background

1.1 Introduction: Electronic Transport in Nanostructure

Electrical conductance of a macroscopic object is described by the well known Ohm's law. The conductance (G) of a conductor is proportional to its cross-sectional area (A) and inversely proportional to its length (L)

$$G = \frac{\sigma A}{L} \tag{1.1}$$

Here σ is the conductivity of the conductor, which depends on the charge carrier density and mean free path.

As the conductor gets smaller, several effects that are negligible in a macroscopic conductor become increasingly important. In very small objects such as nanostructures and molecules, electron transport usually does not follow Ohm's law. There are several reasons why Ohm's law fails at such exceedingly small scale. First, the size is smaller than the mean free path, which is the distance traveled by an electron before its initial momentum is destroyed. Thus electron transport is not a diffusive process as described by Ohm's law. Instead, it is in a ballistic conducting regime, where charge carriers experience no scattering within the conductor. Second, the contact between macroscopic electrodes and the nanoscale conductor strongly affects the over all conductance, depending on the property of the contact, the overall transport behavior can be very different and hence understanding the nature of the contact is extremely important. Third, a nanoscale object has a large charge addition energy and a quantized excitation

spectrum. Both of these strongly affect electron transport especially at low temperature.

Studying transport behavior of these extremely small objects is a very interesting scientific problem, and it also has many practical implications, especially to the micro electronic industry. In recent years, studying electron transport in nanoscale objects has become one of the most active fields in condensed matter physics and has also attracted huge research efforts from various other disciplines of science. To date, many nanoscale systems have been investigated, including solid-state nanostructures as well chemical nanostructures such as carbon nanotubes and nanocrystals. Transport measurements on such system have displayed exciting new behavior that cannot be explained within the framework of conventional macroscopic theory [36].

1.2 Theoretical Approaches

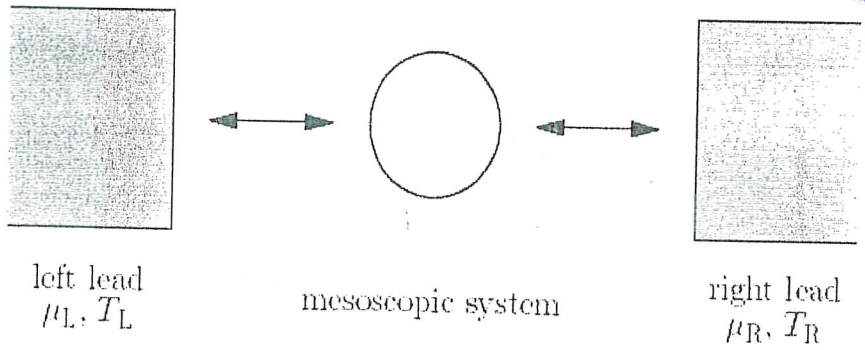
A widely used approach to describe electrical transport through nanoscale systems is the Landauer-Buttiker formalism [21, 22, 23]. Within this framework, the applied voltage drops entirely at the contacts and not within the wire. The Joule dissipation associated with this resistance is assumed to take place far away from the contact, where electrons and holes relax to the Fermi level of the electrodes. This picture is correct for small voltages, and this allows only very small currents. Going beyond, one can use the Kubo formalism [10, 13, 20] to include many body effects. This approach is limited to the linear order in the response. Another approach to transport, especially in the weak coupling regime, where the Coulomb interaction plays an important role [24, 25], makes use of the rate equation to obtain the device currents. In this thesis, we study transport in a regime where we can exclude the presence of charging effects, as we do not consider double occupancy of the electronic levels of the quantum dot. We describe our system within the nonequilibrium Green function formalism (NEGF) [4, 5, 8, 10, 13]. This theory provides a microscopic description for a quantum system out of equilibrium including interactions. It combines quantum dynamics with a statistical description of the interactions. The first approaches within this formalism to calculate transport with an electron-phonon interaction go back to Caroli et al [1, 2, 3]. With the realization of single molecular experiments, this topic has gained great deal of interest [26, 37, 38, 39]. An important development in this regard was the derivation of an expression for the nonequilibrium current through an interacting

region by Wingreen et al. [6, 7, 8].

1.3 Partition Scheme

An approach to the quantum transport problem has been suggested by Caroli et al. [1, 2, 3] who state: "It is usually considered that a description of the system as a whole does not permit the calculation of the current". Their approach is based on a fictitious partition where the left and right leads are treated as two isolated subsystems in the remote past. Then, one can fix a chemical potential μ_α and a temperature β_α^{-1} for each lead, α = L,R. In this picture the initial density matrix is given by $\rho = exp[-\beta_L(H_L - \mu_L N_L)]exp[-\beta_R(H_R - \mu_R N_R))]$, where $H_{L,R}$ and $\mu_{L,R}$ now refer to the isolated L, R lead. The current will flow through the system once the contacts between the device and the leads have been established. Hence, the time-dependent perturbation is a lead-device hopping rather than a local one-particle level-shift. Since the device is a mesoscopic object, it is reasonable to assume that the hopping perturbation does not alter the thermal equilibrium of the left and right charge reservoir and that a non-equilibrium steady state will eventually be reached. This argument is very strong and remains valid even for noninteracting leads. Actually, the partitioned approach by Caroli et al. was originally applied to a tight-binding model describing a metal-insulator-metal tunneling junction and then extended to the case of free electrons subjected to an arbitrary one-body potential. This extension was questioned by Feuchtwang; the controversy was about the appropriate choice of boundary conditions for the uncontacted-system Green functions. In later years the non-equilibrium Green function techniques in the partitioned approach framework were mainly applied to investigate steady-state situations. An important breakthrough in time-dependent non-equilibrium transport was achieved by Wingreen et al [6, 7, 8]. Still in the framework of the partitioned approach, they derived an expression for the fully nonlinear, time-dependent current in terms of the Green functions of the mesoscopic region (this embedding procedure holds only for noninteracting leads). Under the physical assumption that the initial correlations are washed out in the long-time limit, their formula is well suited to study the response to

external time-dependent voltages and contacts.



Basic setup of a transport experiment.

1.4 Outline

We start with the definition of the Green's function in the Heisenberg picture and transform it into the interaction picture. Thereby, we introduce the notation of contour ordered Green's functions. By using formulation of the nonequilibrium theory based on the work of Keldysh and Langreth [4, 5, 14, 27], we derive some important quantities such as the self-energy, which are useful for the derivation of current.

In chapter 3, we derive an exact formula for time-dependent current through the region of interacting electrons coupled to two multi channel leads where the electrons are not interacting. The current is then written in terms of local Green's functions. The general result is then examined in several special cases:

1) We Determine the time independent current from it.

2) It is shown that in the steady state situation for the non interacting region the current is conserved.

3) We derive an exact solution for arbitrary time dependence in a single non interacting level.

In chapter 3 we discuss our model of electrical tunnel junction through a quantum dot cou-

pled to an oscillator, where we have introduced non perturbatively electron phonon interaction and strong dissipation inside system such as when our electron leave the dot-oscillator system then our oscillator comes back to the ground state.

Chapter 2

Nonequilibrium Green's functions: Formalism

In this chapter, we introduce the basic concepts of the nonequilibrium Green function formalism [5, 8, 9, 10, 13, 18]. The nonequilibrium formulation is needed because the system under consideration, a nanostructure between two leads at different chemical potentials, is in a steady state and not in an equilibrium situation.We give the definitions of retarded, advanced, lesser, and greater Green functions and consider some simple examples [34].We also introduce a very important concept of the Schwinger-Keldysh closed-time contour [4, 5, 14, 27, 28], and define contour Green functions. We introduce a general model: two leads, right (R) and left (L) and a single nanostructure such as a quantum dot. We then briefly describe the basic calculations of the time-independent retarded and advanced Green's function and the corresponding self-energy for this model. We move to introduce Langreth's theorem [35] and apply it to derive the time-independent lesser Green's function or the density matrix using the standard Dyson's equation. The expression of the density matrix is equivalent to the Keldysh non-equilibrium Green's function result. This chapter is somewhat technical, but we need these definitions in the chapters to follow.

2.1 Time Ordered Series

Let us consider the full Hamiltonian $H(t)$ as the sum of a free-particle time independent part H_0 and (possibly time-dependent) perturbation $V(t)$ [10, 20] (note that this perturbation may not be necessarily small)

$$H(t) = H_0 + V(t). \tag{2.1}$$

$H(t)$ is in the *Schrodinger picture.* Let Ψ_S be the solution of the time dependent Schrodinger equation then our task is to solve the equation

$$i\frac{d \mid \Psi_s(t) >}{dt} = H_S(t) \mid \Psi_S(t) > . \tag{2.2}$$

We can solve formally by introducing the unitary time evolution operator U_S such that

$$\mid \Psi_s(t) >= U_S(t, t_0) \mid \Psi_s(t_0) > \tag{2.3}$$

where t_0 is arbitrary, and in the time-independent problem one can choose $t_0 = 0$. In general, it is a much better idea taking $H_S(t)$ which depends on time, with the condition that for $t < t_0$, $V \equiv 0$.Assume that the interaction is added very slowly, starting from a time $t \to t_0$, when the Hamiltonian was just H_0 and everything was easy. From Eq. (2.3) and Eq. (2.2)

$$i\frac{d}{dt}U_S(t, t_0) \mid \Psi_s(t_0) >= H_S(t)U_S(t, t_0) \mid \Psi_S(t_0) > . \tag{2.4}$$

Since $\mid \Psi_s(t_0) >$ is arbitrary we find that,

$$i\frac{d}{dt}U_S(t, t_0) = H_S(t)U_S(t, t_0). \tag{2.5}$$

The solution of the above equation is:

$$U_S(t, t_0) = T\exp(-i\int_{t_0}^{t} dt_1 H_S(t_1)). \tag{2.6}$$

Here $Texp$ is a conventional notation that means nothing but the exponential series of time-ordered products.

In the *Heisenberg picture*

$$< A(t) >=< \Psi_H \mid A_H(t) \mid \Psi_H > \tag{2.7}$$

where by definition

$$\mid \Psi_H >= \mid \Psi_S(t_0) > . \tag{2.8}$$

So,

$$\begin{aligned} A_H(t) &= U_S^{\dagger}(t,t_0)A_S(t)U_S(t,t_0) \\ &= T\exp(-i\int_t^{t_0} dt_1 H_S(t_1))A_S(t)T\exp(-i\int_{t_0}^{t} dt_1 H_S(t_1)) \\ &= T_C(\exp(-i\int_t^{t_0} dt_1 H_S(t_1))A_S(t)) \end{aligned} \tag{2.9}$$

where C is an oriented path that goes from t_0 to t at which the operator $A_S(t)$ acts, and subsequent propagating from t to t_0

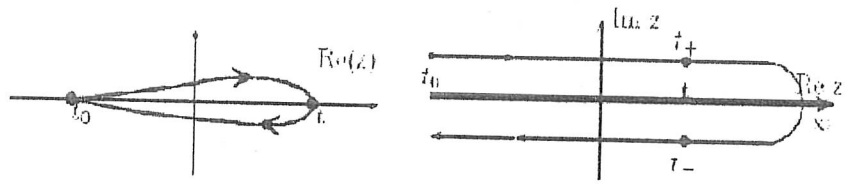


Figure 2-1: a) A contour on the complex time z plane for obtaining <A(t)> from a single particle Schrodinger picture evolution b) The Keldysh contour

The evolution operator satisfies the group property $U(t,t_1)U(t_1,t_2) = U(t,t_2)$; hence the path can be deformed freely as long as it starts and ends at t_0 and goes through t. In time-dependent problems, the most common contour is the Keldysh one from t_0 to $t \to +\infty$ and back to t_0;there are an ascending or positive branch and a descending or negative branch, and a physical time can be taken on any of the two. We write t_+ and t_- the times taken on the

ascending and descending branch respectively;

Now we introduce the *Interaction Picture* in which the operators evolve only with H_0

$$A_I(t) = e^{iH_0 t} A_S e^{-iH_0 t} \tag{2.10}$$

while the wave function is defined by

$$\Psi_I(t) = e^{iH_0 t} \Psi_S(t_0). \tag{2.11}$$

By substituting $\Psi_I(t)$ in the Schrodinger equation we find that

$$i\frac{d}{dt}\Psi_I(t) = V_I(t)\Psi_I(t) \tag{2.12}$$

which is like Schrodinger equation without the obvious part of the dynamics. The evolution operator in the interaction picture from an arbitrary time τ

$$\Psi_I(t) = U_I(t,\tau)\Psi_I(\tau) \tag{2.13}$$

and

$$i\frac{d}{dt}U_I(t,\tau) = V_I(t)U_I(t,\tau). \tag{2.14}$$

The solution

$$U_I(t,t_0) = T\exp(-i\int_{t_0}^{t} dt_1 V_I(t_1)) \tag{2.15}$$

is at the basis of all perturbation theory. In the Heisenberg picture,

$$A_H(t) = U_I^{\dagger}(t,t_0) A_S(t) U_I(t,t_0) \tag{2.16}$$

Having succeeded in writing Heisenberg operator in terms of interaction ones, we can expand them in series of V_I .

2.2 Retarded (G^R) and Advanced (G^A) functions

Retarded Green function for fermions is defined as

$$G^R_{\alpha\beta}(t_1,t_2) = -i\theta(t_1-t_2) < [c_\alpha(t_1), c^\dagger_\beta(t_2)]_+ > \tag{2.17}$$

where $c_\alpha(t_1)$and $c^\dagger_\beta(t_2)$ are creation and annihilation time-dependent (Heisenberg) operators, $[c,d]_+ = cd + dc$ is the anti-commutator, $< .. >$ denotes averaging over the equilibrium state. We use $\alpha, \beta, ...$ to denote single-particle quantum states.

The advanced Green's function for fermions is defined as

$$G^A_{\alpha\beta}(t_1,t_2) = i\theta(t_2-t_1) < [c_\alpha(t_1), c^\dagger_\beta(t_2)]_+ > . \tag{2.18}$$

Retarded and advanced functions for bosons can be defined as,

$$G^R_{\alpha\beta}(t_1,t_2) = -i\theta(t_1-t_2) < [a_\alpha(t_1), a^\dagger_\beta(t_2)]_- > \tag{2.19}$$

$$G^A_{\alpha\beta}(t_1,t_2) = i\theta(t_2-t_1) < [a_\alpha(t_1), a^\dagger_\beta(t_2)]_- > \tag{2.20}$$

where $a_\alpha(t), a^\dagger_\alpha(t)$ are creation and annihilation boson operators, $[a,b]_- = ab - ba$ is the commutator.

Free-particle retarded function for fermions: Now consider the simplest possible example - retarded Green function for free particles (fermions).

The free-particle Hamiltonian has the same form for either Schrodinger or Heisenberg operators:

$$H = H_0 = \sum_\alpha \epsilon_\alpha c^\dagger_\alpha c_\alpha = \sum_\alpha \epsilon_\alpha c^\dagger_\alpha(t) c_\alpha(t) \tag{2.21}$$

If we assume $t_0 = 0$

$$\begin{aligned} c^\dagger_\alpha(t)c_\alpha(t) &= e^{iHt}c^\dagger_\alpha e^{-iHt}e^{iHt}c_\alpha e^{-iHt} \\ &= e^{iHt}c^\dagger_\alpha c_\alpha e^{-iHt} \\ &= c^\dagger_\alpha c_\alpha \end{aligned}$$

where we have used the property that $c_\alpha^\dagger c_\alpha$ commutes with H. Now we use the equation of motion technique to determine the time evolution of the operator $c_\alpha(t)$:

$$\begin{aligned} i\frac{dc_\alpha(t)}{dt} &= [c_\alpha(t), H]_- = \sum_\beta \epsilon_\beta [c_\alpha(t), c_\beta^\dagger c_\beta]_- \\ &= \sum_\beta \epsilon_\beta (c_\alpha c_\beta^\dagger c_\beta - c_\beta^\dagger c_\beta c_\alpha) \\ &= \sum_\beta \epsilon_\beta (c_\alpha c_\beta^\dagger c_\beta + c_\beta^\dagger c_\alpha c_\beta) \\ &= \sum_\beta \epsilon_\beta (c_\alpha c_\beta^\dagger + c_\beta^\dagger c_\alpha) c_\beta \\ &= \sum_\beta \epsilon_\beta \delta_{\alpha\beta} c_\beta \\ &= \epsilon_\alpha c_\alpha(t) \end{aligned} \tag{2.22}$$

So the Heisenberg operator $c_\alpha(t)$ for free fermions can be expressed as

$$c_\alpha(t) = e^{-i\epsilon_\alpha t} c_\alpha(0), \quad c_\alpha^\dagger(t) = e^{i\epsilon_\alpha t} c_\alpha^\dagger(0). \tag{2.23}$$

If we take $t_0 \neq 0$, then Heisenberg operators for free fermions are

$$c_\alpha(t) = e^{-i\epsilon_\alpha (t-t_0)} c_\alpha(t_0), \quad c_\alpha^\dagger(t) = e^{i\epsilon_\alpha (t-t_0)} c_\alpha^\dagger(t_0) \tag{2.24}$$

but the commutator relation in both case is

$$\begin{aligned} &< [c_\alpha(t_1), c_\beta^\dagger(t_2)]_+ > = < c_\alpha(t_1) c_\beta^\dagger(t_2) + c_\beta^\dagger(t_2) c_\alpha(t_1) > \\ &= e^{i\epsilon_\beta (t_2 - t_0)} e^{-i\epsilon_\alpha (t_1 - t_0)} < c_\alpha c_\beta^\dagger + c_\beta^\dagger c_\alpha > \\ &= e^{-i\epsilon_\alpha (t_1 - t_2)} \delta_{\alpha\beta} \end{aligned} \tag{2.25}$$

Therefore

$$G_{\alpha\beta}^R(t_1, t_2) = -i\theta(t_1 - t_2) e^{-i\epsilon_\alpha (t_1 - t_2)} \delta_{\alpha\beta}. \tag{2.26}$$

Similarly,

$$G_{\alpha\beta}^A(t_1, t_2) = i\theta(t_2 - t_1) e^{-i\epsilon_\alpha (t_1 - t_2)} \delta_{\alpha\beta}. \tag{2.27}$$

We define Fourier transform over time difference $(t_1 - t_2)$ as

$$G^R(\epsilon) = \int_0^\infty G^R(t_1 - t_2) e^{-i(\epsilon + i0)(t_1 - t_2)} d(t_1 - t_2) \tag{2.28}$$

where we add infinitely small positive complex part to ϵ to make this integral well defined at the upper limit. Thus,

$$G^R_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha + i0} \tag{2.29}$$

Likewise,

$$G^A(\epsilon) = \int_{-\infty}^0 G^A(t_1 - t_2) e^{-i(\epsilon - i0)(t_1 - t_2)} d(t_1 - t_2)$$

with the result

$$G^A_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha - i0}. \tag{2.30}$$

Now we introduce a useful combination of retarded and advanced functions known as the *spectral or spectral weight function*

$$A_{\alpha\beta}(\epsilon) = i(G^R_{\alpha\beta}(\epsilon) - G^A_{\alpha\beta}(\epsilon)). \tag{2.31}$$

Since $G^A(\epsilon) = (G^R(\epsilon))^*$ this implies $A_{\alpha\beta}(\epsilon) = -2\,\mathrm{Im}\, G^R_{\alpha\beta}(\epsilon)$. For free fermions the spectral function is

$$A_{\alpha\beta}(\epsilon) = -2\,\mathrm{Im}\left(\frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha - i0}\right) = 2\pi\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}. \tag{2.32}$$

Further, the spectral function has a special property

$$\int_{-\infty}^\infty A_{\alpha\beta}(\epsilon)\frac{d\epsilon}{2\pi} = \delta_{\alpha\beta}. \tag{2.33}$$

2.3 Lesser ($G^<$) and Greater ($G^>$) functions

The lesser and greater Green function are defined as:

For Fermions

$$G^<_{\alpha\beta}(t_1, t_2) = i < c^\dagger_\beta(t_2) c_\alpha(t_1) > \tag{2.34}$$

$$G^>_{\alpha\beta}(t_1, t_2) = -i < c_\alpha(t_1) c^\dagger_\beta(t_2) > \tag{2.35}$$

For bosons

$$\begin{aligned} G^{<}_{\alpha\beta}(t_1,t_2) &= i < a^{\dagger}_{\beta}(t_2)a_{\alpha}(t_1) > \\ G^{>}_{\alpha\beta}(t_1,t_2) &= -i < a_{\alpha}(t_1)a^{\dagger}_{\beta}(t_2) > \end{aligned}$$

The origin and utility of these Green functions is apparent if we consider a Green function which is the central element in equilibrium theory which can be calculated by diagrammatic techniques. This is the time-ordered Green function defined by

$$G_{\alpha\beta}(t_1,t_2) = -i < T(c_{\alpha}(t_1)c^{\dagger}_{\beta}(t_2)) > . \tag{2.36}$$

It can be expressed as

$$G_{\alpha\beta}(t_1,t_2) = \begin{cases} -i < c_{\alpha}(t_1)c^{\dagger}_{\beta}(t_2) > & \text{if } t_1 > t_2, \Rightarrow G_{\alpha\beta}(t_1,t_2) \equiv G^{>}_{\alpha\beta}(t_1,t_2) \\ i < c^{\dagger}_{\beta}(t_2)c_{\alpha}(t_1) > & \text{if } t_1 < t_2, \Rightarrow G_{\alpha\beta}(t_1,t_2) \equiv G^{<}_{\alpha\beta}(t_1,t_2) \end{cases} . \tag{2.37a}$$

here additional negative sign appears on account of interchanging of fermionic creation and annihilation operators.Lesser means that $t_1 < t_2$. From the definitions it is clear that the retarded function can be obtained from lesser and greater functions

$$G^{R}_{\alpha\beta}(t_1,t_2) = \theta(t_1 - t_2)[G^{>}_{\alpha\beta}(t_1,t_2) - G^{<}_{\alpha\beta}(t_1,t_2)] \tag{2.38}$$

*Free-particle lesser function for fermions:*Lesser function is

$$\begin{aligned} G^{<}_{\alpha\beta}(t_1,t_2) &= i < c^{\dagger}_{\beta}(t_2)c_{\alpha}(t_1) >= ie^{-i\epsilon_{\alpha}t_1 + i\epsilon_{\beta}t_2} < c^{\dagger}_{\beta}c_{\alpha} > \\ &= ie^{-i\epsilon_{\alpha}t_1 + i\epsilon_{\beta}t_2} f(\epsilon_{\alpha})\delta_{\alpha\beta}. \end{aligned} \tag{2.39}$$

The lesser function is proportional to the distribution function, in equilibrium this is the Fermi distribution function

$$f(\epsilon_{\alpha}) = \frac{1}{e^{\frac{\epsilon-\mu}{T}} + 1} \tag{2.40}$$

Now we define the Fourier-transform for lesser function

$$G^{<}(\epsilon) = \int_{-\infty}^{\infty} G^{<}(\tau) e^{i(\epsilon + 0i(sign\tau))\tau} d\tau.$$

note that here we use $0isign(\tau)$ for convergence.

Applying this transformation we obtain,

$$\begin{aligned} G^{<}_{\alpha\beta}(\epsilon) &= if(\epsilon_\alpha)\delta_{\alpha\beta} \int_{-\infty}^{\infty} e^{i(\epsilon - \epsilon_\alpha + 0i(sign\tau))\tau} d\tau \\ &= 2\pi i f(\epsilon_\alpha)\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}. \end{aligned} \tag{2.41}$$

By comparing Eq. (2.32) and Eq. (2.41) we get

$$\begin{aligned} G^{<}_{\alpha\beta}(\epsilon) &= if(\epsilon_\alpha)A_{\alpha\beta}(\epsilon) \\ &= -f(\epsilon_\alpha)(G^{R}_{\alpha\beta}(\epsilon) - G^{A}_{\alpha\beta}(\epsilon)). \end{aligned} \tag{2.42}$$

For free fermion greater function

$$G^{>}_{\alpha\beta}(\epsilon) = -2\pi i(1 - f(\epsilon_\alpha))\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta} = -i(1 - f(\epsilon_\alpha))A_{\alpha\beta}(\epsilon). \tag{2.43}$$

$f(\epsilon_\alpha)$ describes the thermal occupation of the states.So in the fermionic case $G^{<}$ contains information about the occupied particles(electrons) and $G^{>}$ about the unoccupied states (holes). In the nonequilibrium case the spectral density and the distribution function have to be calculated. By subtracting Eq. (2.42) and Eq. (2.43) and substitute the vale of $A_{\alpha\beta}(\epsilon)$ we get

$$G^{<}_{\alpha\beta}(\epsilon) - G^{>}_{\alpha\beta}(\epsilon) = i(G^{R}_{\alpha\beta}(\epsilon) - G^{A}_{\alpha\beta}(\epsilon)) \tag{2.44}$$

2.4 Contour-Ordered Green Function

Now we will express the Green functions in the interaction representation. Consider, for example, the lesser function

$$G^{<}_{\alpha\beta}(t_1, t_2) = i < c^{\dagger}_{\beta}(t_2)c_\alpha(t_1) >= i < \Psi^H \mid c^{\dagger}_{\beta}(t_2)c_\alpha(t_1) \mid \Psi^H >, \tag{2.45}$$

c-operators here are Heisenberg operators and they should be replaced by operators $c^I(t) \equiv c(t)$ in the interaction representation:

$$\begin{aligned} G^<_{\alpha\beta}(t_1,t_2) &= < U_I^\dagger(t_2,t_0)c_\beta^\dagger(t_2)U_I(t_2,t_0)U_I^\dagger(t_1,t_0)c_\alpha(t_1)U_I(t_1,t_0) > \\ &= < U_I(t_0,t_2)c_\beta^\dagger(t_2)U_I(t_2,t_1)c_\alpha(t_1)U_I(t_1,t_0) > \end{aligned} \tag{2.46}$$

It would still be cumbersome to expand the three U_I factors, but we can do with just one expansion, since for each operator A

$$\begin{aligned} A_H(t) &= U_I^\dagger(t,t_0)A_I(t)U_I(t,t_0) \\ &= T\exp(-i\int_{t_0}^{t} dt_1 V_I(t_1))A_I(t)T\exp(i\int_{t_0}^{t} dt_1 V_I(t_1)) \\ &= T_C(\exp(-i\int_{t_0}^{t} dt_1 V_I(t_1))A_I(t)) \end{aligned} \tag{2.47}$$

where C is any oriented path in complex time through t_0 and t, using the generalized time-ordering T_C along C

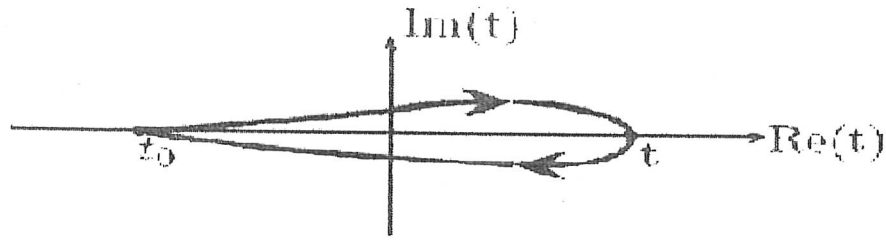


FIG.2.2 A contour on the complex time t plane for obtaining <A(t)> from a single particle interaction evolution picture

Note that $A_I(t)$ is under the action of T_C that places it appropriately. In a similar way, we

can read from left to right $G^<_{\alpha\beta}(t_1,t_2) = i < c^\dagger_\beta(t_2)c_\alpha(t_1) >$ as one story: the system starts at $t_0 \to -\infty$, evolves to t_1, is acted on by c_α, then evolves to receive the action of $c^\dagger$ at time t_2 and eventually it evolves back to t_0. Physically, t_2 can be before or after t_1. In this story, we meet $c^\dagger$ after c because $G^<$ is defined with $c^\dagger$ on the left of c. Thus along the path $C = C_1 U C_2$, t precedes t', we write $t <_C t'$, and

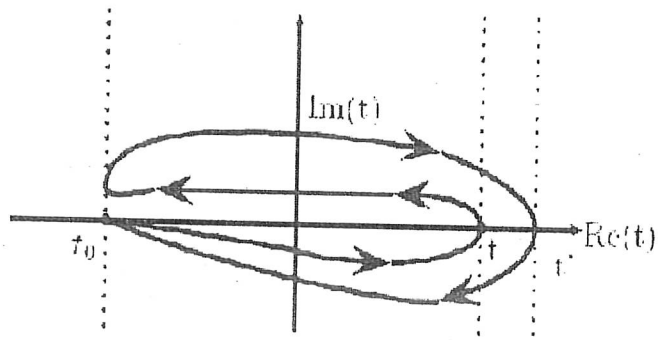


Figure 2.3 The contour C for $g^<$ on the t planewith $t<_c t'$. Note C can be analyzed as a two-step path $C=C_1 \cup C_2$. C_1 starts from t_0 and returns there after visiting t. and C_2 starts from t_0 and returns there after visiting t'

$$G^<(t_1,t_2) = < \{T_C(\exp(-i\int_{t_0}^{t} dt_1 V_I(t_1))c_I^\dagger(t))\}\{T_C(\exp(i\int_{t_0}^{t} dt_1 V_I(t_1))c_I(t)) > \quad (2.48)$$

$$= < T_C(\exp(-i\int_C dt_1 V_I(t_1))c_I^\dagger(t)c_I(t) > \quad (2.49)$$

Because of the group property, the contour C is largely arbitrary. It can go back to t_0 between t and t' any number of times, including 0. The terms arising in the series development of the operators are ordered automatically by T_C with earlier times (on C) to the right. Moreover,

$$G^>(t_1,t_2) =< T_C(\exp(-i\int_C dt_1 V_I(t_1))c_I(t)c_I^\dagger(t) > . \quad (2.50)$$

We can also use the same C in both cases, placing t and t' in opposite orders. As we know, the knowledge of both $G^>$ an $G^<$ gives access to the physically important retarded and advanced Green's functions. We also need to define a time-ordered (on C) Green's function:

$$iG(t_1,t_2) =< T_C c_I(t)c_I^\dagger(t) >= G^>(t_1,t_2)\theta_C(t_1-t_2) - G^<(t_1,t_2)\theta_C(t_2-t_1) \tag{2.51}$$

where the contour C goes through t and t' and $\theta_C(t-t) = 1$ if C is such that $t\prime$ is met first and 0 otherwise.

2.4.1 Complex-Time Integrals by Langreth's Technique

Let A and B denote contour-time-ordered Green's functions expressed in terms of $>$ and $<$ functions as

$$A(t,t') = -ia^>(t,t')\theta_C(t-t') + ia^<(t,t')\theta_C(t'-t) \tag{2.52}$$

$$B(t,t') = -ib^>(t,t')\theta_C(t-t') + ib^<(t,t')\theta_C(t'-t). \tag{2.53}$$

Following Langreth we must develop their combinations in series which is needed to calculate diagrams in this theory. The combination in series $D = AB$ is defined by

$$\begin{aligned} D(t,t') &= AB(t,t') = \int_C d\tau A(t,\tau)B(\tau,t') \\ &= -id^>(t,t')\theta_C(t-t') + id^<(t,t')\theta_C(t'-t) \end{aligned} \tag{2.54}$$

and must be rewritten as a combination of ordinary real-axis integrals. To calculate $d^<(t,t')$ we want t to be earlier on the contour, so we adopt $C = C_1 > C_2$ like in Figure. C_1 starts from t_0 and returns there after visiting t, C_1 starts from t_0 and returns there after visiting t'. Along $C_1, \tau <_C t \Rightarrow B = ib^<$, while along $C_2, \tau >_C t \Rightarrow A = ia^<$, hence

$$d^<(t,t') = -iD = d^<[C_1] + d^>[C_2] \tag{2.55}$$

$$d^<[C_1] = -i\int_C d\tau A(t,\tau)ib^<(\tau,t') \tag{2.56}$$

$$d^>[C_2] = -i\int_C d\tau ia^<(t,\tau)B(\tau,t') \tag{2.57}$$

On $C1$, $A = -ia^>$ on the $t_0 < \tau < t$ branch, $A = ia^<$on the back trip, so

$$\begin{aligned} d^<[C_1] &= \int_{t_0}^{t} d\tau(-i)a^>(t,\tau)b^<(\tau,t') + \int_{t}^{t_0} d\tau i a^<(t,\tau)b^<(\tau,t') \\ &= \int_{t_0}^{t} d\tau(-i)[a^>(t,\tau) - a^<(t,\tau)]b^<(\tau,t') \end{aligned} \tag{2.58}$$

Now we let $t_0 \to -\infty$, and formally extend the integration to the full real axis introducing a theta function. The result is

$$\begin{aligned} d^<[C_1] &= \int_{-\infty}^{\infty} d\tau(-i)\{[a^>(t,\tau) - a^<(t,\tau)]\theta(t-\tau)\}b^<(\tau,t') \\ &= \int_{-\infty}^{\infty} d\tau a_r(t,\tau)b^<(\tau,t') = a_r b^< \end{aligned} \tag{2.59}$$

using Langreth's convenient shorthand notation (product of small letters for real axis integrals). One finds $d^<[C2]$ and $d^>$ in a similar way and get

$$\begin{aligned} d^< &= a_r b^< + a^< b_a \\ d^> &= a_r b^> + a^> b_a. \end{aligned} \tag{2.60}$$

From $d^<$, $d^>$ one finds d_r, d_a:

$$d_r = -i\theta(t-t')[d^< + d^>] = -i\theta(t-t')[a_r b^< + a^< b_a + a_r b^> + a^> b_a], \tag{2.61}$$

that is, more explicitly,

$$d_r(t,t') = -i\theta(t-t')\int_{-\infty}^{\infty} d\tau\{a_r(t-\tau)[b^>(\tau,t')+b^<(\tau,t')]+[a^>(\tau,t')+a^<(\tau,t')]b_a(\tau,t')\} \tag{2.62}$$

Since $g^< + g^> = i(g_r - g_a)$, we can simplify this to read

$$d_r(t,t') = \theta(t-t')\int_{-\infty}^{\infty} d\tau\{a_r(t-\tau)b_r(\tau,t') - a_a(t-\tau)b_a(\tau,t')\} \tag{2.63}$$

However, the second integrand vanishes unless $t > \tau > t$ but then the θ in front of the integral

vanishes; therefore, we conclude that

$$d_r = a_r b_r, \tag{2.64}$$

$$d_a = a_a b_a. \tag{2.65}$$

The series combination $E = ABC$ is immediately obtained:

$$e^{>} = (AB)_r c^{>} + (AB)^{>} c_a = a_r b_r c^{>} + (a_r b^{>} + a^{>} b_a) c_a, \tag{2.66}$$

$$e^{<} = (AB)_r c^{<} + (AB)^{<} c_a = a_r b_r c^{<} + (a_r b^{<} + a^{<} b_a) c_a, \tag{2.67}$$

2.5 General model formulation: Time-independent

We consider the time-independent formulation of our model problem. The system that we model is a molecule/quantum dot connected to leads and analyze electron transport through this system. In the present case, we have two leads, right (R) and left (L) and a single molecule such as a quantum dot. Hamiltonian of our simple system is

$$H = H_0 + \Delta H_\alpha \tag{2.68}$$

$$H_0 = \varepsilon_0 c_0^\dagger c_0 + H_{leads}, \qquad \Delta H_\alpha = H_{dot-leads}$$

where $\alpha = L$ or R stands for each lead and ε_0 is the single energy level of electrons on the dot with $c_0^\dagger, c_0$ the corresponding creation and annihilation operators. The remaining elements of the Hamiltonian are

$$H_{leads} = \sum_j \epsilon_j c_j^\dagger c_j, \tag{2.69}$$

$$H_{leads-dot} = \frac{1}{\sqrt{N}} \sum_j V_\alpha \left(c_j^\dagger c_0 + c_0^\dagger c_j \right), \tag{2.70}$$

where N is the total number of states in the lead, j represents the channels in one of the leads $\alpha = L, R$. For the second lead the Hamiltonian can be written in the same way.

Now the Green's function on the dot due to interaction with the leads can be written as

[see Appendix]

$$G_{00}(E) = g_{00}(E) + \sum_{\alpha} g_{00}(E)\Delta H_{0,\alpha} G_{\alpha,0}(E), \tag{2.71}$$

where the unperturbed Green's function on the dot is g_{00} while the perturbed one on the dot due to the lead (α) is $G_{\alpha,0}(E)$. With the help of $G_{\alpha,0}(E)$, one can write Eq. (2.71) as

$$G_{00}(E) = g_{00}(E) + \sum_{\alpha} g_{00}(E)\Delta H_{0,\alpha}\{g_{\alpha,0}(E) + g_{\alpha,\alpha}(E)\Delta H_{\alpha,0} G_{00}(E)\}. \tag{2.72}$$

Using the fact that $g_{\alpha,0}(E)$ is zero the two sites are uncoupled, Eq. (2.72) is simplified to

$$G_{00}(E) = g_{00}(E) + \sum_{\alpha} g_{00}(E)\Delta H_{0,\alpha} g_{\alpha,\alpha}(E)\Delta H_{\alpha,0} G_{00}(E). \tag{2.73}$$

Using $\Sigma_{00} = \sum_{\alpha} \Delta H_{0,\alpha} g_{\alpha,\alpha}(E)\Delta H_{\alpha,0}$, the self-energy calculated in the next section, the expression Eq. (2.73) may be written as

$$G_{00}(E) = g_{00}(E) + g_{00}(E)\Sigma_{00} G_{00}(E), \tag{2.74}$$

which is the standard Dyson's Green's function expression.

With the help of Eq. (2.74), the retarded (advanced) Green's function may be written as

$$G_{00}^{r(a)}(E) = g_{00}^{r(a)} + g_{00}^{r(a)}(E)\Sigma_{00}^{r(a)} G_{00}^{r(a)}(E) \tag{2.75}$$

$$[1 - g_{00}^{r(a)}(E)\Sigma_{00}^{r(a)}] G_{00}^{r(a)}(E) = g_{00}^{r(a)} \tag{2.76}$$

$$G_{00}^{r(a)}(E) = \frac{g_{00}^{r(a)}}{[1 - g_{00}^{r(a)}(E)\Sigma_{00}^{r(a)}]} \tag{2.77}$$

$$G_{00}^{r(a)}(E) = \frac{1}{[[g_{00}^{r(a)}]^{-1} - \Sigma_{00}^{r(a)}]}. \tag{2.78}$$

Hence, the final result is written as

$$G_{00}^{r(a)}(E) = [E - E_0 - \Sigma_{00}^{r(a)}]^{-1}. \tag{2.79}$$

$G_{00}^{r(a)}(E)$ has poles in one half-plane and are sufficient ingredients for calculating the physical

response of the system. Information about the spectral properties, density of states and scattering rates are contained in these functions. $\Sigma_{00}^{r(a)}$ behaves as an exact contribution to the energy of the dot. Hence, the term "self-energy".

2.5.1 The Self-energy

The self-energy represents the contribution to the dot energy, due to interactions between the dot and the leads it is coupled to. We use the wide-band approximation where the self-energy of the dot due to each lead is considered to be energy independent. The self-energy defined in the previous section can be calculated in the following way

$$\Sigma_{00}^{r} = \Delta H_{0,\alpha} g_{\alpha,\alpha}^{r}(E) \Delta H_{\alpha,0}, \tag{2.80}$$

where

$$\begin{aligned} g_{\alpha,\alpha}^{r}(E) &= \frac{1}{N} \sum_{j} g_{\alpha,j}^{r}(E) \\ &= \frac{1}{N} \int_{-\infty}^{+\infty} N \frac{n_\alpha d\varepsilon_\alpha}{\varepsilon - \varepsilon_\alpha} \end{aligned} \tag{2.81}$$

where $g_{\alpha,\alpha}^{r}(E)$ is the uncoupled Green's function in the leads, $\sum_{j} = \int_{-\infty}^{+\infty} N n_\alpha d\varepsilon_\alpha$, j stands for channels in each lead, and n_α is the density of states in lead α. The retarded self-energy can be rewritten as

$$\Sigma_{00}^{r} = \Delta H_{0,\alpha} \frac{1}{N} \int_{-\infty}^{+\infty} N \frac{n_\alpha d\varepsilon_\alpha}{\varepsilon - \varepsilon_\alpha} \Delta H_{\alpha,0}, \tag{2.82}$$

which can be simplified as follows

$$\begin{aligned}\Sigma^r_{00} &= |V_{0.\alpha}|^2 \int_{-\infty}^{+\infty} \frac{n_\alpha d\varepsilon_\alpha}{\varepsilon - \varepsilon_\alpha} \\ &= -|V_{0,\alpha}|^2 n_\alpha \int_{-\infty}^{+\infty} \frac{d\varepsilon_\alpha}{\varepsilon_\alpha - \varepsilon} \\ &= -|V_{0,\alpha}|^2 n_\alpha \times (2\pi i) \\ &= \frac{-i\Gamma_\alpha}{2},\end{aligned} \tag{2.83}$$

where $\Gamma_\alpha = 4\pi |V_{0,\alpha}|^2 n_\alpha$, and $\Sigma^a_\alpha = (\Sigma^r_\alpha)^* = \frac{i\Gamma_\alpha}{2}$ and α represents the L or R lead.

2.5.2 Dyson's equation and the Lesser Green's function

The standard Dyson's equation (2.74) may be rewritten as

$$G^{r(a)}_{00}(E) = g^{r(a)}_{00}(E) + g^{r(a)}_{00}(E)\Sigma^{r(a)}_{00}G^{r(a)}_{00}(E), \tag{2.84}$$

where G^r_{00} and G^a_{00} are the retarded and advanced Green's functions respectively.

Applying Langreth's theorem (2.67) to equation (2.84) in order to derive a relation for the $G^<_{00}$ on the dot, the above becomes

$$G^<_{00} = g^<_{00}(E) + g^r_{00}(E)\Sigma^r_{00}G^<_{00}(E) + g^r_{00}(E)\Sigma^<_{00}G^a_{00}(E) + g^<_{00}(E)\Sigma^a_{00}G^a_{00}(E), \tag{2.85}$$

which can be rewritten as

$$\{1 - g^r_{00}(E)\Sigma^r_{00}\}G^<_{00} = g^<_{00}(E) + g^r_{00}(E)\Sigma^<_{00}G^a_{00}(E) + g^<_{00}(E)\Sigma^a_{00}G^a_{00}(E) \tag{2.86}$$

$$\{1 - g^r_{00}(E)\Sigma^r_{00}\}G^<_{00} = g^<_{00}(E)\{1 + \Sigma^a_{00}G^a_{00}(E)\} + g^r_{00}(E)\Sigma^<_{00}G^a_{00}(E) \tag{2.87}$$

$$G^<_{00} = \{1 - g^r_{00}(E)\Sigma^r_{00}\}^{-1}[g^<_{00}(E)\{1 + \Sigma^a_{00}G^a_{00}(E)\} + g^r_{00}(E)\Sigma^<_{00}G^a_{00}(E)] \tag{2.88}$$

$$G^<_{00} = \{1-g^r_{00}(E)\Sigma^r_{00}\}^{-1}g^<_{00}(E)\{1+\Sigma^a_{00}G^a_{00}(E)\}+\{1-g^r_{00}(E)\Sigma^r_{00}\}^{-1}g^r_{00}(E)\Sigma^<_{00}G^a_{00}(E)]. \tag{2.89}$$

Eq. (2.89) can be further simplified by using the following relations $\{1 - g^r_{00}(E)\Sigma^r_{00}\}^{-1} =$

$\{1 + G^r_{00}(E)\Sigma^r_{00}\}$, and $\{1 - g^r_{00}(E)\Sigma^r_{00}\}^{-1} g^r_{00}(E) = G^r_{00}(E)$. Hence, the final result is

$$G^<_{00} = \{1 + G^r_{00}(E)\Sigma^r_{00}\} g^<_{00}(E)\{1 + \Sigma^a_{00} G^a_{00}(E)\} + G^r_{00}(E)\Sigma^<_{00} G^a_{00}(E). \tag{2.90}$$

For the unperturbed system, the dot is initially empty due to which $g^<_{00}(E)$ is zero. Thus Eq. (2.90) can be written as

$$G^<_{00} = G^r_{00}(E)\Sigma^<_{00} G^a_{00}(E), \tag{2.91}$$

This is the Keldysh's nonequilibrium Green's function result and is related to the density matrix through the following relation

$$\rho_{00} = -iG^<_{00}. \tag{2.92}$$

This is the central result of this formal development.

The lesser Green's function is called the particle propagator and the greater is called the hole propagator in which the order of the operators (creation & annihilation) is reversed. By using Eq. (2.43)

$$G^> = -i[1 - f(E)](G^a - G^r), \tag{2.93}$$

where $f(E)$ is the Fermi-Dirac distribution function. The lesser and the greater Green's functions are directly linked to physical observables and properties of the system such as dot population and current.

The lesser self-energy may be written as (using Eq. (2.42))

$$\Sigma^<_\alpha = f_\alpha(E)[\Sigma^a_\alpha - \Sigma^r_\alpha] \tag{2.94}$$

From Eq. (2.83)

$$\Sigma^<_\alpha = i\Gamma_\alpha f_\alpha(E), \tag{2.95}$$

where $f_\alpha(E)$ is the Fermi-Dirac distribution function and α represents the L or R leads. Similarly one can calculate the greater self-energy as

$$\Sigma_\alpha^> = -i\Gamma_\alpha[1 - f_\alpha(E)]. \tag{2.96}$$

Chapter 3

Current through a nanosystem: Meir-Wingreen-Jauho formula

In the last chapter, we have developed the formalism to calculate the Green functions for the interacting central region, which is coupled to the leads [5, 6, 7, 8, 29]. Now we have to relate those Green functions to physical quantities such as current. The general result that we shall derive is known as the Meir-Wingreen-Jauho current formula. This important result shows that the current can be calculated, if the spectral (G^r, G^a) and kinetic $(G^<, G^>)$ Green functions of the central region are known, and it is exact in the case of noninteracting leads. Time-independent current can be easily formulated by taking the Fourier transform of time dependent case. Further, we apply the formalism to investigate $I - V$ characteristics of a resonant tunneling diode.

3.1 Model Hamiltonian

We split the total Hamiltonian in three pieces:

$$H = H_c + H_T + H_{cen}, \tag{3.1}$$

where H_c describes the contacts, H_T is the tunneling coupling between contacts and the interacting region, and H_{cen} models the interacting central region, respectively. Below we discuss

each of these terms.

3.1.1 The contact Hamiltonian H_c

We view electrons in the leads as noninteracting except for an overall self-consistent potential. Thus, the contact Hamiltonian is

$$H_c = \sum_{k\alpha \epsilon L,R} \varepsilon_{k\alpha} c^{\dagger}_{k\alpha} c_{k\alpha} \tag{3.2}$$

and the Green functions in the leads for the uncoupled system are:

$$\begin{aligned} g^{<}_{k\alpha}(t-t') &= i < c^{\dagger}_{k\alpha}(t') c_{k\alpha}(t) > \\ &= i f(\epsilon^{0}_{k\alpha}) \exp[-i\varepsilon_{k\alpha}(t-t')]. \end{aligned} \tag{3.3}$$

$$\begin{aligned} g^{r}_{k\alpha}(t-t') &= -i\theta(t-t') < \{c_{k\alpha}(t), c^{\dagger}_{k\alpha}(t')\} > \\ &= -i\theta(t-t') \exp[-i\varepsilon_{k\alpha}(t-t')] \end{aligned} \tag{3.4}$$

and

$$\begin{aligned} g^{a}_{k\alpha}(t-t') &= i\theta(-t+t') < \{c_{k\alpha}(t), c^{\dagger}_{k\alpha}(t')\} > \\ &= -i\theta(-t+t') \exp[-i\varepsilon_{k\alpha}(t-t')]. \end{aligned}$$

Here

$$f(\varepsilon_{k\alpha}) = [exp[(\varepsilon_{k\alpha} - \mu_{\alpha})/k_B T] + 1]^{-1}$$

is the equilibrium distribution in a given lead.The operator $c_{k\alpha}$ ($c^{\dagger}_{k\alpha}$) destroys (creates) an electron with wave vector k in lead α.

3.1.2 Coupling between leads and central region, H_T

The coupling between the lead and the central region can be modified with the time dependent gate voltage. Hence,

$$H_T = \sum_{k\alpha\epsilon L} [V_{k\alpha,n}(t) c^\dagger_{k\alpha} d_n + H.c] \tag{3.5}$$

Here, $\{d^\dagger_n\}$ and $\{d_n\}$ are the single-electron creation and annihilation operators in the central region.

3.1.3 The central region hamiltonian, H_{cen}

The form chosen for the central region Hamiltonian H_{cen} depends on geometry and on the physical behavior being investigated. We take the central region to consist of noninteracting, but time-dependent levels,

$$H_{cen} = \sum_m \varepsilon_m(t) d^\dagger_m d_{m.}, \tag{3.6}$$

Here, $d^\dagger_m(d_m)$ creates (destroys) an electron in state m. The choice made in Eq. (3.6) represents a simple model for time dependent resonant tunneling. Below we shall present general results for an arbitrary number of levels, and analyze the case of a single level, which is exactly solvable in detail.

3.2 General Expression For Current

The current from the left lead contact through the right barrier to the centrel region can be calculated from the time evolution of the occupation number operator of the left contact:

$$J_L = -e < \dot{N}_L >= -\frac{ie}{\hbar} < [H, N_L] > \tag{3.7}$$

where

$$N_L = \sum_{k\alpha\epsilon L} c^\dagger_{k\alpha} c_{k\alpha}$$

and

$$H = H_c + H_T + H_{cen}.$$

Since H_c and H_{cen} commute with N_L we only need to calculate

$$\begin{aligned}
[H_T, N_L] &= [\sum_{\substack{k'\alpha'\epsilon L \\ n}} (V_{k'\alpha',n}(t) c^\dagger_{k'\alpha'} d_n + H.c), \sum_{k\alpha\epsilon L} c^\dagger_{k\alpha} c_{k\alpha}] \\
&= \sum_{\substack{k'\alpha' k\alpha\epsilon L \\ n}} V_{k'\alpha',n}(t) c^\dagger_{k\alpha} d_n [c^\dagger_{k'\alpha'}, c_{k\alpha}] + H.c \\
&= \sum_{\substack{k'\alpha'\epsilon L \\ n}} -V_{k'\alpha',n}(t) c^\dagger_{k\alpha} d_n + V^*_{k'\alpha',n}(t) d^*_n c_{k\alpha} \qquad (3.8)
\end{aligned}$$

and hence,

$$J_L = \frac{ie}{\hbar} \sum_{k'\alpha'\epsilon L} [V_{k'\alpha',n}(t) < c^\dagger_{k\alpha} d_n > - V^*_{k'\alpha',n}(t) < d^*_n c_{k\alpha} >]. \qquad (3.9)$$

Now we define two Green functions

$$\begin{aligned}
G^<_{n,k\alpha}(t,t') &= i < c^\dagger_{k\alpha}(t') d_n(t) > \\
G^<_{k\alpha,n}(t,t') &= i < d^\dagger_n(t') c_{k\alpha}(t) > . \qquad (3.10)
\end{aligned}$$

Using

$$G^<_{n,k\alpha}(t,t) = -[G^<_{n,k\alpha}(t,t)]^* \qquad (3.11)$$

the current can be expressed as

$$J_L = \frac{2e}{\hbar} \mathrm{Re}\{\sum_{\substack{k\alpha\epsilon L \\ n}} V_{k\alpha,n}(t) G^<_{n,k\alpha}(t,t)\}. \qquad (3.12)$$

We now require an expression for $G^<_{n,k\alpha}(t,t')$. For the present case, with non-interacting leads, a general relation for contour-ordered Green function $G_{n,k\alpha}(\tau,\tau')$ can be derived easily with the equation of motion technique as follows: Equation-of-motion for the time-ordered Green function $G_{n,k\alpha}$ in Eq. (3.10) is

$$\begin{aligned}
-i\frac{\partial}{\partial t'} G_{n,k\alpha}(t-t') &= \varepsilon_{k\alpha} G_{n,k\alpha}(t-t') + \sum_m G_{nm}(t-t') V^*_{k\alpha,m}(t) \\
(-i\frac{\partial}{\partial t'} - \varepsilon_{k\alpha}) G_{n,k\alpha}(t-t') &= \sum_m G_{nm}(t-t') V^*_{k\alpha,m}(t).
\end{aligned}$$

We can interpret the factor $(-i\frac{\partial}{\partial t'} - \varepsilon_{k\alpha})$ multiplying $G_{n,k\alpha}(t-t')$ as the inverse of the contact Green function operator and introduce a short-hand notation:

$$G_{n,k\alpha}(t-t')g^{-1}_{k\alpha} = \sum_m G_{nm}(t-t')V^*_{k\alpha,m}(t) \tag{3.13}$$

By operating with $g_{k\alpha}$ from right, we arrive at

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

$$G_{n,k\alpha}(\tau,\tau') = \sum_m \int d\tau_1 G_{nm}(\tau,\tau_1)V^*_{k\alpha,m}(\tau_1)g_{k\alpha}(\tau_1,\tau). \tag{3.14}$$

Here $G_{nm}(\tau,\tau_1)$ is the contour ordered Green function for the central region.

Now using the Langreth technique Eq. (2.60) we find that

$$G^<_{n,k\alpha}(t,t) = \sum_m \int dt_1 V^*_{k\alpha,m}(t_1)[G^r_{nm}(t,t_1)g^<_{k\alpha}(t_1,t) + G^<_{nm}(t,t_1)g^a_{k\alpha}(t_1,t)] \tag{3.15}$$

whereby the current becomes

$$\begin{aligned} J_L(t) &= \frac{2e}{\hbar}\,\mathrm{Re}\{\sum_{\substack{k\alpha\epsilon L\\ m,n}} V_{k\alpha,n}(t)\int dt_1 V^*_{k\alpha,m}(t_1) \\ &\quad [G^r_{nm}(t,t_1)g^<_{k\alpha}(t_1,t) + G^<_{nm}(t,t_1)g^a_{k\alpha}(t_1,t)]\}. \end{aligned} \tag{3.16}$$

$$\begin{aligned} &= \frac{2e}{\hbar}\int dt_1\,\mathrm{Re}\sum_{\substack{k\alpha\epsilon L\\ m,n}} V_{k\alpha,n}(t)V^*_{k\alpha,m}(t_1) \\ &\quad [G^r_{nm}(t,t_1)g^<_{k\alpha}(t_1,t) + G^<_{nm}(t,t_1)g^a_{k\alpha}(t_1,t)]. \end{aligned} \tag{3.17}$$

At this juncture, it is useful to convert the momentum summations to energy integrations and define a level-width function:

$$[\Gamma(\varepsilon,t,t_1)]_{mn} = 2\pi\sum_{\alpha\epsilon L} n_\alpha(\varepsilon)V_{\alpha,n}(\varepsilon,t)V^*_{\alpha,m}(\varepsilon,t_1) \tag{3.18}$$

where $V_{k\alpha,n}(t) = V_{\alpha,n}(\varepsilon,t)$, where $n(\varepsilon)$ is the density of states. There are two terms in the current expression. Consider, for example, the piece involving G^r_{nm}, which we evaluate as

$$J_L(t) = \frac{2e}{\hbar}\int dt_1 \int \frac{d\varepsilon}{2\pi}\,\mathrm{Re}\{\sum_{\substack{k\alpha\epsilon L\\ m,n}} V_{k\alpha,n}(\varepsilon,t)V^*_{n,k\alpha}(\varepsilon,t)[G^r_{nm}(t,t_1)g^<_{k\alpha}(t_1,t) + G^<_{nm}(t,t_1)g^a_{k\alpha}(t_1,t)]\} \tag{3.19}$$

$$\begin{aligned} J_L(t) &= \frac{2e}{\hbar}\int dt_1 \int \frac{d\varepsilon}{2\pi}\Gamma^L(\varepsilon,t,t_1)\,\mathrm{Re}[G^r_{nm}(t,t_1)if_L(\epsilon^0_{k\alpha}) \\ &\quad \exp[-i\varepsilon_{k\alpha}(t_1-t) - G^<_{nm}(t,t_1)i\theta(-t+t')\exp[-i\varepsilon_{k\alpha}(t-t')]] \end{aligned} \tag{3.20}$$

$$\begin{aligned} J_L(t) &= -\frac{2e}{\hbar}\int_{-\infty}^{t} dt_1 \int \frac{d\varepsilon}{2\pi}\exp[-i\varepsilon_{k\alpha}(t_1-t)]\Gamma^L(\varepsilon,t,t_1) \\ &\quad \mathrm{Im}[G^r_{nm}(t,t_1)f_L(\epsilon^0_{k\alpha}) + G^<_{nm}(t,t_1)] \end{aligned} \tag{3.21}$$

$$\begin{aligned} J_L(t) &= -\frac{2e}{\hbar}\int_{-\infty}^{t} dt_1 \int \frac{d\varepsilon}{2\pi}\,\mathrm{Im}\,Tr\{\exp[-i\varepsilon_{k\alpha}(t_1-t)]\Gamma^L(\varepsilon,t,t_1) \\ &\quad [G^<_{nm}(t,t_1) + G^r_{nm}(t,t_1)f_L(\epsilon^0_{k\alpha})]\} \end{aligned} \tag{3.22}$$

This is the central formal result. The current is expressed in term of the local quantities: Green functions of the central region. The first term which is proportional to the lesser function $G^<$ suggests an interpretation as an out-tunneling rate [recall $Im\ G^< = N$]. Likewise, the second term which is proportional to the occupation in the leads and to the density of states in the central region, can be associated to the in-tunneling rate. However, one should bear in mind that all Green functions in the above equation are to be calculated in the presence of tunneling. Thus, $G^<$ may depend on the occupation in the leads. Furthermore, in the presence of interactions, G^r may depend on the central-region occupation. Consequently, the current can be a nonlinear function of the occupation factors.

3.3 Time-independent case

3.3.1 General expression

In the time-independent limit the line-width function simplifies:

$$\Gamma(\varepsilon, t, t_1) \rightarrow \Gamma(\varepsilon)$$

and the t_1 integration is performed and we get the current from the left (right) contact to the central region becomes,

$$J_{L(R)}(t) = \frac{ie}{\hbar}\int \frac{d\varepsilon}{2\pi} Tr\{\Gamma^L(\varepsilon)[G^<(\varepsilon) + [G^r(\varepsilon) - G^r(\varepsilon)]f_L(\varepsilon)]\}. \tag{3.23}$$

In the steady state, the current will be uniform, so that

$$J = J_L = -J_R$$

or the current J is

$$J = \frac{J_L + J_L}{2} = \frac{J_L - J_R}{2}.$$

Thus the general expression for current in this case is

$$J = \frac{ie}{2\hbar}\int \frac{d\varepsilon}{2\pi} Tr\{(\Gamma^L(\varepsilon) - \Gamma^R(\varepsilon))G^<(\varepsilon) + (\Gamma^L(\varepsilon)f_L(\varepsilon) - \Gamma^R(\varepsilon)f_R(\varepsilon))[G^r(\varepsilon) - G^r(\varepsilon)]\}. \tag{3.24}$$

3.3.2 Proportionate coupling

If the left and right line-width functions are proportional to each other, i.e., $\Gamma^L(\varepsilon) = \lambda\Gamma^R(\varepsilon)$, a very simple final result can be acheived. We observe that the current can be written as

$$J \equiv xJ_L - (1-x)J_R$$

which gives, using

$$J = \frac{ie}{\hbar}\int \frac{d\varepsilon}{2\pi} Tr\{\Gamma^R(\varepsilon)[(\lambda x - (1-x))G^<(\varepsilon) + (\lambda x f_L(\varepsilon) - (1-x)f_R(\varepsilon))(G^r(\varepsilon) - G^r(\varepsilon))]\} \tag{3.25}$$

The arbitrary parameter x is now fixed so that the first term vanishes, i.e.,$x = 1/(1+\lambda)$, which results in

$$J = \frac{ie}{\hbar}\int \frac{d\varepsilon}{2\pi}(f_L(\varepsilon) - f_R(\varepsilon)Tr\{\frac{\Gamma^L(\varepsilon)\Gamma^R(\varepsilon)}{\Gamma^L(\varepsilon)+\Gamma^R(\varepsilon)}[G^r(\varepsilon) - G^r(\varepsilon)]\}. \tag{3.26}$$

The ratio is well-defined because the Γ-matrices are proportional. The difference between the retarded and advanced Green functions is essentially the density of states.

3.4 Current Conservation

Any meaningful theory of transport must respect current conservation. Here we examine what implications this necessary requirement has on the derived expressions for the current flowing between the contacts and the central region. To this end, it is convenient to rewrite the current expression Eq. (3.19) as

$$\begin{aligned} J_L(t) &= \frac{2e}{\hbar}\int dt_1 \int \frac{d\varepsilon}{2\pi}\,\mathrm{Re}\{\sum_{\substack{k\alpha\epsilon L\\ m,n}} V_{k\alpha,n}(\varepsilon,t)V^*_{n,k\alpha}(\varepsilon,t) \\ &\quad [G^r_{nm}(t,t_1)g^<_{k\alpha}(t_1,t) + G^<_{nm}(t,t_1)g^a_{k\alpha}(t_1,t)]\} \end{aligned} \tag{3.27}$$

For the time independent case $V_{k\alpha,n}(\varepsilon,t) \to V_{k\alpha,n}(\varepsilon)$ and after doing the integration on t as in the time independent case we get

$$J_L = \frac{2e}{\hbar}\int \frac{d\varepsilon}{2\pi}\,\mathrm{Re}\{\sum_{\substack{k\alpha\epsilon L\\ m,n}} V_{k\alpha,n}(\varepsilon)V^*_{n,k\alpha}(\varepsilon)[G^r_{nm}(\varepsilon)g^<_{k\alpha}(\varepsilon) + G^<_{nm}(\varepsilon)g^a_{k\alpha}(\varepsilon)]\}. \tag{3.28}$$

Using the general relationship $G^r - G^a = G^> - G^<$, valid for both contact and central region Green functions, we re-express

$$J_L = \frac{2e}{\hbar}\int \frac{d\varepsilon}{2\pi}\{\sum_{\substack{k\alpha\epsilon L\\ m,n}} V_{k\alpha,n}(\varepsilon)V^*_{n,k\alpha}(\varepsilon)[G^>_{nm}(\varepsilon)g^<_{k\alpha}(\varepsilon) - G^<_{nm}(\varepsilon)g^>_{k\alpha}(\varepsilon)]\}$$

$$J_L = \frac{2e}{\hbar}\int \frac{d\varepsilon}{2\pi}\{\sum_{\substack{\alpha\epsilon L\\ m,n}}[G^>_{nm}(\varepsilon)\Sigma^<_{\alpha mn}(\varepsilon) - G^<_{nm}(\varepsilon)\Sigma^>_{nm\alpha}(\varepsilon)]\} \tag{3.29}$$

$$J_L = \frac{2e}{\hbar}\int \frac{d\varepsilon}{2\pi}\{Tr[G^{>}(\varepsilon)\Sigma_L^{<}(\varepsilon) - G^{<}(\varepsilon)\Sigma_L^{>}(\varepsilon)]\}$$

where we have defined the tunneling self-energy $\Sigma = \Sigma V^* g V$ with the components

$$\begin{aligned}
\Sigma^{r(a)}_{\alpha mn}(\varepsilon) &= \sum_k V^*_{m,k\alpha}(\varepsilon) g^{r(a)}_{k\alpha}(\varepsilon) V_{k\alpha,n}(\varepsilon) \\
\Sigma^{<}_{\alpha mn}(\varepsilon) &= \sum_k V^*_{m,k\alpha}(\varepsilon) g^{<}_{k\alpha}(\varepsilon) V_{k\alpha,n}(\varepsilon) \\
\Sigma^{<}_{\alpha mn}(\varepsilon) &= \sum_k V^*_{m,k\alpha}(\varepsilon) g^{<}_{k\alpha}(\varepsilon) V_{k\alpha,n}(\varepsilon)
\end{aligned} \tag{3.30}$$

The Green function $G^{<}$ contains the distribution of the occupied electronic states and $G^{>}$ contains information about the empty states, similarly the greater and lesser self-energies from the leads. The product $\Sigma^{>}G^{<}$ represents in this respect the scattering out from the central region, and the other product the in scattering.We next define the total self-energy, which is the sum of tunneling contributions, and the interactions residing in the central region:

$$\Sigma_{tot} = \Sigma_L + \Sigma_R + \Sigma_{int} \tag{3.31}$$

Also the sum of left and right current should vanish.

$$J_L + J_R = \frac{2e}{\hbar}\int \frac{d\varepsilon}{2\pi}\{Tr[G^{>}(\varepsilon)\Sigma^{<}_{tot}(\varepsilon) - G^{<}(\varepsilon)\Sigma^{>}_{tot}(\varepsilon)] - Tr[G^{>}(\varepsilon)\Sigma^{<}_{int}(\varepsilon) - G^{<}(\varepsilon)\Sigma^{>}_{int}(\varepsilon)]\} \tag{3.32}$$

With the Keldysh equations (Eq. (2.91)) for steady state $G^{<} = G^r\Sigma^{<}G^a$

$$\begin{aligned}
\Sigma^{<}_{tot} - \Sigma^{>}_{tot} &= (G^r)^{-1} G^{<} (G^a)^{-1} - (G^r)^{-1} G^{>} (G^a)^{-1} \\
&= (G^r)^{-1} \{G^{<} - G^{>}\} (G^a)^{-1} \\
&= (G^a)^{-1} - (G^r)^{-1}
\end{aligned}$$

so,

$$G^a \left(\Sigma^{<}_{tot} - \Sigma^{>}_{tot}\right) G^r = G^r - G^a = G^{>} - G^{<} \tag{3.33}$$

Now we can show:

$$\begin{aligned} & Tr[G^{>}\Sigma^{<}_{tot} - G^{<}\Sigma^{>}_{tot}] \\ = \; & Tr[\Sigma^{<}_{tot}(G^{>} + G^{a}\Sigma^{>}G^{r} - G^{a}\Sigma^{>}G^{r}) - \Sigma^{>}_{tot}G^{<}] \\ = \; & Tr[\Sigma^{<}_{tot}(G^{r}\Sigma^{>}_{tot}G^{a} + G^{a}\Sigma^{>}_{tot}G^{r} - G^{a}\Sigma^{>}_{tot}G^{r}) - \Sigma^{>}_{tot}G^{a}\Sigma^{<}G^{r}] \\ = \; & 0 \end{aligned} \tag{3.34}$$

the current conservation condition

$$J_L + J_R = 0$$

implies the following constraint on the self-energy Σ_{int}

$$J_L + J_R = \frac{2e}{\hbar}\int \frac{d\varepsilon}{2\pi}\{-Tr[G^{>}(\varepsilon)\Sigma^{<}_{int}(\varepsilon) - G^{<}(\varepsilon)\Sigma^{>}_{int}(\varepsilon)]\} = 0. \tag{3.35}$$

Obviously this shows that if there are no internal interactions the current is conserved.

3.5 Noninteracting Resonant-Level Model

In the noninteracting case (or mean-field models), the Hamiltonian is $H = H_c + H_T + H_{cen}$, where $H_{cen} = \sum_m \varepsilon_m d^{\dagger}_m d_m$. The Dyson and the Keldysh equations are now

$$\begin{aligned} G^{r}(\varepsilon) &= g^{r}(\varepsilon) + g^{r}(\varepsilon)\Sigma^{r}(\varepsilon)G^{r}(\varepsilon) \\ G^{<}(\varepsilon) &= G^{r}(\varepsilon)\Sigma^{<}(\varepsilon)G^{a}(\varepsilon) \end{aligned} \tag{3.36}$$

By taking the Fourier transform of the Green function we get,

$$\begin{aligned} g^{r}(\varepsilon) &= \frac{1}{\varepsilon - \varepsilon_{k\alpha} + i\eta} \\ g^{a}(\varepsilon) &= \frac{1}{\varepsilon - \varepsilon_{k\alpha} - i\eta} \end{aligned} \tag{3.37}$$

where we have defined the self-energy

$$\Sigma^r(\varepsilon) = \sum_{k\alpha\epsilon L,R} V_{k\alpha}^2 g^r(\varepsilon) = \sum_{k\alpha\epsilon L,R} \frac{V_{k\alpha}^2}{\varepsilon - \varepsilon_{k\alpha} + i\eta}. \tag{3.38}$$

Since

$$\Gamma(\varepsilon) = -2\,\mathrm{Im}\,\Sigma^r(\varepsilon) = 2\pi \sum_k \delta(\varepsilon - \varepsilon_{k\alpha}) V_{k\alpha}^2 \tag{3.39}$$

and we define

$$\Lambda(\varepsilon) = \mathrm{Re}\,\Sigma^r(\varepsilon). \tag{3.40}$$

Therefore

$$\Sigma^r(\varepsilon) = \Lambda(\varepsilon) - i\frac{\Gamma(\varepsilon)}{2}. \tag{3.41}$$

Similarly

$$\Sigma^a(\varepsilon) = \Lambda(\varepsilon) + i\frac{\Gamma(\varepsilon)}{2} \tag{3.42}$$

where the real and imaginary parts contain left right contributions: $\Lambda(\varepsilon) = \Lambda^L(\varepsilon) + \Lambda^R(\varepsilon)$ and $\Gamma(\varepsilon) = \Gamma^L(\varepsilon) + \Gamma^R(\varepsilon)$.The lesser self-energy is

$$\begin{aligned} \Sigma^<(\varepsilon) &= \sum_{k\alpha\epsilon L,R} V_{k\alpha}^2 g^<(\varepsilon) \\ &= i[\Gamma^L(\varepsilon) f_L(\varepsilon) + \Gamma^R(\varepsilon) f_R(\varepsilon)]. \end{aligned} \tag{3.43}$$

Using the identity

$$G^r G^a = \frac{G^r - G^a}{G^{a-1} - G^{r-1}} = \frac{A(\varepsilon)}{\Gamma(\varepsilon)} \tag{3.44}$$

where $A(\varepsilon) = i[G^r(\varepsilon) - G^a(\varepsilon)]$,is the spectral function, one can write $G^<$ in a "pseudoequilibrium" form:

$$G^<(\varepsilon) = iA(\varepsilon)\bar{f}(\varepsilon) \tag{3.45}$$

where

$$\begin{aligned} \bar{f}(\varepsilon) &= \frac{\Gamma^L(\varepsilon)f_L(\varepsilon) + \Gamma^R(\varepsilon)f_R(\varepsilon)}{\Gamma(\varepsilon)} \\ A(\varepsilon) &= \frac{\Gamma(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + \left[\frac{\Gamma(\varepsilon)}{2}\right]^2}. \end{aligned} \tag{3.46}$$

The current becomes

$$J = \frac{e}{\hbar}\int \frac{d\varepsilon}{2\pi} \frac{\Gamma^L(\varepsilon)\Gamma^R(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + \left[\frac{\Gamma(\varepsilon)}{2}\right]^2}(f_L(\varepsilon) - f_R(\varepsilon). \tag{3.47}$$

Note that this derivation made no assumptions about proportionate coupling to the leads. The factor multiplying the difference of the Fermi functions is the familiar expression for elastic transmission coefficient $T(\varepsilon)$ through a resonant level [31].

If the level-width and level-shift functions Γ and Λ are energy-independent, it is easy to evaluate the integral in equation (3.47), and get the current–voltage characteristic.However, the model still lacks two essential ingredients before the nonmonotonic IV-curve characteristic of RTD devices can be obtained. The first missing item concerns the band-widths of the contacts: so far the band-width is essentially infinite. This failure can be remedied by considering a model where the contacts have a finite, occupied band-width; we introduce a low energy cutoff $D_{L/R}$, in addition to the upper cutoff provided by the electrochemical potential. Further, we must specify how the central-region energy ε_0 depends on the applied voltage $\mu_L - \mu_R = eV$. However, for present purposes it is sufficient to simply assume that the left chemical potential μ_L defines the zero-point for energy, and that the other two field-dependencies are given by $\mu_R(V) = \mu_R - eV$, and $\varepsilon_0(V) = \varepsilon_0 - eV/2$, respectively. The zero-temperature IV-characteristic is then

$$\begin{aligned} J_{dc}(V) = \frac{e}{\hbar}[&\int_{\mu_L - D_L - \varepsilon_0(V)}^{\mu_L - \varepsilon_0(V)} \frac{d\varepsilon}{2\pi} \frac{\Gamma^L\Gamma^R}{[\varepsilon - \varepsilon_0 - \Lambda]^2 + \left[\frac{\Gamma}{2}\right]^2} \\ &- \int_{\mu_R - D_R - \varepsilon_0(V)}^{\mu_R - \varepsilon_0(V)} \frac{d\varepsilon}{2\pi} \frac{\Gamma^L\Gamma^R}{[\varepsilon - \varepsilon_0 - \Lambda]^2 + \left[\frac{\Gamma}{2}\right]^2}] \end{aligned}$$

$$J_{dc}(V) = \frac{e}{\hbar}\frac{2\Gamma^L\Gamma^R}{\Gamma}[Tan^{-1}(\frac{\mu_L - \varepsilon_0(V)}{\Gamma/2}) - Tan^{-1}(\frac{\mu_L - D_L - \varepsilon_0(V)}{\Gamma/2}) - Tan^{-1}(\frac{\mu_R - \varepsilon_0(V)}{\Gamma/2}) + Tan^{-1}(\frac{\mu_R - D_R - \varepsilon_0(V)}{\Gamma/2})]. \quad (3.48)$$

We note that the strong increase in current, which is observed in experimental systems at very high voltages, is not present in our model: this is because we have ignored the bias-dependence of the barrier heights as well as any higher lying resonances.

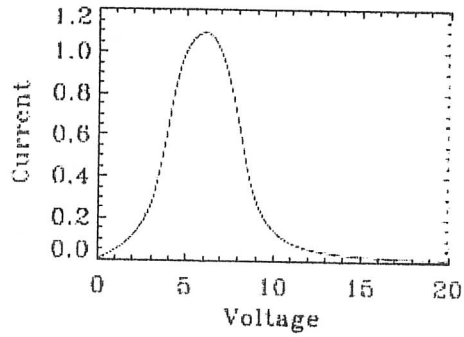


Fig. 3. 1 IV-characteristic for a model resonant tunneling device. The system is defined by parameters $\varepsilon_0(V = 0) = 2$, $\mu_L = \mu_R(V = 0) = 0$, and $D_L = D_R = 2$. The energy parameters are in units of Γ, and the current is shown in units of $e\Gamma/\hbar$

Chapter 4

Single particle quantum transport in a resonant tunnel junction coupled to a nanomechanical oscillator

4.1 Introduction

In this chapter, we apply the formalism introduced in chapter 2 to study electron transport in NanoElectromechanical (NEM) systems. The NEM system that we consider is a single dot and a single oscillator with strong coupling between them [32, 33]. An arbitrary voltage is applied to the tunnel junction and the electrons in the leads are considered to be at zero temperature. We consider the electronic state of the dot as empty/occupied (a two-level system). This chapter is based on the work carried out in [12]. In the present model the system is initially in its ground state and we assume strong dissipation of the nanomechanical oscillator. This means that every independent electron which comes onto the dot finds the oscillator in its ground state. We consider a finite chemical potential difference between the right and left leads. In addition to the main resonant feature due to electrons on the dot, we find satellite features due to creation or annihilation of phonons. These satellite features become sharper and more significant with increasing strength of coupling between the electrons and the oscillator.

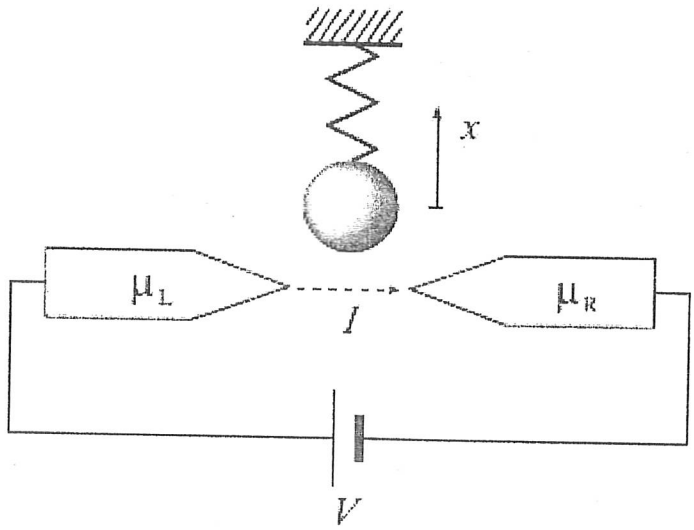


Figure 4-1: Oscillator coupled to an electrical tunnel junction. As a result of an applied voltage V, electrons will tunnel from the left (L) to the right (R) electrode, with tunnel rates depending on the position x of a nearby mechanical oscillator. The electromechanical coupling can be achieved by putting a net non-zero charge (or voltage) on a metallized

4.2 A Simple Model Hamiltonian

In this model, we describe electrons tunneling between a left and a right lead (electron reservoir H_{leads}) through a single dot level ε_0 that is coupled to a single phonon mode with creation operator $b^\dagger$.The total Hamiltonian (system plus coupling to leads) is [12, 16, 17]

$$H = H_{ph-dot} + H_{leads} + H_T \tag{4.1}$$

The system Hamiltonian H_{ph-dot} describes a single dot level ε_0 linearly coupled to a single harmonic oscillator mode,

$$H_{ph-dot} = \left[\varepsilon_0 + \alpha(b^\dagger + b)\right] c_0^\dagger c_0 + H_{ph}\,, \tag{4.2}$$

the second term in the bracket describe a linear coupling between the charge on the dot-level and the vibrational coordinate, where the proportionality constant α is the electron-vibration coupling and

$$H_{ph} = \frac{\widehat{p}^2}{2m} + \frac{1}{2}m\omega^2\widehat{x}^2 = \hbar\omega(b^\dagger b + \frac{1}{2}) \tag{4.3}$$

where we have introduced the phonon creation and annihilation operators $b^\dagger$ b in terms of which the position operator $\widehat{x}$ and the momentum operator $\widehat{p}$ of the oscillator can be expressed as

$$\widehat{x} = \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}(b^\dagger + b), \tag{4.4}$$

$$\widehat{p} = \frac{i}{\sqrt{2}}\sqrt{\hbar m\omega}(b^\dagger - b). \tag{4.5}$$

In the following we want to study electron transport through the device and we therefore assume that the device is connected to two leads kept at different chemical potentials μ_L (left lead) and μ_R (right lead) with $\mu_L > \mu_R$. The potential difference defines a bias drop across the device which causes electrons to propagate through the system from the left lead to the right lead. The electrons of the leads are assumed to be non-interacting, and given in terms of the creation

and annihilation operators $c_j^\dagger$ and c_j with $j = L, R$. The Hamiltonian of the leads is,

$$H_{Leads} = \sum_j \epsilon_j c_j^\dagger c_j \tag{4.6}$$

whereas the tunnelling of electrons between the leads and the device is described by

$$H_T = \frac{1}{\sqrt{N}} \sum_j V_\alpha \left(c_j^\dagger c_0 + c_0^\dagger c_j \right) \tag{4.7}$$

where N is the total number of states in the lead, V_α is the hopping between the dot and the leads $\alpha = L, R$, j represents the channels in one of the leads. For the second lead the Hamiltonian can be written in the same way.

4.2.1 Canonical transformation

The first approach to this new type of problem is to consider a canonical transformation of the dot-level Hamiltonian.

$$H_{ph-dot} = \left[\epsilon_0 + \alpha(b^\dagger + b) \right] c_0^\dagger c_0 + \hbar\omega(b^\dagger b + \frac{1}{2}). \tag{4.8}$$

We introduce a unitary transformation for all operators $\hat{O}$,

$$\hat{O} \rightarrow \bar{O} \equiv e^S \hat{O} e^{-S}, \tag{4.9}$$

$$S = \frac{\alpha}{\omega}(b^\dagger - b) c_0^\dagger c_0. \tag{4.10}$$

The operator $U \equiv e^S$ is unitary because $U^{-1} = U^\dagger, i.e. UU^\dagger = U^\dagger U = 1$. Note that $c_0^\dagger c_0$ in the definition of S is the electron number operator.

For explicit calculations, one has to use the nested commutator expansion

$$\bar{O} = O + [S, O] + \frac{1}{2!}[S, [S, O]] + \frac{1}{3!}[S, [S, [S, O]]] + .. \tag{4.11}$$

We first transform the electron number operator $c_0^\dagger c_0$,

$$\bar{c}_0^\dagger \bar{c}_0 = c_0^\dagger c_0 + [S, c_0^\dagger c_0] + .. = c_0^\dagger c_0 \tag{4.12}$$

because S and $c_0^\dagger c_0$ commute. This is not the case for b

$$\begin{aligned}\bar{b} &= b + [S,b] + \frac{1}{2!}[S,[S,b]] + .. \\ &= b + \frac{\alpha}{\omega} c_0^\dagger c_0 [b^\dagger - b, b] + .. \\ &= b - \frac{\alpha}{\omega} c_0^\dagger c_0 \end{aligned} \tag{4.13}$$

because $[b^\dagger, b] = -1$ is a scalar and all the higher commutators vanish. Correspondingly,

$$\begin{aligned}\bar{b}^\dagger &= b^\dagger + [S,b^\dagger] + \frac{1}{2!}[S,[S,b^\dagger]] + .. \\ &= b^\dagger + \frac{\alpha}{\omega} c_0^\dagger c_0 [b^\dagger - b, b^\dagger] + .. \\ &= b^\dagger + \frac{\alpha}{\omega} c_0^\dagger c_0 . \end{aligned} \tag{4.14}$$

Transforming now all operators individually, the canonical transformed H_{ph-dot} is

$$\begin{aligned}\bar{H}_{ph-dot} &= e^S H_{ph-dot} e^{-S} \\ &= e^S \left(\left[\epsilon_0 + \alpha(b^\dagger + b) \right] c_0^\dagger c_0 + \hbar\omega(b^\dagger b + \frac{1}{2}) \right) e^{-S} \\ &= \left[\epsilon_0 + \alpha(\bar{b}^\dagger + \bar{b}) \right] \bar{c}_0^\dagger \bar{c}_0 + \hbar\omega(\bar{b}^\dagger \bar{b} + \frac{1}{2}) \\ &= \left[\epsilon_0 + \alpha(b^\dagger + \frac{\alpha}{\omega} c_0^\dagger c_0 + b - \frac{\alpha}{\omega} c_0^\dagger c_0) \right] c_0^\dagger c_0 + \hbar\omega((b^\dagger + \frac{\alpha}{\omega} c_0^\dagger c_0)(b - \frac{\alpha}{\omega} c_0^\dagger c_0) + \frac{1}{2}) \\ &= \epsilon_0 c_0^\dagger c_0 + \hbar\omega(b^\dagger b + \frac{1}{2}) - \hbar\omega \left(\frac{\alpha}{\omega} c_0^\dagger c_0 \right)^2 . \end{aligned} \tag{4.15}$$

The square of the number operator is just the number operator itself, $\left(c_0^\dagger c_0\right)^2 = c_0^\dagger c_0$:there is either one or no electron on the level. We can thus write

$$\bar{H}_{ph-dot} = (\epsilon_0 - \hbar\frac{\alpha^2}{\omega}) c_0^\dagger c_0 + \hbar\omega(b^\dagger b + \frac{1}{2}). \tag{4.16}$$

From this result it is clear that the canonical transformation provides a decoupling of the electronic and vibrational degrees of freedom. We write the eigenvalues of H_{ph-dot} as ($\hbar = 1$)

$$\epsilon = \epsilon_0 + \omega(n + \frac{1}{2}) - \Delta \tag{4.17}$$

where

$$\Delta = \frac{\alpha^2}{\omega}.$$

We find from the definition that the Green function

$$\begin{aligned} G(t,t') &= (-i) < Tb(t)b^\dagger(t) > \\ &= (-i) < Tb(t)b^\dagger(t)e^S e^{-S} > \\ &= (-i) < Te^S b(t)b^\dagger(t)e^{-S} > \\ &= (-i) < T\bar{b}(t)\bar{b}^\dagger(t) > \end{aligned} \tag{4.18}$$

in applying the canonical transformation to the individual operators, we obtain

$$\bar{b} = b\chi, \quad where \quad \chi = e^{-\frac{\alpha}{\omega}(b-b^\dagger)} \tag{4.19}$$

$$\bar{b}^\dagger = b^\dagger\chi^\dagger, \quad where \quad \chi^\dagger - e^{\frac{\alpha}{\omega}(b-b^\dagger)} \tag{4.20}$$

So,

$$\begin{aligned} G(t,t') &= (-i) < Tb(t)\chi(t)b^\dagger(t')\chi^\dagger(t') > \\ &= (-i) < Tb(t)b^\dagger(t) >< \chi(t)\chi^\dagger(t') > \\ &= G'(t,t') < \chi(t)\chi^\dagger(t') > \end{aligned} \tag{4.21}$$

The meaning of the above equalities is that we can calculate the properties of the resonant level in the quantum dot as we have done before, but in the Hamiltonian system, and then finally multiply it by the average $< \chi(t)\chi^\dagger(t') >$ This average can be exactly calculated as,

We write the eigenfunctions of H_{dot-ph} in k-space representation as

$$\Phi_n(k, x_0 \neq 0) = A_m \exp[-\frac{l^2k^2}{2}]H_n(k)\exp[-\mathrm{i}kx_0]$$

$$\Phi_n(k, x_0 = 0) = A_m \exp[-\frac{l^2k^2}{2}]H_n(k)$$

for the occupied, $x_0 \neq 0$, and unoccupied, $x_0 = 0$, dots, respectively, where x_0 is the displace-

ment of the oscillator due to the coupling to the electron and $H_n(k)$ are the usual Hermite polynomials. Here we have used the fact that the harmonic oscillator eigenfunctions have the same form in both real and Fourier space.

In order to transform between the representations for the occupied and unoccupied dots, we require the matrix with elements

$$A_{mn} = \int \Phi_n^*(k, x_0 = 0)\Phi_m(k, x_0 \neq 0)\, \mathrm{d}k, \tag{4.22}$$

which may be simplified [15, 30] as

$$\begin{aligned} A_{mn} &= \frac{l}{\sqrt{\pi 2^{m+n} n! m!}} \int \exp\left(-k^2\right) H_m^*(k) H_n(k) \exp\left(\mathrm{i}kx_0\right)\, \mathrm{d}k \\ &= \sqrt{\frac{2^{m-n} n!}{m!}} \exp\left(-\frac{1}{4}x^2\right) \left(\frac{1}{2}\mathrm{i}x\right)^{m-n} L_n^{m-n}\left(\frac{1}{2}x^2\right) \end{aligned} \tag{4.23}$$

for m n, where $x = \frac{\Delta}{\omega_0}$, $\Delta = \frac{\alpha^2}{\omega_0}$, and $L_n^{m-n}(x)$ are the associated Laguerre polynomials. Note that the integrand is symmetric in m and n but the integral is valid only for $m \leq n$. Clearly the result for $m > n$ is obtained by exchanging m and n in Eq. (4.23) to obtain

$$< \chi(t)\chi^\dagger(t') >= A_{nm} = \sqrt{\frac{2^{|m-n|}\, \min[n,m]!}{\max[n,m]!}} \exp\left(-\frac{1}{4}x^2\right) \left(\frac{1}{2}\mathrm{i}x\right)^{|m-n|} L_{\min[n,m]}^{|m-n|}\left(\frac{1}{2}x^2\right) \tag{4.24}$$

where $x = \frac{\Delta}{\omega}$ and $L_n^{m-n}(x)$ are the associated Laguerre polynomials

4.2.2 Green's function and quantum transport

In order to calculate the analytical results and to discuss the numerical quantum dynamics of the nanomechanical system, our focus in this section is to derive an analytical relation for the retarded self-energy. The self-energy represents the contribution to the dot energy, due to interactions between the dot and the leads it is coupled to. In obtaining these results we use the wide–band approximation where the retarded self–energy of the dot due to each lead is considered to be energy independent and is given by

$$\Sigma^r_{n_0,n_0,\alpha} = \Delta H^*_{\alpha} g^r_{\alpha,\alpha}(E - (n_0 + \frac{1}{2})\hbar\omega)\Delta H_{\alpha}, \tag{4.25}$$

where off-diagonal element of matrix, $\Sigma^r_{n_0,n_0',\alpha}$, are zero, and $g^r_{\alpha,\alpha}(E-(n_0+\frac{1}{2})\hbar\omega)$ is the uncoupled Green function in the leads as

$$g^r_{\alpha,\alpha}(E-(n_0+\frac{1}{2}\hbar\omega) = \frac{1}{N}\sum_j g^r_{\alpha,j}(E-(n_0+\frac{1}{2})\hbar\omega) \tag{4.26}$$
$$= \frac{1}{N}\int_{-\infty}^{+\infty}\frac{Nn_\alpha d\varepsilon_\alpha}{E-(n_0+\frac{1}{2})\hbar\omega-\varepsilon_\alpha}$$

where $\sum_j = \int_{-\infty}^{+\infty} Nn_\alpha d\varepsilon_\alpha$, j stands for every channel in each lead, and n_α is the density of states in lead α. With the help of eq. (4.26), the retarded self-energy may be written as

$$\Sigma^r_{n_0,n_0,\alpha} = \Delta H_{0,\alpha}\frac{1}{N}\int_{-\infty}^{+\infty}\frac{Nn_\alpha d\varepsilon_\alpha}{E-(n_0+\frac{1}{2})\hbar\omega-\varepsilon_\alpha}\Delta H_{\alpha,0}, \tag{4.27}$$

which may be simplified as

$$\Sigma^r_{n_0,n_0,\alpha} = |V_{0,\alpha}|^2\int_{-\infty}^{+\infty}\frac{n_\alpha d\varepsilon_\alpha}{E-(n_0+\frac{1}{2})\hbar\omega-\varepsilon_\alpha} \tag{4.28}$$

$$= -|V_{0,\alpha}|^2 n_\alpha\int_{-\infty}^{+\infty}\frac{d\varepsilon_\alpha}{\varepsilon_\alpha-E+(n_0+\frac{1}{2})\hbar\omega} \tag{4.29}$$

$$= -|V_{0,\alpha}|^2 n_\alpha\times(2\pi i) \tag{4.30}$$

$$= \frac{-i\Gamma_\alpha}{2}, \tag{4.31}$$

where $\Gamma_\alpha = 4\pi|V_{0,\alpha}|^2 n_\alpha$, α representing the L or R leads, and the retarded self energy is now independent of the oscillator's index (n_0, n_0). Hence, it can be written as

$$\Sigma^r_{n_0n_0,\alpha} = (\Sigma^a_{n_0,n_0,\alpha})^* = -\frac{i\Gamma_\alpha}{2}. \tag{4.32}$$

We solve Dyson's equation using $H_{dot-lead}$ as a perturbation. For the more general systems we aim to treat in the future, this is a reasonable small parameter. In the present case, however, we can find an exact solution. The retarded and advanced Green's functions on the dot, with the phonon states in the representation of the unoccupied dot, may be written as

$$G^{r(a)}_{nn_0} = \sum_m A_{n,m} g^{r(a)}_m(E) A^*_{n_0,m} , \tag{4.33}$$

where $g^{r,(a)}_m(E)$ is the retarded (advanced) Green's function on the occupied dot,

$$g^{r,(a)}_m(E) = \left[E - \epsilon_0 - (m + \frac{1}{2})\hbar\omega + \Delta \pm \mathrm{i}\Gamma \right]^{-1} , \tag{4.34}$$

with the fact that $\Gamma_L = \Gamma_R = \Gamma$.

The lesser Green's function in the presence of the nanomechanical oscillator including the dot and the leads and is written as

$$G^<_{n,n'} = \sum_{n_0,n'_0} G^r_{n,n_0} \Sigma^<_{n_0 n'_0}(E) G^a_{n'_0,n'} , \tag{4.35}$$

with $\Sigma^<_{n_0,n'_0}(E)$ being the the lesser self energy which is given as

$$\Sigma^<_{n_0,n'_0}(E) = \Sigma^<_{n_0,n'_0,L}(E) + \Sigma^<_{n_0,n'_0,R}(E) , \tag{4.36}$$

where the off-diagonal element of matrix, $\Sigma^r_{n_0,n'_0,\alpha}$, are zero, and the diagonal ($n'_0 = n_0$) element of the lesser self-energy may be written as

$$\Sigma^<_{n_0,n_0,\alpha}(E) = \mathrm{i}\Gamma_\alpha f_\alpha(E) , \tag{4.37}$$

where $f_\alpha(E)$ are the Fermi distribution functions of the left and right leads, which have different chemical potentials under a voltage bias..

The formula for the current through each of the leads given in chapter 3 is written as

$$I_\alpha = \frac{ie}{\hbar}\sum_{n_0,n}\int\{\Sigma^<_{n_0,n,\alpha}(E)(G^r_{n,n_0}-G^a_{n,n_0})+(\Sigma^a_{n_0,n,\alpha}-\Sigma^r_{n_0,n,\alpha})G^<_{n,n_0}]\}dE. \tag{4.38}$$

With the help of the above equation, we calculate the net current through the dot and the leads with the oscillator on the dot, written as

$$I = I_L - I_R \tag{4.39}$$

$$= \frac{e}{4\pi}\sum_{n_0,n}\int\left\{\begin{array}{c}\left[\left(\Sigma^<_{n_0,n,L}(E)-\Sigma^<_{n_0,n,R}(E)\right)\left(G^r_{n,n_0}-G^a_{n,n_0}\right)\right]\\ +\left[\left(\left(\Sigma^a_{n_0,n,L}-\Sigma^r_{n_0,n,L}\right)-\left(\Sigma^a_{n_0,n,R}-\Sigma^r_{n_0,n,R}\right)\right)G^<_{n,n_0}\right]\end{array}\right\}\mathrm{d}E. \tag{4.40}$$

The resulting expression for the net current is

$$I = \frac{e}{4\pi\hbar}\sum_{n_0,n}\int\left(\Sigma^<_{n_0,n,L}(E)-\Sigma^<_{n_0,n,R}(E)\right)\left(G^r_{n,n_0}-G^a_{n,n_0}\right)dE, \tag{4.41}$$

which is derived from equation (4.40) using the same damping factor for each lead ($\Gamma_L = \Gamma_R = \Gamma$).

For the present case of zero temperature the lesser self–energy may be recast in terms of the Heaviside step function $\theta(x)$ as

$$\Sigma^<_{n_0,n_0,\alpha}(E) = \mathrm{i}\Gamma_\alpha\theta\left(\epsilon_{\mathrm{F}\alpha}+(n_0+\frac{1}{2})\hbar\omega-E\right)\delta_{n_0,0}\,, \tag{4.42}$$

where $\epsilon_{\mathrm{F}\alpha}$ is the Fermi energy on lead α and the Kronecker delta, $\delta_{n_0,0}$, signifies that the nanomechanical oscillator is initially in its ground state, $n_0 = 0$.

Using the expression for the retarded and advanced Green's function and the right and left self-energy, the expression for the net current becomes

$$I = \frac{e}{2\pi\hbar}\sum_n |A_{0,n}|^2\int_{\epsilon_{\mathrm{F}R}+\frac{1}{2}\hbar\omega}^{\epsilon_{\mathrm{F}L}+\frac{1}{2}\hbar\omega}\frac{\Gamma^2}{\left[E-\epsilon_0-\left(n+\frac{1}{2}\right)\hbar\omega+\Delta\right]^2+\Gamma^2}dE, \tag{4.43}$$

After performing the integral in the above expression, the final result is written as

$$I = \frac{e\Gamma}{2\pi\hbar}\sum_n |A_{0,n}|^2 \left[\tan^{-1}\left(\frac{\epsilon_{FL} - \epsilon_0 - n\hbar\omega + \Delta}{\Gamma}\right) - \tan^{-1}\left(\frac{\epsilon_{FR} - \epsilon_0 - n\hbar\omega + \Delta}{\Gamma}\right)\right]. \quad (4.44)$$

We calculate the differential conductance by differentiating Eq. (4.44) with respect to ϵ_{FL} and keeping ϵ_{FR} constant. The final expression for the differential conductance is then

$$\frac{dI}{d\epsilon_{FL}} = \frac{e}{2\pi\hbar}\sum_n \frac{\Gamma^2 |A_{0,n}|^2}{[\epsilon_{FL} - \epsilon_0 - n\hbar\omega + \Delta]^2 + \Gamma^2}. \quad (4.45)$$

Obviously one could have obtained the differential conductance directly from Eq. (4.43). without integrating and then differentiating.

4.3 Discussion of results

4.3.1 Current

The $I - V$ characteristics of the NEMS device against applied bias for different values of the coupling strength are shown in Figure 4.2. The main resonance step is the elastic or zero phonon transition. The amplitude of the additional steps is much smaller than the basic resonance step. The electrons that tunnel onto the dot can only excite the oscillator mode as at zero temperature there are no phonons available to be absorbed. Moreover, we have seen that with increasing coupling strength, the number and intensity of the additional steps increases but their intensity always remains much smaller than the main step. The steps in the current characteristics vanish if the upper electrochemical potential is smaller than the dot energy plus the oscillator energy.

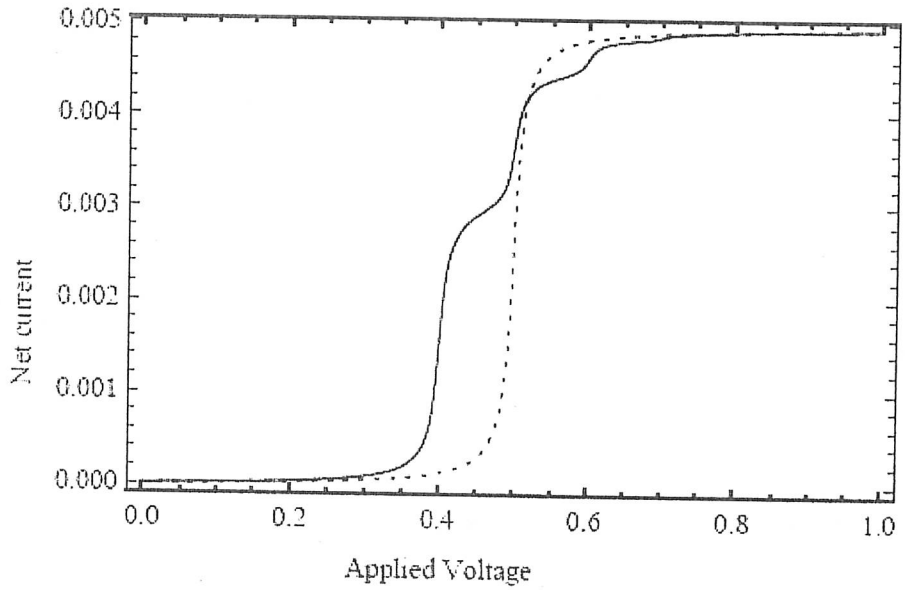


Fig. 4.2 Current-voltage characteristics (dimensionless) as a function of applied voltage μ_{FL} (in arbitrary units), coupling strength $\alpha = 0.1\omega_0$(dotted line), and $1\omega_0$ (solid line).Gate voltage $\varepsilon_0 = 0.5$, oscillator energy $\omega_0 = 0.1$, self-energy $\Gamma = 0.1\omega_0$.

4.3.2 Differential conductance

The differential conductance is shown graphically in figure 4.3 as a function of applied voltage for different values of coupling strength, using the parameters as: the single energy level of the dot $\epsilon_0 = 0.5$, the characteristic frequency of the oscillator $\hbar\omega = 0.3$, the damping factor $\Gamma = 0.3\hbar\omega$ and the chemical potentials $0 \leq \epsilon_{FL} \leq 1$ and $\epsilon_{FR} = 0$. These are chosen to illustrate the physics of such systems rather than to represent a specific implementation. The oscillator induced resonance effects are clearly visible in the numerical results. It must be noted that we have obtained these results in the regime of strong and zero or weak coupling of the oscillator with the electrons on the dot. The coupling between the leads and the dot is considered to be symmetric and we assume that the electrons in the leads are at zero temperature and the leads

have constant density of states. With increasing coupling strength, the number of satellite peaks also increases while for zero or weak coupling we find only the basic resonance. This confirms the effect of the coupling between the electrons on the dot and the single oscillator mode where higher energy electrons are able to drop to the dot energy by creation of phonons. Transport processes involving creation or annihilation of phonons are a common feature of NEMS.

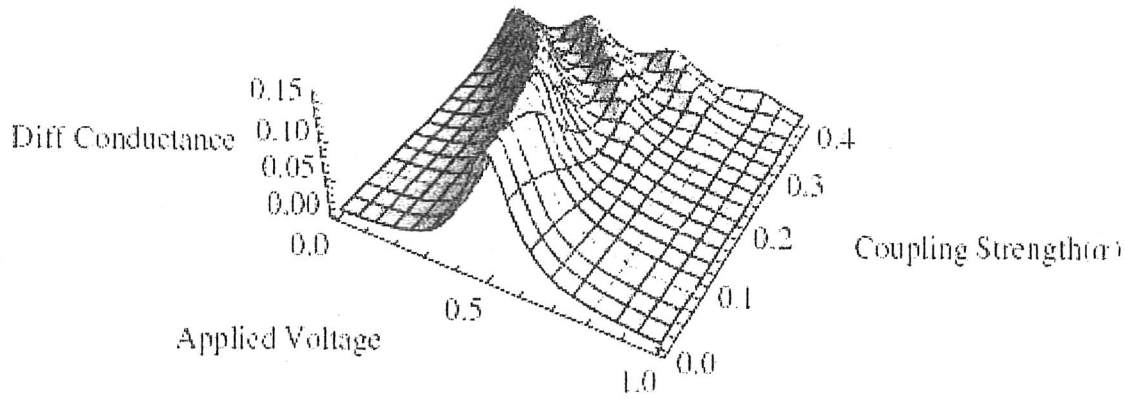


Fig. 4.3 Differential conductance dimensionless as a function of applied voltage μ_{FL} in arbitrary units and coupling strength α. Gate voltage $\epsilon_0 = 0.5$, oscillator frequency $\omega_0 = 0.3$, selfenergy $\Gamma = 0.3\omega_0$.

Closer analytical examination of the expression for the differential conductance shows that the main resonance peaks occur when the applied voltage, ϵ_{FL} is equal to the energy eigenvalues of the coupled dot electron and oscillator. The main peak ($n = 0$) is given by the Lorentzian form with its center at the $\epsilon_{FL} = \epsilon_0 - \Delta$, known as a Breit-Wigner resonance. The satellite peaks due to the emission of phonons can be seen on the positive energy side with $\epsilon_{FL} = \epsilon_0 - \Delta + n\hbar\omega$ where ω is the characteristic frequency of the oscillator.

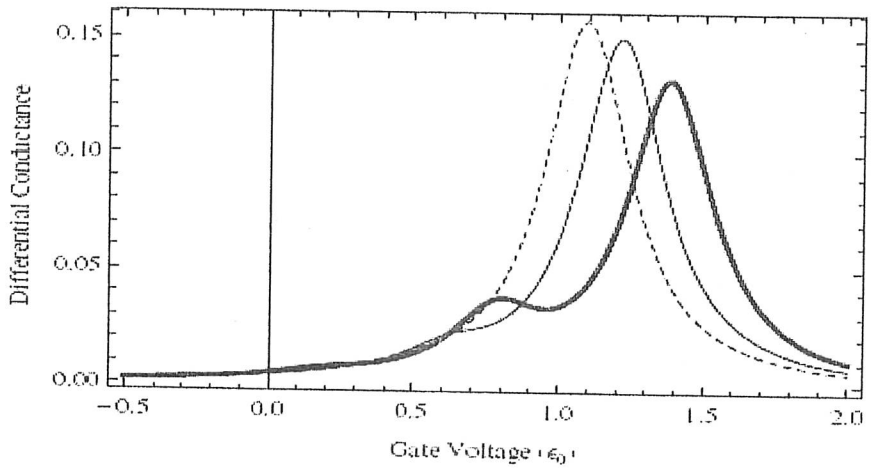


FIG. 4.4 Differential conductance (dimensionless) as a function of gate voltage ϵ_0, with applied voltage $\epsilon_{FL}=1$, oscillator frequency $\omega_0=0.6$, self-energy $\Gamma=0.3\omega_0$, and coupling strength $\alpha=0.4\omega_0$ (dotted line), $0.6\omega_0$ (light solid line), and $0.8\omega_0$ (bold solid line).

Chapter 5

Appendix

5.1 Green's function for one particle Schrodinger equation

Green's functions are useful for problems where we use perturbation theory solutions. Consider the Schrodinger equation,

$$[H_0(r) + V(r)]\Psi = E\Psi \tag{5.1}$$

where we know the eigenstate of $H_0(r)$ and E is the corresponding energy eigenvalue with the eigenstate Ψ, we want to treat $V(r)$ as perturbation. In order to solve the Schrodinger equation, we define the corresponding Green's function by the differential equation

$$\left(E - H_0\left(r\right)\right) G_0\left(r, r', E\right) = \delta\left(r - r'\right) \tag{5.2}$$

with the boundary condiions,$G\left(r, r'\right) = G\left(r', r\right)$ .Here it is obvious that $E - H_0\left(r\right)$ is the inverse of $G_0\left(r, r'\right)$ and therefore we can write

$$G_0^{-1}(r, E) = E - H_0(r) \tag{5.3}$$

or

$$G_0^{-1}(r, E) G_0\left(r, r', E\right) = \delta\left(r - r'\right) \tag{5.4}$$

Now the Shrodinger equation can be written as,

$$[G_0^{-1}(r,E) - V(r)]\Psi = 0 \tag{5.5}$$

The solution may be written as an integral equation

$$\Psi(r) = \Psi^0(r) + \int dr' G_0\left(r, r', E\right) V(r')\Psi(r') \tag{5.6}$$

where Ψ_0 is an eigenstate of H_o. We can solve this equation by iteration, and upto the first order in V the solution is,

$$\Psi(r) = \Psi^0(r) + \int dr' G_0\left(r, r', E\right) V(r')\Psi^0(r') + O(V^2) \tag{5.7}$$

For the static case we can write the solution as

$$\Psi = \Psi^0 + G_0 V\Psi^0 + G_0 V G_0 V\Psi^0 + G_0 V G_0 V G_0 V\Psi^0 + ... \tag{5.8}$$

$$= \Psi^0 + (G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + ...)V\Psi^0 \tag{5.9}$$

where the iteration veriable has been supressed. By comparision with the equation we can write,

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + ... \tag{5.10}$$

$$G = G_0 + (G_0 + G_0 V G_0 + ...)V G_0 \tag{5.11}$$

$$G = G_0 + G V G_0 \tag{5.12}$$

the last equation is the standard Dyson equation [10].

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