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Kondo Effect in Quantum Dots: A Non-crossing Approximation Study

by

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ABSTRACT

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In this thesis, non-equilibrium Green’s function techniques in combination with the time-dependent non-crossing approximation are utilized to calculate the transient currents through a quantum dot in the Kondo regime subject to sudden perturbations. We first present novel numerical algorithms which enable relatively fast calculations. We then employ these algorithms to study the transient current through a quantum dot which is symmetrically coupled to metallic leads and its coupling to the leads is abruptly switched such that the Kondo effect is present in the final state. The timescales for the approach to equilibrium are shown to be the same as the ones when the energy level of the dot is suddenly switched. Finally, we study the transient currents in a quantum dot asymmetrically coupled to metallic leads resulting from the abrupt change of the dot level. We show that for asymmetric coupling, sharp features in the density of states of the leads can induce oscillations in the current through the
dot. The amplitude of these oscillations increases as the temperature is reduced and saturates below the Kondo temperature. We discuss the microscopic origin of these oscillations and comment on the possibility for their experimental detection.
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Chapter 1
Introduction

1.1 Overview of electron transport through quantum dots

The smashing success of semiconductor technology in recent years has mainly been due to the miniaturization of silicon field effect transistors (MOSFET's), thus the increase of density of memory and logic components. The International Technology Roadmap for Semiconductors predicts that the shrinking of silicon MOSFET's and integrated circuits in accordance with Moore's Law will continue for the next 10 years. The extrapolation of the data in Fig. 1.1 clearly shows that the computers which contain transistors with feature size of less than 10 nm will be available by 2016.

Continuation of the Moore Law beyond the 10 nm barrier looks uncertain at the moment though. Theoretical modeling of such nanoscale MOSFET's indicate that such devices would be extremely sensitive to the small deviations of their physical dimensions [1]. Fig. 1.2 depicts the results of such a calculation. It is clear from this figure that the gate length of a 5 nm MOSFET should be controlled better than 0.25 nm, much tighter than the tightest ITRS prediction in order to keep deviations of the transistor threshold voltage $V_t$ below an acceptable limit (50 mV). This kind of sensitivity would result in extra costs in the chip fabrication processes making going below the 10 nm barrier unfeasible. Therefore Si-MOSFET-based Moore law would
Figure 1.1  This figure shows the number of MOSFET transistors per chip and the minimum feature size used in the production of microprocessors and DRAM memory as a function of time. Moore’s law states empirically that the number of transistors doubles roughly in every two years. Extrapolation of the green line in the figure implies that the minimum feature size is going to be around 10 nm by 2016.

de facto stop at around 10 nm.

These predictions provide motivation for scientists to find alternative devices that could potentially replace MOSFET’s beyond the 10 nm barrier providing better performance with less fabrication costs. This thesis explores a viable alternative candidate, namely a quantum dot in great detail. A quantum dot is an artificially fabricated nanostructure. Quantum dots are small regions defined in semiconductor heterostructures. On contrary to what the name ”the dot” suggests, semiconductor quantum dots, in reality, consist of around a million atoms with an equivalent number of atoms, however, all the electrons are bound to the nuclei thus the number of free
electrons in the dot are quite small ranging between one and a few hundred in most cases. A striking property of the quantum dots is that the de Broglie wavelength of the free electrons is on the order of the size of the dot and these electrons occupy discrete quantum states reminiscent of atomic orbitals in atoms. Another interesting property of a quantum dot is that it has a charging energy (i.e. the energy required to add or remove a single electron from the dot) in close analogy with the ionization energy of an atom. Due to these ubiquitous properties, quantum dots are sometimes referred as artificial atoms. The physics of real atoms is studied via their interaction with light. In contrast, the physics of quantum dots is probed by attaching leads and measuring their transport properties. We refer reader to several review articles about quantum dots for more details [5, 6, 7].

We will first investigate the requirements for the Coulomb charging energy to be important for the so called lateral quantum dots. Such a device is schematically shown in Fig. 2. Quantum dot is coupled to three terminals. Electron transport takes place with the source and drain contacts only. The function of the gate electrode is to adjust the discrete dot level and the number of electrons in the dot. The amount of charge the dot contains is quantized and equal to Ne where e is the elementary unit charge.

The first requirement stems from the change in Coulomb energy when tunneling takes place between the dot and the source and drain leads. An extra electron tun-
Figure 1.2  Threshold voltage "roll-off" (reduction relative to the value for \( L \rightarrow \infty \)) as a function of gate length \( L \), for various combinations of oxide thickness \( t_{ox} \) and channel thickness \( t \), calculated for a simple model of an "ultimate MOSFET" [1].

Tunneling on and off the dot changes the electrostatic potential by the charging energy \( E_C = e^2 / C \), where \( C \) is the capacitance of the dot. This charging energy becomes important when it is well above the thermal energy \( k_B T \). Therefore the first requirement is given by

\[
e^2 / C >> k_B T. \tag{1.1}
\]

The second requirement is related to the quantum fluctuations in the number \( N \). The deviation in \( N \) due to the tunneling of electrons through the barriers to the source and drain electrodes should be much smaller than the inverse of the timescale of the measurement. In practice,

\[
R_t >> h / e^2. \tag{1.2}
\]
Figure 1.3  Potential energy landscape through a quantum dot coupled to metallic leads. The states in the 2D reservoirs are filled up to the electrochemical potentials $\mu_{\text{left}}$ and $\mu_{\text{right}}$ which are related via the bias voltage $V_{sd} = (\mu_{\text{left}} - \mu_{\text{right}})/e$. The discrete 0D-states in the dot are filled with $N$ electrons up to $\mu_{\text{dot}}(N)$. The addition of an extra electron to the dot would raise $\mu_{\text{dot}}(N)$ (the highest solid line) to $\mu_{\text{dot}}(N + 1)$ (the lowest dashed line). In this figure, this addition is blocked due to Coulomb blockade.

When these two requirements are met, charge tunneling becomes quantized.

The first requirement can be met by using a small dot since the capacitance of an object scales with its radius $R$, whereas the dot needs to be coupled weakly to the metallic leads for the latter.

Electrons on the dot reside on quantized energy levels in analogy with real atoms. In order to be able to resolve these levels, the energy level spacing $\Delta E$ should be much larger than the thermal energy $k_B T$. The level spacing at the Fermi energy for a box of size $L$ depends on the dimensionality. Including the spin degeneracy, level
spacing is given by

\[ \Delta E = (N/4)\hbar^2 \pi^2 / (mL^2) \]
\[ = (1/\pi)\hbar^2 \pi^2 / (mL^2) \]
\[ = (1/3\pi^2 N)^{1/3} \hbar^2 \pi^2 / (mL^2) \]  
(1.3)

for 1D, 2D and 3D respectively. For instance, the level spacing of a 100 nm 2D dot is around 0.03 meV. Electrons confined in semiconductor heterostructure interfaces can be two dimensional. They also have small effective masses that increase the level spacing even further. Therefore, dots formed in semiconductor heterostructures are true artificial atoms with both experimentally observable quantized charge states and quantized energy levels.

We are now going to investigate the mechanism of the electron transport in lateral quantum dot devices in more detail. Our discussion is rather a simple one following previous works [8, 9, 10, 11], however it is sufficiently involved to explain most experiments. Fig. 1.3 depicts the energy landscape of such a device along the transport direction. Fermi-Dirac distribution function governs the distribution of the electrons in the leads, thus at zero temperature, the states in the left and right leads are filled up to the electrochemical potentials \( \mu_{\text{left}} \) and \( \mu_{\text{right}} \), which are separated from each other by the applied source-drain bias \( eV_{sd} = \mu_{\text{left}} - \mu_{\text{right}} \). The current flowing in this electrical circuit is (non) zero when the number of available states on the dot in the
Figure 1.4  This figure shows the removal of the Coulomb blockade. The addition of an extra electron to the dot level is allowed here since $\mu_{\text{dot}}(N + 1)$ is aligned with the reservoir potentials by adjusting the gate voltage. Left and right panels show two parts of the sequential tunneling process at the same gate voltage with $N$ and $N + 1$ electrons on the dot respectively.
Figure 1.5  Circuit diagram in which the tunnel barriers are represented as a capacitor and resistor. The different gates are represented by a single capacitor $\Sigma C_g$. The charging energy in this circuit is $e^2/(C_l + C_r + \Sigma C_g)$.

energy window between $\mu_{\text{left}}$ and $\mu_{\text{right}}$ is (non) zero. The number of available states is determined by the electrochemical potential $\mu_{\text{dot}}N$ which is the minimum energy for adding the $N$th electron to the dot. It is given by

$$\mu_{\text{dot}}(N) = U(N) - U(N - 1)$$  \hspace{1cm} (1.4)

where $U(N)$ is the total ground state energy for $N$ electrons on the dot at zero temperature.

In order to come up with a formula for $U(N)$, we will make some assumptions. In general, ab initio methods are employed to determine $U(N)$. We will model the
Coulomb interaction among the electrons in the dot and between the electrons in the dot and the ones in the environment by a capacitance $C$. We will assume that neither $C$ nor the quantum levels depend on the number of electrons on the dot. This assumption is justified if the size of the dot is much larger than the screening length. In terms of the circuit diagram shown in Fig. 1.5 the total capacitance $C = C_l + C_r + C_g$ consists of capacitances across the barriers, $C_l$ and $C_r$ and a capacitance between the dot and the gate, $C_g$. This rather simplistic model leads in the linear response regime to an electrochemical potential $\mu_{\text{dot}}(N)$ for $N$ electrons on the dot:

$$\mu_{\text{dot}}(N) = E_N + \frac{(N - N_0 - 0.5)e^2}{C} - e \frac{C_g}{C} V_g$$  \hspace{1cm} (1.5)$$

This expression can be cast in the general form

$$\mu_{\text{dot}}(N) = \mu_{\text{ch}}(N) + e\phi_N$$  \hspace{1cm} (1.6)$$

thus the electrochemical potential is the sum of the chemical potential $\mu_{\text{dot}}(N) = E_N$, where the single-particle state $E_N$ for the $N$th electron is measured from the bottom of the conduction band and the electrostatic potential $\phi_N$, which contains a discrete and continuous part. In our terminology, the integer $N$ represents the number of electrons at a fixed gate volatage $V_g$ and $N=N_0$ when $V_g=0$.

For a given gate voltage $V_g$, the number of electrons on the dot $N$ is the largest integer for which $\mu_{\text{dot}}(N) < \mu_{\text{left}} \cong \mu_{\text{right}}$. When we change the number of electrons
by one at fixed gate voltage, the change electrochemical potential is given by

$$\mu_{dot}(N + 1) - \mu_{dot}(N) = \Delta E + \frac{e^2}{C},$$

where $\Delta E = E_{N+1} - E_N$ between 0D states. This addition energy is large for small capacitance or large energy splitting. Many body contribution $e^2/C$ to the energy gap exists only at the Fermi energy. Below $\mu_N$, the energy state separation is just the single-particle energy difference $\Delta E$. Technically, $\Delta E$ is the excitation energy of a dot with fixed $N$.

An important consequence of this addition energy is the possible blockade of the electron transport on and off the dot. This situation is schematically shown in Fig. 1.3. $N$ electrons are localized on the dot here and the $(N+1)$th electron cannot tunnel on the dot since the resulting electrochemical potential $\mu_{dot}(N+1)$ would be higher than the potentials of the source and drain leads. Consequently, the electron transport is blocked as long as $\mu_{dot}(N) < \mu_{left}, \mu_{right} < \mu_{dot}(N + 1)$. This phenomenon is called the Coulomb blockade.

Aligning $\mu_{dot}(N + 1)$ between $\mu_{left}$ and $\mu_{right}$ by changing the gate voltage removes the Coulomb blockade. This situation is depicted in Fig. 1.4, where the electrostatic increase $e\phi(N + 1) - e\phi(N) = e^2/C$ is shown as a change in the conduction band bottom. In this case, an electron can tunnel from the left reservoir onto the dot since $\mu_{left} > \mu_{dot}(N + 1)$. This electron can also tunnel off the dot to the right reservoir since $\mu_{dot}(N + 1) > \mu_{right}$. This drops the electrochemical potential back
to $\mu_{\text{dot}}$ allowing another electron to tunnel onto the dot from the left reservoir, thus repeating the cycle $N \to N + 1 \to N$. This device, which functions with successive discrete charging and discharging of the dot is called *single electron transistor* or *SET* [12, 13, 14].

The conductance oscillates between zero (Coulomb blockade) and non-zero (no Coulomb blockade) when the gate voltage is swept. In Coulomb blockade valleys, the number of electrons $N$ is fixed. The situation is shown in Fig. 1.6. It is clear from this figure that when conductance $G$ goes over a maximum,

1. $N$ changes by one
2. the electrochemical potential $\mu_{\text{dot}}$ shifts by $\Delta E + e^2/C$
3. the electrostatic potential $e\phi$ shifts by $e^2/C$

From Eq. FIRST and the condition that $\mu_{\text{dot}}(N_g, V_g) = \mu_{\text{dot}}(N + 1, V_g + \Delta V_g)$, the distance in gate voltage $\Delta V_g$ is given by

$$\Delta V_g = \frac{C}{eC_g} \left( \Delta E + \frac{e^2}{C} \right)$$

(1.8)

and the position of the $N$th conductance peak is

$$V_g(N) = \frac{C}{eC_g} \left( E_N + (N - 0.5)\frac{e^2}{C} \right)$$

(1.9)

For vanishing energy splitting $\Delta E \simeq 0$, the classical ohmic voltage-capacitance relation $\Delta V_g = e/C$ is recovered.

There are three distinct temperature regimes:
Figure 1.6 Schematic comparison, as a function of gate voltage $V_g$, of the Coulomb blockade oscillations in the conductance, the number of of electrons in the dot $N$, the electrochemical potential in the dot $\mu_{\text{dot}}(N)$ and the electrostatic potential $\phi$ from top to bottom respectively.
1. $e^2/C \ll k_B T$, where charge discreteness cannot be distinguished

2. $\Delta E \ll k_B \ll e^2/C$, the classical Coulomb blockade regime. Several discrete levels are excited by thermal fluctuations

3. $k_B T \ll \Delta E \ll e^2/C$, the quantum Coulomb blockade regime. Only one or a few discrete levels take part in the electron transport.

We will be dealing with the last situation throughout the rest of this work.

1.2 Kondo effect in quantum dots

Physicists' interest in the Kondo effect started with Japanese theorist Jun Kondo's groundbreaking discovery in 1964. It subsided until the advent of the state-of-the art nanotechnology techniques which enabled unprecedented control over Kondo systems.

The electrical resistance of a pure metal generally drops as its temperature decreases since the electrons can travel through a metallic crystal more easily when the lattice vibrations are tiny. The resistance saturates as the temperature drops below around 10 K because the static defects in the metal are insensitive to the temperature variations.

Some metals like lead, niobium and aluminium suddenly lose all their resistance and become superconducting. This phase transition from a conducting to a superconducting state takes place at a critical temperature $T_c$.

When magnetic atoms, such as cobalt, are added, the electrical resistance increases as the temperature is lowered further rather as opposed to the saturation
in pure metals. Although this behaviour does not involve a phase transition unlike superconductivity, the so-called Kondo temperature governs the low-temperature electronic properties of the material. This anomalous increase has been observed experimentally since 1930's, however, a convincing theoretical explanation did not come until 1964.

It is possible to calculate theoretically the probability of backscattering from defects within the metal, which prevents the propagation of electrons through the crystal, when the defect is small. The calculation can only be carried out perturbatively for large defects though. In 1964, Jun Kondo found out that the second term in the perturbation series could be much larger than the first while he was considering the scattering from a magnetic ion that interacts with the spins of the conduction electrons. The implication of this result was that the resistance of a metal increases logarithmically in low temperatures.

It turns out that Kondo's theory accurately describes the experimentally observed upturn of resistance at low temperatures. On the other hand, the resistance would go to infinity at zero temperature according to this theory and it is obviously wrong. Subsequent investigations showed that Kondo's result was valid only above a certain energy scale, which was called the Kondo temperature $T_k$.

The main difference between a quantum dot and a bulk metal lies in their different geometries. In a metal, the electron states are plane waves and scattering from
Figure 1.7  Upper panel shows the resistance as a function of temperature in bulk geometry. In metals that contain magnetic impurities, such as cobalt-in copper systems, the electrons are scattered by the impurity resulting in an increased resistance below the Kondo temperature(red curve). In the absence of magnetic impurities, it saturates for normal metals(blue curve) and drops to zero for superconductors at $T_c$(green). The lower panel shows the conductance as a function of temperature for a quantum dot. When the number of electrons in the dot is odd(red curve), conductance increases below Kondo temperature since a new channel for transport opens. When the number of electrons is even, it drops to zero(blue curve).
impurities in the metal mixes electron waves with different momenta. This momentum transfer increases the resistance. In a quantum dot, all the electrons have to travel through the device since there is no electrical path around it. In this case, the Kondo resonance makes it easier for states belonging to the two opposite leads to mix. This mixing increases the conductance when the dot contains odd number of electrons thus the Kondo effect produces the opposite behaviour in a quantum dot in contrast with a bulk metal.

The Kondo effect arises only when the defects are magnetic, i.e. the total spin of all the electrons in the impurity is non-zero. These electrons interact with the electrons in the metal which act like a Fermi liquid in which the distribution of the electrons are governed by a Fermi-Dirac distribution function.

Phillip Anderson introduced a model Hamiltonian in 1961 that has one electron level denoted by $\varepsilon_0$. In this model, the electron can tunnel quantum mechanically from the impurity and escape if its energy lies above the Fermi level, otherwise it remains trapped. The net spin of the defect is 1/2 and its z-component is fixed as either "up" or "down" initially. Exchange processes can effectively change the initial orientation of the net spin in the impurity (from up to down or vice versa) while generating a reverse process in the Fermi sea. In quantum mechanics, Heisenberg uncertainty principle allows an electron to be taken from the localized impurity state and put into an occupied energy state at the surface of the Fermi sea for a very
Figure 1.8  The single level Anderson Hamiltonian assumes the impurity has one discrete state with energy level $\epsilon_0$ below the Fermi level of the metal. This state is occupied by a spin-degenerate electron (blue arrow). Adding another electron is forbidden by the intrasite Coulomb repulsion energy $U$. The electron in the dot may tunnel onto one of the leads to briefly occupy a classically prohibited "virtual state" and then be replaced by an electron from the other lead with the opposite spin. This process effectively flips the spin of the impurity. Many such events combine to produce the "Kondo effect", which gives rise to a sharp resonance at the Fermi level in the impurity density of states.
short period time-on the order of $\hbar/|\varepsilon_0|$ even though this is a classically forbidden process without putting energy into the system. Another electron must tunnel from the Fermi sea back to the impurity within this timescale and the spin orientation of this electron may be opposite to the first one resulting in a flip of the net spin of the impurity. When many such processes come together, a novel many-body state called Kondo resonance is generated at the Fermi level.

The Kondo resonance is pinned to the Fermi level so it is always "on resonance". Even when the location of the discrete state $\varepsilon_0$ is very far away from the Fermi level, the Kondo effect adjusts the energy of the system so that it is always on resonance. The only requirement for the effect to occur is that the system is cooled below the Kondo temperature $T_k$, which characterizes the strength of the Kondo effect. An expression for the [15]

$$T_k = \frac{1}{2} \sqrt{U \Gamma} \exp \left( \frac{\pi \varepsilon_0 (\varepsilon_0 + U)}{\Gamma U} \right)$$

(1.10)

The main advantage of the quantum dots is the tunability. While it is extremely difficult to change the parameters of the bulk metals, external knobs enable the discrete energy level of the structure to be swept as well as the number of electrons confined in the dot. In terms of the Anderson Hamiltonian, the energy level $\varepsilon_0$, of the discrete state, its linewidth $\Gamma$ and the intasite Coulomb repulsion energy $U$ can easily be adjusted by changing the voltages on the gates. One common feature between quantum dots and the bulk metals is the universality. The conductance of a quantum
Figure 1.9  This is the scanning electron microscope image showing top view of the quantum dot. Three gate electrodes, the one on the right and the upper and lower ones on the left, control the tunnel barriers between reservoirs of two-dimensional electron gas (at top and bottom) and the droplet of electrons. The middle electrode on the left is used as a gate to change the energy of the droplet relative to the two-dimensional electron gas. Source and drain contacts at the top and bottom are not shown.
dot and a bulk metal in the Kondo regime depends only on $T/T_k$. In quantum dots, this universality can easily be changed because the parameters that define $T_k$ can easily be changed.

The first pioneering experiment demonstrating the Kondo effect in quantum dots was carried out by David Goldhaber-Gordon and his coworkers at MIT and by the Delft group shortly thereafter [2, 16]. Fig. 1.9 shows the quantum dot fabricated by the first group using multiple metallic gates deposited on a GaAs/AlGaAs heterostructure containing a two-dimensional electron gas. The electrons were first trapped in a plane by differences in the electronic properties of the heterostructure’s layers. They were subsequently isolated from regions of the plane under the gates when negative volatages are applied to those gates. This process creates an island of electrons separated from the leads by tunnel junctions. The smaller size of the SET’s which is crucial to the observation of the Kondo effect was achieved by fabricating shallower 2DEG heterostructures and finer metallic gate patterns by electron-beam lithography.

Fig. 1.9 depicts the behaviour of the Coulomb blockade peaks for this device as a function of gate voltage $V_g$ for large $\Gamma$. Panels a and b show that these peaks form pairs with large inter-pair spacing and small intra-pair spacing. Between paired peaks, $N$ is odd and it is even between adjacent pairs. Intrapair and interpair space are proportional to the $U$ and $U + \Delta\varepsilon$ respectively. The conduction mechanism is
also different within pairs from between pairs. The conductance is enhanced for odd number intrapair valleys at low temperatures whereas it is suppressed for even number interpair valleys. This is an unambiguous evidence of Kondo physics. In panel c, the Kondo effect is suppressed as $\Gamma$ is reduced and peak pairing disappears too.

The subsequent experiments at Delft demonstrated that the conductance can indeed reach the quantum limit of conductance $2e^2/h$ so that the electrons are transmitted perfectly through the dot making it completely transparent.

Fig. 1.11 shows the results of that experiment [17]. The upper panel displays the conductance for several temperatures as a function of gate voltage $V_g$. As the temperature goes down, the conductance $G$ in the valleys where the dot has odd number of electrons starts increasing due to the Kondo effect eventually hitting unitarity limit. On the other hand, the conductance decreases in the valleys where odd number of electrons are trapped in the dot.

The lower panel on the left in Fig. 1.11 shows conductance as a function of temperature for three different gate voltages. Red curves are fits to

$$G(T) = G_0 \left( \frac{T^2_K}{T^2_K + T^2} \right)$$

with $T'_k = T_k/\sqrt{2^{1/s} - 1}$. The fit parameter $s \approx 0.2$ for a spin half system [18, 19]. The Kondo temperature $T_K$ for the different gate voltages can be calculated from these fits. When these curves are replotted as a function of $T/T_K$, they lie on top of each other, illustrating that electronic transport in the Kondo regime is described
Figure 1.10  Temperature dependence of infinitesimal-bias conductance $G$ through two different spatial states on the dot as a function of gate voltage $V_g$. Panels a and b show the situation when $\Gamma$ is large so that the Coulomb blockade peaks corresponding to the two spin states for each spatial state is paired. Full, dashed and dotted lines correspond to 90 mK, 400 mK and 800 mK respectively. Panel c depicts the case when $\Gamma$ is reduced thus the peak pairing disappears. Full line is for 90 mK and dotted line is for 800 mK.[2]

by a universal function that depends only on $T/T_K$. This universality is a property quantum dot systems share with bulk metals, however, their advantage is that the parameters that define $T_K$ can easily be changed so that the universality can be checked readily.

Kondo effect has also been observed in STM experiments probing magnetic impurities attached to surfaces in so called quantum corrals [20]. A fascinating result of these investigations was that a Kondo impurity localized on one of the foci of an
Figure 1.11  Upper panel shows $G$ versus $V_{gl}$ at $B=0.4$ T for temperature ranging from 15 mK (thick black line) up to 800 mK (thick red trace). Left lower panel shows $G(T)$ at fixed gate voltages $V_{gl}=-411(\circ),-414(\circ)$ and $-418(\Delta)$ mV. Red curves are fits to Eqs. (1.11). Right lower panel shows $G$ versus $T/T_K$ for $V_{gl}=-411(\circ), -412(\Box), -413(\times), -414(\circ), -415(\circ), -416(\Delta)$ mV. The blue curve is a fit to Eqs. (1.11) with fixed $T_K=1$ and $G_0 = 2e^2/h$. $s=0.29$ is the only fitting parameter.
ellipse can induce a "mirage" Kondo resonance on the other foci even when the latter one contains no impurity at all [21]. This phenomenon was explained as an interference pattern due to single particle wave mechanics. A rigorous theory invoking non-equilibrium Green's function techniques for STM experiments probing magnetic impurities on surfaces has also been developed [22]. These studies are beyond the scope of this thesis and will not be discussed any further here.
2.1 Anderson Hamiltonian

We describe the interaction between the atomic states and the metal's conduction electrons by a time-dependent Anderson Hamiltonian [23, 24]

\[
H(t) = \sum_{\sigma} \varepsilon_{\sigma}(t)n_{\sigma} + \frac{1}{2} \sum_{\sigma} U_{\sigma,\sigma'} n_{\sigma} n_{\sigma'} + \sum_{k\sigma} \varepsilon_{k} n_{k\sigma} + \sum_{\sigma k} [V_{\sigma k}(t)c_{k\sigma}^\dagger c_{\sigma} + \text{h.c.}]. \tag{2.1}
\]

In this equation, \(\varepsilon_{\sigma}(t)\) denotes the instantaneous energies of the different atomic levels while \(\varepsilon_{k}\) represents the energies in the continuum of levels in the substrate metal's conduction band. The subscripts \(\sigma\) denote spin for both the atomic states and the conduction electrons, \(k\) refers to the spatial quantum numbers of the metal's conduction electrons. The components in \(k\) referring to a common symmetry for both the atom and metal are conserved. The first summation describes the bare atomic states, the second describes intra-atomic correlation (the primed summation here excludes the term in which \(\sigma = \sigma'\)). The third summation represents the surface conduction electrons and the fourth summation describes the tunneling between the atomic states and the surface conduction band of the metal. The abbreviation h.c. denotes the Hermitian conjugate. Eq. (2.1) represents an extension of the conventional Anderson model to the case where multiple atomic orbitals are included. Unless disallowed by symmetry considerations, different atomic orbitals can interact via tunneling to
the substrate and back. This results in off-diagonal components of the impurity self-
energies and Green's functions, which will be discussed in some detail later in this
paper, thus generalizing the equations of Ref. [25].

The significance of the intra-atomic Coulomb interaction $U$ has been discussed
previously [25] and as was done there, we assume that $U$ is sufficiently large enough,
thus it can be taken to be infinite, so that we can apply the slave-boson method
[25, 26]. Introducing a creation operator $b^\dagger$ satisfying boson commutation relations,
we can write the bosonized version of (2.1) as

$$H(t) = \sum_\sigma \varepsilon_\sigma(t)n_\sigma + \sum_k \varepsilon_k n_{k\sigma} + \sum_{\sigma k} \left[ V_{\sigma k}(t)c_{k\sigma}^\dagger b^\dagger c_\sigma + \text{H.c.} \right]. \tag{2.2}$$

In addition to the total electron number, a conserved "charge" $Q_B$ of the above
Hamiltonian is given by

$$Q_B \equiv \sum_\sigma n_\sigma + n_B, \tag{2.3}$$

where $n_B = b^\dagger b$. Since only the $Q_B = 1$ subspace of (2.2) is physically relevant, we
use the Langreth-Nordlander method [25] for accomplishing the projection onto this
subspace.

To treat the non-equilibrium aspects we use the approach introduced by Kadanoff
and Baym [27], in a form summarized by Langreth [28] and used by Langreth and
Nordlander (LN) [25]. The procedure is to 1) develop an approximation for the self
energies, 2) solve the the time-dependent Dyson equation [Eq. (2.9) in LN] for the
advanced and retarded Green's functions $G^A$ and $G^R$, 3) solve the Kadanoff-Baym equations for $G^< [\text{Eq. (2.6)}$ and (2.7) in LN] with the appropriate boundary conditions, using the values of $G^A$ and $G^R$ obtained in step 2. The instantaneous probability $n_i(t)$ for finding an electron in the atomic state $|i\rangle$ is given by the diagonal matrix element

$$n_i(t) = \langle i | G^< (t,t) | i \rangle. \quad (2.4)$$

In this thesis, the $|i\rangle$ is either the state $|l\sigma\rangle$ or the slave boson state. Although we typically speak about the $n_i$'s as if they were "populations", we should remember that $G^<$ is thermally averaged over all initial configurations of the substrate electrons, so that more properly $n_i$ is an ensemble average, which, because it is necessarily between 0 and 1 inclusive, can be interpreted as the probability that there is an electron in state $|i\rangle$.

### 2.2 Non-crossing approximation

We will make the same type of approximation for the self-energies as LN. This is diagrammatically represented in Fig. 2.1. This approximation contains the leading terms in $1/N$, where $N$ is the effective degeneracy of the atomic level involved. It also contains the leading terms in a perturbation series in the size of the tunneling matrix element $V$.

We generally follow the notation of LN and use the notation $B$ for the slave boson functions ($>$, $<$, $A$, or $R$), that is "greater", "less", advanced, or retarded, as the case
may be) and reserve $G_\sigma$ for the corresponding atomic state functions and $G_{kk'\sigma}$ for the substrate electron functions. The self-energy term for the atomic states becomes

$$
\Sigma^\Xi_\sigma(t, t') = K^\Xi_\sigma(t, t') B^\Xi(t, t'), \tag{2.5}
$$

and the self-energy for the slave boson takes the form

$$
\Pi^\Xi(t, t') = \sum_\sigma K^\Xi_\sigma(t', t) G^\Xi_\sigma(t, t'), \tag{2.6}
$$

where $K^\Xi_\sigma(t, t')$ is defined in terms of the Green's function for the conduction electrons and the tunneling matrix elements as

$$
K^\Xi_\sigma(t, t') = \sum_k \tilde{V}_{\sigma k}(t) f^\Xi(\varepsilon_k) \tilde{V}_{\sigma k}(t'), \tag{2.7}
$$

with $\tilde{V}_{\sigma k}(t) = V_{\sigma k}(t) \exp(i\varepsilon_k t)$. Similarly the advanced and retarded self-energies are given by

$$
\Sigma^{R,A}_\sigma(t, t') = K^{R,A}_\sigma(t, t') B^{R,A}_\sigma(t, t'), \tag{2.8}
$$

$$
\Pi^{R,A}_\sigma(t, t') = \sum_\sigma K^{<,>}_\sigma(t', t) G^{R,A}_\sigma(t, t'). \tag{2.9}
$$

The above quantities have been projected onto the $Q_B = 1$ subspace using the method of LN, according to which one removes all terms of order $(Q_B)^2$ or higher in the "less than" correlation functions. One aspect of this projection is that we replaced the substrate functions $G^\Xi_{kk'T}(t, t')$ by their unperturbed forms $\delta_{kk'} f^\Xi(\varepsilon_k) \exp(-i\varepsilon_k(t-t'))$ in the expression (2.7) for $K^\Xi$, where $f^<(\varepsilon)$ is the Fermi function $f^<(\varepsilon) = (e^{\beta \varepsilon} + 1)^{-1}$, and $f^>(\varepsilon) = 1 - f^<(\varepsilon)$. Corrections to this are proportional either to $B^<$ or $G^<_\sigma$ and
hence to \((Q_B)^1\). \(K^\bar{z}\) appears in the Dyson equations of the next section in such a way that any correction to it of order \((Q_B)^1\) causes a correction of order \((Q_B)^2\) to the physical quantities \(B^<\) or \(G_{w \sigma}^<\). Therefore these corrections must be neglected. We emphasize that this neglect, which turns out to be an enormous simplification, is required, and is not an additional approximation. This should not be construed to imply that there is no correction to the substrate electron functions themselves, and these do indeed have a correction of order \((Q_B)^1\) which could be used, for example, to calculate the energy transfer to the substrate, an important subject which should be a matter for a future investigation.

2.3 Dyson Equations

With the above expressions for the self-energies, the Dyson equations for the atomic states and the slave-boson state can be constructed. Dyson's equation for the advanced or retarded Green's functions related to atomic states \(\ket{\sigma}\) and \(\bra{\sigma}\) now takes the form

\[
\left[i \frac{\partial}{\partial t} - \varepsilon_{\sigma}(t)\right] G_{\sigma}^{R}(t,t') = \delta(t - t') + \int_{-\infty}^{\infty} d\bar{\tau} K_{\sigma}^{\bar{z}}(t,\bar{\tau}) B^{R}(t,\bar{\tau}) G_{\sigma}^{R}(\bar{\tau},t'),
\]

while Dyson equation for the slave-boson propagator takes the form

\[
i \frac{\partial}{\partial t} B^{R}(t,t') = \delta(t - t') + \sum_{\sigma} \int_{-\infty}^{\infty} d\bar{\tau} K_{\sigma}^{\bar{z}}(\bar{\tau},t) G_{\sigma}^{R}(t,\bar{\tau}) B^{R}(\bar{\tau},t'),
\]

where \(K_{\sigma}^{\bar{z}}\) are defined in Eq. (2.7). The advanced Green's function can be obtained directly from the retarded Green's function using \(G_{\sigma}^{A}(t,t') = (G_{\sigma}^{R}(t',t))^{*}\), where the
Figure 2.1  This figure shows the Feynman diagrams representing the self energy of the impurity electron and slave boson. The perturbative expansion is truncated after the leading term which includes only the non-crossing propagators.
asterisk denotes the complex conjugate.

The Dyson equations for the "less than" Green's functions may be written explicitly using (2.5) and (2.8) for the atomic states and (2.6) and (2.9) for the slave boson. The "less than" Green's function for the states \(|\sigma\rangle\) and \(|\sigma\rangle\) satisfies

\[
\left[ i \frac{\partial}{\partial t} - \varepsilon_\sigma(t) \right] G^<(\sigma, t, t') = \int_{-\infty}^{\infty} d\bar{t} K^<(\sigma, t, \bar{t}) B^R(\sigma, \bar{t}) G^<(\sigma, \bar{t}, t') + \int_{-\infty}^{\infty} d\bar{t} K^<(\sigma, t, \bar{t}) B^<(\sigma, \bar{t}) G^A(\sigma, \bar{t}, t'), \tag{2.12}
\]

while the "less than" Green's function for the slave-boson state satisfies

\[
i \frac{\partial}{\partial t} B^<(t, t') = \sum_\sigma \int_{-\infty}^{\infty} d\bar{t} \left[ K^<(\bar{t}, t) G^R(\sigma, t, \bar{t}) B^<(\sigma, \bar{t}, t') + K^<(\bar{t}, t) G^A(\sigma, t, \bar{t}) B^A(\bar{t}, t') \right]. \tag{2.13}
\]

The Dyson equations can be simplified by introducing \(\tilde{G}\) defined by the relation

\[
G_\sigma(t, t') \equiv \tilde{G}_\sigma(t, t') \exp \left[ -i \int_{t_0}^{t} d\tau \varepsilon_\sigma(\tau) + i \int_{t_0}^{t'} d\tau \varepsilon_\sigma(\tau) \right], \tag{2.14}
\]

where \(t_0\) can be any fixed time and \(G\) can be a Green's function or \(K^\pm\) defined in Eq. (2.7). The retarded Green's functions can be further simplified by introducing \(g_\sigma(t, t')\) through

\[
\tilde{G}^R_\sigma(t, t') \equiv -i\theta(t - t') g_\sigma(t, t'), \tag{2.15}
\]

and \(b(t, t')\) through

\[
B^R(t, t') \equiv -i\theta(t - t') b(t, t'), \tag{2.16}
\]

\[
B^A(t, t') \equiv i\theta(t' - t) b(t, t'),
\]
with the supplemental conditions that \( g_\sigma(t, t) = 1 \) and \( b(t, t) = 1 \), which arise from the equal-time commutation relations. Notice the following relation:

\[
\begin{align*}
g_\sigma(t', t) &= g_\sigma^*(t, t'), \\
b(t', t) &= b^*(t, t').
\end{align*}
\]

(2.17)

We only calculate the retarded functions and then obtain the advanced ones through complex conjugation, using (2.15), (2.16), and (2.27). The Dyson equations for \( g_\sigma(t, t') \) and \( b(t, t') \) for \( t \geq t' \) become

\[
\begin{align*}
\frac{\partial}{\partial t} g_\sigma(t, t') &= - \int_{t'}^t dt' \bar{K}_\sigma^>(t, t') b(t, t') g_\sigma^*(t', t'), \\
\frac{\partial}{\partial t} b(t, t') &= - \sum_\sigma \int_{t'}^t dt' \bar{K}_\sigma^<(t, t') g_\sigma(t, t') b(t', t'),
\end{align*}
\]

(2.18) \hspace{1cm} (2.19)

which fully determine the functions \( g_\sigma(t, t') \) and \( b(t, t') \) for \( t \geq t' \). For \( t < t' \) they can then be determined using (2.27). In this notation the Dyson equations for the “less than” Green’s functions take the following form

\[
\frac{\partial}{\partial t} \bar{G}_\sigma^<(t, t') = \int_{-\infty}^{t'} dt' \bar{K}_\sigma^<(t, t') B^<(t, t') g_\sigma^*(t', t) - \int_{-\infty}^t dt' \bar{K}_\sigma^>(t, t') b(t, t') \bar{G}_\sigma^<(t', t'),
\]

(2.20)

and

\[
\frac{\partial}{\partial t} B^<(t, t') = \sum_\sigma \left[ \int_{-\infty}^{t'} dt' \bar{K}_\sigma^>(t', t') \bar{G}_\sigma^<(t, t') b^*(t', t) - \int_{-\infty}^t dt' \bar{K}_\sigma^<(t, t') g_\sigma(t, t') B^<(t', t') \right],
\]

(2.21)

where \( g_\sigma^*(t', \bar{t}) \) and \( b^*(t', \bar{t}) \), the complex conjugates of \( g_\sigma(\bar{t}, t') \) and \( b(\bar{t}, t') \) respectively, are from the advanced Green’s functions. The instantaneous population of the atomic
state $|\sigma\rangle$ is then given according to (2.4) by

$$n_\sigma(t) = \tilde{G}_\sigma^<(t,t) = G_\sigma^<(t,t),$$

while the instantaneous population of the slave-boson state is given by

$$n_B(t) = B^<(t,t).$$

It is straightforward to show that $\frac{d}{dt} Q_B(t) = 0$, by using Eqs. (2.20), (2.21), (2.22), (2.23) and (2.3), plus the following identity:

$$\frac{dn(t)}{dt} \equiv \frac{\partial}{\partial t} G^<(t,t') \bigg|_{t'=t} + \frac{\partial}{\partial t'} G^<(t,t') \bigg|_{t'=t},$$

where $n$ and $G^<$ could either refer to atomic states [Eq. (2.22)] or the slave boson [Eq. (2.23)]. Therefore the Dyson equations explicitly conserve $Q_B$.

### 2.4 Discretization of Dyson equations

In this section, we present an improved version of the algorithm for numerical solution of the Dyson equations introduced in [29]. Here we will follow the notation of Shao et al. [29]. Let us start from a consideration of retarded Green's functions. The Dyson equations for $g_\sigma(t,t')$ and $b(t,t')$ for $t \geq t'$ are

$$\frac{\partial}{\partial t} g_\sigma(t,t') = - \int_{t'}^{t} d\tilde{t} \tilde{K}_\sigma^>(\tilde{t}, t) b(\tilde{t}, t') g_\sigma(\tilde{t}, t'),$$

$$\frac{\partial}{\partial t} b(t,t') = - \sum_\sigma \int_{t'}^{t} d\tilde{t} \tilde{K}_\sigma^<=(\tilde{t}, t) g_\sigma(t, \tilde{t}) b(\tilde{t}, t').$$
For \( t < t' \) the \( g_\sigma(t, t') \) and \( b(t, t') \) functions can be determined by
\[
\begin{align*}
g_\sigma(t', t) & = g^*_\sigma(t, t'), \\
               b(t', t) & = b^*(t, t').
\end{align*}
\]
(2.27)

We can represent the Green’s functions as
\[
\begin{align*}
g_\sigma(t, t') & = g^f_\sigma(t, t') e^{i\omega_g(t-t')}, \\
b(t, t') & = b^f(t, t') e^{i\omega_h(t-t')},
\end{align*}
\]
(2.28)

where \( e^{i\omega_g(t-t')} \) and \( e^{i\omega_h(t-t')} \) are the oscillatory “carrier” parts and \( g^f_\sigma(t, t') \) and \( b^f(t, t') \) denote smooth, envelope-like modulating functions. By substituting Eqs. (2.28) in Eqs. (2.25) and (2.26) one can obtain
\[
\begin{align*}
\frac{\partial}{\partial t} \left[ g^f_\sigma(t, t') e^{i\omega_g(t-t')} \right] & = - \int_{t'}^t d\bar{t} \tilde{K}^>(t, \bar{t}) e^{i\omega_h(t-\bar{t})} e^{i\omega_g(\bar{t}-t')} \\
& \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad b^f(t, \bar{t}) g^f_\sigma(\bar{t}, t'), \\
\frac{\partial}{\partial t} \left[ b^f(t, t') e^{i\omega_h(t-t')} \right] & = - \sum_\sigma \int_{t'}^t d\bar{t} \tilde{K}^<(\bar{t}, t) e^{i\omega_g(\bar{t}-t)} e^{i\omega_h(\bar{t}-t')} \\
& \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad g^f_\sigma(\bar{t}, t) b^f(\bar{t}, t').
\end{align*}
\]
(2.29)

(2.30)

In steady state, both kernels depend only on the time difference rather than on individual values of \( t \) and \( \bar{t} \). The kernels can be combined with the oscillatory parts in the following manner
\[
\begin{align*}
\tilde{K}^>_\sigma(t, \bar{t}) e^{i\omega_h(t-\bar{t})} e^{i\omega_g(\bar{t}-t')} & = \tilde{K}^>_\sigma(t, \bar{t}) e^{i(\omega_h-\omega_g)(t-\bar{t})} e^{i\omega_g(t-t')} \\
& = \tilde{K}^>_\sigma(t - \bar{t}) e^{i\omega_g(t-t')},
\end{align*}
\]
(2.31)
and
\[
\tilde{K}_\sigma^<(\bar{t}, t) e^{i\omega_g(t-r)} e^{i\omega_b(t-t')} = \tilde{K}_\sigma^<(\bar{t}, t) e^{i(\omega_g - \omega_b)(t-r)} e^{i\omega_b(t-t')}
\]
\[
= \tilde{K}_\sigma^<_{\omega}(\bar{t} - t) e^{i\omega_b(t-t')}. \tag{2.32}
\]

Let us illustrate our discretization scheme on the integral part of equation (2.30).

First we split the \([t', t]\) range in pieces
\[
\int_{t'}^t d\bar{t} \tilde{K}_\sigma^<(\bar{t}, t) g^f_d(t, \bar{t}) b^f(\bar{t}, t') =
\]
\[
\left[ \int_{t'}^{t'+\Delta t_{\text{lin}}} + \int_{t'-\Delta t_{\text{lin}}}^t + \int_{t'+\Delta t_{\text{lin}}}^{t'-\Delta t_{\text{lin}}} \right] d\bar{t} \tilde{K}_\sigma^<_{\omega}(\bar{t}, t) g^f_d(t, \bar{t}) b^f(\bar{t}, t'). \tag{2.33}
\]

We will refer to the intervals \([(t - \bar{t}) < \Delta t_{\text{lin}} \text{ or } (\bar{t} - t') < \Delta t_{\text{lin}}]\) and \([(t - \bar{t}) > \Delta t_{\text{lin}} \text{ and } (\bar{t} - t') > \Delta t_{\text{lin}}]\) as \(\mathcal{C}\) and \(\mathcal{L}\), respectively. For the \(\mathcal{C}\) interval, we use trapezoidal quadrature on the fine grid (grid size \(\delta\))
\[
\int_{t'}^{t'+\Delta t_{\text{lin}}} d\bar{t} \tilde{K}_\sigma^<(\bar{t}, t) g^f_d(t, \bar{t}) b^f(\bar{t}, t') =
\]
\[
\delta \sum_{j=n}^k c_j \tilde{K}_\sigma^<_{\omega}(m, j)b^f(m, j)g^f_d(j, n). \tag{2.34}
\]

Here we use integers \(j, n, k,\) and \(m\) for the time arguments, \(c_j = 1/2\) for \(j = n, k\) and \(c_j = 1\) in all other cases. In the \(\mathcal{L}\) interval we employ the following decomposition
\[
\int_{t'-\Delta t_{\text{lin}}}^{t-\Delta t_{\text{lin}}} d\bar{t} \tilde{K}_\sigma^<(\bar{t}, t) g^f_d(t, \bar{t}) b^f(\bar{t}, t') =
\]
\[
\Delta \sum_i \int_{\Delta_i} d\bar{t} \tilde{K}_\sigma^<(\bar{t}, t) g^f_d(t, \bar{t}) b^f(\bar{t}, t') =
\]
\[
\Delta \sum_i g^f_d(t, \bar{\xi}_i)b^f(\bar{\xi}_i, t') \int_{\Delta_i} d\bar{t} \tilde{K}_\sigma^<(\bar{t}, t), \tag{2.35}
\]

where \(\Delta_i = [\bar{t}_i, \bar{t}_{i+1}]\) is the \(i\)th coarse grid interval and \(\bar{\xi}_i \in \Delta_i\). We assume that
\[
g^f_d(t, \bar{\xi}_i)b^f(\bar{\xi}_i, t') \approx \frac{1}{2} \left[ g^f_d(t, \bar{t}_i)b^f(\bar{t}_i, t') + g^f_d(t, \bar{t}_{i+1})b^f(\bar{t}_{i+1}, t') \right]. \tag{2.36}
\]
This approximation is valid because the $g^f_\sigma$ and $b^f$ functions behave almost linearly.

To obtain an accurate estimate for the oscillatory kernel integration in equation (2.35) we use a finer grid with spacing $\delta$ and Simpson’s quadrature

$$
\int_{\Delta_i} \tilde{K}_{\sigma \omega}^> (t, \bar{t}) d\bar{t} \cong \delta \sum_j w_j \tilde{K}_{\sigma \omega}^> (t - \bar{t}_j) = \tilde{K}_{\sigma p}^> (t, \bar{t}_i),
$$

(2.37)

and

$$
\int_{\Delta_i} \tilde{K}_{\sigma \omega}^< (t, \bar{t}) d\bar{t} \cong \delta \sum_j w_j \tilde{K}_{\sigma \omega}^< (\bar{t}_j - t) = \tilde{K}_{\sigma p}^< (\bar{t}_i, t),
$$

(2.38)

where $w_j$ are the weights. Due to the translational invariance of the kernels one can precompute $\tilde{K}_{\sigma p}^> (t, \bar{t}_i)$ and $\tilde{K}_{\sigma p}^< (\bar{t}_i, t)$ values and keep them in the core memory during the calculation. In the differential part we use the finite difference method only for the non-periodic part

$$
\frac{\partial}{\partial \bar{t}} \left[ g^f_\sigma (t, t') e^{i \omega_\sigma (t-t')} \right] \cong e^{i \omega_\sigma (t-t')} \left[ i \omega_\sigma g^f_\sigma (t, t') + \frac{g^f_\sigma (t, t') - g^f_\sigma (t - \delta, t')}{\delta} \right].
$$

(2.39)

The discretized version of Eqs. (2.29) and (2.30) can be written as

$$
\left( 1 + \frac{i \delta \omega_\sigma}{2} \right) g^f_\sigma (m, n) = \left( 1 - \frac{i \delta \omega_\sigma}{2} \right) g^f_\sigma (m - 1, n)
$$

$$
-\frac{1}{2} \delta^2 \sum_{j=m}^n c_j \tilde{K}_{\sigma \omega}^> (m, j) b^f (m, j) g^f_\sigma (j, n)
$$

$$
-\frac{1}{2} \Delta \delta \sum_{j=p+1}^r c_j \tilde{K}_{\sigma \omega}^> (m, j) b^f (m, j) g^f_\sigma (j, n)
$$

$$
-\frac{1}{2} \delta^2 \sum_{j=r+1}^m c_j \tilde{K}_{\sigma \omega}^> (m, j) b^f (m, j) g^f_\sigma (j, n)
$$
\[-\frac{1}{2} \delta^2 e^{-i\delta \omega_y} \sum_{j=n}^{p} c_j \tilde{K}_{\sigma \omega}^{>}(m - 1, j)b^f(m - 1, j)g^f_\sigma(j, n)\]
\[-\frac{1}{2} \Delta \delta e^{-i\delta \omega_y} \sum_{j=p+1}^{r} c_j \tilde{K}_{\sigma P}^{>}(m - 1, j)b^f(m - 1, j)g^f_\sigma(j, n)\]
\[-\frac{1}{2} \delta^2 e^{-i\delta \omega_y} \sum_{j=r+1}^{m-1} c_j \tilde{K}_{\sigma \omega}^{>}(m - 1, j)b^f(m - 1, j)g^f_\sigma(j, n)\] (2.40)

and

\[\left(1 + \frac{i\delta \omega_b}{2}\right)b^f(m, n) = \left(1 - \frac{i\delta \omega_b}{2}\right)b^f(m - 1, n)\]
\[-\frac{1}{2} \delta^2 \sum_{\sigma} \sum_{j=n}^{p} c_j \tilde{K}_{\sigma \omega}^{<}(j, m)g^f_\sigma(m, j)b^f(j, n)\]
\[-\frac{1}{2} \Delta \delta \sum_{\sigma} \sum_{j=p+1}^{r} c_j \tilde{K}_{\sigma P}^{<}(j, m)g^f_\sigma(m, j)b^f(j, n)\]
\[-\frac{1}{2} \delta^2 \sum_{\sigma} \sum_{j=r+1}^{m} c_j \tilde{K}_{\sigma \omega}^{<}(j, m)g^f_\sigma(m, j)b^f(j, n)\]
\[-\frac{1}{2} \delta^2 e^{-i\delta \omega_b} \sum_{\sigma} \sum_{j=n}^{p} c_j \tilde{K}_{\sigma \omega}^{<}(j, m - 1)g^f_\sigma(m - 1, j)b^f(j, n)\]
\[-\frac{1}{2} \Delta \delta e^{-i\delta \omega_b} \sum_{\sigma} \sum_{j=p+1}^{r} c_j \tilde{K}_{\sigma P}^{<}(j, m - 1)g^f_\sigma(m - 1, j)b^f(j, n)\]
\[-\frac{1}{2} \delta^2 e^{-i\delta \omega_b} \sum_{\sigma} \sum_{j=r+1}^{m-1} c_j \tilde{K}_{\sigma \omega}^{<}(j, m - 1)g^f_\sigma(m - 1, j)b^f(j, n)\] (2.41)

where we use integers \(i, j, m,\) and \(n\) for the time arguments, with consecutive integers representing a time difference of \(\Delta,\) the coarse grid spacing. In Eqs. (2.40) and (2.41) we use trapezoidal quadrature, thus \(c_j = 1/2\) for \(j = n, m, m - 1\) and 1 in all other cases. These equations have the same algebraic structure as reported before (see [29]). The computational scaling of the equations solving is \(N^3,\) where \(N\) is the number of coarse mesh grid points. Therefore, it is crucial for the computational
Figure 2.2  Real part of retarded Green's functions $g_\sigma(t, t')$ (black), $g_\delta(t, t')$ (red), $b(t, t')$ (blue), and $b'(t, t')$ (green) for S1 with $N = 1000$, and fixed $t$.

performance to reduce $N$ as much as possible without losing accuracy. We therefore reformulate Dyson's equations with respect to the almost linearly behaving functions $g_\sigma(t, t')$ and $b'(t, t')$. This procedure allows us to use the coarse grid for discretized equations and fine grid $\delta$ for the preintegration of the kernels. To find good estimates for the frequencies $\omega_g$ and $\omega_b$ we use the previous implementation [29] with coarse grid discretization and then extract frequencies from the Green's functions. We found that the values of $\omega_g$ and $\omega_b$ are not sensitive to the quality of discretization and that even the coarse grid is sufficient for the frequency estimation.

The same preintegration scheme is valid for the "less than" Green's functions, therefore we present only the final discretized equations for them. In the $t \neq t'$ case
we have the following system of equations

\[
\left(1 + \frac{i\delta \omega_g}{2}\right)G^\sigma_\sigma(m, n) + \frac{\delta^2}{4} \tilde{K}^\sigma_\sigma(m, m) G^\sigma_\sigma(m, n) - \\
\frac{\delta^2}{4} \tilde{K}^\sigma_\sigma(m, n) B^\sigma(m, n) = G^\sigma_\sigma(m, n) + \\
\frac{\delta^2}{4} \tilde{K}^\sigma_\sigma(m - 1, n) B^\sigma(m - 1, n)e^{-i\delta \omega_g} + \left(1 - \frac{i\delta \omega_g}{2}\right) G^\sigma_\sigma(m - 1, n),
\]

(2.42)

\[
\left(1 + \frac{i\delta \omega_b}{2} + \frac{\delta^2}{4} \tilde{K}^\sigma_\sigma(m, n)\right) B^\sigma(m, n) - \\
\sum_\sigma \frac{\delta^4}{4} \tilde{K}^\sigma_\sigma(n, m) G^\sigma_\sigma(m, n) = \sum_\sigma B^\sigma(m, n) + \\
\sum_\sigma \frac{\delta^4}{4} \tilde{K}^\sigma_\sigma(n, m - 1) G^\sigma_\sigma(m - 1, n)e^{-i\delta \omega_b} + \left(1 - \frac{i\delta \omega_b}{2}\right) B^\sigma(m - 1, n),
\]

(2.43)

where

\[
G^\sigma_\sigma(m, n) = -\frac{\delta^2}{4} \tilde{K}^\sigma_\sigma(m - 1, m - 1) G^\sigma_\sigma(m - 1, n)e^{-i\delta \omega_g} + \\
\frac{\delta^2}{2} \sum_{j=1}^{p} \tilde{K}^\sigma_\sigma(m, j) B^\sigma(m, j) g^j_\sigma(n, j)^* + \\
\frac{\Delta \delta}{2} \sum_{j=p+1}^{r} \tilde{K}^\sigma_\sigma_p(m, j) B^\sigma(m, j) g^j_\sigma(n, j)^* + \\
\frac{\delta^2}{2} \sum_{j=r+1}^{n-1} \tilde{K}^\sigma_\sigma(m, j) B^\sigma(m, j) g^j_\sigma(n, j)^* + \\
\frac{\delta^2}{2} \sum_{j=1}^{p} \tilde{K}^\sigma_\sigma(m - 1, j) B^\sigma(m - 1, j) g^j_\sigma(n, j)^* e^{-i\delta \omega_g} + \\
\frac{\Delta \delta}{2} \sum_{j=p+1}^{r} \tilde{K}^\sigma_\sigma_p(m - 1, j) B^\sigma(m - 1, j) g^j_\sigma(n, j)^* e^{-i\delta \omega_g} + \\
\frac{\delta^2}{2} \sum_{j=r+1}^{n-1} \tilde{K}^\sigma_\sigma(m - 1, j) B^\sigma(m - 1, j) g^j_\sigma(n, j)^* e^{-i\delta \omega_g} - \\
\frac{\delta^2}{2} \sum_{j=1}^{p} \tilde{K}^\sigma_\sigma(m, j) b^j_\sigma(m, j) G^\sigma_\sigma(j, n) -
\]
\[ \frac{\Delta \delta}{2} \sum_{j=p+1}^{r} K_{\sigma \rho}^{\geq}(m, j)b^\dagger(m, j)G_{\sigma}^{\leq}(j, n) - \]
\[ \frac{\delta^2}{2} \sum_{j=r+1}^{m-1} K_{\sigma \omega}^{\geq}(m, j)b^\dagger(m, j)G_{\sigma}^{\leq}(j, n) - \]
\[ \frac{\delta^2}{2} \sum_{j=1}^{p} K_{\sigma \rho}^{\geq}(m - 1, j)b^\dagger(m - 1, j)G_{\sigma}^{\leq}(j, n)e^{-i\delta\omega_{g}} - \]
\[ \frac{\Delta \delta}{2} \sum_{j=p+1}^{r} K_{\sigma \rho}^{\geq}(m - 1, j)b^\dagger(m - 1, j)G_{\sigma}^{\leq}(j, n)e^{-i\delta\omega_{g}} - \]
\[ \frac{\delta^2}{2} \sum_{j=r+1}^{m-2} K_{\sigma \omega}^{\geq}(m - 1, j)b^\dagger(m - 1, j)G_{\sigma}^{\leq}(j, n)e^{-i\delta\omega_{g}}, \] (2.44)

and

\[ B_{\sigma}(m, n) = -\frac{\delta^2}{4} K_{\sigma \omega}^{\leq}(m - 1, m - 1)B^{\leq}(m - 1, n)e^{-i\delta\omega_{b}} + \]
\[ \frac{\delta^2}{2} \sum_{j=1}^{p} K_{\sigma \omega}^{\geq}(m, j)G_{\sigma}^{\leq}(m, j)b^*(n, j) + \]
\[ \frac{\Delta \delta}{2} \sum_{j=p+1}^{r} K_{\sigma \rho}^{\geq}(m, j)G_{\sigma}^{\leq}(m, j)b^*(n, j) + \]
\[ \frac{\delta^2}{2} \sum_{j=r+1}^{n-1} K_{\sigma \omega}^{\geq}(m, j)G_{\sigma}^{\leq}(m, j)b^*(n, j) + \]
\[ \frac{\delta^2}{2} \sum_{j=1}^{p} K_{\sigma \rho}^{\geq}(m - 1, j)G_{\sigma}^{\leq}(m - 1, j)b^*(n, j)e^{-i\delta\omega_{b}} + \]
\[ \frac{\Delta \delta}{2} \sum_{j=p+1}^{r} K_{\sigma \rho}^{\geq}(m - 1, j)G_{\sigma}^{\leq}(m - 1, j)b^*(n, j)e^{-i\delta\omega_{b}} + \]
\[ \frac{\delta^2}{2} \sum_{j=r+1}^{n-1} K_{\sigma \omega}^{\geq}(m - 1, j)G_{\sigma}^{\leq}(m - 1, j)b^*(n, j)e^{-i\delta\omega_{b}} - \]
\[ \frac{\delta^2}{2} \sum_{j=1}^{p} K_{\sigma \omega}^{\leq}(j, m)g_{\sigma}^{\dagger}(m, j)B^{\leq}(j, n) - \]
\[ \frac{\Delta \delta}{2} \sum_{j=p+1}^{r} K_{\sigma \rho}^{\leq}(j, m)g_{\sigma}^{\dagger}(m, j)B^{\leq}(j, n) - \]
\[ \frac{\delta^2}{2} \sum_{j=r+1}^{m-1} K_{\sigma \omega}^{\leq}(j, m)g_{\sigma}^{\dagger}(m, j)B^{\leq}(j, n) - \]
\[ \frac{\delta^2}{2} \sum_{j=1}^{p} \tilde{K}_{\sigma\omega}^<(j, m-1)g^f_\sigma(m-1, j)B^<(j, n)e^{-i\delta\omega_b} - \]
\[ \frac{\Delta\delta}{2} \sum_{j=p+1}^{r} \tilde{K}_{\sigma\omega}^p(j, m-1)g^f_\sigma(m-1, j)B^<(j, n)e^{-i\delta\omega_b} - \]
\[ \frac{\delta^2}{2} \sum_{j=r+1}^{m-2} \tilde{K}_{\sigma\omega}^<(j, m-1)g^f_\sigma(m-1, j)B^<(j, n)e^{-i\delta\omega_b}. \]

(2.45)

For the \( t = t' \) case

\[ G_\sigma^<(m, m) + \text{Re}\left( \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^>(m, m)G_\sigma^<(m, m) \right) - \]
\[ \text{Re}\left( \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^<(m, m)B^<(m, m) \right) = G_\sigma^<(m-1, m-1) + \]
\[ \text{Re}\left( \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^<(m-1, m-1)B^<(m-1, m-1) \right) - \]
\[ \text{Re}\left( \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^>(m-1, m-1)G_\sigma^<(m-1, m-1) \right) + \text{Re}\left( G_\sigma(m) \right), \]
\[ (2.46) \]
\[ - \sum_{\sigma} \text{Re}\left( \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^>(m, m)G_\sigma^<(m, m) + \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^<(m, m)B^<(m, m) \right) + \]
\[ B^<(m, m) = - \sum_{\sigma} \text{Re}\left( \frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^<(m-1, m-1)B^<(m-1, m-1) \right) - \]
\[ \sum_{\sigma} \text{Re}\left( -\frac{\delta^2}{2} \tilde{K}_{\sigma\omega}^>(m-1, m-1)G_\sigma^<(m-1, m-1) + G_\sigma(m) \right) + \]
\[ B^<(m-1, m-1), \]
\[ (2.47) \]

where

\[ G_\sigma(m) = \delta^2 \sum_{i=m-1}^{m} \sum_{j=1}^{p} c_{j} \tilde{K}_{\sigma\omega}^<(j, i)B^<(j, i)g^f_\sigma(i, j) + \]
\[ \Delta\delta \sum_{i=m-1}^{m} \sum_{j=p+1}^{r} c_{j} \tilde{K}_{\sigma\omega}^p(j, i)B^<(j, i)g^f_\sigma(i, j) + \]
\[ \delta^2 \sum_{i=m-1}^{m} \sum_{j=r+1}^{i-1} c_{j} \tilde{K}_{\sigma\omega}^<(j, i)B^<(j, i)g^f_\sigma(i, j) - \]
Figure 2.3 Imaginary part of retarded Green's functions $g_\sigma(t,t')$ (black), $g_\sigma^f(t,t')$ (red), $b(t,t')$ (blue), and $b^f(t,t')$ (green) for S1 with $N = 1000$, and fixed $t$.

\[
\delta^2 \sum_{i=m-1}^m \sum_{j=1}^p c_j \tilde{K}_{\sigma\omega}(i,j) b^f(i,j) G_{\sigma}(j,i) - \\
\Delta \delta \sum_{i=m-1}^m \sum_{j=p+1}^r c_j \tilde{K}_{\sigma\rho}(i,j) b^f(i,j) G_\sigma(j,i) - \\
\delta^2 \sum_{i=m-1}^m \sum_{j=r+1}^{i-1} c_j \tilde{K}_{\sigma\omega}(i,j) b^f(i,j) G_{\sigma}(j,i). \tag{2.48}
\]

As in the case of the retarded Green's functions, these systems of linear equations can be treated by methods developed by Shao et al. [29].

Smooth retarded electron and slave boson green's functions obtained by using the new numerical procedure are plotted away from the equal time diagonal in Fig. 2.2 and Fig. 2.3 alongside with the oscillatory ones. These figures clearly show the advantage of the new scheme.
If we want to take into account the abrupt change of the dot-lead tunneling rate or the position of the dot level, we need to modify equations (2.28) as

\[
\begin{align*}
g_\sigma(t, t') &= g_\sigma^f(t, t')e^{i\omega_1(t-t')} + \theta(t - t_1)\theta(t' - t_1) \\
g_\sigma^f(t, t')(e^{i\omega_2(t-t')} - e^{i\omega_1(t-t')}), \\
b(t, t') &= b^f(t, t')e^{i\omega_1(t-t')} + \theta(t - t_1)\theta(t' - t_1) \\
b^f(t, t')(e^{i\omega_2(t-t')} - e^{i\omega_1(t-t')}). \\
\end{align*}
\tag{2.49}
\]

In Eqs. (2.49), \(\omega_1\) and \(\omega_2\) correspond to the oscillation frequencies of the first and second state respectively and \(t_1\) is the time of the sudden change. One can apply the two grid scheme for this case as well.
Chapter 3
Quantum dot symmetrically coupled to metallic leads

3.1 Introduction

The understanding of the nonequilibrium real-time evolution of quantum many-body systems is much less advanced than the understanding of systems in equilibrium. Nonequilibrium effects are responsible for important phenomena such as dissipation and decoherence in electron transport through nanodevices. Quantum dots and qubits fall into this category where a mesoscopic device interacts with a fermionic or bosonic bath. Advances in nanofabrication of quantum dots have made it possible to study nonequilibrium transport phenomena in quantum dots in a controlled manner. Recently Elzerman et al. have emphasized the practical importance of real-time dynamics in quantum dots for quantum computation [30]. This type of system constitutes an ideal platform to study the Kondo effect out of equilibrium, since one can electrically tune the parameters of quantum dots.

The Kondo effect was first discovered in bulk metals with magnetic impurities providing localized unpaired spins [31] and observed later in semiconductor quantum dots [2, 18, 16]. It is a many-body effect in which conduction electrons in the vicinity of a spin impurity screen the spin to form a collective entangled ground state at low temperatures [32]. The most evident manifestation of Kondo physics in quantum dots
occurs when an odd number of electrons are confined within the dot. The resulting net spin is coupled to the fermionic bath at low temperatures and a sharp peak forms at the Fermi level in the dot density of states. The consequence of this Kondo peak is a large enhancement of the dot's conductance. This enhancement strongly depends on temperature, bias, and magnetic field [33, 34, 35, 36, 37].

Several theoretical groups have considered the effects of time-dependent AC perturbations of the bias and gate potentials on the transport trough quantum dots in the Kondo regime [38, 39, 40, 41, 42, 43, 44]. Kondo sidebands induced by AC perturbations of the dot have recently been observed in transport experiments on a single dot [45].

The application of abrupt perturbations by step-like switching the gate potential or bias [3, 46, 47, 48, 49, 50, 51] can determine the intrinsic timescales associated with the Kondo problem more precisely than AC modulation. Three timescales have recently been identified in the transient currents after the sudden shift of the dot level in a quantum dot coupled to two leads [3, 46]. The fastest (and trivial) timescale corresponds to charge relaxation and it is associated with the reshaping of the dot level due to its interaction with the conduction bands of the leads. This is a non-universal non-Kondo timescale and it is inversely proportional to the life time broadening of the dot level. The second timescale is the time it takes for the conductance of the dot to reach within a few percent of its equilibrium value. The third and longest timescale,
which is only present for finite bias across the dot, is the time it takes for the Split Kondo Peak (SKP) oscillations caused by the interference of the Kondo resonances on each lead to dampen out.

Here, we analyze the conductance of a quantum dot subject to a sudden change of coupling to its leads. We develop an efficient implementation of our numerical approach for the solution of the time-dependent Non-Crossing Approximation (NCA) equations [29]. This numerical improvement allows us to investigate the time-dependent response of quantum dots for lower temperatures and smaller biases and with greater speed than in our previous applications [3]. A comparison of the transient currents following a sudden shift in the coupling of the dot level to its leads with the transient currents following a sudden shift of the dot level into the same state shows that the response is almost identical. The two longer timescales are found to be the same.

The quantum dot is modeled by a single spin degenerate level of energy $\varepsilon_{\text{dot}}$ coupled to leads through tunnel barriers. This system is described by the Anderson Hamiltonian given by

$$H(t) = \sum_{\sigma} \varepsilon_{\text{dot}}(t)n_{\sigma} + \sum_{k\sigma} \varepsilon_k n_{k\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} U_{\sigma,\sigma'} n_{\sigma} n_{\sigma'} + \sum_{\sigma k} \left[ V_k(t) c_{k\sigma}^\dagger c_{\sigma} + \text{H.c.} \right],$$

(3.1)

where $c_{\sigma}^\dagger$ creates an electron of spin $\sigma$ in dot level, with $n_{\sigma}$ the corresponding number operator; $c_{k\sigma}^\dagger$ creates an electron in the leads and $V_k(t)$ is the hopping term. The
Coulomb repulsion energy is given by $U$, which we assume to be infinitely large, preventing the dot from being doubly occupied.

The dot density of states consists of two features when the dot level $\epsilon_{dot}$ is well below the Fermi level. First, there is a broad resonance of half-width

$$\Gamma(\epsilon, t) = 2\pi \sum_k |V_k(t)|^2 \delta(\epsilon - \epsilon_k)$$  \hspace{1cm} (3.2)

centered around the dot level. This is inhomogeneous broadening due to the tunneling of electrons between the dot and the leads and is sometimes referred to as the Fano resonance.

In addition to the Fano resonance, there is a sharp temperature sensitive Kondo peak at the Fermi level. It is characterized by a low energy scale called the Kondo temperature, which is given by

$$T_K(t) = D(t) \left( \frac{\Gamma(t)}{4D(t)} \right)^{\frac{1}{2}} \exp \left( -\frac{\pi |\epsilon_{dot}|}{\Gamma(t)} \right),$$  \hspace{1cm} (3.3)

where $D(t)$ is equal to half bandwidth when modeled by a symmetric flat band and $\Gamma(t)$ is defined as $\Gamma(\epsilon_{Fermi}, t)$. A symmetric parabolic band is used in our model with half bandwidth $D_0(t)=9\Gamma(t)$ and $D(t) \simeq D_0(t)/\sqrt{\epsilon}$. This choice gives the correct normalization for the leading logarithmic corrections in the Kondo model[29].

We investigate the physical observables as a function of $T/T_K$ and $\Gamma t$ when $T_K$, $T$, and $V$ are much smaller than $\epsilon_{dot}$ and $\Gamma$ by using the non-crossing approximation (NCA), which is reliable for temperatures down to $T < T_K$ [52]. We make the quantity
dimensionless by appropriate factors of $T_K$ and $G_0 \equiv 2(e^2/2\pi \hbar)$ and use atomic units with $\hbar = k_B = e = 1$ throughout this work.

In this section, we compute the electric currents through a dot which has left-right symmetry. The current into the dot depends on the time $t$ as

$$I_{\text{in}}(t) = i \sum_{k\sigma} V_k(t) \langle c^\dagger_{k\sigma}(t) c_\sigma(t) \rangle + \text{c.c.} \quad (3.4)$$

where $\langle c^\dagger_{k\sigma}(t) c_\sigma(t) \rangle$ is the Keldysh propagator. $I_{\text{in}}(t)$ can be divided into contributions $I_{\text{left}}(t)$ and $I_{\text{right}}(t)$ by restricting the $k$ summations to the appropriate lead. The transport current is given by $I(t) = \frac{1}{2}[I_{\text{left}}(t) - I_{\text{right}}(t)]$.

In the universal timescale where Kondo resonance formation takes place, we compare the conductance results of two systems which have different Kondo temperatures. We refer to them as system one and system two. These two systems have a constant dot level and their dot-lead tunneling constant is abruptly switched at $t = t_1$ from $\Gamma_1$, for which the current at the applied bias is small, and $T_K \ll T$, to $\Gamma_2$ for which the Kondo effect is present. In fact, this amounts to abruptly changing the hopping term in the Hamiltonian as it can be clearly seen from Eq. (4.2). In final state, system one has $T_K = 0.0022 \Gamma_2$ and system two has $T_K = 0.0011 \Gamma_2$. For both systems, the Kondo temperature of the dot is much smaller than the system temperature when the tunneling constant is $\Gamma_1$, therefore, the Kondo resonance does not exist in this state for all practical purposes. The spectral function consists of the broad virtual level of width $\sim 2\Gamma_1$ centered roughly at $\epsilon_{\text{dot}}$. When the tunneling constant is abruptly
switched, a new virtual-level resonance of width $\sim 2\Gamma_2$ is formed around the dot level in the non universal timescale. The time scale for the formation of this resonance is $\Gamma_2[48]$. The Kondo resonance is formed in the universal timescale.

We use the Kadanoff-Baym time dependent Green functions method which results in coupled integro-differential equations for the time loop Green functions. In the previous implementation, these equations were solved on a uniform discrete grid. This implementation works quite efficiently when we do calculations at temperatures and biases well above $T_K$, however it requires huge matrix sizes in order to account for the strong correlations properly when the temperature and bias is well below $T_K$ and this results in CPU times on the order of months. In order to overcome this difficulty and to be able to access very low temperatures within this formalism, we absorbed the oscillation frequencies of retarded and less than time loop Green functions into the kernel in the coupled integro-differential equations and thus obtained smooth Green's functions. This allowed us to use a coarse grid for the elements in the tails of the matrix that are responsible for the strong correlations and a fine grid for the elements close to the diagonal that account for the non-universal timescale. The resulting scheme is roughly half the coarse grid size faster than the previous implementation and this brings down the CPU time from months to a few days in an IBM p690 machine. Mathematical details of our numerical scheme are explained in the appendix.
3.2 Non-universal timescale

First of all, we would like to make the distinction between changing the dot-lead tunneling constant and changing the dot level which was considered before [3]. In Fig. 3.1, we plot the instantaneous conductance for both cases for \textit{system one} at a temperature well above $T_K$ in infinitesimal bias to be able to make both the non-universal and universal timescales visible. We intentionally use slightly different $\epsilon_{\text{dot}}/\Gamma_1$ in initial states for two cases to be able to shift the curves so that the difference would be visible. The final $\epsilon_{\text{dot}}/\Gamma_2$ is the same for both cases therefore both curves gradually merge in the universal timescale. If we pick the same $\epsilon_{\text{dot}}/\Gamma_1$ for both cases, the instantaneous conductances in the universal timescale perfectly overlap, thus the only difference between changing the dot-lead constant and changing the dot level lies in the non-universal timescale.

We start our analysis with the conductance results in the non-universal timescale. In the inset of Fig. 3.1, we show the instantaneous conductance in this timescale for the two cases mentioned above. It is quite clear from these results that we have robust oscillations reminiscent of Rabi oscillations. We observe these oscillations at all temperatures. In order to understand the origin of these fast oscillations, we have to recall that the spin flips that give rise to the Kondo resonance are absent in this timescale and the only process that takes place is the charge relaxation. This implies that we can neglect the spin dependent terms in Eq. (4.1) and solve the remaining
Figure 3.1  Comparison of instantaneous conductance for the cases of changing dot-lead coupling constant and the energy of the dot level. We show the rise of the conductance in the final state for $S1$. The calculation was carried out at $T=0.005\Gamma$ to make both timescales visible. The red curve corresponds to changing the dot level abruptly and the black curve is for changing the dot-lead tunneling constant. In the inset, we show the initial non-universal response on a magnified scale.
part. There are various ways of doing this. Here, we follow the master equation approach[25]. In this approach, one can come up with an exact solution for \( U=0 \) in Eq. (4.1) in the wide band limit. The master equation is given by

\[
\frac{dn(t)}{dt} + \Gamma(t)n(t) = -\sqrt{\Gamma(t)} \int_{t_0}^{t} d\tilde{t} \sqrt{\Gamma(\tilde{t})} \frac{\sin(\varepsilon_{\text{dot}}(\tilde{t} - \tilde{t}))}{\beta \sinh(\frac{\pi(\tilde{t} - \tilde{t})}{\beta})} e^{-\int_{\tilde{t}}^{t} d\eta \frac{\Gamma(\eta)}{2}}, \tag{3.5}
\]

where \( \Gamma(t) \) is the linewidth of the Fano resonance in Eq. (4.2) and \( n(t) \) is the instantaneous probability for finding an electron in the dot level,

\[
n(t) = \sum_{\sigma} \langle \sigma | G^{<}(t, t) | \sigma \rangle, \tag{3.6}
\]

where \( | \sigma \rangle \) correspond to the spin up and down states of the dot level and \( G^{<}(t, t) \) is the equal time component of the double time less than Green’s function[25].

We refer to \( n(t) \) as the population from now on. In order to solve Eq. (3.5) for the case where we abruptly change the lifetime broadening of discrete state at \( t = t_1 \), we use

\[
\Gamma(t) = \begin{cases} 
\Gamma_1 & \text{if } t_0 < t \leq t_1 \\
\Gamma_2 & \text{if } t > t_1 
\end{cases}
\]

together with the initial condition \( n(t_0) = n_0 \). Therefore, if \( t > t_1 \), Eq. (3.5) becomes

\[
\frac{dn(t)}{dt} + \Gamma_2 n(t) = -\sqrt{\Gamma_2} \int_{t_1}^{t} d\tilde{t} \sqrt{\Gamma_1} \sin(\varepsilon_{\text{dot}}(t - \tilde{t})) \frac{1}{\beta \sinh(\frac{\pi(t - \tilde{t})}{\beta})} e^{-\frac{\Gamma_2}{2}(t - \tilde{t})} - \sqrt{\Gamma_2} \int_{t_0}^{t_1} d\tilde{t} \sqrt{\Gamma_1} \sin(\varepsilon_{\text{dot}}(t - \tilde{t})) \frac{1}{\beta \sinh(\frac{\pi(t - \tilde{t})}{\beta})} e^{-\frac{\Gamma_2}{2}(t - \tilde{t}) - \frac{\Gamma_1}{2}(t_1 - \tilde{t})}. \tag{3.7}
\]

In Eq. (3.7), the first term on the right-hand side accounts for the evolution of the unperturbed system, hence we can discard its effect in the transient region. Since we
are interested in the region where $t \gg t_1$, we can safely approximate the hyperbolic sine in the second term on the right hand side with an exponential. After these simplifications and integrating the right hand side, Eq. (3.7) becomes

$$\frac{dn(t)}{dt} + \Gamma_2 n(t) = -\sqrt{\Gamma_1 \Gamma_2} e^{-\frac{\Gamma_1}{2} (t-t_1)} \frac{2}{\beta} e^{-\frac{\Gamma_1}{2} t_1 - \frac{\pi}{3} t} \left( e^{\frac{\Gamma_1}{2} + \frac{\pi}{3} t_1} (\epsilon_{dot} \cos(\epsilon_{dot}(t-t_1)) + \frac{\Gamma_1}{2} + \frac{\pi}{3}) \sin(\epsilon_{dot}(t-t_1))) - \frac{(\frac{\Gamma_1}{2} + \frac{\pi}{3})^2 + \epsilon_{dot}^2}{(\frac{\Gamma_1}{2} + \frac{\pi}{3} + \frac{\pi}{3})^2 + \epsilon_{dot}^2} \right).$$

(3.8)

This is an inhomogeneous first-order differential equation and it can be solved in a straightforward way. Time evolution of $n(t)$ in the second region becomes

$$n(t) = -a \epsilon_{dot} e^{\left(-\frac{\Gamma_1}{2} - \frac{\pi}{3}\right)t} \cos(\epsilon_{dot}(t-t_1) - \arctan(\frac{\epsilon_{dot}}{\epsilon_{dot}'})) \sqrt{(\frac{\Gamma_1}{2} - \frac{\pi}{3})^2 + \epsilon_{dot}^2}$$

$$-a \left(\frac{\Gamma_1}{2} + \frac{\pi}{3}\right) e^{\left(-\frac{\Gamma_1}{2} - \frac{\pi}{3}\right)t} \cos(\epsilon_{dot}(t-t_1) - \pi - \arctan(\frac{\epsilon_{dot}}{\epsilon_{dot}'})) \sqrt{(\frac{\Gamma_1}{2} - \frac{\pi}{3})^2 + \epsilon_{dot}^2}$$

$$b \epsilon_{dot} e^{\left(-\frac{\Gamma_1}{2} - \frac{\pi}{3}\right)t} \cos(\epsilon_{dot}(t-t_0) - \arctan(\frac{\epsilon_{dot}}{\epsilon_{dot}'})) \sqrt{(\frac{\Gamma_1}{2} - \frac{\pi}{3})^2 + \epsilon_{dot}^2}$$

$$b \left(\frac{\Gamma_1}{2} + \frac{\pi}{3}\right) e^{\left(-\frac{\Gamma_1}{2} - \frac{\pi}{3}\right)t} \cos(\epsilon_{dot}(t-t_0) - \pi - \arctan(\frac{\epsilon_{dot}}{\epsilon_{dot}'})) \sqrt{(\frac{\Gamma_1}{2} - \frac{\pi}{3})^2 + \epsilon_{dot}^2}$$

(3.9)

where

$$a = \frac{2 \sqrt{\Gamma_1 \Gamma_2} e^{\left(\frac{\Gamma_1}{2} + \frac{\pi}{3}\right)t_1}}{\beta \left(\frac{\Gamma_1}{2} + \frac{\pi}{3}\right)^2 + \beta \epsilon_{dot}^2}$$

(3.10)

and

$$b = \frac{2 \sqrt{\Gamma_1 \Gamma_2} e^{\left(\frac{\Gamma_1}{2} + \frac{\pi}{3}\right)t_0} e^{\frac{\Gamma_1}{2} - \frac{\pi}{3} t_1}}{\beta \left(\frac{\Gamma_1}{2} + \frac{\pi}{3}\right)^2 + \beta \epsilon_{dot}^2}.$$ 

(3.11)
Figure 3.2  Evolution of the population in the non-universal timescale. Dashed curves show the numerical data right after the dot-lead tunneling constant is switched to its final value at $T=0.005\Gamma_2$ and solid curves are the result of the analytic solution of the spinless Anderson Hamiltonian for the same parameters. The black curves correspond to system one. $\epsilon_{dot}$, $\Gamma_1$ and $\Gamma_2$ are half of system one for red curves. $\epsilon_{dot}$ and $\Gamma_1$ are half of system one and $\Gamma_2=2\Gamma_1$ for blue curves.
In Fig. 3.2, we display the numerically obtained population immediately after the dot-lead tunneling constant was switched to its final value together with the analytical solution obtained above for the spinless Anderson Hamiltonian. The same parameters were used for both cases. First, we compare the results for system one and another configuration whose dot level and coupling constants are exactly half of system one, thus $\varepsilon_{\text{dot}}/\Gamma_1$ and $\varepsilon_{\text{dot}}/\Gamma_2$ are the same for both. It is obvious from Fig. 3.2 that the oscillation frequency of system one is twice as much as the new configuration in both analytical and numerical solutions. The oscillation frequency of the numerical and analytical solutions are the same as well. We reduced $\Gamma_2$ of the new configuration such that $\Gamma_2=2\Gamma_1$ to test the amplitudes and this reduces the amplitude of the oscillations keeping the frequency constant in both numerical and analytical solutions. Therefore, the qualitative analytical solution mimics the behaviour of the numerical population remarkably well even though the actual numerical values differ slightly due to the simplicity of the analytical approach.

Since the instantaneous conductance is related to the population by

$$G(t) \propto \frac{dn(t)}{dt},$$

we reach the conclusion that the instantaneous conductance in the non-universal timescale is governed by the spinless Anderson Hamiltonian and that the instantaneous conductance oscillates sinusoidally with a frequency equal to the dot level as it can be seen from Eq. (4.17). The magnitude of the oscillations have more complicated
Figure 3.3  Rise rate, which is defined as the time it takes for instantaneous conductance to reach its final value, for S1 and S2 versus temperature $T$ for infinitesimal bias. The solid dots are for S1 and open circles are for S2. Black circles and dots represent the data obtained previously [3]. Red circles and dots correspond to the data taken with the new numerical scheme. The straight line has a slope of $\pi$ and passes through the origin.
Figure 3.4  Convergence of the calculated time-dependent conductance curves for S2 as a function of grid size. Solid curves are for $T=0.0005\Gamma$ and the dashed curves are for $T=0.0015\Gamma$. Black, red and blue curves correspond to grid sizes of 20, 40 and 80 respectively. Panels b and c magnify the long time part of panel a.

form and they depend on $\Gamma_1$, $\Gamma_2$ and $\varepsilon_{dot}$ as Eq. (3.10) and (3.11) show.

3.3 Universal timescale

Even though universal scaling behaviour was demonstrated in steady state nonequilibrium by using the perturbative renormalization group [4], it is not obvious that the same arguments can be extended to a time dependent situation. A preliminary investigation has been carried out previously for the latter [3] and it turns out that the universality arguments seem to hold for time dependent situation as well even though these calculations have been done at temperatures around and above $T_K$. 
Figure 3.5  The large time limit of $G(t)/G_0$ vs. temperature for system one and system two. These are the final steady state conductance values in infinitesimal bias. Open circles correspond to system one and solid dots are for system two. Black circles and dots correspond to the data obtained previously [3] and red dots represent the data taken with the new numerical scheme. The blue line is the large $T$ asymptote.
In this work, we want to investigate this thoroughly at temperatures well below $T_K$. We are now in the Kondo timescale where spin relaxation takes place and it is governed by the full Anderson Hamiltonian therefore there is no closed form solution here due to strong correlations unlike the situation for the non-universal timescale. In order to demonstrate the universal scaling behaviour in this regime we use systems with different $T_K$ and compare the resulting instantaneous conductance curves. One slight complication is that we have to rescale the results for different systems since the rise time, which is defined as the time to reach the steady state value in the final state, is different for each system therefore we have to find the correct scaling factor.

We show the rise rates extracted from system one and system two in Fig. 3.3. The new numerical scheme allows us to go down to a fraction of $T_K$ which was previously unavailable. The procedure we follow to extract these rates is identical to the one used previously [3] and we combined the results obtained there with our results for the sake of consistency. It is clear from these results that the rise rate of system two is almost twice as much as system one. This suggests that rise rate scales with $T_K$ in general. Another important conclusion is that the rise rate saturates around $1.3T_K$ after $T/T_K$ gets smaller than approximately 0.1. This is very close to the theoretically predicted Korringa rate for NCA [3, 53].

In Fig. 3.4 we demonstrate the convergence of the instantaneous conductance curves for system two for two different temperatures right after the dot-lead tun-
Figure 3.6 Rise of the instantaneous conductance in the universal timescale in finite bias for system one at $T=0.17T_K$ right after the coupling to the leads is switched. Black, dark blue, light blue, green, red and dashed black curves correspond to $V=0.04\Gamma_2$, $0.06\Gamma_2$, $0.08\Gamma_2$, $0.11\Gamma_2$, $0.15\Gamma_2$, $0.2\Gamma_2$ respectively in panel a. In panel b, we show the instantaneous conductance for $V=0.2\Gamma_2$ in magnified scale.
Figure 3.7 Decay of SKP oscillations vs. bias $V$ for system one. Solid circles represent the analytical calculations of $2\gamma$ at zero temperature [4]. Black squares, diamonds and downwards triangles are previous results[3] and correspond to $T=1.4T_K$, $0.69T_K$ and $0.34T_K$ respectively. Red open circles and upwards triangles are for $T=0.17T_K$ and $0.08T_K$.

neling constant is switched to its final value. In order to do so, we plotted the instantaneous conductance curves for different coarse grid sizes while keeping all other numerical parameters constant. As we see in the magnified panels, we achieve good convergence as we reduce the grid size. We also would like to point out that a comparison of the x axis values for Fig. 3.4 and the inset of Fig. 3.1 reveals quite clearly that the universal timescale is much longer than non-universal timescale.

In Fig. 3.5, we plot the final steady state conductances obtained from the converged curves in Fig. 3.4 alongside with the exact asymptotic curve at large $\ln(T/T_K)$. 
It is given by:

\[
\frac{G}{G_0} = \frac{3\pi^2}{16 \ln^2(T/T_K)}.
\]  \hfill (3.13)

This asymptote was first calculated by Abrikosov [54] and later adapted to quantum dots [41]. We again plotted the results obtained previously [3] together with the results taken with the new numerical scheme. The new scheme allows us to handle temperatures well below \( T_K \) for \( T_K \) as low as 1 K. The results in Fig. 3.5 clearly demonstrate that the universality is preserved for temperatures down to a fraction of \( T_K \). Our conductance results for temperatures lower than \( T/T_K = 0.1 \) in Fig. 3.5 exceed the unitarity limit thus they are not shown. This is a pathology of NCA and it was pointed out before[4].

We believe the tiny deviations observed in the final steady state would disappear if we could study a system for which the Fano resonance has negligible overlap with the Fermi level. This is presently out of our reach. This is mainly due to the fact that the rise time scales with \( T_K \) as we demonstrated above. We need to study a system which has \( T_K \) around a few nanokelvin to make the overlap of the Fano resonance with the Fermi level less than one percent since the broadening has a lorentzian lineshape. This is computationally not feasible at the moment.

We finally would like to investigate the instantaneous conductance at large bias. When we apply finite bias to the system, Kondo resonances that form at each lead's Fermi level split. Due to the finite bias, these resonances are broadened compared to
the infinitesimal bias situation [55]. It has recently been established that the quantum beating between these split Kondo peaks gives rise to sinusoidal oscillations in the instantaneous conductance after it reaches its final state [55, 56] and the frequency of these oscillations is equal to the magnitude of the bias [3].

In this work, we investigate these SKP oscillations close to zero temperature. In Fig. 3.6, we display the instantaneous conductance right after the tunneling constant is switched to its final state for a variety of biases at constant temperature. As the bias increases, so does the frequency of the SKP oscillations, however, the final steady state value of the conductance goes down. This is due to the fact that decoherence destroys the Kondo effect. We also show the instantaneous conductance for the largest bias in a magnified scale. Damped sinusoidal oscillations are visible clearly here.

It is intriguing to investigate to what extent the decay rate of these oscillations changes as we reduce the temperature. We follow the same procedure used previously [3] to determine the decay rate. We plot the difference between the final steady state value of the conductance and the values at each minima in a logarithmic scale and the slope of the linear best fit curve gives the decay rate. We display half the decay rates together with the previously obtained values at higher temperatures [3] in Fig. 3.7. The decay rates of SKP oscillations saturate as the temperature approaches zero. We also show the zero temperature analytical decoherence rates, $\gamma$, obtained from perturbative renormalization group [4] in the same figure. We find that half the decay
rates obtained from our NCA calculations correspond to roughly $2\gamma$ even though our low temperature decay rates move somewhat further away from the previous high temperature results. This definitely rules out the possibility that there is a one to one correspondence between perturbative renormalization group decoherence rates and NCA decay rates.
Chapter 4
Quantum dot asymmetrically coupled to metallic leads

4.1 Introduction

Quantum effects are likely to play an increasing role in electronic devices as the physical size of their components continues to shrink. Quantum dots and qubits are examples of devices where quantum effects play a direct role in their function. In a Single Electron Transistor (SET), i.e., a quantum dot coupled to two metallic leads, the conductance can be drastically enhanced by the Kondo effect which can occur when the quantum dot is populated by an odd number of electrons [33, 32, 35, 2, 16, 36, 57, 58]. The Kondo effect is a quantum-coherent many-body state in which a spin singlet state is formed between the unpaired localized electron and delocalized electrons at the Fermi energy at low temperatures [31].

An important issue for the function of any electronic device is how fast it can respond to time-dependent perturbations and bias [30, 59]. Several studies of time-dependent response of symmetrically-coupled SET have been performed using a variety of methods [38, 39, 42, 48, 43, 50, 45, 51, 60]. In the case of a sudden switching of the dot level, the transient current has been found to exhibit several distinct timescales [47, 3, 46, 61]. The fastest timescale is associated with charge relaxation and the other much slower timescales are associated with the formation of a Kondo
state, i.e. spin dynamics. The detailed evolution of the instantaneous currents following a sudden change of the dot level has been shown to depend sensitively on external parameters such as source-drain bias, external temperature, dot-lead coupling and position of the dot level. These above mentioned time-dependent studies have all been concerned with quantum dots which are symmetrically coupled to their leads. While the effect of asymmetric coupling on the steady-state conductance of an SET has been studied both theoretically and experimentally,[62, 63] to our knowledge, the transient transport properties of an asymmetrically coupled dot in the Kondo regime have not been investigated previously.

In this section, we use our recently developed multi-scale many-body transport method to study the effect of asymmetric dot-lead coupling on the transient transport in a quantum dot [64]. We show that for a quantum dot asymmetrically coupled to two leads with sharp features in their density of states, the current can display sinusoidal modulations for timescales well beyond the fast charge relaxation timescale. The frequency of these sinusoidal modulations is given by the energy difference between the Kondo resonance and the density of states feature. The amplitude of the oscillations is found to increase with decreasing temperature and source-drain bias and saturate for temperatures below the Kondo scale. We attribute this phenomenon to an interference effect between the Kondo resonance at the Fermi level of the leads and the conduction electrons around the density of state feature. The magnitude of
the oscillations depends sensitively on the structure of the density of state features of the leads. We show that these oscillations also can occur for leads with a smooth density of states but with finite bandwidth.

4.2 Time dependent current in infinite-U Anderson model

The SET is modeled as a single spin degenerate level of energy $\varepsilon_{\text{dot}}$ coupled to leads through tunnel barriers,

$$H(t) = \sum_{\sigma} \varepsilon_{\text{dot}}(t)n_{\sigma} + \sum_{\kappa,\sigma} \varepsilon_{\kappa}\! n_{\kappa\sigma} + \frac{i}{2}\sum_{\sigma,\sigma'} U_{\sigma,\sigma'} n_{\sigma} n_{\sigma'} +$$

$$\sum_{\kappa,\sigma} \left[ V_{\alpha}(\varepsilon_{\kappa\alpha},t)c_{\kappa\alpha\sigma}^\dagger c_{\sigma} + \text{H.c.} \right], \quad (4.1)$$

where $c_{\sigma}^\dagger$ ($c_{\sigma}$) and $c_{\kappa\sigma}^\dagger$ ($c_{\kappa\sigma}$) with $\alpha=L,R$ create (annihilate) an electron of spin $\sigma$ in the dot level and in the left(L) and right(R) leads respectively. The $n_{\sigma}$ and $n_{\kappa\sigma}$ are the corresponding number operators and $V_{\alpha}$ are the hopping amplitudes for the left and right leads. The Coulomb repulsion energy $U$ is assumed to be sufficiently large that double occupancy of the dot level is prohibited. In the following, we will use atomic units with $\hbar = k_B = e = 1$.

The Green functions of the dot levels are calculated using the Non Crossing Approximation (NCA) by numerical integration on a multi-scale time grid [64]. When the dot level $\varepsilon_{\text{dot}}$ lies well below the Fermi level $\varepsilon_F$, the spectral function of the dot (local density of states) exhibit two features: a broad Fano-like resonance of full-width

$$\Gamma_{\text{tot}}(\varepsilon, t) = 2\pi \sum_{k} (|V_{L}(\varepsilon_k, t)|^2 + |V_{R}(\varepsilon_k, t)|^2)\delta(\varepsilon - \varepsilon_k) \quad (4.2)$$
around the dot level, and a sharp temperature sensitive resonance at the Fermi level (the Kondo peak), characterized by a low energy scale \( T_K \) (the Kondo temperature)

\[
T_K \propto \left( \frac{D \Gamma_{\text{tot}}}{4} \right)^{1/2} \exp \left( -\frac{\pi |\varepsilon_{\text{dot}}|}{\Gamma_{\text{tot}}} \right),
\]

(4.3)

where \( D \) is a high energy cutoff equal to half bandwidth of the conduction electrons and \( \Gamma_{\text{tot}} \) corresponds to the value of \( \Gamma_{\text{tot}}(\varepsilon, t) \) at \( \varepsilon = \varepsilon_F \). All energy units in this section will be given in terms of \( \Gamma_{\text{tot}} \).

The current flowing through the SET can be calculated as the difference between the currents from the left and right leads as

\[
I(t) = I_L(t) - I_R(t),
\]

(4.4)

The most general expression for the net current flowing from the left(right) lead is given by [65]

\[
I_{L(R)}(t) = -2\text{Im} \left( \int_{-\infty}^{t} dt_1 \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1-t)} \Gamma_{L(R)}(\varepsilon, t_1, t) \right.
\]

\[
\left. e^{i \int_{t_1}^{t} d\tau \Delta_{L(R)}(\tau) \left[ G^<(t, t_1) + f_{L(R)}(\varepsilon) G^R(t, t_1) \right]} \right)
\]

(4.5)

where the coupling functions \( \Gamma_{L(R)} \)

\[
\Gamma_{L(R)}(\varepsilon, t, t_1) = 2\pi \rho(\varepsilon) V_{L(R)}(\varepsilon, t) V_{L(R)}^*(\varepsilon, t_1),
\]

(4.6)

depend on the density of states of the leads \( \rho(\varepsilon) \) and the hopping matrix elements in Eq.(4.1). The quantity \( \Delta_{L(R)} \) represents the time-dependence of the single particle
Figure 4.1  This figure shows the different density of state functions $\xi(\varepsilon)$ used to model the leads. Panel a) correspond to a rectangular band, b) to a parabolic band, and c) and d) to a parabolic band with a Lorentzian feature located at $\varepsilon=-D/2$ and $\varepsilon=-3D/4$ respectively.

energies in the left and right leads. In this section, we consider the case of a small constant bias across the leads.

Separable matrix elements are assumed in the following analysis. This implies that

$$V_{L(R)}(\varepsilon, t) = \nu_{L(R)}(\varepsilon)u_{L(R)}(t),$$

(4.7)

therefore resulting in

$$\Gamma_{L(R)}(\varepsilon, t, t_1) = u_{L(R)}(t)u_{L(R)}^*(t_1)\xi_{L(R)}(\varepsilon),$$

(4.8)

where

$$\xi_{L(R)}(\varepsilon) = 2\pi\rho_{L(R)}(\varepsilon)|\nu_{L(R)}(\varepsilon)|^2.$$  (4.9)
We consider a situation where the hopping terms $V_{L(R)}(\epsilon, t)$ in the Hamiltonian have no explicit energy and time dependence. This means Eq. (4.8) can be simplified to

$$\Gamma_{L(R)}(\epsilon) = \tilde{\Gamma}_{L(R)}\xi_{L(R)}(\epsilon)$$  \hspace{1cm} (4.10)

where $\tilde{\Gamma}_{L(R)} = |u_{L(R)}|^2$.

In Fig. 4.1 we show the different density of states functions $\xi(\epsilon)$ that will be used to model the leads. The function has been normalized so that the bands contain the same number of electrons. The bandwidth of the leads is assumed to be $2D$ with the Fermi energy at $\epsilon = 0$.

The expression for the current can then be written as

$$I(t) = -2\tilde{\Gamma}_L Im\left( \int_{-\infty}^{t} dt_1 (G^<(t, t_1)h(t - t_1) + G^R(t, t_1)f_L(t - t_1)) \right)$$

$$+ 2\tilde{\Gamma}_R Im\left( \int_{-\infty}^{t} dt_1 (G^<(t, t_1)h(t - t_1) + G^R(t, t_1)f_R(t - t_1)) \right),$$ \hspace{1cm} (4.11)

where

$$h(t - t_1) = \int_{-D}^{D} \frac{d\epsilon}{2\pi} \xi(\epsilon)e^{i\epsilon(t-t_1)},$$ \hspace{1cm} (4.12)

$$f_L(t - t_1) = \int_{-D}^{D} \frac{d\epsilon}{2\pi} \xi(\epsilon) \frac{e^{i\epsilon(t-t_1)}}{1 + e^{\beta[\epsilon - \frac{\nu}{2}]}};$$ \hspace{1cm} (4.13)

and

$$f_R(t - t_1) = \int_{-D}^{D} \frac{d\epsilon}{2\pi} \xi(\epsilon) \frac{e^{i\epsilon(t-t_1)}}{1 + e^{\beta[\epsilon + \frac{\nu}{2}]}}.$$ \hspace{1cm} (4.14)

In these expressions, $V$ represents the source-drain bias.

We need to express the physical Green's functions in Eq. (4.11) in terms of pseudofermion and slave boson Green's functions. This is simply due to the fact that we
rewrite the Hamiltonian for the infinite-$U$ Anderson model in the slave boson representation and the Green’s functions we obtain after solving the resulting Dyson equations correspond to pseudofermion and slave boson operators. In this procedure, the terms that have $Q^2$ dependency must be projected out as previously noted [29]. This yields

$$G^<(t,t_1) = G^<_{pseudo}(t,t_1)B^R(t_1,t)$$  \hspace{1cm} (4.15)

for "less than" Green’s function and

$$G^R(t,t_1) = -i\theta(t-t_1) < c(t)c^\dagger(t_1) + c^\dagger(t_1)c(t) >$$

$$= -i\theta(t-t_1) \left( G^R_{pseudo}(t,t_1)B^<(t_1,t) + G^<_{pseudo}(t,t_1)B^R(t_1,t) \right)$$  \hspace{1cm} (4.16)

for the retarded Green’s function. Here, $G^R_{pseudo}$ and $B^R_{<}$ are pseudofermion and slave boson Green functions respectively.

The final expression for the current is then

$$I(t) = -2\bar{\Gamma}_L Im\left( \int_{-\infty}^{t} dt_1 (G^<_{pseudo}(t,t_1)B^R(t_1,t)h(t-t_1)$$

$$-i((G^R_{pseudo}(t,t_1)B^<(t_1,t) + G^<_{pseudo}(t,t_1)B^R(t_1,t))f_L(t-t_1)))$$

$$+2\bar{\Gamma}_R Im\left( \int_{-\infty}^{t} dt_1 (G^<_{pseudo}(t,t_1)B^R(t_1,t)h(t-t_1)$$

$$-i((G^R_{pseudo}(t,t_1)B^<(t_1,t) + G^<_{pseudo}(t,t_1)B^R(t_1,t))f_R(t-t_1))) \right)$$.  \hspace{1cm} (4.17)

This is the main result of this section and will be used in the calculations presented below.
4.3 Results

In this section we will analyze the instantaneous current following a sudden change of the dot level from a position at $\varepsilon_1 = -5\Gamma_{tot}$ below the Fermi level where, for the present finite temperatures, the Kondo effect will be absent to a position at $\varepsilon_2 = -2\Gamma_{tot}$ closer to the Fermi energy where the Kondo effect will be present. For a parabolic density of states function (Fig. 1b) with $D = 9\Gamma_{tot}$, the Kondo temperature in the final state is approximately $T_K = 0.0016\Gamma_{tot}$.

We begin our analysis by investigating the effect of asymmetric coupling to the leads. We define the asymmetry factor as the the ratio $\tilde{\Gamma}_L/\tilde{\Gamma}_{tot}$ where $\tilde{\Gamma}_{tot} = \tilde{\Gamma}_L + \tilde{\Gamma}_R$. In Fig. 4.2, the instantaneous conductance is plotted as a function of time after the dot level is switched for various asymmetry factors with small bias. The final steady state conductances are in perfect agreement with previous theoretical results [55].

The transient increase of the conductances on the short timescale $\Gamma$ shown in panel a of Fig. 4.2 is due to the formation of the broad Fano-like resonance at $\varepsilon_2$. Panel b in Fig. 4.2 shows the instantaneous conductances for larger times on a magnified scale. It is clear from this panel that the current exhibits sinusoidal modulations at timescales well beyond $\Gamma_L$ or $\Gamma_R$. As we reduce the asymmetry factor, the amplitude of these sinusoidal modulations starts decreasing and eventually disappear for symmetric coupling. The frequency of the conductance oscillations is equal to the bandwidth $D$ of the leads. External parameters such as the energy or width of the dot level,
**Figure 4.2** Black(dotted), blue(dashed) and red(dot dashed) curves in panel a show the instantaneous conductance vs. time for rectangular density of states in Fig. 1.3 immediately after the dot level is switched to its final position for asymmetry factors of 0.95, 0.9 and 0.85 respectively with fixed $\Gamma_{\text{tot}}$ and $D=9\Gamma_{\text{tot}}$ at $T=0.0093\Gamma_{\text{tot}}$ with $V=T_K$. The beginning of the oscillations is clearly visible in this panel. Black(dotted), blue(dashed) and red(dot dashed) curves in panel b are the continuation of the ones in the first panel in the long timescale for the same parameters.
Figure 4.3  Effect of the density of states function on the instantaneous conductance. Red(dotted), dark blue(dot dashed), black(solid) and green(dashed) curves display the instantaneous conductance vs. time in the long timescale for cases a, b, c and d respectively in Fig.1 when the source-drain bias is equal to \( V = T_K \) with fixed \( \Gamma_{tot} \). All curves are for asymmetry factor of 0.9, \( D = 9\Gamma_{tot} \) at \( T = 0.0093\Gamma_{tot} \), asymmetry factor, and ambient temperature and source-drain bias only influence the amplitude of the oscillations.

In Fig. 4.3, we show the effect of the the density of states function of the leads \( \xi(\epsilon) \) on the conductance oscillations. The figure reveals that the density of states can have a pronounced effect on the conductance oscillations. The largest oscillations occur for a density of states with a peak feature as in panels c and d of Fig. 4.1. For a parabolic density of states function, conductance oscillations are still present but
not discernible on the scale of the figure. The frequency of the current oscillations is equal to the energy difference between the Fermi level of the leads and and the feature in their density of state function. For the rectangular and parabolic density of states function, where the density of states feature is the band cut-off, the period is equal to $1/D=1/9$ and for the density of state functions depicted in panels c and d of Fig. 4.1, where the density of states feature is the narrow Lorentzian peak, the periods are $2/D$ and $4/3D$ respectively.

We have also investigated other shapes of DOS functions. For instance, for a triangular DOS, $\xi(\varepsilon) = 2(1 + \varepsilon/D)$, the conductance displays oscillations whose frequency is equal to $D$ very similar to what was obtained for the parabolic DOS in panel b of Fig. 4.1. For two sharp features at different energies $D_1$ and $D_2$ in the DOS we obtain conductance modulations of frequencies proportional to $(D_1 + D_2)$ and $(D_1 - D_2)$. This suggests the presence of "beating" phenomenon and is understandable since there are two distinct oscillation frequencies in the system now. Higher harmonics start to appear when we have more than two lorentzians superimposed on parabolic density of states.

Fig. 4.4 shows the effect of temperature and source-drain bias on the conductance oscillations. The figure demonstrates that the amplitude of the oscillations decrease with temperature and bias across the dot but their frequency remain unchanged. The figure shows two important effects. First, it takes longer for the current and
thus the damped oscillations to decay as the temperature or source-drain bias is reduced. Second, the amplitude of the damped oscillations increases with decreasing temperature or source-drain bias and but saturates for temperatures and bias below the Kondo temperature, which we estimate to be around $T_K = 0.0016 \Gamma_{tot}$ in these systems.

### 4.4 Discussion

Our numerical calculations clearly show that the timescale for the decay of the conductance oscillations is much larger than the fast timescales set by the couplings of the dot level to the leads, $\Gamma_L$ or $\Gamma_L$. The timescale does not depend on the width or shape of the DOS feature in the leads. It appears that the timescale is related to the Kondo resonance. When the Kondo resonance is fully formed at times around $1/T_K$, the oscillations disappears.

The saturation of the conductance oscillations for temperatures and source-drain bias below the Kondo temperature suggests that the Kondo resonance at the Fermi level of the leads may play a role in this phenomenon. The effect of temperature and source-drain bias on the Kondo resonance in an SET was recently investigated in detail.[3] For values smaller than the Kondo temperature, the Kondo resonance is fully formed just above the Fermi Level. Increasing the temperature above $T_K$ broaden and reduce the magnitude of the resonance. Increasing the source-drain bias results in the formation of a split Kondo resonance with strongly reduced intensi-
Figure 4.4  Panel a shows the instantaneous conductance for several different temperatures with asymmetry factor of 0.9, fixed $\Gamma_{tot}$, $D=9\Gamma_{tot}$ and rectangular density of states. Dark blue (dot dot dashed), red (dot dashed), green (dashed), light blue (dotted) and black (solid) curves represent the conductance at $T=0.0186$, 0.0093, 0.0046, 0.0023, and 0.0009$\Gamma_{tot}$ respectively. Red (dot dashed), black (dotted) and dark blue (dashed) curves in panel b display the instantaneous conductance vs. time in the long timescale for rectangular density of states when the source-drain bias is equal to $V=T_K$, $V=5T_K$ and $V=10T_K$ respectively with fixed $\Gamma_{tot}$ and $D=9\Gamma_{tot}$ for asymmetry factor of 0.9 at $T=0.0093\Gamma_{tot}$. 
ties. For temperatures or source-drain bias well above the Kondo temperature, the Kondo resonance is completely suppressed. Since the frequency of the oscillations is determined by the energy difference between the Fermi level and the density of states feature, we believe that the oscillations reflect an interference process between the conduction electrons associated with the Kondo resonance and the conduction electrons associated with the density of states feature. In order to substantiate this explanation we used a simple analytical noninteracting Anderson model to calculate the instantaneous conductance following the sudden switching of a dot level of a width $\Gamma_{eff}$ equal to that of the final Kondo resonance in the interacting model. This effective resonance was switched to a position just above the Fermi level of the leads. The instantaneous conductance was found to display the same conductance oscillations with frequencies determined by the bandwidth $D$ as in the original interacting model. The oscillations are found to decay over a long timescale determined by $\Gamma_{eff}$.

While the Kondo temperature depends only on the total coupling to the leads $\Gamma_{tot}$, the total current depends on the asymmetry factor. The reason why the conductance oscillations only show up for asymmetric couplings is that the total current through the dot is the difference of the currents from the left and right leads Eq. (4.4). The interference effect shows up both in the the right and left currents. For symmetric coupling, the current oscillations from the right and left leads are out of phase resulting in a cancellation of the oscillations in the total current. For asymmetric
coupling the left and right current oscillations do not cancel resulting in the observed conductance oscillations.

For dots coupled to leads with very weak density of states features, the conductance oscillations will be very small. In Fig. 4.5, we show the time-derivative of the instantaneous current for leads with a parabolic density of states function for three different values of the bandwidth $D$. The conductance oscillations here results from the interference of the Kondo resonance in the final state and the weak discontinuity in the density of states at the lower band edge of the leads. The figure clearly demonstrates oscillations of the instantaneous currents with a frequency equal to $D$ in the long timescale.

The experimental study of the conductance oscillations could possibly be made using previously suggested techniques, i.e., by measuring the total charge transport as function of pulse duration.[48] For a bandwidth of $D=1$ eV, the oscillation period will be of an order of $10^{-14}$ seconds. Since the current oscillates, electromagnetic radiation will be emitted at a rate proportional to $\left| \frac{dI(t)}{dt} \right|^2$. For a suitably designed system it may be possible to detect the emitted light. For $D=1$ eV the emission would occur in the infrared at a photon energy of 0.1 eV.

4.5 Conclusion

In this chapter, we employed time dependent non-crossing approximation to analyze the transient current in a single electron transistor in the Kondo regime asymmet-
Figure 4.5 Time-derivative of the instantaneous current in the long timescale for parabolic density of states (Fig. 1b). Black (solid), red (dashed) and dark blue (dot dashed) curves correspond to $D=6.75\Gamma_{tot}$, $D=9\Gamma_{tot}$ and $D=13.5\Gamma_{tot}$ for asymmetry factor of 1.0 at $T=0.0093\Gamma_{tot}$. 
rically coupled to two metallic leads with features in their density of states. We show that for asymmetric coupling, the conductance can exhibit oscillations which persist for times much longer than the timescale for charge relaxation. The origin of these oscillations is an interference between the conduction electrons associated with the Kondo resonance and those associated with the density of states feature. The amplitude of the oscillations are found to depend strongly on temperature and source-drain bias when those exceed the Kondo temperature. We hope that our predictions will motivate further theoretical and experimental studies.
Chapter 5
Outlook

Investigations into the Kondo effect are far from complete. The holy grail for research on the Kondo effect is twofold these days. The first aspect is to understand the time evolution of this many-body quantum state. In this thesis, we tried to answer this open question by invoking non-crossing approximation applied to a slave boson Hamiltonian in combination with double time Green’s function techniques. This sheds light on questions like how this highly nontrivial many body state builds up and whether it is possible to suddenly switch on the exchange interaction in a quantum-dot experiment.

Another ongoing debate is related to the formation of the so-called Kondo cloud [66, 67, 68]. The many electrons that participate in the spin-flip processes give rise to the sharp Kondo resonance at the Fermi level. The Kondo cloud consists of electrons that have previously interacted with the same impurity. Since each of these electrons contains information about the same impurity, they effectively have information about each other. In other words, the electrons are mutually correlated.

The interest in this topic also focuses on questions like whether experiments would allow us to measure how the accompanying Kondo cloud forms. Detection of this elusive Kondo cloud would also provide a possible mechanism to investigate the in-
teractions between impurities. It is of significant interest to determine how the two many-body states that are formed around two separated localized moments merge. A well controlled experiment probing interacting localized spins could provide us a clear perspective on extended Kondo systems such as spin glasses.

The state-of-the-art nanotechnology for fabricating interacting Kondo systems like scanning tunneling microscopy and quantum-dot devices enabled to study this highly-correlated many body state with unprecedented tunability unlike bulk metals and it is reasonable to expect that it will soon give birth to yet another Kondo revival.
References


