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MASTER'S THESIS

**Quantum transport in
non-equilibrium impurity models at
exactly solvable points**

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Abstract

Quantum dot devices may be tuned to Kondo models which each have a non-interacting limit called the Toulouse limit. At sufficiently low temperatures the Toulouse limit can be used to make predictions for charge transport in such devices driven away from equilibrium, e.g. with an ac bias. We investigate non-equilibrium transport in a resonant level model with a single lead which may be mapped onto the Toulouse limit of the Kondo model. The main results are expressions for the charge current that are exact in the tunnelling couplings, while remaining in the linear response regime of the time-dependent voltage bias. We also show how the line of enquiry directly extends to the tunnelling junction studied by A. Schiller and S. Hershfield in which a Kondo impurity interacts separately with two leads.

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Chapter 1

Introduction

Pervasive challenges in theoretical physics include finding fundamental descriptions for the collective behaviour of electrons in systems where they are strongly interacting. A related question is how these descriptions change when such systems are driven far away from equilibrium. Due to the rapid progress in recent decades in the fabrication of small electronics on the nanoscale it is possible to engineer nanostructures to directly test different theoretical models.

The theoretical work developed in this thesis is connected to experiments on semiconductor quantum dot devices which are tuned to the Kondo regime. Traditionally the Kondo problem concerns the many body effects of a single localised spin-1/2, representing a magnetic impurity, in an otherwise non-magnetic metal. Curiously the spin-1/2 strongly interacts under exchange with the spins of the conduction electrons, and this effect leads to a minimum in the resistivity-temperature plot for temperatures below the Kondo scale T_K . For quantum transport experiments the Kondo effect leads to a boost in the conductance through nanostructures.. In a 1997 review on electron transport in quantum dots [1], L. P Kouwenhoven et al. wrote of the Kondo effect:

‘This is particularly interesting since parameters like the exchange coupling and the Kondo temperature should be tunable with a gate voltage. However, given the size of present day quantum dots, the Kondo temperature is hard to reach, and no experimental results have been reported to date.’

Less than a year after this remark was made the situation changed dramatically. The year of 1998 saw the first publication for observation of the Kondo effect in a quantum dot approximately 100 nm across [2], by 2007 the first observation of two-channel Kondo physics was reported in a similarly sized device [3], and recently, in 2015, a fully tuneable ‘charge’ two-channel Kondo effect has been observed on the relative macroscale where the role of the ‘dot’ is played by a metallic island of several microns in diameter (consisting of billions of electrons) which combine to have an overall pseudospin-1/2 [4].

Earlier theoretical research towards exact solutions of models for strongly correlated electrons in a sense anticipated the progress in nanostructure fabrication. In particular Meir and Wingreen [5], and later Jauho, Wingreen and Meir [6], exactly solved for the charge current through different resonant level models with two leads, in and away from equilibrium, including the most physically relevant case with a harmonically modulating bias. This showed that a general formula for tunnelling through an arbitrary mesoscopic region exists, provided that one treats the connecting leads as non-interacting.

In a similar manner, and more related to the present research, A. Schiller and S. Hershfield investigated transport through a Kondo impurity interacting with two separate leads away from equilibrium [7, 8], including time-dependent transport with the sinusoidal

voltage bias [9]. This was done by studying the non-interacting Toulouse limit of the spin-anisotropic two-channel Kondo model, extended to include anisotropic exchange between the channels. Beyond a motivation from the point of view of basic research, a search for exact solutions is important for quantum dot experiments in the Kondo regime because the tunnelling between the dot and surrounding reservoirs of electrons does not necessarily have to be weak. One should therefore aim to work non-perturbatively in the Kondo exchange couplings.

In this thesis we will examine the physics of electron transport in Kondo impurity models away from equilibrium by using Keldysh functional integrals, inspired by the theoretical studies above. The main line of investigation studies a one-channel Kondo (1CK) model at the Toulouse limit, where it is described by a resonant level (RL) model with a single lead. By allowing for a height difference between the Fermi energy and the d level, and modulating the single particle energies of the lead electrons with a sinusoidal voltage bias, we will study an extension of the Toulouse limit 1CK model that is driven away from equilibrium. The system may be loosely thought of as half of a tunnelling junction. The main results are expressions for the current which are exact in the tunnelling couplings within the linear response regime in the amplitude of the bias. We also show how the procedure carries over to the two-channel model studied by Schiller and Hershfield.

1.1 Outline

Chapter 2 introduces a selection of useful subjects. This includes theoretical concepts: many body physics tools in one-dimension, Keldysh functional integrals and linear response; as well as phenomenology: transport in quantum dots, and Kondo impurity physics topics.

Chapter 3 prepares for the research in chapters IV and V by showing the mappings of the one-channel and two-channel Kondo models to the resonant level and Majorana resonant level models in their respective Toulouse limits. This is mainly done by filling in details from the book by Gogolin et al. [10].

Chapter 4 investigates ac transport through a RL model, i.e. the non-interacting Anderson model. The toy-version of the model here considers a single metallic lead of spinless electrons attached to a quantum dot. The current into the dot is calculated for any temperature and driving frequency in the sinusoidal voltage bias. This is mapped to a non-equilibrium version of the 1CK model at the Toulouse limit.

Chapter 5 considers ac transport in the two-channel Kondo (2CK) model at the Toulouse limit. Here a free Majorana fermion controls the behaviour near a non-trivial fixed point in the RG flow. By this we mean the Toulouse limit for the 2CK model interpolates between the familiar RL model and a Majorana RL model in the space of exchange couplings, making potential experiments a robust way to observe Majorana physics. We outline how the methods of Chapter 4 extend to the tunnelling junction studied by Schiller and Hershfield [8].

Chapter 6 summarises the findings in the thesis. An important feature to the research is that our conductance calculations are exact in the tunnelling amplitudes (while staying within linear response in the time dependent voltage bias). This is crucial because for quantum dot experiments tuned to the Kondo regime the role of “tunnelling amplitude” is played by the transverse Kondo coupling J_{\perp} which may be $\mathcal{O}(1)$.

Chapter 2

Preliminaries

Here we devote a chapter to background material to help the thesis become accessible to the reader not working in the field of quantum transport, or who may not be familiar with some of the techniques we employ such as Keldysh functional integrals.

2.1 Impurity physics and quantum transport topics

The first half of the chapter focuses on selected topics in quantum transport.

2.1.1 Quantum dots and transport

A quantum dot is a spatially isolated island, quantum confined in all three orthogonal directions, that supports discrete energy levels. A simple model for a dot would be to consider a single energy level:

$$H_{\text{dot}} = \sum_{\sigma \in (\uparrow, \downarrow)} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow} \quad (2.1)$$

where $d_{\sigma}, d_{\sigma}^{\dagger}$ are creation/annihilation operators for a spin- σ electron on the dot, ϵ_d is the onsite energy, $n_{d\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$ and $U > 0$ is a repulsive Hubbard-type potential which provides an energy penalty for double occupancy. To investigate transport through a quantum dot

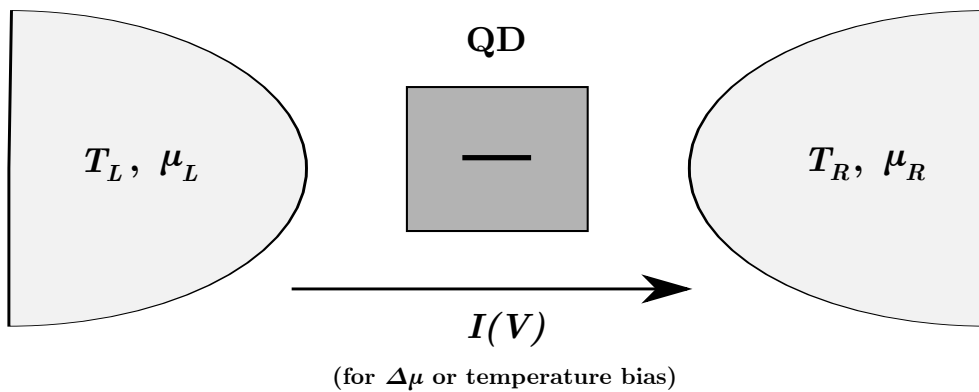


Figure 2.1: Schematic for the prototypical single impurity Anderson model (2.4) used for investigating transport through quantum dots.

we can put metallic leads to the left and right which have the Hamiltonians:

$$H_L = \sum_{k\sigma} \xi_{kL} c_{kL}^\dagger c_{kL} \quad H_R = \sum_{k\sigma} \xi_{kR} c_{kR}^\dagger c_{kR}, \quad (2.2)$$

where we have neglected interaction effects in the leads and assumed that they have the single particle energies $\xi_{k,\alpha} = \epsilon_k - \mu_\alpha$ where α labels the channel in the left (L) or right (R) lead. Since the leads and the dot are close together the electrons can hop between the dot and each lead separately. For this we have a tunnelling Hamiltonian:

$$H_{\text{tun}} = \sum_{\alpha=R,L} \sum_{k\sigma} (V_{k\alpha} c_{k\alpha\sigma}^\dagger d_\sigma + \text{h.c.}) \quad (2.3)$$

where $V_{k,L(R)}$ are complex hopping amplitudes which are often assumed to be momentum-independent.

The whole set-up comprises the single impurity Anderson model:

$$H_{\text{And.}} = H_{\text{dot}} + H_L + H_R + H_{\text{tun}}, \quad (2.4)$$

sketched in Fig. 2.1. The leads act as reservoirs for the electrons so by holding them at different chemical potentials (with a gate voltage V) the electrons hop from one lead to the dot and then onto the next, thus leading to an observable current $I(V)$. This is what is meant by ‘‘out of equilibrium’’ for charge transport¹. The dot can accommodate up to two electrons that are strongly interacting due to the finite onsite Coulomb repulsion U . The current will be a complicated function of the applied voltage, the tunnelling amplitudes $V_{k,L(R)}$ and the interaction U .

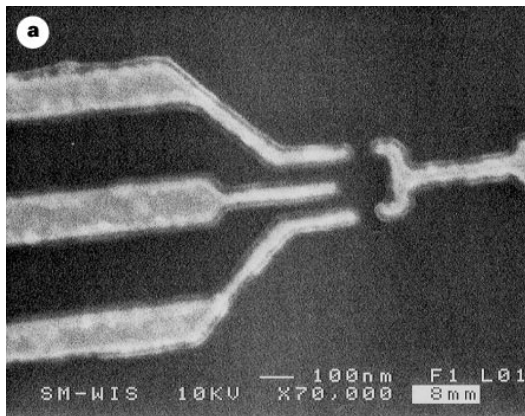


Figure 2.2: Scanning electron microscope image of a semiconductor quantum dot device extracted from Goldhaber-Gordon et al. [2], in which the Kondo effect was first observed in quantum dots. Typical energy scales for such experiments are of the order 1 meV.

For comparison to an experimental system, consider Fig. 2.2 from Ref. [2]. The quantum dot is in the confined region between the electrodes, or metallic ‘gates’, shown in white. By placing semiconductors with different band structures together, e.g. GaAs and AlGaAs, the conduction bands and valence bands bend at the interface so to create a two dimensional electron gas (2DEG) where the electrons have a very high mobility. This

¹Another possibility is a a heat current from a non-zero temperature gradient between the leads.

is the dark background. In this case the outer two gates tune the tunnelling coupling between the dot and the 2DEG, while the ‘back gate’ in the middle controls the levels of the dot compared to the Fermi energy of the conduction band electrons. Two further ‘source’ and ‘drain’ contacts may also be placed on the heterostructure in order to measure a current through the device.

In this thesis we will investigate non-equilibrium charge transport that fits into this framework.

2.1.2 Transport regimes for quantum dots

The field of quantum transport can be divided into different regimes by energy scales. Two important ones are the level spacing δ_s (\sim the inverse of the DOS per energy interval) and the charging energy E_c (the cost to add an electron into the nanostructure). Other than energy, the other important quantity is the conductance in terms of the conductance quantum $G_Q = 2e^2/h$ which gives us an idea about the scattering behaviour. Often experimentalists investigate the conductance lineshape for a device, which shows the conductance in units of G_Q versus an applied voltage bias for different temperatures, e.g. Fig. 2.3.

For experiments addressing transport through quantum dots the conductance is often low, $G \ll G_Q$, the scale of E_c becomes important, and electron-electron interactions are strong. As a consequence electrons tunnel one-by-one as infrequent discrete events, with corrections for ‘co-tunnelling’ where they tunnel two at a time. This is known as Coulomb blockade. Moving towards lower energies one enters the Kondo regime characterised by

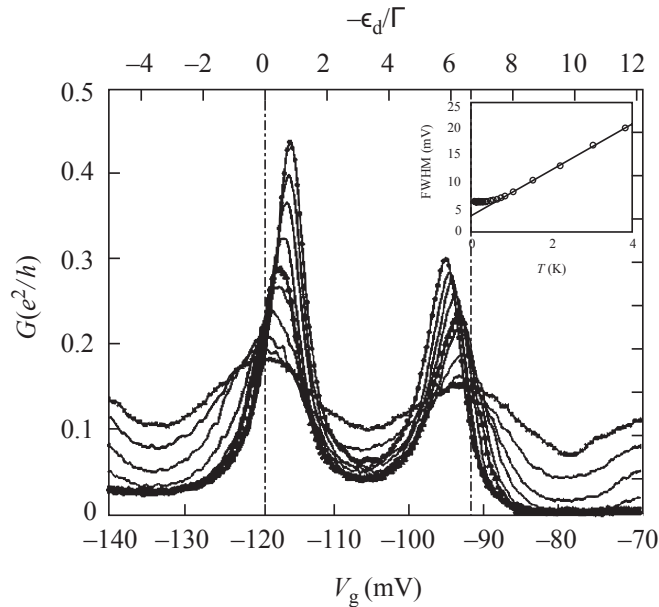


Figure 2.3: Conductance versus gate voltage at different temperatures for a single electron transistor. An increased peak in the conductance with decreased temperature is an unmistakable sign of the Kondo effect. The curves range from 100 mK (at the highest) to 3800 mK (at the lowest) here. Figure reproduced from Ref. [11]

an energy scale T_K which, theoretically, should be much less than bare energy scales like the electron bandwidth D . As we will see later the conductance depends exponentially on

T_K . An important difficulty that experimentalists must confront which is buried in words like ‘moving towards lower temperature one enters the Kondo regime’ is that for Kondo physics one needs to design the device such that it has a degenerate ground state. This makes it very difficult in general for transport experiments in semiconductor quantum dot devices to access the Kondo regime and in practice can lead to a narrow range of tunnelling conductances.

2.1.3 The Kondo effect

Long before the advent of semiconductor quantum dot devices like in Fig. 2.2, the phenomenon called the Kondo effect was found in metals: Usually the resistivity ρ is approximately flat at low temperatures T towards some residual $T = 0$ value ρ_0 . Then at higher T electron-phonon scattering effects are important giving a $\rho_{ep} \propto T^5$ contribution, for $T \ll \theta_D$ where θ_D denotes is the Debye scale, and at even higher T the behaviour is Ohmic. In the 1930s, however, the resistivity of gold was found to increase at low T . The anomalous behaviour was due to magnetic impurities; doping a metallic host with magnetic ions, such as iron, contributes a Curie component to the susceptibility

$$\chi_{\text{imp}} \propto J(J+1)/T \quad (2.5)$$

where J is the total angular momentum of the impurities. This indicates the formation of a localised magnetic moment because free spins also show the $\chi \propto 1/T$ decay.

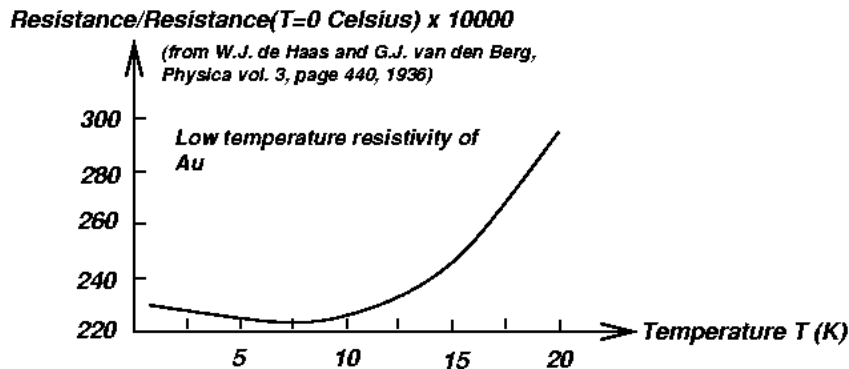


Figure 2.4: The Kondo effect. A resistivity minimum appears at low temperatures for metals doped with magnetic impurities.

Kondo explained the resistivity minimum, Fig. 2.4, by virtual spin flip scattering processes between the conduction electrons and the impurities. He did this by going up to third order perturbation theory in the interaction of his effective model, which describes a single localised magnetic moment at the origin interacting with a sea of conduction electrons via spin exchange.

$$H = H_0[\psi] + JS \cdot \mathbf{s}(\mathbf{0}), \quad J > 0 \quad (2.6)$$

with

$$H_0 = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}, \quad \mathbf{s}(\mathbf{0}) = \sum_{\sigma,\sigma'} \psi_\sigma^\dagger(\mathbf{0}) \boldsymbol{\sigma}_{\sigma\sigma'} \psi_{\sigma'}(\mathbf{0}) \quad (2.7)$$

Here \mathbf{S} is the spin-1/2 operator such that $\mathbf{S}^2 = S(S+1)$, J is the antiferromagnetic exchange coupling, ψ_σ are the conduction electron field operators, $\mathbf{s}(\mathbf{0})$ is the spin density

of the conduction electrons and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^\top$ is the vector of Pauli matrices. Kondo's perturbative solution, however, diverges logarithmically in the zero temperature limit and further corrections diverge ever more rapidly. Seeking an understanding of this became known as the Kondo problem, while the resulting characteristic behaviour such as the resistivity minimum at low T is due to the 'Kondo effect'.

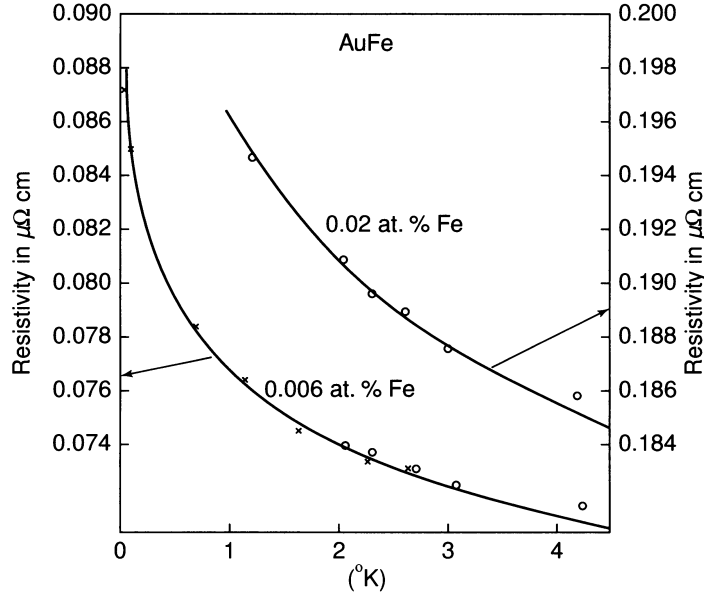


Figure 2.5: Resistivity of dilute iron alloys as a function of temperature close to $T = 0\text{K}$. Image reproduced from [12].

The Kondo effect is associated with a condensation of the conduction electrons spins to 'screen' the localised moment. This phenomenon becomes stronger the lower the temperature and the greater the dilution of magnetic moments, Fig. 2.5. Screening means that the bare interaction becomes replaced by an effective one which is shorter ranged. For instance, in any electronic medium the electric fields are always screened on a macroscopic scale since current must not flow in thermodynamic equilibrium. The extreme end of this is the Hubbard U where only zero ranged potentials are retained, described as 'total screening'.

Local moment formation

The notion of a localised spin interacting under exchange with the spins of many conduction electrons in a surrounding bath emerges from a microscopic description. Starting with a single lead version of the Anderson model (2.3), we may arrange the parameters such that the energy of the singly occupied state of the dot is lower than both the empty and the doubly-occupied states, Fig. 2.6. Given this starting point the low energy limit of the Hamiltonian is an effective Kondo model.

This is achieved by the Schrieffer-Wolff transformation, a canonical transformation that projects the Hamiltonian onto the subspace where only one electron is on the dot. The idea is that excitations to the empty or doubly occupied subspace exist as virtual

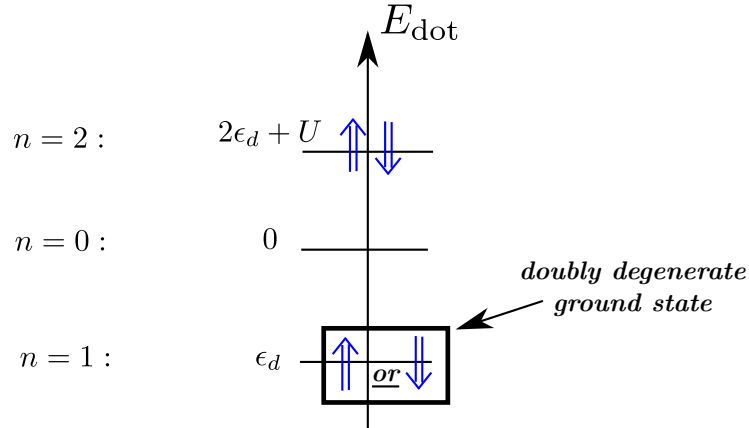


Figure 2.6: Arrangement of parameters for the local moment regime, where the Fermi energy for the conduction band is set at zero. Virtual processes, e.g. where a single dot electron in the ground state hops to the conduction band for a short period of time, leads to Kondo spin flips. This is accurate for isolated transition metal atoms with unfilled f-shells.

processes which are integrated out in a kind of one-step renormalisation process,

$$\begin{aligned}
 H_{\text{And.}} &\xrightarrow{\text{S-W}} \sum_{k,k'} V_k^* V_{k'} \left[\frac{1}{(\epsilon_k - \epsilon_d)} + \frac{1}{(U + \epsilon_d - \epsilon_{k'})} \right] c_{k\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{k'\beta} \cdot d_\lambda^\dagger \boldsymbol{\sigma}_{\lambda\mu} d_\mu + \dots \\
 &= \sum_{k,k'} J_{kk'} \mathbf{S} \cdot c_{k\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{k'\beta} + \dots, \tag{2.8} \\
 &\text{(repeated spin indices summed)}
 \end{aligned}$$

where the dots indicate a discarded potential scattering term² and the pseudofermionic representation of the spin-1/2 is: $\mathbf{S} = d_\lambda^\dagger \boldsymbol{\sigma}_{\lambda\mu} d_\mu$. Since only electrons near the Fermi level $\epsilon_k = 0$ contribute to the low energy properties, the k dependence may be neglected, giving precisely the Kondo model. Further details for this procedure may be found in textbooks (e.g. Hewson [13], Ch. 1.7).

As a consequence one finds that the exchange coupling which emerges is antiferromagnetic, such that it is favourable for neighbouring spins to be anti-parallel:

$$J \simeq V^2 \left(\frac{1}{|\epsilon_d|} + \frac{1}{|\epsilon_d + U|} \right) > 0 \tag{2.9}$$

2.1.4 Scaling and screening for Kondo models

The Wilsonian numerical renormalisation group (NRG) as a non-perturbative method fully solves the Kondo problem. Historically, Anderson’s “poor man’s scaling” came as one of the important advances towards this and is in exact agreement with a perturbative RG analysis to leading order in the β -function expansion. We will briefly outline the scaling features for the Kondo models and how this fits in with the screening picture.

²which vanishes in the particle-hole symmetric case.

Isotropic 1CK model

In renormalisation group procedures one progressively adjusts the coupling J while slowly lowering a cutoff energy scale D such that the Hamiltonian retains its form, i.e. $H(J, D) \rightarrow H(J, \tilde{D})$ where $J(D) \rightarrow J(\tilde{D}) + \delta J$ for the rescaling $D \rightarrow \tilde{D} < D$. This is also referred to as integrating out the excitations $E \in [\tilde{D}, D]$. This tells us whether or not the theory has a well defined low energy limit. Since J is being tuned in this case and it depends on the cutoff it is said to be a running coupling constant. For the Kondo model starting at high temperatures the result is that $J = 0^+$ flows to a $J = \infty$ strong coupling fixed point, Fig. 2.7 (a):

$$\frac{\partial g}{\partial \log(D)} = -2g^2 + 2g^3 + O(g^4) \quad (2.10)$$

Here the dimensionless coupling $g = \nu J$ has been introduced where ν is the density of states which is assumed to be constant near the Fermi level. In plain English, ‘flowing to an infinite fixed point’ means that the Kondo interaction strength always grows as the energy scale is reduced in the renormalisation group (RG) transformation. This behaviour is known as asymptotic freedom - it is said that the local moment coupled to the conduction sea through J is asymptotically free - which is famously known as a feature of quantum chromodynamics describing the quark-gluon interactions found in nuclear matter. The Kondo model is the simplest example of this idea in physics.

Solving the RG equation to leading order, choosing appropriate integration boundaries, gives

$$g(D) = \frac{g_0}{1 + 2g_0 \log(D/D_0)}, \quad (2.11)$$

from which we may estimate the Kondo temperature T_K , the point at which we need to use more advanced techniques than perturbation theory, by a rewriting

$$\frac{1}{g(D)} = 2 \log \left(\frac{D}{D_0 e^{-\frac{1}{2g_0}}} \right). \quad (2.12)$$

The running coupling diverges when D approaches $D_0 e^{-1/2g_0}$, which gives an approximation for T_K as

$$T_K = D_0 e^{-\frac{1}{2g_0}}. \quad (2.13)$$

For quantum dot experiments the Kondo temperature is in the range of a few millikelvin and is estimated from the width of the zero bias peak, which is smeared out and reduced in height with increased temperature. The Kondo resonance is destroyed when the temperature goes above T_K .

The ground state for the Kondo model is a local many body singlet between the spin-1/2 and the conduction electron spins, Fig. 2.7 (b). The idea is that as the temperature is lowered, provided J is initially positive, the conduction band gains a net spin-polarisation which screens the spin-1/2 impurity. A consequence is the spectral function of the impurity develops a peak at the Fermi energy of the conduction band electrons due to resonant spin-flip scattering, and the effects of this have been experimentally confirmed in quantum dot systems such as the one shown in the earlier figure from Goldhaber-Gordon et. al, Fig. 2.2.

In addition, the spin singlet ground state for the Kondo effect in metals can be deduced from an analysis of specific heat data. For combining two spin 1/2 particles there is only

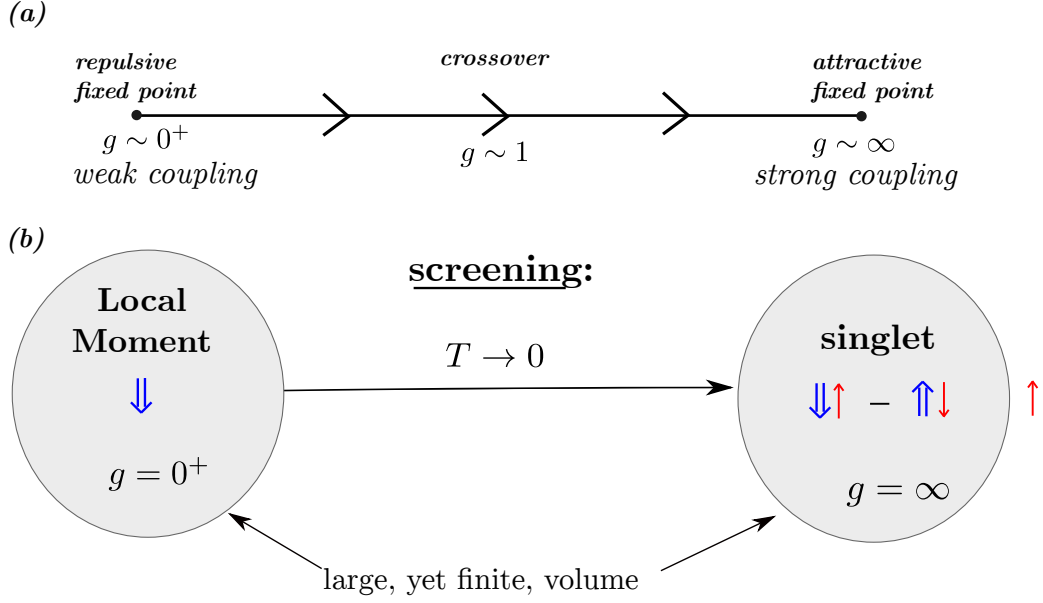


Figure 2.7: (a) The renormalisation group flow for the isotropic Kondo model. (b) Corresponding illustration of the many body state where the blue arrow represents the spin-1/2 impurity, and the red arrow is the collective spin of the bath of conduction electrons. The ground state is a many body singlet.

one possible way to make a singlet³, so the degeneracy is one and the predicted residual entropy is $S = k_B \ln(1) = 0$. In contrast for a free spin-1/2, as in the local moment regime, the spin is either up or down so the prediction in that case would be $S = k_B \ln(2)$. Nozières showed that towards the strong coupling fixed point with $T \ll T_K$ the conduction band electrons behave like a local Fermi liquid near the local singlet. This acts as static scatterer with an associated phase shift near the Fermi energy of $\delta = \pi/2$ per spin [14].

Anisotropic 1CK

The Kondo model can also be generalised to allow anisotropy of the exchange interaction:

$$\begin{aligned}
 \hat{V} &= J_a S^a \psi_\alpha(0)^\dagger \sigma_{\alpha,\beta}^a \psi_\beta(0) \\
 &= \psi_\uparrow^\dagger \psi_\downarrow (J_x S^x - i J_y S^y) + \psi_\downarrow^\dagger \psi_\uparrow (J_x S^x + i J_y S^y) + J_z (\psi_\uparrow^\dagger \psi_\uparrow - \psi_\downarrow^\dagger \psi_\downarrow) S^z \\
 &= J_\perp (\psi_\uparrow^\dagger \psi_\downarrow S^- + \psi_\downarrow^\dagger \psi_\uparrow S^+) + J_z (\psi_\uparrow^\dagger \psi_\uparrow - \psi_\downarrow^\dagger \psi_\downarrow) S^z
 \end{aligned} \tag{2.14}$$

where all field operators are implicitly evaluated at $\mathbf{x} = 0$, the $S^\pm = S^x \pm i S^y$ are ladder operators, we have defined $J_x = J_y \equiv J_\perp$ and the repeated indices were summed over. In this situation there are two coupled flow equations:

$$\frac{\partial J_z}{\partial \log(D)} = -2\nu J_\perp^2 + O(J^3) \tag{2.15}$$

$$\frac{\partial J_\perp}{\partial \log(D)} = -2\nu J_z J_\perp + O(J^3) \tag{2.16}$$

³So the Fermi sea is not really ‘one’ electron. ‘One’ is accurate for considering the problem on a 1D lattice, on the other hand, where the impurity traps a single electron at say site zero and hopping onto it is excluded.

To leading order these are also in the form of the Kosterlitz RG equations originally found for the Berezinskii-Kosterlitz-Thouless (BKT) phase transition in the two-dimensional XY model. The anisotropic version of the Kondo model is the one we will be most concerned with in later chapters.

A qualitatively different approach than the perturbative analysis, such as NRG, is necessary to fully determine all possible fixed points. In the simple example of the isotropic 1CK model, for instance, suppose it is only known that there is the repulsive (trivial) fixed point at $J = 0$ and an attractive fixed point at $J \rightarrow \infty$. Then in principle it is possible, though it seems unlikely, that such an arrangement has any even number of fixed points in between since these would all be topologically consistent situations. Due to NRG, which is numerically exact, we know that this is not the case and that the asymptotic freedom characterisation is accurate.

Two-channels and non-Fermi-Liquid physics

The two channel Kondo model includes a second species of fermions which also interact with the localised spin:

$$H_{2CK} = \sum_{\alpha=L,R} \sum_{k\sigma} \epsilon_k c_{k\sigma\alpha}^\dagger c_{k\sigma\alpha} + J_L \mathbf{S} \cdot \mathbf{s}_L(0) + J_R \mathbf{S} \cdot \mathbf{s}_R(0) \quad (2.17)$$

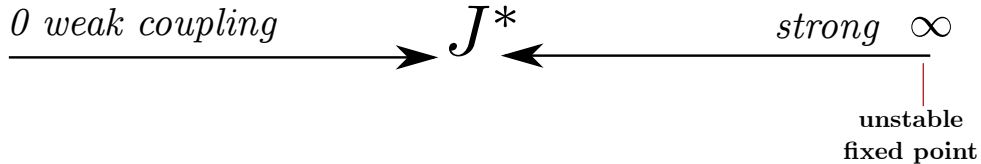


Figure 2.8: RG flow for the two-channel Kondo model when $J_L = J_R = J > 0$. The infinite coupling fixed point is now repulsive and a single intermediate fixed point exists at finite coupling. This is confirmed by numerically exact techniques like the NRG.

Sticking with the spin-isotropic case, for simplicity, and choosing $J_L = J_R = J > 0$, we may compare the RG flow Fig. 2.8 to the earlier single-channel diagram Fig. 2.7 (a). The infinite coupling fixed point is now unstable and there is a new non-trivial attractive fixed point at finite coupling. This leads to different physics because the low energy properties of the model are no longer in essence like the Fermi-liquid. Instead correlators now decay with power laws. This situation is also described as ‘overscreened’. What this means is that both baths compete to screen the spin-1/2 and, loosely speaking, each only interacts with ‘half’ of the impurity spin, Fig. 2.9.

The low energy properties are well described by the the non-interacting limit of the Hamiltonian, a ‘Majorana resonant level model’, that we will see in more detail in Chapter 3. By an analysis of the free energy for this theory, a frustrated ground state with non-integer degeneracy is revealed by a non-vanishing residual entropy:

$$S(T \rightarrow 0) = \frac{1}{2} \ln(2). \quad (2.18)$$

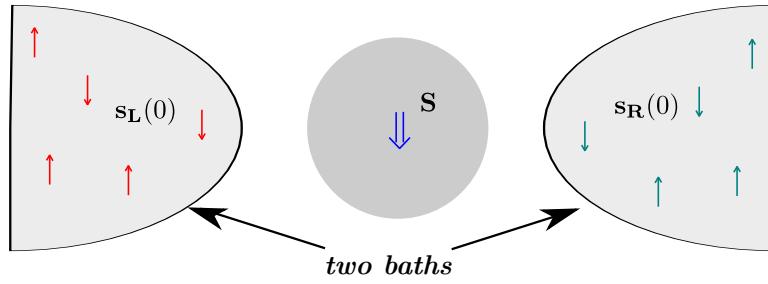


Figure 2.9: In the two-channel case both conduction baths try to screen the spin leading to a non-trivial fixed point in the RG flow. There is a frustrated ground state (non-integer degeneracy) manifested by a non-zero residual entropy.

2.2 Many body physics techniques

In this section we cover the essential techniques used in the rest of the thesis. This includes bosonization, Keldysh functional integrals and linear response theory.

2.2.1 One dimensional techniques (bosonization)

There are two features of one-dimensional Fermi systems which are responsible for the main differences which allow for bosonization, the local fermion-boson correspondence we will use later to set up our transport problems:

- (i) No low-lying energy states for particle-hole excitations with momentum $0 \leq q \leq 2k_F$
- (ii) Linear dispersion in the limit $q \rightarrow 0$.

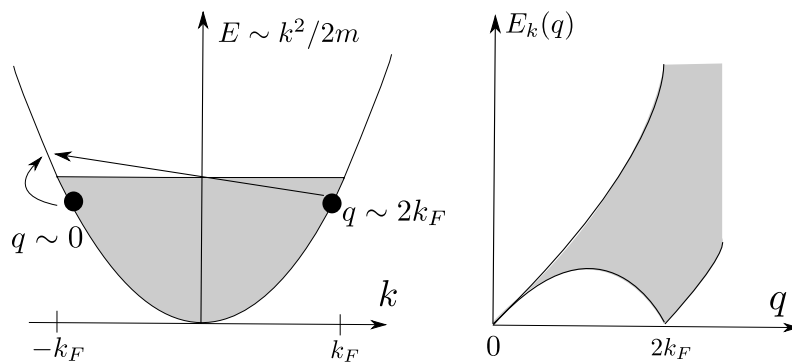


Figure 2.10: Massive particle dispersion (left) and excitation spectrum (right) for a $d = 1$ system (right) with excitation momentum q . Increasing q requires moving away from the Fermi points. For $d > 1$ however there is a continuum of low E states which are accessible for $|q| < 2k_F$.

The corresponding excitation spectrum $E_k(q) = E(k + q) - E(k)$ and dispersion $E(k)$ is shown in Fig 2.10. They may be thought of as a direct result of the reduced phase space of the particle-hole excitations, since they are confined to move along a line with no

freedom of angles to increase their momentum. In addition we know from fundamental results (Mermin-Wagner-Hohenberg-Coleman theorem) that no ordering can exist at finite temperature in one dimension. In the following we present a very short overview of bosonization for non-interacting models.

Free Tomonaga-Luttinger model (FTLM)

We shall start by linearising the free electron Hamiltonian. This is always allowed when there is a one-dimensional excitation spectrum, Fig. 2.10. Expanding around the points $\pm k_F$ where we impose a finite bandwidth of 2Λ , one finds

$$\begin{aligned} H &= \sum_k \epsilon_k c_k^\dagger c_k \approx \sum_{k=k_F-\Lambda}^{k_F+\Lambda} \left. \frac{\partial \epsilon(k)}{\partial k} \right|_{k_F} (k - k_F) c_k^\dagger c_k + \sum_{k=-k_F-\Lambda}^{-k_F+\Lambda} \left. \frac{\partial \epsilon(k)}{\partial k} \right|_{-k_F} (k + k_F) c_k^\dagger c_k \\ &= \sum_{-\Lambda \leq k < \Lambda} v_F k c_{k+k_F}^\dagger c_{k+k_F} + \sum_{-\Lambda \leq k < \Lambda} -v_F k c_{k-k_F}^\dagger c_{k-k_F}. \end{aligned}$$

Extending the momenta range $\Lambda \rightarrow \infty$ and inserting normal ordering signs, we have

$$H \rightarrow H_F = \sum_{k=-\infty}^{\infty} v_F k (: c_{kR}^\dagger c_{kR} : - : c_{kL}^\dagger c_{kL} :). \quad (2.19)$$

$$H_F = \sum_{k,r \in (-1,1)} r v_F k : c_{\alpha_r k}^\dagger c_{\alpha_r k} : \quad (2.20)$$

where $\alpha_r \in (\alpha_1, \alpha_{-1}) = (R, L)$. This is the free Tomonaga-Luttinger model (FTLM). Here the symbols R and L correspond to right- and left-moving electrons. With the finite bandwidth it is known just as the Tomonaga model. Extending the k values is justified provided the higher energy states never take part in any physical excitation. The normal ordering signs are inserted because the states below the lower $-\Lambda$ cutoff are unphysical; the (Dirac) sea of electrons is unbounded from below. The left-moving and right-moving c operators obey the usual fermionic algebra and different species R and L always anticommute with each other, regardless of their creation or annihilation nature.

$$\{c_{\alpha_r k}, c_{\alpha_{r'} k'}^\dagger\} = \delta_{r,r'} \delta_{k,k'}, \quad \{c_{\alpha_r k}, c_{\alpha_{r'} k'}\} = \{c_{\alpha_r k}^\dagger, c_{\alpha_{r'} k'}^\dagger\} = 0 \quad (2.21)$$

Field description (Massless Dirac theory)

Later we will often work at the level of field operators. The fermion field operator splits into left and right moving parts ψ_L and ψ_R . This comes by restricting attention to states near the Fermi momentum and isolating the parts ψ_L and ψ_R which are slowly varying in space compared to $\exp(\pm i k_F x)$:

$$\begin{aligned} \psi(x_j, \tau) &= \frac{1}{\sqrt{L\hbar\beta}} \sum_{kn} e^{ikx_j - i\omega_n \tau} c_k \approx \frac{1}{\sqrt{L\hbar\beta}} \left[\sum_{n,k=k_F-\Lambda}^{k_F+\Lambda} e^{ikx_j - i\omega_n \tau} c_k + \sum_{n,k=\Lambda-k_F}^{-k_F-\Lambda} e^{ikx_j - i\omega_n \tau} c_k \right] \\ &\xrightarrow{\Lambda \rightarrow \infty} \frac{1}{\sqrt{L\hbar\beta}} \sum_{kn} (e^{ik_F x_j} e^{ikx_j - i\omega_n \tau} c_{k,R} + e^{-ik_F x_j} e^{ikx_j - i\omega_n \tau} c_{k,L}) \\ &= e^{ik_F x_j} \psi_R(x_j, \tau) + e^{-ik_F x_j} \psi_L(x_j, \tau) \end{aligned} \quad (2.22)$$

Eq. (2.22) above is for discrete systems with a length $L = Na$, with N sites and a lattice spacing a where sites are enumerated by $x_j = ja$ with $1 \leq j \leq N$. Again the continuum limit is allowed for low energy processes $|q \pm k_F| \ll k_F$. The spatial part taken alone is

$$\psi(x) = e^{ik_F x} \psi_R(x) + e^{-ik_F x} \psi_L(x) \quad (2.23)$$

where

$$\psi_{\alpha_r}(x) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} c_{k,\alpha_r}, \quad c_{k,\alpha_r} = \frac{1}{\sqrt{L}} \int_0^L dx e^{-ikx} \psi_{\alpha_r}(x) \quad (2.24)$$

with the periodic boundary conditions $k = 2\pi n/L$, ($n = 0, \pm 1, \pm 2, \dots$). For this convention the anticommutator is normalized as a delta function:

$$\{\psi_{\alpha_r}(x), \psi_{\alpha_{r'}}^\dagger(y)\} = \delta_{r,r'} \delta(x-y). \quad (2.25)$$

Rewritten on the level of the fermion fields using the definitions above the FTLM is the massless Dirac Hamiltonian:

$$H_F = -iv_F \int dx : [\psi_R^\dagger(x) \partial_x \psi_R(x) - \psi_L^\dagger(x) \partial_x \psi_L(x)] : \quad (2.26)$$

where the Fermi velocity plays the role of the speed of light.

Fermion-boson correspondence between the massless free theories

Chiral fermion densities J_L and J_R may be used to rewrite the FTLM. In field-theoretic language we may also refer to $J_{L(R)}$ as currents. The currents are:

$$\begin{aligned} J_{\alpha_r}(p) &= \sum_k : c_{\alpha_r, k+p}^\dagger c_{\alpha_r, k} : \\ &= \sum_k \left(c_{\alpha_r, k+p}^\dagger c_{\alpha_r, k} - \delta_{k,0} \langle c_{\alpha_r, 0}^\dagger c_{\alpha_r, 0} \rangle \right), \end{aligned} \quad (2.27)$$

such that:

$$J_L(p > 0)|0\rangle = 0, \quad J_R(p < 0)|0\rangle = 0, \quad (2.28)$$

where $0 < p \leq 2\pi$ and $\alpha_r \in (\alpha_{-1}, \alpha_1) = (L, R)$. They form an Abelian Kac-Moody algebra:

$$[J_{\alpha_r}(p), J_{\alpha_{r'}}(-p')] = -\delta_{p,p'} \delta_{r,r'} \frac{rLp}{2\pi} \quad (2.29)$$

The Hamiltonian may be written in this new basis up to an unimportant constant.

$$H_F = \frac{\pi v_F}{L} \sum_q (: J_R(q) J_R(-q) : + : J_L(q) J_L(-q) :) \quad (2.30)$$

$$= \pi v_F \int dx : (J_R(x)^2 + J_L(x)^2) : \quad (2.31)$$

This is equal to a theory of massless chiral bosons $\phi_{L(R)}$ which are compactified on a circle⁴:

$$H_B = -v \int dx ((\partial_x \phi_L(x))^2 + \partial_x (\phi_R(x))^2) \quad (2.32)$$

⁴e.g. $\phi_{L(R)}(x+a) = \phi_{L(R)}(x)$. The U(1) symmetry motivates the name Abelian bosonization.

The equivalence comes by using the famous bosonization formulae:

$$\psi_L(x) = \frac{1}{\sqrt{2\pi a_0}} : e^{-i\sqrt{4\pi}\phi_L(x)} :, \quad \psi_R(x) = \frac{1}{\sqrt{2\pi a_0}} : e^{i\sqrt{4\pi}\phi_R(x)} :, \quad (2.33)$$

where a_0 is a short-distance cut-off. In this case the corresponding bosonization formulae for the currents are more useful for showing the mapping:

$$J_L(x) = \frac{i}{\sqrt{\pi}} \partial_x \phi_L(x), \quad J_R(x) = -\frac{i}{\sqrt{\pi}} \partial_x \phi_R(x), \quad (2.34)$$

The details of the correspondence $H_F = H_B$ and the equivalence of the local operator algebras for the above bosonization formulae (2.33)-(2.34) may be found in Appendix A.2. More straightforwardly, one can also establish the correspondence by ensuring that H_B and H_F generate equivalent correlation functions. This is a common trick which will be seen again shortly in the context of the Keldysh formalism which describes the many body physics of systems out of equilibrium.

Note that the label of ‘chiral’ for the Bose fields $\phi_{L(R)}$ is not only to indicate which kind of Weyl fermion it bosonizes. It also indicates that the fields only move in one direction in (τ, x) space, because they are defined as the left and right moving parts of $\Phi(x, \tau)$ which solve the wave equation from the Gaussian model:

$$H_B(\tau) = \frac{v}{2} \int dx (\Pi(x, \tau))^2 + (\Phi(x, \tau))^2. \quad (2.35)$$

We will exclusively use the definitions (2.33)-(2.34) for the bosonization formulae throughout this thesis with the exception of Chapter VI, where we elect to adopt notations from Schiller and Hershfield in Ref. [8].

Inclusion of spin: Klein factors

For upgrading our discussion to the case of more than one fermion species, which we will need later for the two-channel Kondo model, we have to deal with the fact that the different species should anti-commute. In addition the different spin species of the same fermionic field should also anti-commute. This is afforded by introducing ‘Klein factors’ $\eta_{L(R)\mu}$ such that

$$\psi_{R\mu}(x) = \frac{1}{\sqrt{2\pi a_0}} \eta_{R\mu} e^{i\sqrt{4\pi}\phi_R(x)} \quad \psi_{L\mu}(x) = \frac{1}{\sqrt{2\pi a_0}} \eta_{L\mu} e^{-i\sqrt{4\pi}\phi_L(x)}, \quad (2.36)$$

where $\alpha, \beta \in (L, R)$ and $\nu, \mu \in (1, 2, 3 \dots)$ are labels for the fermion species (or spins). These obey a Clifford algebra.

$$\{\eta_{\alpha,\mu}, \eta_{\beta,\nu}\} = 2\delta_{\alpha\beta}\delta_{\mu\nu} \quad (2.37)$$

As a consequence the chiral currents associated to three spin components for right-movers are:

$$J^z(x) = \frac{1}{2} \psi_\alpha^\dagger (\sigma_3)_{\alpha\beta} \psi_\beta = \frac{i}{\sqrt{2\pi}} \partial_x \phi_s(x) \quad (2.38)$$

$$J^x(x) = \frac{1}{2} \psi_\alpha^\dagger (\sigma_1)_{\alpha\beta} \psi_\beta = \frac{i}{2\pi} \eta_\uparrow \eta_\downarrow \sin(8\pi\phi_s(x)) \quad (2.39)$$

$$J^y(x) = \frac{1}{2} \psi_\alpha^\dagger (\sigma_2)_{\alpha\beta} \psi_\beta = -\frac{i}{2\pi} \eta_\uparrow \eta_\downarrow \cos(8\pi\phi_s(x)) \quad (2.40)$$

where the spin-sector chiral Bose field ϕ_s is defined by $\phi_s = \phi_\uparrow - \phi_\downarrow$ and we dropped the subscript R everywhere for neatness. For completeness the even combination is called the charge-sector: $\phi_c = \phi_\uparrow + \phi_\downarrow$. The fact that this description is not spin-rotation invariant⁵ motivates the extension to non-Abelian bosonization where the corresponding bosonized descriptions are Wess-Zumino-Witten models [15], but this goes beyond the material we will need.

2.2.2 Local scattering and reduced dimensionality

The features of one-dimensional many body physics as sketched above are applicable to isolated impurities in a three dimensional Fermi liquid. Due to the local nature of potential scattering off the impurities, or indeed the spin exchange interaction as in the Kondo model, one can make progress by using a spherical wave basis rather than a plane wave basis,

$$\psi_\lambda(\mathbf{x}) = \int_0^\infty \frac{dk}{2\pi} \sum_{lm} \chi_{klm}(\mathbf{x}) c_{klm,\lambda} \quad (2.41)$$

where

$$\chi_{klm}(\mathbf{x}) = R_{kl}(|\mathbf{x}|) Y_{lm} \left(\frac{\mathbf{x}}{|\mathbf{x}|} \right), \quad R_{kl}(|\mathbf{x}|) = 2k j_l(k|\mathbf{x}|) \quad (2.42)$$

are the expansion coefficients, Y_{lm} are spherical harmonics and R_{kl} are radial functions in terms of spherical Bessel functions $j_l(x)$.^{6,7} By considering s -wave scattering as the dominant contribution, so $\chi_{klm}(\mathbf{x}) = 0$ for $l > 0$, the only important term is

$$\chi_{k00}(\mathbf{x}) = \frac{2 \sin(k|\mathbf{x}|)}{|\mathbf{x}|}. \quad (2.43)$$

and the chiral fermion field evaluated at the location $\mathbf{x} = 0$ of a single impurity is

$$\psi_\lambda(0) = \int_0^\infty \frac{dk}{2\pi} 2k c_{k\lambda} + (l \geq 1 \text{ waves}). \quad (2.44)$$

This approximation is exact for point-like scattering off a static impurity, where ‘static’ means that there are no internal degrees of freedom (e.g. spin):

$$\hat{V} = \int d\mathbf{x} V \delta(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) = V \psi^\dagger(0) \psi(0) \quad (2.45)$$

As a side remark, such terms arise the passage from the Anderson model to the Kondo model via the Schrieffer-Wolff transformation. These are typically discarded because static potential scattering is not important for the Kondo effect. Nevertheless, scattering potentials with an electron spin index s can always be reduced to (2.45) through a general decomposition:

$$\hat{V} = \sum_{s,s'} V(s, s') \psi_s^\dagger(0) \psi_{s'}(0), \quad V(s, s') = V \delta_{ss'} + \mathbf{J} \mathbf{S} \cdot \boldsymbol{\sigma}_{ss'}. \quad (2.46)$$

⁵While the current-current correlators $\langle J^\alpha(x) J^\alpha(0) \rangle$ decay with the same power law, J^z has a different normalisation, somewhat unsatisfactorily.

⁶See e.g. Landau and Lifshitz Vol. 3 Ch. 5 [16].

⁷For convenience we are choosing a different normalisation of the fields for this subsection alone, with $\{\psi_\lambda(\mathbf{x}), \psi_\rho^\dagger(\mathbf{x}')\} = (2\pi)^3 \delta_{\lambda\rho} \delta(\mathbf{x} - \mathbf{x}')$

consisting of the potential scattering $V\delta_{s,s'}$ and the spin-exchange term controlled by J . In summary, this is therefore an accurate tool for studying the Kondo problem; the spin-1/2 impurity acts as a boundary which scatters electrons and we unfold it into a one-dimensional picture with artificial length.⁸ The crucial point is that only one spin channel (the s-wave) couples to the Kondo impurity for the mapping to the one-dimensional model to be applicable.

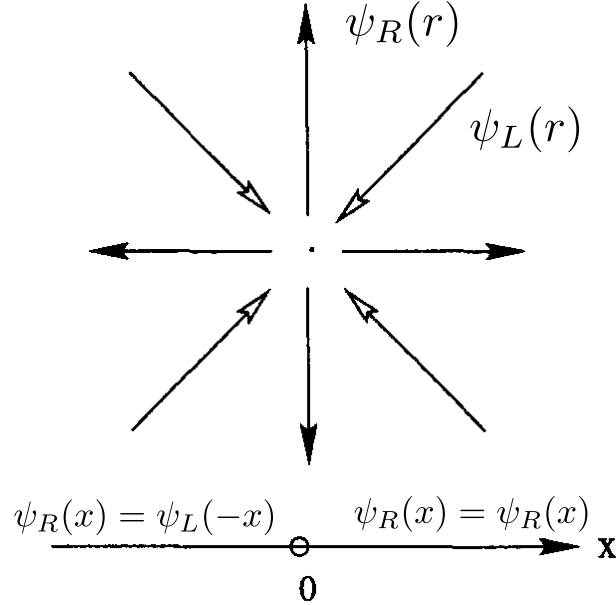


Figure 2.11: Local Hamiltonians like the Kondo model can be mapped to an effective one-dimensional picture with species of chiral fermion that defined along the whole real line, given that it is a good approximation to consider only the s-wave channel.

In practice, a way forward to accomplish this is to define a new chiral field ψ_σ (a right-mover) which is defined in general on the whole line $-\infty < x < \infty$ through

$$\psi_\sigma(x) = \begin{cases} \psi_{R\sigma}(x), & x > 0 \\ \psi_{L\sigma}(-x), & x < 0 \end{cases} \quad (2.47)$$

where x is a fictitious coordinate which is conjugate to k and σ is the spin index (Fig. 2.11).

2.2.3 Keldysh functional integrals and non-interacting transport

Equilibrium statistical field theory methods often rely on Matsubara expansions for Green functions. These are ineffective when there is broken time translation symmetry in a model, in the same way that Fourier transformations in momentum space are futile when there is broken spatial translation symmetry. This happens whenever systems are driven out of equilibrium by arbitrary time-dependent potentials $V(t)$. Examples of physical systems include electrons in a quantum wire when an alternating voltage bias is applied or when lasers are applied to the same effect in a cold atom set-up. The Keldysh technique circumvents relying on any symmetries so it is the proper theoretical tool for investigating time-dependent many body physics.

⁸Appendix A.3 contains an example scattering amplitude calculation for Kondo's spin-flips.

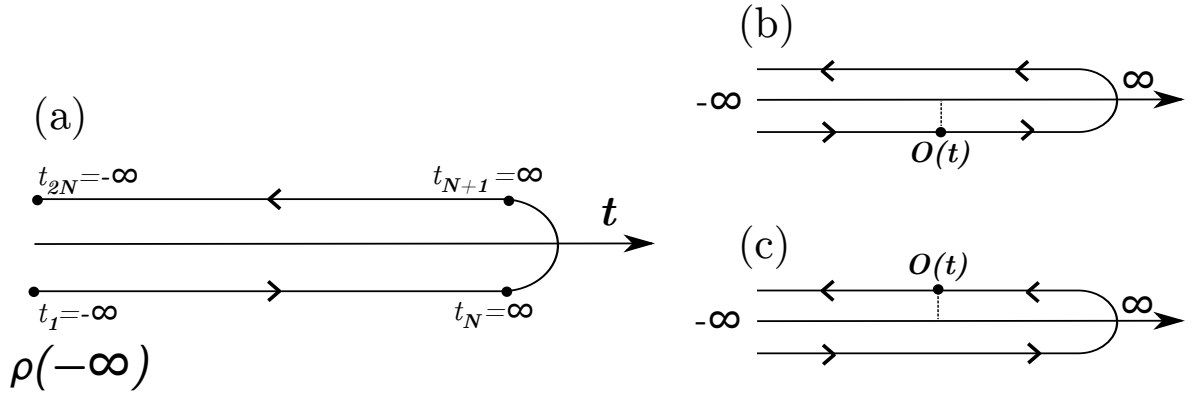


Figure 2.12: (a) The closed time contour is broken up into $2N$ pieces to define the discrete path integral. (b) Calculating the observable $O(t)$ on the forwards path, Eq. (2.55). (c) Calculating $O(t)$ on the backwards path, Eq. (2.56).

The unique fact about the Keldysh technique is that it does not rely on interactions being switched on adiabatically (the Gell-Mann and Low theorem). Instead it views the averages of observables as properties which are calculated along a closed-time contour C , Fig. 2.12 (a). This traces the evolution of a many-body state in real time from $t = -\infty$, at which point it is in equilibrium, to $t = \infty$ and back again to $t = -\infty$ where the final state no longer has to coincide with the initial one. The Matsubara formalism, in contrast, assumes that at some time in the distant past there was an equilibrium state from which the full interacting system evolves adiabatically and we only propagate forwards in imaginary time τ towards a final state which is the same up to a phase as the initial one.

The framework we will use for the Keldysh technique is based on coherent state functional integrals. It is of course possible to work only in the operator formalism instead. We will adhere to conventions in the book by Kamenev [17].

Short overview

The von Neumann equation is

$$\partial_t \hat{\rho}(t) = -i[H(t), \hat{\rho}(t)] \quad (2.48)$$

where the quantum system has density matrix $\hat{\rho}$, a Hamiltonian $H(t)$ and we work in units such that $\hbar = 1$. At $t = -\infty$ assume the system is described by a many body density matrix $\hat{\rho}(-\infty)$. The formal solution is

$$\hat{\rho}(t) = \hat{U}_{t,-\infty} \hat{\rho}(-\infty) \hat{U}_{-\infty,t} \quad (2.49)$$

where the evolution operator, up to a phase, is the time ordered exponent:

$$\hat{U}_{t,t'} = \mathcal{T} \exp \left(-i \int_{t'}^t H(s) ds \right) = \lim_{N \rightarrow \infty} e^{-iH(t)\delta t} e^{-iH(t-\delta t)\delta t} \dots e^{-iH(t'+\delta t)\delta t} \quad (2.50)$$

where the infinitesimal time step is $\delta t = (t - t')/N$. In non-equilibrium systems the final state does not have to coincide with the initial one in expectation values, and the

correct evolution takes place on a closed time contour C . This leads to considering a unit partition function:

$$Z = \frac{\text{Tr}(U_c \hat{\rho}_0)}{\text{Tr}(\hat{\rho}_0)} = 1 \quad (2.51)$$

where the initial equilibrium density matrix is

$$\hat{\rho}_0 = e^{-\beta(\hat{H} - \mu \hat{N})} \quad (2.52)$$

and the evolution along the closed time contour is

$$\begin{aligned} U_c &= U_{-\infty, \infty} U_{\infty, -\infty} \\ &= 1 \quad (\text{trivially by Eq. (2.50)}). \end{aligned} \quad (2.53)$$

Even though $Z = 1$ it is still useful for setting up a coherent state path integral. From it, $Z = 1$ also provides a useful consistency check. Averages of observables O are calculated as:

$$\langle \hat{O}(t) \rangle = \frac{\text{Tr}[U_{-\infty, t} \hat{O} U_{t, -\infty} \rho_0(-\infty)]}{\text{Tr}[\rho_0(t)]} \quad (2.54)$$

which can proceed in one of two ways when introducing the closed time contour:

$$\langle \hat{O}(t) \rangle = \frac{\text{Tr}[U_{-\infty, \infty} U_{\infty, t} \hat{O} U_{t, -\infty} \rho_0(-\infty)]}{\text{Tr}[\rho_0(-\infty)]} \quad (2.55)$$

or, similarly,

$$\langle \hat{O}(t) \rangle = \frac{\text{Tr}[U_{-\infty, t} \hat{O} U_{t, \infty} U_{\infty, -\infty} \rho_0(-\infty)]}{\text{Tr}[\rho_0(-\infty)]} \quad (2.56)$$

corresponding to evaluating the average on the forwards or backwards path respectively, Figs 2.12 (b) and (c). The accepted wisdom is to combine half of each option by making the Hamiltonian different on each half of the contour with a source term $W(t)$.

$$H_W^\pm(t) \equiv H(t) \pm \hat{O}W(t) \quad (2.57)$$

where the Hamiltonian is $H_W^{+(-)}$ on the forwards (backwards) part. Then $U_c[W] \neq 1$ and we may define a generating functional:

$$Z[W] = \frac{\text{Tr}[U_c[W] \rho_0(-\infty)]}{\text{Tr} \rho_0(-\infty)} \quad (2.58)$$

The form for $\langle \hat{O}(t) \rangle$ involving functional differentiation of $Z[W]$ from this is:

$$\langle \hat{O}(t) \rangle \equiv \frac{\text{Tr}(\hat{O}(t) \rho_0)}{\text{Tr}(\rho_0)} = \left. \frac{i}{2} \frac{\delta Z[W]}{\delta W(t)} \right|_{W=0}. \quad (2.59)$$

If \hbar is restored it is $\langle \hat{O}(t) \rangle = \left. \frac{i\hbar}{2} \frac{\delta Z[W]}{\delta W(t)} \right|_{W=0}$. The factor of one half in the formula arises from adding the source twice along the contour.

where $h_{\pm} = 1 \pm i\epsilon_0\delta_t$ and the four $N \times N$ blocks are:

$$(iG^{\mathbb{T}}) = \begin{pmatrix} 1 & -\rho h_+^{N-1} h_-^{N-2} & \dots & -\rho h_+^{N-1} h_- & -\rho h_+^{N-1} \\ h_- & 1 & \dots & \cdot & \rho h_+^{N-1} h_- \\ \vdots & & \ddots & & \vdots \\ h_-^{N-2} & \cdot & \cdot & 1 & -\rho h_-^{N-1} h_+^{N-2} \\ h_-^{N-1} & h_-^{N-2} & \dots & h_- & 1 \end{pmatrix} \\ = [(iG^{\tilde{\mathbb{T}}}), \text{ provided } h_+ \leftrightarrow h_-], \quad (2.66)$$

$$(iG^{<}) = \begin{pmatrix} -\rho h_+^{N-1} & -\rho h_+^{N-2} & \dots & -\rho h_+ & -\rho \\ -\rho h_- h_+^{N-1} & \cdot & \cdot & \cdot & -\rho h_- \\ \vdots & \cdot & \cdot & \cdot & \vdots \\ -\rho h_-^{N-2} h_+^{N-1} & \cdot & \cdot & \cdot & \rho h_-^{N-2} \\ -\rho h_-^{N-1} h_+^{N-1} & -\rho h_-^{N-1} h_+^{N-2} & \dots & -\rho h_-^{N-1} h_+ & \rho h_-^{N-1} \end{pmatrix} \\ = [-\rho(iG^{>}), \text{ provided } h_+ \leftrightarrow h_-]. \quad (2.67)$$

Indexing the $2N \times 2N$ matrix as $j = 1, 2, \dots, N, N, \dots, 2, 1$, the components of these may be written as:

$$\langle \psi_j^+ \bar{\psi}_{j'}^- \rangle \equiv iG_{jj'}^{<} = \frac{-\rho h_+^{j-1} h_-^{j'-1}}{\det(iG^{-1})} \quad (2.68)$$

$$\langle \psi_j^- \bar{\psi}_{j'}^+ \rangle \equiv iG_{jj'}^{>} = \frac{h_+^{N-j} h_-^{N-j'}}{\det(iG^{-1})} \quad (2.69)$$

$$\langle \psi_j^+ \bar{\psi}_{j'}^+ \rangle \equiv iG_{jj'}^{\mathbb{T}} = \frac{h_-^{j-j'}}{\det(iG^{-1})} \times \begin{cases} 1 & j \geq j' \\ -\rho(h_+ h_-)^{N-1} & j < j' \end{cases} \quad (2.70)$$

$$\langle \psi_j^- \bar{\psi}_{j'}^- \rangle \equiv iG_{jj'}^{\tilde{\mathbb{T}}} = \frac{h_+^{j-j'}}{\det(iG^{-1})} \times \begin{cases} -\rho(h_+ h_-)^{N-1} & j > j' \\ 1 & j \leq j' \end{cases} \quad (2.71)$$

and in the continuum limit $N \rightarrow \infty$ these become:

$$\langle \psi^+(t) \bar{\psi}^-(t') \rangle \equiv iG^{<}(t, t') = -n_F(\epsilon_0) \exp[-i\epsilon_0(t - t')] \quad (2.72)$$

$$\langle \psi^-(t) \bar{\psi}^+(t') \rangle \equiv iG^{>}(t, t') = (1 - n_F(\epsilon_0)) \exp[-i\epsilon_0(t - t')] \quad (2.73)$$

$$\langle \psi^+(t) \bar{\psi}^+(t') \rangle \equiv iG^{\mathbb{T}}(t, t') = (\theta(t - t') - n_F(\epsilon_0)) \exp[-i\epsilon_0(t - t')] \quad (2.74)$$

$$\langle \psi^-(t) \bar{\psi}^-(t') \rangle \equiv iG^{\tilde{\mathbb{T}}}(t, t') = (\theta(t' - t) - n_F(\epsilon_0)) \exp[-i\epsilon_0(t - t')] \quad (2.75)$$

where $\theta(n) = 1$ for $n \geq 1$ and 0 otherwise, and n_F is the Fermi distribution coming from $n_F = \rho/(1 + \rho)$. All four continuum limit correlators combine into one Green matrix¹⁰:

$$G_{(t,t')} = -i \langle \begin{pmatrix} \psi_t^+ \\ \psi_t^- \end{pmatrix} \begin{pmatrix} \bar{\psi}_{t'}^+ & \bar{\psi}_{t'}^- \end{pmatrix} \rangle = -i \begin{pmatrix} \langle \psi_t^+ \bar{\psi}_{t'}^+ \rangle & \langle \psi_t^+ \bar{\psi}_{t'}^- \rangle \\ \langle \psi_t^- \bar{\psi}_{t'}^+ \rangle & \langle \psi_t^- \bar{\psi}_{t'}^- \rangle \end{pmatrix}. \quad (2.76)$$

Up to the present point with the toy model we have only reviewed a coherent state functional integral for a single fermion set up on the closed time contour. The Keldysh

¹⁰The change from $G(t, t')$ to the subscript notation $G_{(t,t')}$ is just for convenience.

formalism exploits a redundancy in the description of the two point functions for unequal times:

$$G^{\mathbb{T}}(t, t') + G^{\tilde{\mathbb{T}}}(t, t') - G^{<}(t, t') - G^{>}(t, t') = 0 \quad \text{for } t \neq t'. \quad (2.77)$$

(the right hand side is 1 if $t = t'$). This motivates a rotation of the fields such that this combination explicitly appears in the rotated version of the full Green matrix. The choice for fermions (due to Larkin and Ovchinnikov) is the non-unitary transformation:

$$\psi_1(t) = \frac{1}{\sqrt{2}}(\psi^+(t) + \psi^-(t)), \quad \psi_2(t) = \frac{1}{\sqrt{2}}(\psi^+(t) - \psi^-(t)) \quad (2.78)$$

$$\bar{\psi}_1(t) = \frac{1}{\sqrt{2}}(\bar{\psi}^+(t) - \bar{\psi}^-(t)), \quad \bar{\psi}_2(t) = \frac{1}{\sqrt{2}}(\bar{\psi}^+(t) + \bar{\psi}^-(t)) \quad (2.79)$$

This is also conveniently written as:

$$\psi' = U\psi, \quad \bar{\psi}' = \bar{\psi}\sigma_3U \quad (2.80)$$

where $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, $\psi' = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ and $\bar{\psi}' = (\bar{\psi}_1 \quad \bar{\psi}_2)$. Consequently the transformed Green matrix for unequal times is

$$G \rightarrow G(t, t') = \begin{pmatrix} G^r(t, t') & G^K(t, t') \\ 0 & G^a(t, t') \end{pmatrix} \quad \text{where } t \neq t' \quad (2.81)$$

where the retarded (r), advanced (a) and Keldysh (K) Green functions are defined:

$$G^r_{(t,t')} = \frac{1}{2}(G^{\mathbb{T}}_{(t,t')} + G^{>}_{(t,t')} - G^{<}_{(t,t')} - G^{\tilde{\mathbb{T}}}_{(t,t')}) \quad (2.82)$$

$$G^a_{(t,t')} = \frac{1}{2}(G^{\mathbb{T}}_{(t,t')} - G^{>}_{(t,t')} + G^{<}_{(t,t')} - G^{\tilde{\mathbb{T}}}_{(t,t')}) \quad (2.83)$$

$$G^K_{(t,t')} = \frac{1}{2}(G^{\mathbb{T}}_{(t,t')} + G^{>}_{(t,t')} + G^{<}_{(t,t')} + G^{\tilde{\mathbb{T}}}_{(t,t')}). \quad (2.84)$$

They have the properties:

$$[G^r(t, t')]^\dagger = G^a(t, t'), \quad [G^K(t, t')]^\dagger = -G^K(t, t'). \quad (2.85)$$

Equations (2.81-2.85) are general expressions that are not restricted to the single-fermion toy model. For the free fermion the functions are:

$$G^r_{(t,t')} = -i\theta(t - t')e^{-i\epsilon_0(t-t')} \rightarrow G^R(\epsilon) = (\epsilon - \omega_0 + i\delta^+)^{-1} \quad (2.86)$$

$$G^a_{(t,t')} = i\theta(t' - t)e^{-i\epsilon_0(t-t')} \rightarrow G^A(\epsilon) = (\epsilon - \omega_0 - i\delta^+)^{-1} \quad (2.87)$$

$$G^K_{(t,t')} = -i(1 - 2n_F(\epsilon_0))e^{-i\epsilon_0(t-t')} \rightarrow G^K(\epsilon) = -2\pi i(2n_F(\epsilon_0) - 1)\delta(\epsilon - \epsilon_0) \quad (2.88)$$

where we also wrote the Fourier transforms¹¹, since they are all only functions of the difference in times. The first two Fourier transforms are easily proved using the Heaviside function $\delta(t) = \frac{1}{2\pi i} \int ds \frac{e^{its}}{s - i\delta^+}$. A further extremely useful result is:

$$G^K(\epsilon) = \tanh\left(\frac{\epsilon - \mu}{2T}\right) [G^r(\epsilon) - G^a(\epsilon)] \quad (2.89)$$

which is a fluctuation-dissipation relation. This form is true for any fermionic system in equilibrium.

¹¹ $\hbar = 1$ FT convention: $f(\epsilon) = \int dt e^{i\epsilon t} f(t)$, $f(t) = \int \frac{d\epsilon}{2\pi} e^{-i\epsilon t} f(\epsilon)$.

Keldysh causality structure for fermions:

The essence of the Keldysh technique is that we construct a second (inequivalent) Gaussian action in the Keldysh rotated basis which generates the same two point functions (2.81) as the continuum limit of our original problem, and then we study that simpler QFT instead. The price to pay is that we have to double the number of fields.

The inverse of $G_{(t,t')}$, (2.81), is the operator matrix defined by $\int dt_1 \hat{G}_{(t,t_1)}^{-1} G_{(t_1,t')} = \delta(t - t')$. We may propose a form such that:

$$\int dt_1 \begin{pmatrix} \left(\hat{G}_{(t,t_1)}^{-1} \right)^r & \left(\hat{G}_{(t,t_1)}^{-1} \right)^K \\ 0 & \left(\hat{G}_{(t,t_1)}^{-1} \right)^a \end{pmatrix} \begin{pmatrix} G_{(t_1,t')}^R & G_{(t_1,t')}^K \\ 0 & G_{(t_1,t')}^A \end{pmatrix} = \delta(t - t'). \quad (2.90)$$

The form is valid provided the anti-hermitian Keldysh component G^K is parameterised by a hermitian matrix F :

$$G_{(t,t')}^K = \int dt_1 \left(G_{(t,t_1)}^r F_{(t_1,t')} - F_{(t,t_1)} G_{(t_1,t')}^a \right), \quad (2.91)$$

thus satisfying the anti-hermiticity property. As a consequence the R and A components of \hat{G}^{-1} are simply the operator inverses of G^R and G^A .

$$\hat{G}_{(t,t')}^{-1} = \begin{pmatrix} \left(\hat{G}_{(t,t')}^r \right)^{-1} & \left(\hat{G}_{(t,t')}^{-1} \right)^K \\ 0 & \left(\hat{G}_{(t,t')}^a \right)^{-1} \end{pmatrix} \quad (2.92)$$

In thermal equilibrium for fermions one always has

$$F(\epsilon) = 1 - 2n_F(\epsilon) = \tanh((\epsilon - \mu)/k_B T), \quad (2.93)$$

as found for the single-fermion Hamiltonian previously, and specific to the non-interacting model one has $(\hat{G}^{-1})^K = 2i0^+ F$. Equation (2.92) defines the so-called causality structure. This form is very general; it extends to the many body case and is even robust for interacting models (in which case $(\hat{G}^{-1})^K$ is no longer infinitesimally small).

A broad reason why we have no need to worry about the equal time possibility spoiling this nice framework is that observables in many body physics are always found using time ordered correlation functions due to a causality restriction: switching on external fields should not affect properties of the system in the past. This explains the origin of the ‘causality structure’ name.

The kinetic equation for F

For systems away from equilibrium, instead of the fluctuation-dissipation theorem relation we have to calculate the non-equilibrium distribution function $F(t, t')$ explicitly. For this we need a quantum kinetic equation. In general for a dressed Fermionic Green function we have to solve a Dyson equation:

$$(\hat{G}_0^{-1} - \hat{\Sigma}) \circ \hat{G} = \hat{1} \quad (2.94)$$

where the subscript “0” indicates the bare inverse Green function, and “ \circ ” indicates to trace over the intermediate arguments. The self energy matrix Σ shares the same

structure as (2.92), with the difference that the Keldysh component is now finite. For the one-dimensional theories we will investigate, the dressed components $G^{r,a}$ obey the equation

$$(i\partial_t - iv\partial_x - \Sigma^{r,a})G^{r,a} = \delta(t - t')\delta(x - x'), \quad (2.95)$$

and the Keldysh component may be written in the form

$$-[(i\partial_t - iv\partial_x); F] = \Sigma^K - (\Sigma^r \circ F - F \circ \Sigma^a). \quad (2.96)$$

This last equation is the quantum kinetic equation for the distribution F .

Keldysh technique example: non-interacting transport in one-dimension

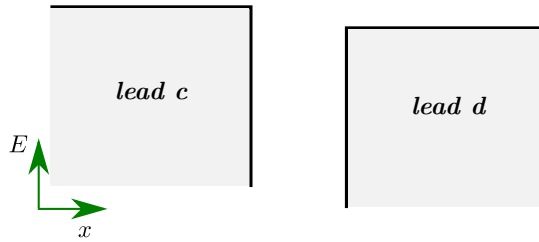


Figure 2.13: Schematic of two connected leads.

As an instructive example of the Keldysh technique, here we will demonstrate an explicit derivation of the tunnelling current in a set-up of two connected leads¹² following [18], where interactions in the leads are neglected, Fig. 2.13. All dimensionful quantities will be retained in the calculation. The Hamiltonian is

$$H = H_0 + H_{\text{tun}} = \sum_k (\epsilon_k^{(c)} c_k^\dagger c_k + \epsilon_k^{(d)} d_k^\dagger d_k) + \sum_{k,k'} (t_{k,k'} c_k^\dagger d_{k'} + t_{k,k'}^* d_k^\dagger c_{k'}). \quad (2.97)$$

where c_k and $d_{k'}$ describe fermions in left and right leads respectively and $t_{k,k'}$ are tunnelling matrix elements between the two. From this we can find an expression for the current operator for electrons in the left lead via the Heisenberg equation of motion:

$$\hat{I}(t) = -e \frac{dN_c(t)}{dt} = \frac{ie}{\hbar} \sum_{k,k'} [t_{k,k'} c_k^\dagger(t) d_{k'}(t) - t_{k,k'}^* d_k^\dagger(t) c_k(t)] \quad (2.98)$$

where

$$N_c = \sum_k c_k^\dagger c_k \quad (2.99)$$

is the number operator of electrons in the left lead and $e > 0$ is the elementary charge. From the Hamiltonian we can also construct the Grassmann action:

$$\begin{aligned} S &= \int_{-\infty}^{\infty} dt \sum_{k,k'} \begin{pmatrix} \bar{c}_k(t) \\ \bar{d}_k(t) \end{pmatrix}^\top \left[\begin{pmatrix} i\hbar\partial_t - \epsilon_k^{(c)} & 0 \\ 0 & i\hbar\partial_t - \epsilon_k^{(d)} \end{pmatrix} \delta_{k,k'} - \begin{pmatrix} 0 & t_{k,k'} \\ t_{k,k'}^* & 0 \end{pmatrix} \right] \begin{pmatrix} c_{k'}(t) \\ d_{k'}(t) \end{pmatrix} \\ &= \int_{-\infty}^{\infty} dt \sum_{k,k'} \begin{pmatrix} \bar{c}_k(t) \\ \bar{d}_k(t) \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hbar\hat{G}_{0k(c)}^{-1} & -t_{k,k'} \\ -t_{k,k'}^* & \delta_{k,k'} \hbar\hat{G}_{0k(d)}^{-1} \end{pmatrix} \begin{pmatrix} c_{k'}(t) \\ d_{k'}(t) \end{pmatrix}. \end{aligned} \quad (2.100)$$

¹²The ‘connected leads’ do not need to be wires, nor do they have to be touching. One just needs that electrons can tunnel from one conducting material to another. The conductors may be separated by an insulating oxide material for instance, or, in the case of a scanning tunnelling microscope, by the vacuum.

Next we may construct the Keldysh version of S and J . First of all the action has to be put on the Keldysh contour,

$$S = \int dt L \rightarrow \int_{\mathcal{C}} dt L = \int_{-\infty}^{\infty} L^+ dt + \int_{\infty}^{-\infty} L^- dt \quad (2.101)$$

where $L^{+(-)}$ indicates the fields inherit plus (minus) subscripts which doubles their number. Then we apply the rotation (2.80). This leads to:

$$S = \int_{-\infty}^{\infty} dt \sum_{k,k'} \bar{\Psi}_k (\delta_{k,k'} \hbar \hat{G}_{0k}^{-1} - \hat{T}_{k,k'}) \Psi_{k'} \quad (2.102)$$

where we defined the matrices:

$$\hat{G}_{0k}^{-1} = \begin{pmatrix} \hat{\gamma}^{cl} \hat{G}_{0k(c)}^{-1} & 0 \\ 0 & \gamma^{cl} \hat{G}_{0k(d)}^{-1} \end{pmatrix}, \quad \hat{T}_{k,k'} = \begin{pmatrix} 0 & t_{k,k'} \gamma^{cl} \\ t_{k,k'}^* \gamma^{cl} & 0 \end{pmatrix}, \quad (2.103)$$

$$\gamma^q = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^{cl} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (2.104)$$

along with a four component spinor $\bar{\Psi}_k = (\bar{\psi}_{1k}^{(c)}, \bar{\psi}_{2k}^{(c)}, \bar{\psi}_{1k}^{(d)}, \bar{\psi}_{2k}^{(d)})$ and a similar one for the fields without the bar (explicit details of the steps may be found in Appendix A.4).

According to the agreed-upon convention, Eq. (2.57), to calculate the current we should add $\hat{I}(t)$ to the Hamiltonian with a source $W(t)$ which takes different values $W_+(t)$ and $W_-(t)$ on the forwards and backwards parts of the closed time contour. Going through the same algebra and replacing H with $H_{W_+}^+$ and $H_{W_-}^-$ on the corresponding parts of the contour leads to (2.102) plus the following source action:

$$S_W = - \int dt \sum_{k,k'} \bar{\Psi}_k W_\alpha \hat{I}_{k,k'}^\alpha \Psi_{k'} \quad (2.105)$$

where

$$\hat{I}_{k,k'}^\alpha = \begin{pmatrix} 0 & \frac{ie}{\hbar} t_{k,k'} \\ -\frac{ie}{\hbar} t_{k,k'}^* & 0 \end{pmatrix} \otimes \gamma^\alpha, \quad W_{cl}(t) = \frac{1}{2}(W_+ + W_-), \quad W_q(t) = \frac{1}{2}(W_+ - W_-) \quad (2.106)$$

and $\alpha \in (cl = 1, q = 2)$ is summed over. The full action $S_{\text{tot}} = S + S_W$ for the generating functional is therefore:

$$S_{\text{tot}}[\{\bar{\Psi}_k\}, \{\Psi_k\}, W_{cl}, W_q] = \int dt \sum_{k,k'} \bar{\Psi}_k (\delta_{k,k'} \hbar \hat{G}_{0k}^{-1} - \hat{T}_{k,k'} - W_\alpha \hat{I}_{k,k'}^\alpha) \Psi_{k'}. \quad (2.107)$$

To calculate averages, the generating functional has to be differentiated with respect to the quantum component of the source, called W_q . It can be shown quite generally that contributions from non-zero W_{cl} do not change the normalisation, $Z[W_{cl}, W_q = 0] = 1$. We may therefore discard W_{cl} as it serves no future purpose for this problem. The full Keldysh generating functional is:

$$\begin{aligned} Z[W_q] &= \frac{1}{\text{Tr}(\hat{\rho})} \int \mathcal{D}(\bar{\psi}, \psi) e^{\frac{i}{\hbar} S_{\text{tot}}[\bar{\psi}, \psi, W_q]} \\ &= \frac{1}{\text{Tr}(\hat{\rho})} \int \mathcal{D}(\bar{\psi}, \psi) e^{\frac{i}{\hbar} \int dt \sum_{k,k'} \bar{\Psi}_k (\delta_{k,k'} \hbar \hat{G}_{0k}^{-1} - \hat{T}_{k,k'} - W_q \hat{I}_{k,k'}^\alpha \otimes \gamma^q) \Psi_{k'}} \end{aligned} \quad (2.108)$$

Side-remark: For non-interacting theories the majority of the steps for Keldysh set-ups such as (2.108) above can be short-circuited; doubling the fields and Keldysh-rotating amounts to the substitutions:

$$S = \sum_{k,k'} \int_{\mathcal{C}} dt \bar{\psi}_k \hbar G_{k,k'}^{-1} \psi_{k'} \rightarrow \sum_{k,k'} \int_{-\infty}^{\infty} dt \bar{\Psi}_k (\hbar G_{k,k'}^{-1} \otimes \gamma^{cl}) \Psi_{k'}, \quad (2.109)$$

and

$$S_{W_q} = - \int_{-\infty}^{\infty} dt \sum_{k,k'} W_q(t) \bar{\Psi}_k (\hat{O}_{k,k'} \otimes \gamma^q) \Psi_{k'}. \quad (2.110)$$

for an observable $\hat{O}_{k,k'}$.

At this point we could evaluate the Gaussian integral and then take the derivative with respect to W_q to find the current, but this turns out to be quite impractical for the problem with two connected leads. A better choice is to settle for an approximation by making an expansion in $\hat{T}_{k,k'}$ before integrating. In effect, this means partitioning the system into an unmixed part S_0 and the tunnelling perturbation S_T that breaks particle number conservation and which we are assuming to be weak:

$$\begin{aligned} \langle \hat{J}(t) \rangle &= \frac{i\hbar}{2} \frac{\delta}{\delta W_q(t)} \Big|_{W_q=0} \frac{1}{\text{Tr}[\hat{\rho}_0]} \int \mathcal{D}(\bar{\psi}, \psi) e^{\frac{i}{\hbar} S_{\text{tot}}[\bar{\psi}, \psi, W_q]} \\ &= \frac{1}{\text{Tr}(\hat{\rho}_0)} \int \mathcal{D}(\bar{\psi}, \psi) \left[\frac{1}{2} \sum_{k,k'} \bar{\Psi}_k(t) \hat{I}_{k,k'} \Psi_{k'}(t) \right] \sum_{n=0}^{\infty} \frac{\left(-\frac{i}{\hbar} \int dt' \sum_{k_1, k_2} \bar{\Psi}_{k_1}(t') \hat{T}_{k_1, k_2} \Psi_{k_2}(t') \right)^n}{n!} e^{\frac{i}{\hbar} S_0} \\ &= \left\langle \frac{1}{2} \sum_{k,k'} \bar{\Psi}_k(t) \hat{I}_{k,k'} \Psi_{k'}(t) - \frac{i}{\hbar} \sum_{k_1, k_2} \int dt' \bar{\Psi}_{k_1}(t') \hat{T}_{k_1, k_2} \Psi_{k_2}(t') \right\rangle_0 + \mathcal{O}[(\hat{T}_{k,k'})^2] \end{aligned} \quad (2.111)$$

The expectation $\langle \hat{I}(t) \rangle_0$ coming from the $n = 0$ term in the perturbation series vanished because the average is weighted by $\exp(\frac{i}{\hbar} S_0)$ and S_0 just describes two disconnected leads. Equivalently, $[\hat{H}_0, \hat{N}_c] = 0$ so there is no contribution from this term in the perturbation theory. Focusing on the leading order term, we have to calculate:

$$I(t) = \frac{-i}{2\hbar} \sum_{k,k',k_1,k_2} \int dt' \left\langle \bar{\Psi}_k(t) \hat{I}_{k,k'} \Psi_{k'}(t) \bar{\Psi}_{k_1}(t') \hat{T}_{k_1, k_2} \Psi_{k_2}(t') \right\rangle_0 \quad (2.112)$$

Now we can use a trick from linear algebra: $x^\top A x = \text{Tr}(A x x^\top)$ for square matrices A and vectors x . Identifying $A = \hat{I}_{k,k'} \Psi_{k'}(t) \bar{\Psi}_{k_1}(t') \hat{T}_{k_1, k_2}$ leads to

$$\begin{aligned} I(t) &= \frac{-i}{2\hbar} \sum_{k,k',k_1,k_2} \int dt' \text{Tr} \left[\left\langle \hat{I}_{k,k'} \Psi_{k'}(t) \bar{\Psi}_{k_1}(t') \hat{T}_{k_1, k_2} \Psi_{k_2}(t') \bar{\Psi}_k(t) \right\rangle_0 \right] \\ &= \frac{-i}{2\hbar} \sum_{k,k',k_1,k_2} \int dt' \text{Tr} \left[\hat{I}_{k,k'} \left\langle \Psi_{k'}(t) \bar{\Psi}_{k_1}(t') \right\rangle_0 \hat{T}_{k_1, k_2} \left\langle \Psi_{k_2}(t') \bar{\Psi}_k(t) \right\rangle_0 \right] \end{aligned} \quad (2.113)$$

where we applied Wick's theorem, dropping the (unphysical) disconnected Feynman graph. In the above we have Green matrices:

$$G_{0(k,t;k',t')} = -i \langle \Psi(k,t) \bar{\Psi}(k',t') \rangle_0 = \begin{pmatrix} \gamma^{cl} G_{0(k,t;k',t')}^{(c)} & 0 \\ 0 & \gamma^{cl} G_{0(k,t;k',t')}^{(d)} \end{pmatrix}. \quad (2.114)$$

These are diagonal in k space, $G_{0(k,t;k',t')} = \delta_{k,k'} G_{0k(t,t')}$, due to spatial translational symmetry of the action S_0 .

$$\begin{aligned} I(t) &= \frac{i}{2\hbar} \sum_{k,k'} \int dt' \text{Tr} \left[\hat{I}_{kk'} G_{0k'(t,t')} \hat{T}_{k'k} G_{0k(t',t)} \right] \\ &= \frac{e}{2\hbar^2} \int dt' \sum_{k,k'} |t_{kk'}|^2 \text{Tr} [\gamma^q G_{0k(t,t')}^{(c)} \gamma^{cl} G_{0k'(t',t)}^{(d)} - \gamma^q G_{0k'(t,t')}^{(d)} \gamma^{cl} G_{0k(t',t)}^{(c)}] \end{aligned} \quad (2.115)$$

where $|t_{kk'}|^2 = t_{kk'} t_{k'k}^*$ and we took a partial trace. At this point we may make use of the Keldysh structure for the 2×2 s:

$$\gamma^{cl} G_{0k(t,t')}^{(x)} \rightarrow \begin{pmatrix} G_{k(t,t')}^{(x)R} & G_{k(t,t')}^{(x)K} \\ 0 & G_{k(t,t')}^{(x)A} \end{pmatrix} \quad (2.116)$$

where $x \in (c, d)$. We also dropped the ‘0’ subscript referring to the pre-Keldysh-rotated action S_0 . This leads to:

$$I(t) = \frac{e}{2\hbar^2} \int dt' \sum_{kk'} |t_{kk'}|^2 \left[G_{k(t,t')}^{(c)r} G_{k'(t',t)}^{(d)K} + G_{k(t,t')}^{(c)K} G_{k'(t',t)}^{(d)a} - G_{k'(t,t')}^{(d)r} G_{k(t',t)}^{(c)K} - G_{k'(t,t')}^{(d)K} G_{k(t',t)}^{(c)a} \right] \quad (2.117)$$

This is the leading order term in the perturbation series in $t_{k,k'}$ for finding the tunnelling current. One can go further than this for certain limiting cases. As a simple example, for a stationary situation where the Green functions only depend on the time difference, due to time-independent single particle energies, it is advantageous to work in energy space¹³:

$$\begin{aligned} I &= \frac{e}{4\pi\hbar^3} \int d\epsilon \sum_{k,k'} |t_{k,k'}|^2 (G_{k,\epsilon}^{(c)r} G_{k',\epsilon}^{(d)K} + G_{k,\epsilon}^{(c)K} G_{k',\epsilon}^{(d)a} - G_{k',\epsilon}^{(d)r} G_{k,\epsilon}^{(c)K} - G_{k',\epsilon}^{(d)K} G_{k,\epsilon}^{(c)a}) \\ &= \frac{e}{4\pi\hbar^3} \int d\epsilon \sum_{k,k'} |t_{k,k'}|^2 [(G_{k,\epsilon}^{(c)r} - G_{k,\epsilon}^{(c)a}) G_{k',\epsilon}^{(d)K} - (G_{k',\epsilon}^{(d)r} - G_{k',\epsilon}^{(d)a}) G_{k,\epsilon}^{(c)K}] \end{aligned} \quad (2.118)$$

We proceed by using the earlier expressions for the non-interacting Green functions in energy space for free fermions¹⁴. This comes with the assumption that the electrons in the leads are in local thermal equilibrium. The result is:

$$I = \frac{2\pi e}{\hbar} \sum_{k,k'} |t_{k,k'}|^2 \delta(\epsilon_{k'}^{(d)} - \epsilon_k^{(c)}) \left[n_F^{(d)}(\epsilon_{k'}) - n_F^{(c)}(\epsilon_k) \right] \quad (2.119)$$

where we have different occupation factors associated to the different leads because they may be at different chemical potentials, e.g. due to a dc bias.

$$n_F^{(c)}(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu_c)} + 1}, \quad n_F^{(d)}(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu_d)} + 1}. \quad (2.120)$$

In conclusion we see that there are problems even in perturbation theory where the functional Keldysh framework is very useful. For instance we did not need to do any analytic continuation to real time, a calculation that becomes cumbersome with increasingly complicated set-ups.

¹³FT convention when $\hbar \neq 1$: $G(t-t') = \int \frac{d\epsilon}{2\pi\hbar} \exp[-\frac{i\epsilon}{\hbar}(t-t')] G(\epsilon)$, $G(\epsilon) = \int dt \exp[\frac{i\epsilon}{\hbar}(t-t')] G(t-t')$

¹⁴Each of $G^{r,a,K}$ for single particles acquires an overall factor of \hbar when recovering SI units.

2.2.4 Linear response techniques

The generalised susceptibility χ_{ij} which describes the response of an observable A_i to weak perturbations V_j is defined by the linear response formula:

$$A_i(\mathbf{x}, t) = \sum_j \int d\mathbf{x}' \int dt' \chi_{ij}(\mathbf{x}, t; \mathbf{x}', t') V_j(\mathbf{x}', t') + \mathcal{O}(\tilde{V}^2) \quad (2.121)$$

In addition we demand the causality constraint:

$$\chi_{ij}(\mathbf{x}, \mathbf{x}'; t, t') = 0 \quad t < t' \quad (2.122)$$

This ensures that the perturbation only has influence at later times and characterises χ as a retarded function. For a conservative system, $H \neq H(t)$, we can work in frequency space as χ will only depend on the differences in times: $\chi_{ij}(\mathbf{x}, \mathbf{x}'; t, t') = \chi_{ij}(\mathbf{x}, \mathbf{x}'; t - t')$. From this, (2.121) becomes:

$$A_i(\mathbf{x}, \omega) = \int d\mathbf{x}' \chi_{ij}(\mathbf{x}, \mathbf{x}'; \omega) V_j(\mathbf{x}', \omega) + \mathcal{O}(V^2) \quad (2.123)$$

(adopting the summation convention for repeated indices from now on). If there is also translational invariance in space, then similarly one writes $\chi_{ij}(\mathbf{x}, \mathbf{x}'; t, t') = \chi_{ij}(\mathbf{x} - \mathbf{x}'; t - t')$ such that:

$$A_i(\mathbf{q}, \omega) = \chi_{ij}(\mathbf{q}; \omega) V_j(\mathbf{q}, \omega) + \mathcal{O}(V^2) \quad (2.124)$$

Averages of observables can be found with functional field integrals. Consider for example the average of a single particle operator:

$$A(\tau) = \sum_{\alpha, \alpha'} \langle \bar{\psi}_\alpha(\tau) A_{\alpha, \alpha'} \psi_{\alpha'}(\tau) \rangle \quad (2.125)$$

where the average $\langle (\dots) \rangle$ is defined by functional integration over Grassmann fields $\bar{\psi}$ and ψ with weight e^{iS_V} :

$$\langle (\dots) \rangle = Z_V^{-1} \int \mathcal{D}(\bar{\psi}, \psi) (\dots) \exp(-S[V, \bar{\psi}, \psi]) \quad (2.126)$$

Here the Euclidean action is $S_V = S[V, 0, \bar{\psi}, \psi]$ such that:

$$S[V, \tilde{V}, \bar{\psi}, \psi] = S_0[\bar{\psi}, \psi] + \delta S[V, \bar{\psi}, \psi] + \delta \tilde{S}[\tilde{V}, \bar{\psi}, \psi] \quad (2.127)$$

where the perturbation is

$$\delta S[V, \bar{\psi}, \psi] = \int d\tau V(\tau) \sum_{\alpha, \alpha'} \bar{\psi}_\alpha(\tau) A_{\alpha, \alpha'} \psi_{\alpha'}(\tau). \quad (2.128)$$

and similar for $\delta \tilde{S}[\tilde{V}, \bar{\psi}, \psi]$. This fixes the generating functional:

$$Z[V, \tilde{V}] = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S[V, \tilde{V}, \bar{\psi}, \psi]}. \quad (2.129)$$

Equation (2.125) is then expressed through functional differentiation:

$$A(\tau) = - \left. \frac{\delta \ln(Z[V, \tilde{V}])}{\delta V(\tau)} \right|_{V=0} \quad (2.130)$$

We can see from (2.130) that the reason for including a second copy of the perturbation, the term $\delta\tilde{S}$ in equation (2.127), was in order to ensure the correct Boltzmann weight, or otherwise the expectation would vanish over the unperturbed action (a standard assumption which arises because the imagined system described by S_0 is in thermal equilibrium). In other words the Z_V in the definition (2.126) is $Z[V, 0]$.

Equations (2.125) through to (2.130) are in principle exact for averages over any distribution S . To narrow it down to just the linear response, the generating functional is expanded about $\tilde{V}(\tilde{\tau}) = 0$ to first order:

$$\ln Z[V, \tilde{V}] = \ln Z[V] + \int d\tilde{\tau} \left. \frac{\delta \ln Z[V, \tilde{V}]}{\delta \tilde{V}(\tilde{\tau})} \right|_{\tilde{V}=0} \tilde{V}(\tilde{\tau}) + \mathcal{O}(\tilde{V}^2) \quad (2.131)$$

Substitution into (2.130) gives:

$$A(\tau) \approx - \left. \frac{1}{Z[0, 0]} \frac{\delta Z[V]}{\delta V(\tau)} \right|_{V=0} - \int d\tilde{\tau} \left. \frac{\delta^2 \ln Z[V, \tilde{V}]}{\delta V(\tau) \delta \tilde{V}(\tilde{\tau})} \right|_{V=\tilde{V}=0} \tilde{V}(\tilde{\tau}) \quad (2.132)$$

where the first term is an average over the unperturbed (equilibrium) distribution with weight $\exp(iS_0)$ and is therefore assumed to be zero: $\langle \hat{A}(\tau) \rangle_0 = 0$. From the second term we identify the linear response function χ , which can be simplified:

$$\begin{aligned} \chi(\tau, \tilde{\tau}) &= - \left. \frac{\delta}{\delta V(\tau)} \left(\frac{1}{Z[V, 0]} \frac{\delta Z[V, \tilde{V}]}{\delta \tilde{V}(\tilde{\tau})} \right) \right|_{V=0} \bigg|_{V=0} \\ &= - \left. \frac{1}{Z[V, 0]} \frac{\delta^2 Z[V, \tilde{V}]}{\delta V(\tau) \delta \tilde{V}(\tilde{\tau})} \right|_{V=\tilde{V}=0} + \left. \frac{1}{Z[0, 0]} \frac{\delta Z[V, 0]}{\delta V(\tau)} \right|_{V=0} \left. \frac{1}{Z[0, 0]} \frac{\delta Z[0, \tilde{V}]}{\delta \tilde{V}(\tilde{\tau})} \right|_{\tilde{V}=0} \\ &= - \left. \frac{1}{Z[V, 0]} \frac{\delta^2 Z[V, \tilde{V}]}{\delta V(\tau) \delta \tilde{V}(\tilde{\tau})} \right|_{V=\tilde{V}=0} \end{aligned} \quad (2.133)$$

By applying this to the path integral (2.129) we are led to the conclusion:

$$A(\tau) = \sum_{\alpha, \alpha'} \langle \bar{\psi}_\alpha(\tau) A_{\alpha, \alpha'} \psi(\tau) \rangle \approx - \sum_{abcd} \int d\tilde{\tau} \langle \bar{\psi}_a(\tau) A_{a,b} \psi_b(\tau) \bar{\psi}_c(\tilde{\tau}) A_{c,d} \psi_d(\tilde{\tau}) \rangle \tilde{V}(\tilde{\tau}) \quad (2.134)$$

i.e. the response function is a 4-point correlation function.

The version of linear response that we will employ in the following research is a twist on the description above. Instead of considering the generating functional or its logarithm in a series expansion we will calculate observables by expanding the Green functions to linear order in a potential $V(t)$. This is an entirely equivalent choice which is more traditional in the spirit of operator formalism diagrammatic perturbation theory. Furthermore since we will work in the Keldysh functional formalism where $Z[V, 0] = 1$, the instances of $\ln Z[V, \tilde{V}]$ are replaced everywhere by $Z[V, \tilde{V}]$ and then the discussion follows identically.

Chapter 3

Non-interacting limits for Kondo impurity models

Here we include mappings of anisotropic Kondo impurity models to their exactly solvable points. We elect to use the letter I for the various Kondo couplings, (e.g. I_z , I_\perp for one-channel Kondo) to avoid confusion with the spin density operators for the conduction electrons which traditionally take the letter J .

3.1 Introduction

An initial remark is that the descriptions we outline are not unique. The technique followed is the Abelian bosonization procedure applied to the one-dimensional formulation of the Kondo model which comes by projecting out the s-wave channel. Affleck and Ludwig, by contrast, used boundary conformal field theory techniques to study the general over-screened multichannel case [19], and one may also make progress for exact results for some observables by using the Bethe-Ansatz.

3.2 Mapping for the anisotropic one-channel Kondo (1CK) model

Recasting the anisotropic Kondo model as a one-dimensional theory with the spin densities for the conduction electrons as $J^a(x) = \sum_{\alpha,\beta} \frac{1}{2} : \psi_\alpha^\dagger(x) \sigma_{\alpha,\beta}^a \psi_\beta(x) :$, where $a \in (x, y, z)$, gives:

$$H = H_0[\psi] + \frac{I_\perp}{2} [s_+ J^-(0) + \text{h.c.}] + I_z s_z J^z(0) \quad (3.1)$$

with

$$H_0[\psi] = -iv_F \sum_{s \in \{\uparrow, \downarrow\}} \int dx \psi_s(x)^\dagger \partial_x \psi_s(x) \quad (3.2)$$

where the exchange couplings are now written with the symbols I_\perp and I_z , adopting notations from Ch. 28 of Ref. [10]. For convenience the currents in (3.1) above are¹:

$$J^-(x) =: \psi_\downarrow^\dagger(x) \psi_\uparrow(x) :, \quad J^z(x) = \frac{1}{2} : [\psi_\uparrow^\dagger(x) \psi_\uparrow(x) - \psi_\downarrow^\dagger(x) \psi_\downarrow(x)] : \quad (3.3)$$

This model only depends on right movers ψ_s where $s \in \{\uparrow, \downarrow\}$. The electrons are therefore chiral and we have dropped the subscript R for neatness. This was allowed due to the

¹We discard Klein factors by assuming suitable zero modes in the mode expansion of the Bose fields which preserve the anticommutation algebra. This kind of simplification can sometimes be dangerous.

local nature of the Hamiltonian: the chiral right-moving field ψ_s is defined in general on the whole line $-\infty < x < \infty$ through

$$\psi_\sigma(x) = \begin{cases} \psi_{R\sigma}(x), & x > 0 \\ \psi_{L\sigma}(-x), & x < 0 \end{cases} \quad (3.4)$$

where x is a fictitious coordinate which is conjugate to k . We will outline, following [10], the mapping of (3.1) onto a refermionized resonant level model. There are three steps to this:

1. **Bosonization:** The chiral fermion field ψ_s is a vertex operator $\psi_s \propto e^{i\phi_s}$ of the chiral boson ϕ_s . Only the spin-sector (the antisymmetric combination of Bose fields ϕ_s) will turn out to be coupled to the impurity spin.
2. **Canonical transformation** (a rotation $H \rightarrow U^\dagger H U$): In order to ensure we can refermionize the contributions to exchange the scaling dimensions of new fermion fields should be $\Delta = 1/2$. This fixes the rotation parameter α .
3. **Refermionization:** By defining new Fermi fields (ψ, ψ^\dagger) including a pseudo-fermionic (d, d^\dagger) representation for the spin-1/2 operators, and ensuring that the canonical anticommutation relations still hold, we map to a resonant level model.

The details of the steps are slightly cumbersome so only the main features will be sketched here (elaboration is provided in Appendix B.1).

Step (1): The bosonized electron fields are defined as:

$$\psi_\sigma(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi_\sigma(x)} \quad (3.5)$$

where ϕ_s is a right-moving Bose field with spin σ and a_0 is a short distance cutoff (e.g. lattice spacing). The Kac-Moody $SU(2)$ currents may be expressed in terms of just the ‘spin-sector’ Bose field $\phi(x) = [\phi_\uparrow(x) - \phi_\downarrow(x)]/\sqrt{2}$:

$$J^-(x) = \frac{1}{2\pi a_0} e^{i\sqrt{8\pi}\phi(x)}, \quad J^z(x) = \frac{1}{\sqrt{2\pi}} \partial_x \phi(x). \quad (3.6)$$

Using these the bosonized Hamiltonian is

$$H = H_0[\phi] + \frac{I_\perp}{4\pi a_0} [s_+ e^{i\sqrt{8\pi}\phi(0)} + \text{h.c.}] + \frac{I_z}{\sqrt{2\pi}} s_z \partial_x \phi(0), \quad (3.7)$$

with

$$H_0[\phi] = v_F \int dx [\partial_x \phi(x)]^2 \quad (3.8)$$

where a contribution $H_0[\phi_c]$ from the decoupled charge field $\phi_c(x) = [\phi_\uparrow(x) + \phi_\downarrow(x)]/\sqrt{2}$ has been discarded and $H_0[\phi]$ is the non-interacting contribution from the spin-sector which is retained. The fact that only the spin sector remains coupled to the impurity immediately reveals the power of the bosonization approach for this problem.

Step (2): The unitary transformation is achieved by $U = e^{i\sqrt{4\pi}\alpha s_z \phi(0)}$. For the s_+ part by employing the standard $SU(2)$ algebra we have

$$U^\dagger s_+ U = s_+ e^{-i\sqrt{4\pi}\alpha \phi(0)} \quad (3.9)$$

The result for the transverse exchange, therefore, is

$$U^\dagger \left[\frac{I_\perp}{4\pi a_0} (s_+ e^{i\sqrt{8\pi}\phi(0)} + \text{h.c.}) \right] U = \frac{I_\perp}{4\pi a_0} (s_+ e^{i\sqrt{4\pi}(\sqrt{2}-\alpha)\phi(0)} + \text{h.c.}) \quad (3.10)$$

The new scaling dimension for this term is $\Delta = \frac{1}{2}(\sqrt{2}-\alpha)^2$. Choosing $\alpha = \sqrt{2}-1$ ensures we can define the new fermionic fields with $\Delta = \frac{1}{2}$, required for the one-dimensional theory by a simple dimensional analysis. For H_0 combined with the longitudinal exchange term we find:

$$U^\dagger \left[H_0 + \frac{I_z}{\sqrt{2\pi}} s_z \partial_x \phi(0) \right] U = H_0 + \frac{s_z}{\sqrt{\pi}} \left(\frac{I_z}{\sqrt{2}} - 2\pi v_F \alpha \right) \partial_x \phi(0) + \left(\alpha \pi v_F - \frac{I_z}{\sqrt{2}} \right) \frac{\alpha}{4} \delta(0) \quad (3.11)$$

by using the canonical algebra $[\partial_x \phi(x), \phi(y)] = \frac{i}{2} \delta(x-y)$. The transformed Hamiltonian now reads

$$H = H_0[\phi] + \frac{I_\perp}{4\pi a_0} [s_+ e^{i\sqrt{4\pi}\phi(0)} + \text{h.c.}] + \frac{\lambda}{\sqrt{\pi}} s_z \partial_x \phi(0) \quad (3.12)$$

with

$$\lambda = \frac{I_z}{\sqrt{2}} - 2(\sqrt{2}-1)\pi v_F \quad (3.13)$$

where the shift to the longitudinal coupling arises due to the contribution

$$U^\dagger \partial_x \phi(x) U = \partial_x \phi(x) - \sqrt{\pi} \alpha s_z \delta(x). \quad (3.14)$$

Step (3): The new fermion fields to refermionize the problem are

$$\psi(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\pi d^\dagger d} e^{i\sqrt{4\pi}\phi(x)} \quad (3.15)$$

where the $\{d, d^\dagger\}$ construct a pseudo-fermionic representation for the impurity spin 1/2 via

$$s_+ = d^\dagger, \quad s_z = d^\dagger d - \frac{1}{2}. \quad (3.16)$$

It may be easily checked with the redefinition of the fields that the canonical algebra (e.g. $\{\psi(x), d\} = 0$) holds due to the inclusion of the phase $e^{i\pi d^\dagger d}$. Using these the Hamiltonian finally becomes:

$$H_{RL} = H_0[\psi] + \frac{I_\perp}{2\sqrt{2\pi a_0}} [d^\dagger \psi(0) + \text{h.c.}] + \lambda (d^\dagger d - \frac{1}{2}) : \psi^\dagger(0) \psi(0) : . \quad (3.17)$$

We can see that this is a type of interacting resonant level model for spinless particles with an interaction controlled by the parameter λ , where the resonant d level is situated at the Fermi energy (i.e. $\epsilon_d = 0$). This is in contrast to the Anderson model where there is an energy penalty U for double occupancy.

3.2.1 Toulouse limit

The important non-interacting limit which we are interested in is the Toulouse limit $I_z = I_z^*$ when the interaction with the Fermi sea vanishes ($\lambda = 0$) but there is still hybridisation present:

$$I_z^* = 2\sqrt{2}(\sqrt{2}-1)\pi v_F. \quad (3.18)$$

No restriction is put on I_\perp so this limit forms a line in the parameter space.

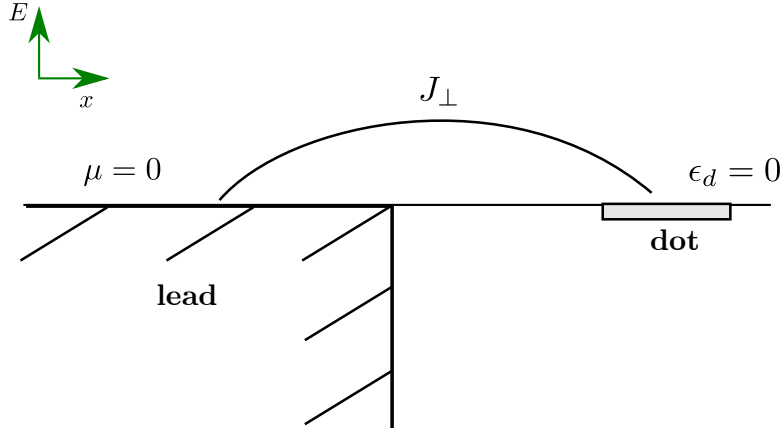


Figure 3.1: The Toulouse point Kondo model may be loosely thought of as half of a tunnelling junction, where the resonant d level sits at the Fermi energy of the conduction electrons in the lead.

3.3 Mapping for the anisotropic two-channel Kondo (2CK) model

The mapping for the two-channel model was accomplished by Emery and Kivelson [20] and proceeds in a similar spirit. Upon refermionization it also leads to models of the resonant level type. We will just show an outline. The starting point for the anisotropic 2CK model mapping is essentially the double of Eq. (3.1):

$$H = \sum_{\alpha=1,2} \left\{ H_0[\psi_\alpha] + \frac{I_{\perp\alpha}}{2} [s_+ J_\alpha^-(0) + \text{h.c.}] + I_{z\alpha} s_z J_\alpha^z(0) \right\} \quad (3.19)$$

We could instead have named the different channels L and R for consistency with the 2CK introduction in Chapter 2, but it is easy to see how this could be confused with the left/right notion for the chiral movers. The J operators follow the same representation as (3.3) with the addition of a channel index for the electron fields.

From this point the steps, in a guiding fashion, are:

1. Bosonization: Bosonize fermions in each channel and discard the decoupled charge-sector contribution to the non-interacting Hamiltonian.
 - This is identical to Step (1) from before.
2. Basis change: Introduce channel-symmetric and channel-antisymmetric Bose fields (i.e. linear combinations of the two different boson species).
 - Symmetric (dubbed ‘spin’): $\phi_s(x) = \frac{1}{\sqrt{2}}[\phi_1(x) + \phi_2(x)]$
 - Antisymmetric (dubbed ‘spin-flavour’): $\phi_{sf}(x) = \frac{1}{\sqrt{2}}[\phi_1(x) - \phi_2(x)]$
 - Couplings: $I_{\perp\pm} = \frac{1}{2}(I_{\perp 1} \pm I_{\perp 2})$ and $I_{z\pm} = \frac{1}{2}(I_{z 1} \pm I_{z 2})$
3. Canonical transformation: The correct unitary $U(\alpha)$ this time depends on the channel-symmetric Bose field so this is more cumbersome than the 1CK model. The free rotation parameter is $\alpha = 1$ in order for the scaling dimension of the transverse exchange coupling to remain fermionic.

4. Refermionization: Carefully define the new Fermi fields ψ_s and ψ_{sf} , and pick the same pseudofermionic description for the spin-1/2, to map to another resonant-level type of model.

$$\bullet \psi_s(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi_s(x)}, \text{ and } \psi_{sf}(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\pi d^\dagger d} e^{i\sqrt{4\pi}\phi_{sf}(x)}$$

This gives a resonant level type model where the d -level is hybridised and interacting with the conduction electrons:

$$\begin{aligned} H = & H_0[\psi_s] + H_0[\psi_{sf}] + \frac{I_{\perp+}}{\sqrt{8\pi a_0}} (d^\dagger - d) [\psi_{sf}^\dagger(0) + \psi_{sf}(0)] \\ & + \frac{I_{\perp-}}{\sqrt{8\pi a_0}} (d^\dagger + d) [\psi_{sf}^\dagger - \psi_{sf}(0)] + (d^\dagger d - \frac{1}{2}) [\lambda_+ : \psi_s^\dagger(0)\psi_s(0) : + \lambda_- : \psi_{sf}^\dagger(0)\psi_{sf}(0) :] \end{aligned} \quad (3.20)$$

where

$$\lambda_+ = I_{z+} - 2\pi v_F, \quad \text{and} \quad \lambda_- = I_{z-}. \quad (3.21)$$

3.3.1 Toulouse limit

We may see that this model becomes quadratic in the fields for $\lambda_\pm = 0$ such that the Toulouse limit is given by fixed values of the original longitudinal couplings:

$$I_{z1} = I_{z2} = 2\pi v_F \quad (3.22)$$

For further choices of the couplings there are two neat options. The trivial one is the case of $I_{\perp 2} = 0$ which reduces to the usual resonant level model:

$$H_{\text{RL}} = H_0[\psi_{sf}] + \frac{I_{\perp 1}}{\sqrt{8\pi a_0}} [d^\dagger \psi_{sf}(0) + \text{h.c.}] \quad (3.23)$$

where we discarded the decoupled $H_0[\psi_s]$ contribution. More exciting is the observation that the d -level fields combine in the Toulouse limit Hamiltonian in a convenient way when cast in the Majorana basis:

$$\psi_{sf}(x) = \frac{1}{\sqrt{2}} [\xi_{sf}(x) + i\zeta_{sf}(x)], \quad \psi_s(x) = \frac{1}{\sqrt{2}} [\xi_s(x) + i\zeta_s(x)] \quad (3.24)$$

$$d = \frac{1}{\sqrt{2}} [\psi_{sf}(x) + i\zeta_{sf}(x)]. \quad (3.25)$$

In particular for the channel symmetric case, $I_{\perp 1} = I_{\perp 2} \equiv I_\perp$, this gives the Emery-Kivelson Hamiltonian which is a Majorana-resonant level model:

$$H_{\text{MRL}} = H_0[\xi_{sf}] - i \frac{I_\perp}{\sqrt{2\pi a_0}} b \xi_{sf}(0) \quad (3.26)$$

In the space of couplings, given we are pinned to the Toulouse line, the two channel Kondo model therefore interpolates between the Majorana resonant level model and the resonant level model.

Chapter 4

Transport in a non-equilibrium resonant level model

In this chapter we investigate electron transport in a resonant level (RL) toy model with a sinusoidal voltage bias. The time-dependent tunnelling conductance is calculated using non-equilibrium Green functions, which was first accomplished for resonant level models by Jauho, Wingreen and Meir [6]. We take a different approach to the problem by using Keldysh functional integrals. The main results are explicit expressions for the alternating current in the linear response regime in V_0 which are exact in the tunnelling coupling g .

4.1 Introduction

The picture we will investigate has a single lead coupled to the resonant d level Fig. 4.1. This has a direct connection to the one-channel Kondo model at the Toulouse point as discussed in Chapter 3.

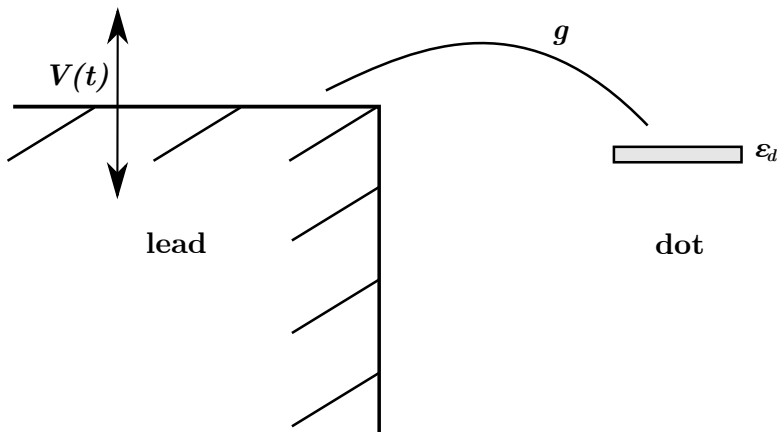


Figure 4.1: The resonant level toy model studied in this chapter. If the dot is put at the Fermi energy of the conduction electrons in the lead, $\epsilon_d = \mu$, then we recover the one-channel Kondo model at the Toulouse point.

We take as a starting point the one-dimensional Hamiltonian $H(t)$,

$$H(t) = H_c(t) + H_{\text{tun}} + H_{\text{cen}}$$

$$H_c(t) = \sum_k \epsilon_k(t) c_k^\dagger c_k, \quad H_{\text{tun}} = g[c^\dagger(0)d + d^\dagger c(0)], \quad H_{\text{cen}} = \epsilon_d d^\dagger d, \quad (4.1)$$

where the conduction electron energy and voltage bias as a function of time are:

$$\epsilon_k(t) = \hbar v_F k - eV(t), \quad V(t) = V_0 \cos(\omega_0 t). \quad (4.2)$$

The resonant d level is localised in real space at the origin, it has energy ϵ_d and is populated by electrons created by d^\dagger , while c_k^\dagger creates a conduction electron with momentum k . The elementary charge is $e > 0$. The tunnelling matrix elements g are assumed to be real numbers that are independent of k . They have SI units:

$$[g] = \text{Jm}^{1/2}. \quad (4.3)$$

Notice that we are considering a single species of (spinless) fermions. Thus the label “resonant” is artificial because there is only one lead in the picture represented by this Hamiltonian, Fig. 4.1. Usually one considers two-terminal conductance set-ups with left and right channels L and R . We provide an appendix for the differences that arise when adding a second lead.

The non-linear time-dependent current through a system described by Eq. (4.1) is given by

$$I(t) \equiv -e\langle \dot{N}_c(t) \rangle = \frac{2eg}{\hbar} \text{Re} \left[\langle c^\dagger(0, t)d(t) \rangle \right] \quad \text{with} \quad N_c = \sum_k c_k^\dagger c_k. \quad (4.4)$$

which comes from the Heisenberg equation of motion for the particle number $\dot{N}_c(t) = -\frac{i}{\hbar}[N_c, H]$:

$$\hat{I}(t) \equiv -e\dot{N}_c(t) = -\frac{ieg}{\hbar} (d^\dagger(t)c(0, t) - c^\dagger(0, t)d(t)) \quad (4.5)$$

and the property $G_{k(t,t)}^< = -(G_{k(t,t)}^>)^\dagger$ for the mixed Green functions $G_{k(t,t)}^< = -i\langle d(t)c_k^\dagger(t) \rangle$.

We need the Heisenberg versions of the different H_c , H_{tun} , H_{cen} in order to construct an action. In real space the kinetic term for the conduction electrons is:

$$H_c(t) = \int dx c^\dagger(x, t) (-i\hbar v_F \partial_x - eV(t)) c(x, t) \quad (4.6)$$

where the Fermion field operator is

$$c(x, t) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} c_k(t), \quad c_k(t) = \frac{1}{\sqrt{L}} \int dx e^{-ikx} c(x, t) \quad (4.7)$$

where L is the size of the system and k takes values $2\pi n/L$, ($n = 0, \pm 1, \pm 2 \dots$). In the transformation $c(x) \rightarrow c(x, t) = e^{iHt/\hbar} c(x) e^{-iHt/\hbar}$ the annihilation operator c_k is promoted to being time dependent. The total Hamiltonian mixes the c and d operators so this t -dependence is not a simple usual phase. Similarly, for the tunnelling Hamiltonian:

$$H_{\text{tun}}(t) = g[c^\dagger(0, t)d(t) + d^\dagger(t)c(0, t)]. \quad (4.8)$$

and for the central region with the impurity:

$$H_{\text{cen}}(t) = \epsilon_d d^\dagger(t)d(t) \quad (4.9)$$

To find the Lagrangian density we need the canonical momenta conjugate to $c(x, t)$ and $d(t)$. These are:

$$\Pi_c(x, t) \equiv \frac{\partial \mathcal{L}}{\partial \dot{c}(x, t)} = i\hbar c^\dagger(x, t), \quad \Pi_d(x, t) \equiv \frac{\partial \mathcal{L}}{\partial \dot{d}(t)} = i\hbar \delta(x) d^\dagger(t). \quad (4.10)$$

which satisfy the canonical algebra:

$$\{\Pi_c(x, t), c(x', t')\} = i\hbar\delta(x - x')\delta(t - t') \quad (4.11)$$

$$\{\Pi_d(x, t), d(t')\} = i\hbar\delta(x)\delta(t - t'). \quad (4.12)$$

The associated action is:

$$\begin{aligned} S[c, d] &= \int dt dx \begin{pmatrix} c^\dagger(x, t) & d^\dagger(t) \end{pmatrix} \begin{pmatrix} i\hbar\partial_t + i\hbar v_F\partial_x + eV(t) & -g\delta(x) \\ -g\delta(x) & \delta(x)(i\hbar\partial_t - \epsilon_d) \end{pmatrix} \begin{pmatrix} c(x, t) \\ d(t) \end{pmatrix} \\ &= \int dt dx dt' dx' \begin{pmatrix} c^\dagger(x, t) & d^\dagger(t) \end{pmatrix} \hbar\hat{G}^{-1}(x, t; x', t') \begin{pmatrix} c(x', t') \\ d(t') \end{pmatrix} \\ &\equiv (\psi|\hbar G^{-1}|\psi). \end{aligned} \quad (4.13)$$

For a simple consistency check, it may be seen that the Euler-Lagrange equations for this Lagrangian generate the same equations of motion as the Heisenberg equations for the original Hamiltonian (Appendix C.1). The inverse Green function \hat{G}^{-1} for the theory is read off as the 2×2 matrix:

$$\begin{aligned} \hat{G}^{-1}(x, t; x', t') &= \delta(x - x')\delta(t - t')\hat{G}^{-1}(x, t) \\ &= \delta(x - x')\delta(t - t')\frac{1}{\hbar} \begin{pmatrix} i\hbar\partial_t + i\hbar v_F\partial_x + eV(t) & -g\delta(x) \\ -g\delta(x) & \delta(x)(i\partial_t - \epsilon_d) \end{pmatrix} \end{aligned} \quad (4.14)$$

such that the Green function $G(x, t; x', t')$ is defined by the inverse matrix equation:

$$\int dt_1 dx_1 \hat{G}^{-1}(x, t; x_1, t_1)G(x_1, t_1; x', t') = \delta(x - x')\delta(t - t') \quad (4.15)$$

$$\implies \hat{G}^{-1}(x, t)G(x, t; x', t') = \delta(x - x')\delta(t - t'). \quad (4.16)$$

Note that the $1/\hbar$ that is absorbed into \hat{G}^{-1} is the one which multiplies S in the partition function:

$$Z = \int \mathcal{D}(\bar{c}, c) d\bar{d} dd \exp\left(\frac{i}{\hbar}S[\bar{c}, c, \bar{d}, d]\right), \quad \mathcal{D}(\bar{c}, c) = \prod_{i=1}^N d\bar{c}_i dc_i. \quad (4.17)$$

Due to the time dependence in $V(t)$ the solution for G cannot be written using a usual Matsubara expansion. This motivates turning to the Keldysh formalism.

Before proceeding to the Keldysh set-up it will be useful to review why constructing an action for the problem helps with calculating the current (4.4). The idea is to construct the generating functional,

$$Z[J_d, J_c] = \int \mathcal{D}(\bar{c}, c) d\bar{d} dd e^{\frac{i}{\hbar}S[c, d] + (J_c|c) + (c|J_c) + (J_d|d) + (d|J_d)}, \quad (4.18)$$

where the short-hand notation is

$$(J_c|c) = \int dx dt \bar{J}_c(x, t)c(x, t) \quad (4.19)$$

and the $c(x)$ fields are expressed as vectors of Grassmann variables. With this in place, the correlator $\langle c_k^\dagger(t)d(t) \rangle$ which we need for finding the current in Eq. (4.4) comes from

4.2. Conversion to a local theory

taking the appropriate derivatives of Z with respect to the (Grassmann) sources $\bar{J}_{c(d)}$ and then taking the Fourier transform:

$$\langle c^\dagger(x, t)d(t) \rangle = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \langle c_k^\dagger(t)d(t) \rangle = -\frac{1}{Z_0} \frac{\delta^2 Z[J_c, J_d]}{\delta \bar{J}_d \delta \bar{J}_c} \Big|_{\bar{J}, J=0} \quad (4.20)$$

$$\langle c_k^\dagger(t)d(t) \rangle = \frac{1}{\sqrt{L}} \int_0^L dx e^{-ikx} \langle c^\dagger(x, t)d(t) \rangle \quad (4.21)$$

where $Z_0 = Z[0, 0]$. Since Eq. (4.20) is just a two-point function it can be read off from the off-diagonal element of the corresponding Green function G due to well known results for Grassmann Gaussian functional integrals:

$$Z_0 \equiv \text{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}] = \int \mathcal{D}(\bar{\phi}, \phi) e^{-\phi|(iG)^{-1}|\phi} = \det[(iG)^{-1}] \quad (4.22)$$

$$Z[\bar{J}, J] = \int \mathcal{D}(\bar{\phi}, \phi) e^{-\phi|(iG)^{-1}|\phi + (J|\phi) + (\phi|\bar{J})} = \det[(iG)^{-1}] e^{(J|iG|J)} \quad (4.23)$$

$$\langle \phi_i \bar{\phi}_j \rangle = -\frac{1}{Z_0} \frac{\delta^2 Z[\bar{J}, J]}{\delta \bar{J}_i \delta J_j} \Big|_{\bar{J}, J=0} = iG_{ij} \quad (4.24)$$

As already explained, however, it is not straightforward to invert the 2×2 matrix \hat{G}^{-1} due to the time dependent potential $V(t)$.

4.2 Conversion to a local theory

Rewriting the action (4.13) in momentum space we find:

$$S = \sum_k \int_{-\infty}^{\infty} dt \begin{pmatrix} \bar{c}_k(t) \\ \bar{d}(t) \end{pmatrix}^\top \begin{pmatrix} i\hbar\partial_t - \epsilon_k(t) & -g/\sqrt{L} \\ -g/\sqrt{L} & \delta_{k,0}(i\hbar\partial_t - \epsilon_d) \end{pmatrix} \begin{pmatrix} c_k(t) \\ d(t) \end{pmatrix}. \quad (4.25)$$

By integrating out all of the fermions from the partition function except the one at site zero we can derive an effective action with just two fermionic fields (four when counting the bar fields). For ease of notation let us denote the operators for the unmixed c and d theories by

$$\hat{\mathcal{L}}_{0k}^{-1} = \frac{1}{\hbar} [i\hbar\partial_t - \epsilon_k(t)], \quad \hat{\mathcal{D}}_0^{-1} = \frac{1}{\hbar} [(i\hbar\partial_t - \epsilon_d)], \quad (4.26)$$

and a discrete Fourier representation for the lead electrons, e.g:

$$\hat{\mathcal{L}}_{0k}^{-1} = \sum_x e^{-ikx} \hat{\mathcal{L}}_0^{-1}(x) \quad (4.27)$$

where the coefficients $\hat{\mathcal{L}}_0^{-1}(x)$ are unknowns. Denoting $f(x, x') = \bar{c}(x)\hbar\hat{\mathcal{L}}_0^{-1}(x-x')c(x)$ we may write:

$$\sum_k \bar{c}_k \hbar \hat{\mathcal{L}}_k^{-1} c_k = \sum_{\substack{x \neq 0 \\ x' \neq 0}} f(x, x') + \sum_{x \neq 0} [f(0, x) + f(x, 0)] + f(0, 0) \quad (4.28)$$

Using this full action is

$$S = S_a + S_{\text{bath}} \quad (4.29)$$

where:

$$S_a = \int_{-\infty}^{\infty} dt \begin{pmatrix} \bar{c}(0) \\ \bar{d} \end{pmatrix}^\top \begin{pmatrix} \hbar \hat{\mathcal{L}}_0^{-1}(0) & -g \\ -g & \hbar \hat{\mathcal{D}}_0^{-1} \end{pmatrix} \begin{pmatrix} c(0) \\ d \end{pmatrix} \quad (4.30)$$

and,

$$S_{\text{bath}} = \int dt \int dt' \sum_{\substack{x \neq 0 \\ x' \neq 0}} \bar{c}(x) \hbar \hat{\mathcal{L}}_0^{-1}(x-x') c(x') + \hbar \sum_{x \neq 0} [\bar{c}(0) \hat{\mathcal{L}}_0^{-1}(-x) c(x) + \bar{c}(x) \hat{\mathcal{L}}_0^{-1}(x) c(0)] \quad (4.31)$$

where we suppressed the time arguments for ease of notation. The partition function is:

$$Z = \int \mathcal{D}(c_0, d) e^{\frac{i}{\hbar} S_a} \underbrace{\int \mathcal{D}(c(x \neq 0)) e^{\frac{i}{\hbar} S_{\text{bath}}}}_{Z_B[c(0)]}, \quad (4.32)$$

We may now integrate out all the fermions from the ‘bath’, by treating $J(x) = i \hat{\mathcal{L}}_0(x) c(0)$ and $\bar{J}(x) = i \bar{c}(0) \hat{\mathcal{L}}_0^{-1}(-x)$ as source terms and applying (4.23), giving:

$$Z_B = \mathcal{N} \exp \left[-i \int dt \int dt' \sum_{\substack{x \neq 0 \\ x' \neq 0}} \bar{c}(0) \hat{\mathcal{L}}_0^{-1}(-x') [\hat{\mathcal{L}}_0^{-1}(x-x')]^{-1} \hat{\mathcal{L}}_0^{-1}(x) c(0) \right] \quad (4.33)$$

where $\mathcal{N} = \det \left[-i \left(\hat{\mathcal{L}}_0^{-1}(x \neq 0, x' \neq 0) \right)^{-1} \right]$. Then the effective theory is

$$Z = \mathcal{N} \int \mathcal{D}(c(0), d) e^{\frac{i}{\hbar} S_{\text{eff}}}. \quad (4.34)$$

where

$$S_{\text{eff}} = \int dt \int dt' \begin{pmatrix} \bar{c}(0) \\ \bar{d} \end{pmatrix}_t^\top \begin{pmatrix} \hbar \hat{\mathcal{L}}'^{-1} & -g \\ -g & \hbar \hat{\mathcal{D}}_0^{-1} \end{pmatrix}_{t,t'} \begin{pmatrix} c(0) \\ d \end{pmatrix}_{t'}, \quad (4.35)$$

and

$$\hat{\mathcal{L}}'^{-1} = \hat{\mathcal{L}}^{-1}(0) - \sum_{\substack{x \neq 0 \\ x' \neq 0}} \bar{c}(0) \hat{\mathcal{L}}_0^{-1}(-x') [\hat{\mathcal{L}}_0^{-1}(x-x')]^{-1} \hat{\mathcal{L}}_0^{-1}(x) c(0). \quad (4.36)$$

The matrix element (4.36), unlike the other three, is not diagonal in time. We will see that this plays an important role for the following investigation.

Crucially it does not matter if we do not know the precise operator form of (4.36) which generates the site zero propagator. According to the original action the two point functions for the electrons in the absence of tunnelling are:

$$\langle c_k \bar{c}_{k'} \rangle_0 = i \delta_{k,k'} \mathcal{L}_{0k} \quad (4.37)$$

and, consequently, the propagator for the lead electrons in the local theory is given by the momentum integral over the single particle Green functions \mathcal{L}_{0k} :

$$\mathcal{L}' \equiv -i \langle c(0) \bar{c}(0) \rangle_0 = \frac{1}{L} \sum_k e^0 \langle c_k \bar{c}_{k'} \rangle = \frac{1}{L} \sum_k \mathcal{L}_{0k} \rightarrow \int \frac{dk}{2\pi} \mathcal{L}_{0k} \quad (4.38)$$

In the following sections we revert to a more traditional notation, i.e. $\mathcal{L}'_0 \equiv G_{co}$ and $\mathcal{D}_0 \equiv G_{do}$ for the unmixed propagators.

4.3 Keldysh action and expression for the current

Doubling the fermionic fields and performing the Keldysh rotation gives:

$$S_{\text{eff}} \rightarrow S = \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \bar{\psi}(t) \left[\begin{pmatrix} \hbar \hat{G}_{co}^{-1} & -g \\ -g & i\hbar \partial_t - \epsilon_d \end{pmatrix}_{t,t'} \otimes \mathbb{1}_{2 \times 2} \right] \psi(t') \quad (4.39)$$

where we have defined a four component spinor $\psi = (\psi_1^{(c)}, \psi_2^{(c)}, \psi_1^{(d)}, \psi_2^{(d)})^\top$ and a similar one for the bar fields, and $\mathbb{1}_{2 \times 2}$ is a 2×2 unit matrix. By similar manipulations one finds the source action for the current:

$$S_W = - \int dt W_q(t) \bar{\psi} \left(\frac{eg}{\hbar} \sigma_y \otimes \gamma^q \right) \psi \quad (4.40)$$

Thus the generating functional is:

$$Z[W_q] = \mathcal{N} \int \mathcal{D}(\bar{\psi}, \psi) e^{\frac{i}{\hbar} S_W} e^{\frac{i}{\hbar} S} \quad (4.41)$$

where N accounts for a constant prefactor coming from integrating out the fields from the lead. We call to mind from Chapter 2 that the ‘quantum’ γ^q matrix above is just the Pauli x -matrix. Following the prescription for averages on the Keldysh contour, the time-dependent current is:

$$\begin{aligned} I(t) \equiv \langle \hat{I}(t) \rangle &= \frac{i\hbar}{2} \frac{\delta Z[W_q(t')]}{\delta W_q(t)} \Big|_{W_q=0} \\ &= \frac{1}{2} \langle \bar{\psi}(t) \left(\frac{eg}{\hbar} \sigma_y \otimes \gamma^q \right) \psi(t) \rangle \end{aligned} \quad (4.42)$$

where the expectation sign $\langle (\dots) \rangle$ indicates that the average is taken over the whole theory with weight $\mathcal{N} \exp(iS/\hbar)$. Recall that the $1/2$ in front originates from adding two copies of the observable on the closed time contour, once in the forwards direction and once going back. Now we can use the identity $x^\top A x = \text{Tr}(A x x^\top)$ for square matrices A and column vectors x :

$$\begin{aligned} I(t) &= \frac{eg}{2\hbar} \langle \text{Tr}(\sigma_y \otimes \gamma^q) \psi(t) \bar{\psi}(t) \rangle \\ &= \frac{eg}{2\hbar} (G_{dc(t,t)} - G_{cd(t,t)})^K \end{aligned} \quad (4.43)$$

where we used the (as-yet-unknown) 4×4 Green matrix^{1,2}:

$$G_{(t,t)} \equiv \begin{pmatrix} G_{cc} & G_{cd} \\ G_{dc} & G_{dd} \end{pmatrix}_{t,t} = -i \langle \psi(t) \bar{\psi}(t) \rangle \quad (4.44)$$

and the Keldysh causality structure $G_{ij} = \begin{pmatrix} G_{ij}^r & G_{ij}^K \\ 0 & G_{ij}^a \end{pmatrix}$ where $i, j \in (c, d)$. The K in equation (4.43) indicates that we are taking the Keldysh component. The forms of G_{cd} and G_{dc} may be found using the block inversion formula:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}, \quad (4.45)$$

¹The (t, t') -arguments were put in the subscripts simply for neatness. The ‘ $\otimes \mathbb{1}_{2 \times 2}$ ’ notation will also be dropped for convenience where it is unambiguous.

²This Green matrix is *exact* in the hybridisation coupling g .

true for any block matrix with non-singular A and $D - CA^{-1}B$. We may therefore write G at site zero in terms of the components of its inverse \hat{G}^{-1} which has the known form

$$\hat{G}_{(t,t')}^{-1} = \begin{pmatrix} \delta(t-t')\hat{G}_{co}^{-1}(t') & -(\frac{g}{\hbar})_{t,t'} \\ -(\frac{g}{\hbar})_{t,t'} & \frac{1}{\hbar}\delta(t-t')[i\hbar\partial_{t'} - \epsilon_d] \end{pmatrix} = \begin{pmatrix} \hat{G}_{co}^{-1} & -\frac{g}{\hbar} \\ -\frac{g}{\hbar} & \hat{G}_{do}^{-1} \end{pmatrix}_{t,t'} \quad (4.46)$$

where: $(\frac{g}{\hbar})_{t,t'} = \delta(t-t')\frac{g}{\hbar}$. Hence:

$$G_{(t,t')} = \begin{pmatrix} (G_{co}^{-1} - \frac{g^2}{\hbar^2}G_{do})^{-1} & G_{co}\frac{g}{\hbar}(G_{do}^{-1} - \frac{g^2}{\hbar^2}G_{co})^{-1} \\ (G_{do}^{-1} - \frac{g^2}{\hbar^2}G_{co})^{-1}\frac{g}{\hbar}G_{co} & (G_{do}^{-1} - \frac{g^2}{\hbar^2}G_{co})^{-1} \end{pmatrix}_{t,t'} = \begin{pmatrix} G_{cc} & G_{co}\frac{g}{\hbar}G_{dd} \\ G_{dd}\frac{g}{\hbar}G_{co} & G_{dd} \end{pmatrix}_{t,t'} \quad (4.47)$$

such that $\int dt_1 \hat{G}_{t,t_1}^{-1} G_{t_1,t'} = \delta(t-t')$.

We need to calculate the off-diagonal blocks and isolate their Keldysh components. Substituting G_{dc} and G_{cd} into the expression for the current gives:

$$\begin{aligned} I(t) &= \frac{eg^2}{2\hbar^2} \int dt' (G_{dd(t,t')}G_{co(t',t)} - G_{co(t,t')}G_{dd(t',t)})^K \\ &= \frac{eg^2}{2\hbar^2} \int dt' (G_{dd(t,t')}^r G_{co(t',t)}^K + G_{dd(t,t')}^K G_{co(t',t)}^a - G_{co(t,t')}^r G_{dd(t',t)}^K - G_{co(t,t')}^K G_{dd(t',t)}^a). \end{aligned} \quad (4.48)$$

The different $G_{co}(t, t')$ in the above integral for the current are the local Green functions corresponding to the single electron at site zero which is correlated with the impurity. The prescription from single-particle Green functions, which we call $\mathcal{G}_{co}(k, t, t')$, to the local functions $G_{co}(t, t')$ in the above formula, as recently discussed, is:

$$G_{co}(t, t') = \frac{1}{L} \sum_k \mathcal{G}_{co}(k; t, t') \rightarrow \int \frac{dk}{2\pi} \mathcal{G}_{co}(k; t, t') \quad (4.49)$$

The resonant level model just has one d -fermion so this is not necessary for the impurity Green functions:

$$\mathcal{G}_{do}(t, t') \equiv G_{do}(t, t'), \quad (4.50)$$

yet it is for the mixed functions G_{dd} which are dressed by the hybridisation:

$$G_{dd}(t, t') = \frac{1}{L} \sum_k \mathcal{G}_{dd}(k; t, t') \rightarrow \int \frac{dk}{2\pi} \mathcal{G}_{dd}(k; t, t'). \quad (4.51)$$

4.4 Linear response calculations

In this section the current $I(t)$ is calculated by doing linear response in the time dependent potential with the parameter V_0 , the amplitude of the ac bias. This is necessary because it is too difficult to find the fully time dependent G_{dd} functions analytically. Instead, the approach we take is to apply the different Green functions in linear response where they are only functions of the difference in times $\pm(t-t')$.

4.4.1 Approximation for the current

The retarded/advanced versions of functions \mathcal{G}_{co} , G_{do} and G_{dd} must satisfy the inverse equations:

$$\hbar\delta(t-t') = \int ds\delta(t-s)(i\hbar\partial_s - \epsilon_k(s) \pm i0^+)\mathcal{G}_{co(k;s,t')}^{r,a} \quad (4.52)$$

$$\hbar\delta(t-t') = \int ds\delta(t-s)(i\hbar\partial_s - \epsilon_d \pm i0^+)G_{do(s,t')}^{r,a} \quad (4.53)$$

$$\hbar\delta(t-t') = \int ds[\delta(t-s)(i\hbar\partial_s - \epsilon_d \pm i0^+) - \frac{1}{\hbar}g^2G_{co(t,s)}^{r,a}]G_{dd(s,t')}^{r,a}, \quad (4.54)$$

where the upper (lower) sign corresponds to the leftmost (rightmost) superscripts. The Keldysh versions, meanwhile, are constructed from these according to the usual recipe³ described in Chapter II, i.e.:

$$\mathcal{G}_{co(k;t,t')}^K = (\mathcal{G}_{co(k;t,t')}^r - \mathcal{G}_{co(k;t,t')}^a)(1 - 2n_F(\epsilon_k)) \quad (4.55)$$

The fully time dependent results, as far as possible, are:

$$\mathcal{G}_{co(k;t,t')}^{r,a} = \mp i\theta[\pm(t-t')]e^{-\frac{i\epsilon_k}{\hbar}(t-t')}e^{-\frac{ie}{\hbar}\int_t^{t'}V(s)ds}, \quad (4.56)$$

$$G_{co(t,t')}^{r,a} = \mp i\theta[\pm(t-t')] \int \frac{dk}{2\pi} e^{-\frac{i\epsilon_k}{\hbar}(t-t')}e^{-\frac{ie}{\hbar}\int_t^{t'}V(s)ds}, \quad (4.57)$$

$$G_{co(t,t')}^K = -i \int \frac{dk}{2\pi} (1 - 2n_F(\epsilon_k))e^{-\frac{i\epsilon_k}{\hbar}(t-t')}e^{-\frac{ie}{\hbar}\int_t^{t'}V(s)ds}, \quad (4.58)$$

$$G_{do(t-t')}^{r,a} = \mp i\theta[\pm(t-t')]e^{-\frac{ie_d}{\hbar}(t-t')}. \quad (4.59)$$

By contrast, the full hybridisation-dressed functions $G_{dd}^{r,a}$ cannot be written so simply. This motivates turning to an approximation for the $I(t)$ integral by doing linear response in V_0 . By examining the current Eq. (4.48) we see that we need expansions for $G_{co}^{r,a,K}$ and $G_{dd}^{r,a,K}$. Expanding around $V_0 = 0$ gives⁴:

$$G_{co(t,t';V_0)}^{r,a,K} = G_{co(t,t';0)}^{r,a,K} \left(1 - \frac{ie}{\hbar} \int_t^{t'} dsV(s)\right) + \mathcal{O}(V_0^2) \quad (4.60)$$

$$G_{dd(t,t';V_0)}^{r,a} = G_{dd(t,t';0)}^{r,a} - \frac{ieg^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} dsV(s) \right) G_{dd(t,t_1;0)}^{r,a} G_{co(t_1,t_2;0)}^{r,a} G_{dd(t_2,t';0)}^{r,a} + \mathcal{O}(V_0^2)$$

$$G_{dd(t,t';V_0)}^K = G_{dd(t,t';0)}^K - \frac{ieg^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} dsV(s) \right) \left[G_{dd(t,t_1;0)}^r G_{co(t_1,t_2;0)}^r G_{dd(t_2,t';0)}^K \right. \\ \left. + G_{dd(t,t_1;0)}^r G_{co(t_1,t_2;0)}^K G_{dd(t_2,t';0)}^a + G_{dd(t,t_1;0)}^K G_{co(t_1,t_2;0)}^a G_{dd(t_2,t';0)}^a \right] + \mathcal{O}(V_0^2) \quad (4.61)$$

All of the Green functions on the right hand side of the expansions have $V_0 = 0$. They therefore only depend on the difference in times and may be referred to as equilibrium functions:

$$G_{co,dd}^{r,a,K}(t, t', V_0 = 0) \equiv G_{co,dd}^{r,a,K}(t - t'). \quad (4.62)$$

³This comes with the assumption that the lead is in local thermal equilibrium.

⁴The interested reader may find derivations in Appendix C.3.1.

Kinetic equation for the dot: The dot, unlike the lead which we assume to be in thermal equilibrium, comes with a kinetic equation to solve to find the Keldysh component. Through it enters the filling factor of the electrons in the lead. From the Dyson equation for the dot we find that:

$$G_{dd}^K = G_{dd}^r \Sigma_d^K G_{dd}^a \quad (4.63)$$

where Σ_d^K is the Keldysh component of the self energy matrix, which is proportional to the lead Keldysh function:

$$\Sigma_d^K = \frac{g^2}{\hbar^2} G_{co}^K \quad (4.64)$$

This may be determined by the diagram technique (there is only one irreducible diagram) or by an explicit calculation (e.g. integrating out all fermions except d from the theory).

It will be advantageous to work in the energy domain. The results are given in Table 4.1, where $v_F > 0$ is the Fermi velocity and Λ is a UV cutoff. For the Keldysh functions $G_{dd(\epsilon)}^K$ and $G_{co(\epsilon)}^K$ we will sometimes substitute the hyperbolic tangents for $1 - 2n_F^{(c)}(\epsilon)$ with chemical potential μ .

Table 4.1: Equilibrium Green functions

Mixed Green functions	Local Green functions
$G_{dd(\epsilon)}^{r,a} = \frac{\hbar}{\epsilon - \epsilon_d \pm i \frac{g^2}{2\hbar v_F}} + \mathcal{O}(\Lambda^{-1})$	$G_{co(\epsilon)}^{r,a} = \frac{\epsilon}{\pi \hbar v_F^2 \Lambda} \mp \frac{i}{2v_F} + \mathcal{O}(\Lambda^{-2})$
$G_{dd(\epsilon)}^K = \frac{-\frac{ig^2}{v_F}}{(\epsilon - \epsilon_d)^2 + (\frac{g^2}{2\hbar v_F})^2} \tanh\left(\frac{\epsilon - \mu}{2k_B T}\right) + \mathcal{O}(\Lambda^{-1})$	$G_{co(\epsilon)}^K = \frac{1}{iv_F} \tanh\left(\frac{\epsilon - \mu}{2k_B T}\right) + \mathcal{O}(\Lambda^{-1})$

Substituting the expansions for the Green functions into Eq. (4.48) leads to the following perturbation series for the charge current:

$$I(t) = \underbrace{I_0(t)}_{\sim g^2 \int dt(\dots)} + \underbrace{I_1(t)}_{\sim g^4 \int dt(\dots)} + \underbrace{I_2(t)}_{\sim g^4 \int dt(\dots)} + \mathcal{O}(V_0^2) \quad (4.65)$$

where the three contributions are:

$$I_0(t) = \frac{eg^2}{2\hbar^2} \int dt' \left[G_{dd(t-t')}^r G_{co(t'-t)}^K + G_{dd(t-t')}^K G_{co(t'-t)}^a - G_{co(t-t')}^r G_{dd(t'-t)}^K - G_{co(t-t')}^K G_{dd(t'-t)}^a \right], \quad (4.66)$$

$$I_1(t) = \frac{-ie^2 g^2}{2\hbar^3} \int dt' \left(\int_{t'}^t V(s) ds \right) \left[G_{dd(t-t')}^r G_{co(t'-t)}^K + G_{dd(t-t')}^K G_{co(t'-t)}^a + G_{co(t-t')}^r G_{dd(t'-t)}^K + G_{co(t-t')}^K G_{dd(t'-t)}^a \right], \quad (4.67)$$

$$I_2(t) = \frac{-ie^2 g^4}{2\hbar^5} \int dt' \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) \left[G_{dd(t-t_1)}^r G_{co(t_1-t_2)}^r G_{dd(t_2-t')}^r G_{co(t'-t)}^K + G_{dd(t-t_1)}^r G_{co(t_1-t_2)}^K G_{dd(t_2-t')}^a G_{co(t'-t)}^a + G_{dd(t-t_1)}^K G_{co(t_1-t_2)}^a G_{dd(t_2-t')}^r G_{co(t'-t)}^K + G_{dd(t-t_1)}^K G_{co(t_1-t_2)}^r G_{dd(t_2-t')}^a G_{co(t'-t)}^a - G_{co(t-t')}^r G_{dd(t'-t_1)}^r G_{co(t_1-t_2)}^r G_{dd(t_2-t)}^a - G_{co(t-t')}^r G_{dd(t'-t_1)}^K G_{co(t_1-t_2)}^a G_{dd(t_2-t)}^a - G_{co(t-t')}^K G_{dd(t'-t_1)}^r G_{co(t_1-t_2)}^r G_{dd(t_2-t)}^a - G_{co(t-t')}^K G_{dd(t'-t_1)}^a G_{co(t_1-t_2)}^a G_{dd(t_2-t)}^a \right]. \quad (4.68)$$

4.4.2 The I_0 (equilibrium) contribution

The first of these, $I_0(t)$, is the equilibrium contribution since V_0 is absent. It is accurate to all orders in the coupling g . By making use of the following useful identity,

$$G_{dd,co(t-t')}^X G_{co,dd(t'-t)}^Y = \int \frac{d\epsilon}{2\pi\hbar} \int \frac{d\epsilon_1}{2\pi\hbar} G_{dd,co(\epsilon)}^X G_{co,dd(\epsilon-\epsilon_1)}^Y e^{-\frac{i}{\hbar}\epsilon_1(t-t')}, \quad (4.69)$$

the contribution $I_0(t)$ becomes:

$$I_0(t) = \frac{eg^2}{2\hbar^2} \int \frac{d\epsilon}{2\pi\hbar} [(G_{dd(\epsilon)}^r - G_{dd(\epsilon)}^a) G_{co(\epsilon)}^K - (G_{co(\epsilon)}^r - G_{co(\epsilon)}^a) G_{dd(\epsilon)}^K] \quad (4.70)$$

Inserting the Green functions immediately gives zero, as we would expect in equilibrium.

$$I_0 = 0 \quad (4.71)$$

4.4.3 The $I_1(t)$ contribution

The next contribution, $I_1(t)$, is the first out of the two pieces for the leading order term in V_0 . Only when combined with I_2 does it become accurate to all orders in g . The Fourier transform $\tilde{I}_1(\omega)$ is:

$$\tilde{I}_1(\omega) = \frac{-ie^2g^2}{2\hbar^3} \int dt \int dt' \left(\int_{t'}^t ds V(s) \right) e^{i\omega t/\hbar} \int \frac{d\epsilon_1}{2\pi\hbar} \int \frac{d\epsilon_2}{2\pi\hbar} e^{-i\epsilon_2(t-t')/\hbar} f(\epsilon_1, \epsilon_2) \quad (4.72)$$

where we have defined a new function f :

$$f(\epsilon_1, \epsilon_2) = G_{dd(\epsilon_1)}^r G_{co(\epsilon_1-\epsilon_2)}^K + G_{dd(\epsilon_1)}^K G_{co(\epsilon_1-\epsilon_2)}^a + G_{co(\epsilon_1)}^r G_{dd(\epsilon_1-\epsilon_2)}^K + G_{co(\epsilon_1)}^K G_{dd(\epsilon_1-\epsilon_2)}^a. \quad (4.73)$$

We may complete all of the time integrals to find:

$$I_1(t) = \frac{-V_0e^2g^2}{8\pi\hbar^4\omega_0} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} \int d\epsilon (h_1(\epsilon, \zeta\hbar\omega_0) + h_2(\epsilon, \zeta\hbar\omega_0)) \quad (4.74)$$

where we have reorganised the integral with new functions:

$$h_1(\epsilon, \zeta\hbar\omega_0) = G_{dd(\epsilon)}^K (G_{co(\epsilon+\zeta\hbar\omega_0)}^r + G_{co(\epsilon-\zeta\hbar\omega_0)}^a - G_{co(\epsilon)}^r - G_{co(\epsilon)}^a). \quad (4.75)$$

$$h_2(\epsilon, \zeta\hbar\omega_0) = G_{co(\epsilon)}^K (G_{dd(\epsilon+\zeta\hbar\omega_0)}^r - G_{dd(\epsilon)}^r + G_{dd(\epsilon-\zeta\hbar\omega_0)}^a - G_{dd(\epsilon)}^a) \quad (4.76)$$

by making appropriate integration shifts. The first piece of Eq. (4.74), $h_1(\epsilon, \zeta\hbar\omega_0)$, is vanishingly small with the UV cutoff Λ . By inserting the Green functions $I_1(t)$ becomes:

$$I_1(t) = \frac{iV_0e^2g^2}{4\pi\hbar^2v_F} \sum_{\zeta,\alpha=-1,1} \alpha e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon \frac{n_F^{(c)}(\epsilon + \epsilon_d)}{(\epsilon + i\alpha\frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\alpha\frac{g^2}{2\hbar v_F})}. \quad (4.77)$$

One integral was immediately discarded because all of the poles lie in one half of the complex plane⁵. By transferring to a Matsubara sum we can trade the remaining ϵ -integral for infinite sums by further treatment with the residue theorem. The sums may then be expressed in a closed form in terms of the digamma function Ψ .

$$I_1(t) = \frac{V_0 e^2 g^2}{4\pi \hbar^2 v_F} \sum_{\zeta=-1,1} i e^{-i\zeta\omega_0 t} X_\zeta \quad (4.78)$$

where:

$$X_\zeta = \frac{-\zeta}{\hbar\omega_0} \left\{ \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu - \zeta\hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] + \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} - i(\epsilon_d - \mu + \zeta\hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} - i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \right\} \quad (4.79)$$

We may rewrite this in a nicer form, that is more obviously real, by using the conjugation property for polygamma functions $\Psi^{(n)}(z^*) = (\Psi^{(n)}(z))^*$. The final result is

$$I_1(t) = \frac{eV_0}{\hbar\omega_0} \frac{e \cdot (\frac{g^2}{2\hbar v_F})}{\pi\hbar} \text{Im} \left\{ e^{-i\omega_0 t} \sum_{\alpha=1,-1} \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i\alpha(\epsilon_d - \mu - \alpha\hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i\alpha(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \right\}. \quad (4.80)$$

Explicit details for this calculation may be found in Appendix C.4.

The $I_1(t)$ dc limit at finite temperature

For the dc limit, by expanding the summations in (4.78)-(4.79) and taking $\omega_0 \rightarrow 0$, we find:

$$I_1(\omega_0 \rightarrow 0) = V_0 \frac{-2e^2}{\pi\hbar} \frac{\frac{g^2}{2\hbar v_F}}{2\pi k_B T} \text{Re} \left[\Psi^{(1)} \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \quad (4.81)$$

The $I_1(t)$ zero temperature limit:

Picking up from (4.77) we can find the zero temperature limit $I_1(t, T) \rightarrow I_1(t, 0)$. The Fermi function becomes a step function and the integral simplifies:

$$\begin{aligned} I_1(t, T=0) &= \frac{iV_0 e^2 g^2}{4\pi \hbar^2 v_F} \sum_{\zeta, \alpha=-1,1} \alpha e^{-i\zeta\omega_0 t} \int_{-\infty}^{\mu - \epsilon_d} d\epsilon \frac{1}{(\epsilon + i\alpha \frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\alpha \frac{g^2}{2\hbar v_F})} \\ &= \frac{-eV_0}{\hbar\omega_0} \frac{e \cdot (\frac{g^2}{2\hbar v_F})}{\pi\hbar} \text{Im} \left\{ e^{-i\omega_0 t} \ln \left[\frac{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F} + \hbar\omega_0)^2}{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F})^2} \right] \right\} \end{aligned} \quad (4.82)$$

⁵We may enclose the empty half with a standard semi-circular contour (giving zero by Cauchy-Goursat) that yields the desired form in the radius $\rightarrow \infty$ limit.

4.4.4 The $I_2(t)$ contribution

Going through the algebra as done for $I_1(t)$ (see ‘Useful identities’ in Appendix C.3.3) to write the $I_2(t)$ integral (4.68) in energy space, we find:

$$I_2(t) = \frac{-e^2 g^4 V_0}{8\pi \hbar^6 \omega_0} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} \int d\epsilon (h_1(\epsilon, \zeta \hbar \omega_0) + h_2(\epsilon, \zeta \hbar \omega_0) + h_3(\epsilon, \zeta \hbar \omega_0)) \quad (4.83)$$

where we have defined the functions:

$$h_1(\epsilon_1, \epsilon_2) = \sum_{\alpha=1,-1} G_{dd(\epsilon_1)}^K G_{dd(\epsilon_1+\alpha\epsilon_2)}^{\xi\alpha} (G_{co(\epsilon_1)}^{\xi-\alpha} - G_{co(\epsilon_1+\alpha\epsilon_2)}^{\xi\alpha}) \underline{(G_{co(\epsilon_1)}^{\xi\alpha} - G_{co(\epsilon_1+\alpha\epsilon_2)}^{\xi\alpha})}, \quad (4.84)$$

$$h_2(\epsilon_1, \epsilon_2) = \sum_{\alpha=1,-1} G_{co(\epsilon_1)}^K (G_{dd(\epsilon_1)}^{\xi\alpha} \underline{(G_{co(\epsilon_1)}^{\xi\alpha} - G_{co(\epsilon_1+\alpha\epsilon_2)}^{\xi\alpha})} G_{dd(\epsilon_1+\alpha\epsilon_2)}^{\xi\alpha}), \quad (4.85)$$

$$h_3(\epsilon_1, \epsilon_2) = \sum_{\alpha=1,-1} G_{co(\epsilon_1)}^K G_{dd(\epsilon_1)}^{\xi\alpha} (G_{co(\epsilon_1)}^{\xi\alpha} - G_{co(\epsilon_1-\alpha\epsilon_2)}^{\xi-\alpha}) G_{dd(\epsilon_1-\alpha\epsilon_2)}^{\xi-\alpha}, \quad (4.86)$$

where $(\xi_1, \xi_{-1}) = (r, a)$.

As found in the case of the I_1 contribution we notice that large parts of the integral (underlined) vanish with the UV cutoff Λ , since, for all ϵ_1, ϵ_2 :

$$G_{co(\epsilon_1)}^{r,a} - G_{co(\epsilon_2)}^{r,a} = \frac{1}{\Lambda} \rightarrow 0 \quad \text{as} \quad \Lambda \rightarrow \infty \quad (4.87)$$

The third part, (4.86), however, does not vanish with the cutoff since, for all ϵ_1, ϵ_2 :

$$G_{co(\epsilon_1)}^{r,a} - G_{co(\epsilon_2)}^{a,r} = \mp \frac{i}{v_F} \quad \text{as} \quad \Lambda \rightarrow \infty \quad (4.88)$$

This leads to a potentially non-zero contribution:

$$I_2(t) = \frac{-e^2 g^4 V_0}{4\pi \hbar^6 v_F \omega_0} \text{Im} \left\{ e^{-i\omega_0 t} \int_{-\infty}^{\infty} d\epsilon (G_{dd(\epsilon)}^r G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a G_{dd(\epsilon+\hbar\omega_0)}^r) G_{co(\epsilon)}^K \right\} \quad (4.89)$$

by making use of the properties $G_{dd(\epsilon)}^r = (G_{dd(\epsilon)}^a)^\dagger$ and $G_{dd(\epsilon)}^K = -(G_{dd(\epsilon)}^K)^\dagger$.

Inserting the Green functions and performing the integrals, in an identical manner as done for $I_1(t)$, gives the final result:

$$I_2(t) = \frac{-eV_0}{\hbar\omega_0} \frac{e}{2\pi\hbar} \frac{(\frac{g^2}{\hbar v_F})^2}{(\frac{g^2}{\hbar v_F})^2 + (\hbar\omega_0)^2} \text{Im} \left\{ e^{-i\omega_0 t} \left(\frac{g^2}{\hbar v_F} + i\hbar\omega_0 \right) \right. \quad (4.90)$$

$$\left. \cdot \sum_{\alpha=1,-1} \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i\alpha(\epsilon_d - \mu - \alpha\hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i\alpha(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \right\} \quad (4.91)$$

Further details are located in Appendix C.5, and the dc and zero temperature limits are still in progress at the time of writing.

4.5 Translation of results to the 1CK model Toulouse limit

For the 1CK model at the Toulouse limit the resonant d level is pinned to the Fermi energy of the conduction band which can be set equal to zero (recall Fig. 3.1):

$$H_{\text{Toulouse}}^{\text{1CK}} = H_0[\psi] + \frac{J_{\perp}}{2\sqrt{2\pi}a_0}[d^{\dagger}\psi(0) + \text{h.c.}]. \quad (4.92)$$

If we consider the I_1 solution alone then this leads to the zero temperature prediction:

$$I_1^{\text{1CK}}(t, T=0) = \frac{-eV_0}{\hbar\omega_0} \frac{e \cdot \left(\frac{g^2}{2\hbar v_F}\right)}{\pi\hbar} \text{Im} \left[e^{-i\omega_0 t} \ln \left(1 - \frac{i\hbar\omega_0}{(g^2/2\hbar v_F)} \right) \right] \quad (4.93)$$

where we could also write $g \rightarrow \frac{J_{\perp}}{2\sqrt{2\pi}a_0}$ for an exact mapping. The dc conductance at zero temperature may now be found. It is approximated by

$$G_{\text{dc}(T=0)} = \lim_{\omega_0 \rightarrow 0} \frac{I_1(t, 0)}{V_0}, \quad (4.94)$$

leading to a result which is independent of model parameters:

$$G_{\text{dc}(T=0)}^{\text{1CK}} = \frac{4e^2}{h} \quad (4.95)$$

In this limit we expect the Kondo enhanced conductance to be equal to the conductance quantum e^2/h for just a single channel, corresponding to perfect transmission into the dot. Since we did not yet complete the calculation for I_2 , it is possible that this gives a correction. Nevertheless we have found a first approximation for the peak Kondo resonance⁶ at zero bias and near the right order of magnitude. Furthermore we point out that when taken with a possible I_2 correction this should be the exact zero bias dc result because higher order terms than linear response vanish for $V_0 = 0$.

4.6 Discussion and conclusion

In this chapter we calculated the alternating current in a resonant level toy model for any temperature by doing linear response in the amplitude V_0 of a sinusoidal voltage bias, and for all driving frequencies ω . We also extracted several limits. Notably, the dc limit for I_1 is in the same form as the two-channel Kondo literature result (up to a numerical prefactor). This quantitatively reproduces the hallmark Kondo resonance peak at zero bias, as measured in recent experiments [4], Fig. 4.2.

An obvious question to ask is what would change if we added another lead so that the RL model has two non-interacting channels that are coupled to the dot. This is a well known problem that was successfully solved *exactly* by Jauho, Wingreen and Meir in a variety of situations, [5, 6], even including the time-dependent harmonic bias, so it would be interesting to see how to do the equivalent derivation with functional integrals. This also suggests that, actually, it ought to be possible to go beyond linear response for the problem at hand. A potential extension could be to add another lead which also has the time dependent bias in it and then compare explicitly to a linear response result that can be extracted from Jauho, Wingreen and Meir.

⁶Insofar as a single channel model can be ‘resonating’ at all.

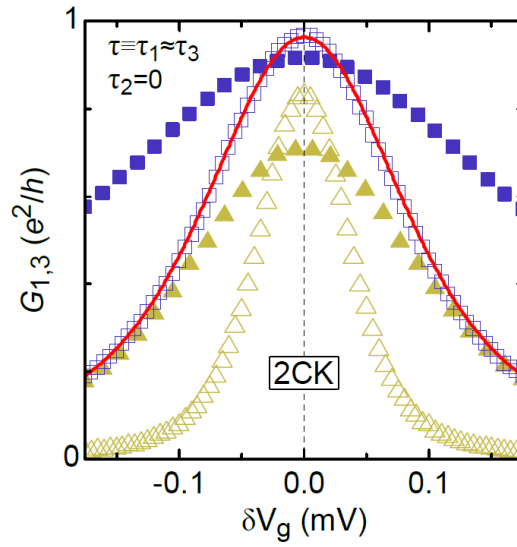


Figure 4.2: The Kondo resonance peak around zero bias from the recent (2015) experiments of the Pierre group [4]. The points are experimental data and the solid red line is the analytical result in terms of the trigamma function.

Chapter 5

Extension: ac transport through a Kondo impurity

Using the methods of the previous chapter we outline how the procedure for calculating the current in the toy resonant level model may be applied to the tunnelling junction studied by Schiller and Hershfield.

5.1 Motivation from a common low energy crossover

An effective anisotropic two-channel Kondo model for a spin-1/2 impurity is:

$$H_K = \sum_{\alpha=L,R} \left[J_\alpha \sum_{k,k'} (c_{\alpha\uparrow k}^\dagger c_{\alpha\downarrow k'} \hat{S}^- + c_{\alpha\downarrow k}^\dagger c_{\alpha\uparrow k'} \hat{S}^+) + \sum_{k,\sigma} \epsilon_{\alpha\sigma k} c_{\alpha\sigma k}^\dagger c_{\alpha\sigma k} \right] + \Delta E \hat{S}^Z \quad (5.1)$$

By numerical renormalization group calculations on this particular model, A. K. Mitchell et. al [21] were able to reproduce the curve for the conductance line shape in an ingenious recent experiment by the Pierre group in Marcoussis, France [4] for over nine orders of magnitude.

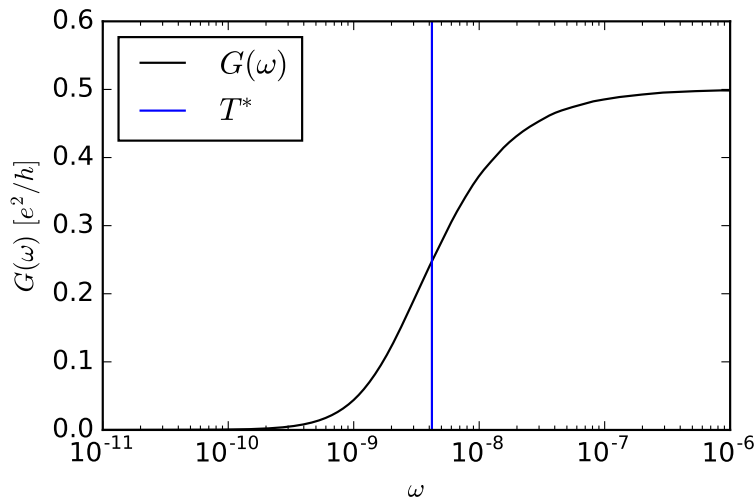


Figure 5.1: NRG calculation for the $T = 0$ ac conductance in linear response for the Hamiltonian (5.1). For the model parameters used, $T^* = 4.2 \times 10^{-9}D$, $J_L = 1.5D$, $J_R = 1.5001D$ with D being the conduction electron bandwidth and T^* the FL crossover scale (see text). Data courtesy of A. K. Mitchell.

Like the anisotropic two-channel Kondo model, the Hamiltonian we will focus on in this chapter is not an effective theory that may be derived from an Anderson model by

the Schrieffer-Wolff transformation. It does, however, display universal features at low temperatures and bias, and belongs to the same universality class of Hamiltonians as the Anderson impurity model. The general idea is that any solvable model with the same low energy physics can be used to study the universal behaviour near the common fixed point, even though the results far away from it will be generally model dependent. For the 2CK model there is the non-Fermi liquid (NFL) quantum critical point involving the Majorana fermion (with the frustrated ground state), and, due to an instability in the RG flow for $J_L \neq J_R$, there is also a crossover scale T^* towards a universal FL ground state.

Consider for instance Fig. 5.1 which shows conductance versus an energy scale ω . Provided the crossover scale T^* is below the Kondo temperature T_K , and T_K is much less than the bare energy scales, i.e. the electron bandwidth D , then towards zero temperature there should be universal Fermi-liquid like behaviour for the conductance $G(T/T_K)$. For the particular lineshape above the exchange couplings are intentionally high in order to focus in on the low energy flow away from the 2CK fixed point below T^* . The practical message to take from this is that we can compare the low ω asymptote of the NRG calculation based on the model (5.1) to analytics from the Toulouse limit.

5.2 S&H's Model: Kondo impurity interacting with two separate leads

By extending the findings of Emery and Kivelson of the Toulouse point for the two-channel Kondo model to include channel anisotropy, in a series of papers in the 1990s Schiller and Hershfield (S&H) conducted some of the first exact transport calculations for problems with strong correlations. The 2CK model with a general non-equilibrium condition Y_0 adapted from the paper by S&H [8] is:

$$H_{2\text{CK}} = i\hbar v_F \sum_{\alpha=L,R} \sum_{\sigma=\uparrow,\downarrow} \int_{-\infty}^{\infty} \psi_{\alpha\sigma}^\dagger(x) \partial_x \psi_{\alpha\sigma}(x) dx + \sum_{\alpha,\beta=L,R} \sum_{\lambda=x,y,z} J_{\lambda}^{\alpha\beta} s_{\alpha\beta}^{\lambda} \tau^{\lambda} + Y_0, \quad (5.2)$$

where

$$Y_0 = \frac{eV(t)}{2} \sum_{\sigma} \int_{-\infty}^{\infty} dx [\psi_{L\sigma}^\dagger \psi_{L\sigma} - \psi_{R\sigma}^\dagger \psi_{R\sigma}], \quad s_{\alpha\beta}^{\lambda} = \frac{1}{2} \sum_{\sigma,\sigma'} \psi_{\alpha\sigma}^\dagger(0) \sigma_{\sigma\sigma'}^{\lambda} \psi_{\beta\sigma'}(0) \quad (5.3)$$

where the elementary charge is $e > 0$, the conduction-electron spin densities at the origin are $s_{\alpha\beta}^{\lambda}$ in terms of the one-dimensional fields $\psi_{\alpha\sigma}(x)$ and the τ^{λ} components form the spin-1/2 impurity moment¹. This describes a spin-1/2 impurity coupled separately to two non-interacting leads of conduction electrons L and R via spin exchange in a tunnel junction, Fig. 5.2. An exactly solvable point for this model is known for special values of the exchange couplings:

$$J_x^{\alpha\beta} = J_y^{\alpha\beta} \equiv J_{\perp}^{\alpha\beta} \quad (5.4)$$

$$J_z^{LR} = J_z^{RL} = 0 \quad (5.5)$$

$$J_z^{LL} = J_z^{RR} \equiv J_z = 2\pi\hbar v_F. \quad (5.6)$$

Equation (5.6), in particular, constitutes the generalisation of the Toulouse point where the model becomes non-interacting.

¹We have changed $-Y_0 \rightarrow +Y_0$ for ease of comparison to calculations in the last chapter in certain limits. For comparison to the findings of S&H we may simply write $eV_0 \rightarrow -eV_0$ at the end.

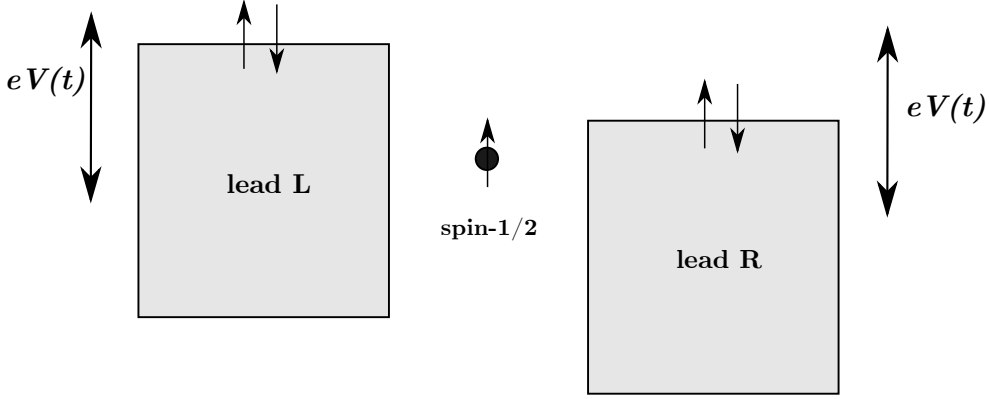


Figure 5.2: Schematic of the physical system for this chapter, adopted from [8]. The tunnel junction has a spin-1/2 impurity moment with two leads of spin-1/2 electrons on either side. Tunnelling across the junction takes place via the exchange interaction between the conduction electrons and the impurity spin. We choose to put an ac voltage bias in both leads.

We adapt as our starting point the reformed Hamiltonian from Eqs. (4.4) and (4.5) in Ref. [8], which is derived from (5.2)-(5.6) with Abelian bosonization techniques (see Chapter 3):

$$\begin{aligned}
 H = \sum_k \left[\epsilon_k \psi_{s,k}^\dagger \psi_{s,k} + \epsilon_k(t) \psi_{f,k}^\dagger \psi_{f,k} + i \frac{J^+}{2\sqrt{\pi a_0 L}} (\psi_{s,k}^\dagger + \psi_{s,k}) b \right. \\
 \left. + \frac{J_\perp^{LR}}{2\sqrt{\pi a_0 L}} (\psi_{f,k}^\dagger - \psi_{f,k}) a + \frac{J^-}{2\sqrt{\pi a_0 L}} (\psi_{s,k}^\dagger - \psi_{s,k}) a \right], \quad (5.7)
 \end{aligned}$$

where

$$J^\pm = \frac{1}{2}(J_\perp^{LL} \pm J_\perp^{RR}), \quad (5.8)$$

$$\epsilon_k(t) = \epsilon_k + eV(t), \quad \epsilon_k = \hbar v_F k, \quad V(t) = V_0 \cos(\omega_0 t), \quad (5.9)$$

where L is the size of the system and a_0 is a short-distance cutoff. The flavor and spin-flavor fields, $\psi_{f,k}$ and $\psi_{s,k}$ respectively, are fermionic channels, chiral left-movers emerging from the bosonization, and a and b are Majorana operators coming from the d -level fermions:

$$a = \frac{d + d^\dagger}{\sqrt{2}}, \quad b = \frac{d^\dagger - d}{i\sqrt{2}} \quad (5.10)$$

so $a^2 = b^2 = 1/2$. Two further quadratic parts coming from charge-sector and spin-sector fermions have been discarded because they do not affect the dynamics.

This is a non-equilibrium analogue of the Toulouse limit with a sinusoidal voltage bias. A prominent feature is that the bias only affects the flavour fermions, despite being initially put in both leads. In reference [8] the authors study many different properties for a dc bias $V(t) \rightarrow V_0$, while the ac bias was investigated in an earlier publication, [9]. To some extent this chapter provides a re-examination of the latter problem, although we do not investigate the effects of a magnetic field.

The Emery-Kivelson limit is given by conditions when only one Majorana fermion is coupled to the ψ fermions:

$$J_\perp^{LR} = 0 \quad \text{and} \quad J_\perp^{LL} = J_\perp^{RR}, \quad (5.11)$$

or,

$$J_{\perp}^{RR} = -J_{\perp}^{LL}, \quad (5.12)$$

which we henceforth call case (a) and case (b) respectively (coupling only to the a or b).

For the equilibrium case with $V_0 = 0$ they are *also* the only two situations when $J_z^{LR} = 0$ and $J_z^{LL} = J_z^{RR} \equiv J_z$ remain stable when reducing the bandwidth. For any other values a nonzero J_z^{LR} coupling is generated upon rescaling [8]:

$$\frac{dJ_z^{LL}}{dl} = \frac{1}{2\pi\hbar v_F} [(J_{\perp}^{LL})^2 + (J_{\perp}^{LR})^2], \quad (5.13)$$

$$\frac{dJ_z^{RR}}{dl} = \frac{1}{2\pi\hbar v_F} [(J_{\perp}^{RR})^2 + (J_{\perp}^{LR})^2], \quad (5.14)$$

$$\frac{dJ_z^{LR}}{dl} = \frac{1}{2\pi\hbar v_F} (J_{\perp}^{LL} + J_{\perp}^{RR}) J_{\perp}^{LR}, \quad (5.15)$$

These weak-coupling RG equations (derived by S&H with the ‘poor man’s scaling’ technique) provide the necessary justification that Eq. (5.5), in which we set one coupling to zero, has no consequence on the low-energy physics.

For convenience we will relabel the couplings:

$$v_1 = -\frac{J_{\perp}^{LR}}{2\sqrt{\pi a_0}}, \quad v_2 = -\frac{J^-}{2\sqrt{\pi a_0}}, \quad v_b = -\frac{iJ^+}{2\sqrt{\pi a_0}}. \quad (5.16)$$

In the new variables the Emery Kivelson limits for case (a) and case (b) are

$$v_1 = 0 \quad \text{and} \quad v_2 = 0. \quad (5.17)$$

or,

$$v_b = 0. \quad (5.18)$$

Recast as an action with Grassmann variables, the model we will investigate is:

$$S = \sum_k \int dt \begin{pmatrix} \bar{\psi}_{f,k} \\ \bar{\psi}_{s,k} \\ \bar{a} \\ \bar{b} \end{pmatrix}^{\top} \begin{pmatrix} i\hbar\partial_t - \epsilon_k(t) & 0 & v_1/\sqrt{L} & 0 \\ 0 & i\hbar\partial_t - \epsilon_k & v_2/\sqrt{L} & v_b/\sqrt{L} \\ v_1/\sqrt{L} & v_2/\sqrt{L} & \delta_{k,0}i\hbar\partial_t & 0 \\ 0 & v_b^*/\sqrt{L} & 0 & \delta_{k,0}i\hbar\partial_t \end{pmatrix} \begin{pmatrix} \psi_{f,k} \\ \psi_{s,k} \\ a \\ b \end{pmatrix} \quad (5.19)$$

The charge current $I(t)$ measures the rate at which electric charge increases on the left lead (or, equivalently for Kondo models, increases on the right one):

$$\hat{I}(t) = I_{\uparrow}(t) + I_{\downarrow}(t) \quad (5.20)$$

with

$$I_{\sigma}(t) = -e \frac{d(N_{tot,\sigma})}{dt} = ie \left[\frac{N_{L\sigma} - N_{R\sigma}}{2}, H_{2CK} \right] \quad (5.21)$$

where $N_{\alpha\sigma}$ is the number operator for electrons with spin σ on lead α . In the (f, sf) refermionized basis for the Hamiltonian (5.7), this transforms to:

$$\begin{aligned} \hat{I}(t) &= \frac{ie}{\hbar} \sum_k [\psi_{f,k}^{\dagger} \psi_{f,k}, H] = -\frac{iev_1}{\hbar\sqrt{L}} \sum_k (\psi_{fk}^{\dagger} + \psi_{fk}) a \\ &= \frac{-iev_1}{\hbar\sqrt{L}} \sum_k \begin{pmatrix} \psi_{f,k}^{\dagger} \\ \psi_{s,k}^{\dagger} \\ a \\ b \end{pmatrix}^{\top} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_{f,k} \\ \psi_{s,k} \\ a \\ b \end{pmatrix} \end{aligned} \quad (5.22)$$

by using the standard fermionic anticommutators. The global prefactor of v_1 immediately shows that the current is zero in the second Emery Kivelson limit, Eq. (5.17), so we only need to be concerned with the first limit with $v_b = 0$.

5.3 Setting up the Keldysh action and current

In an identical procedure to the RL chapter, we may convert to a local problem, put the action on the closed time contour and Keldysh-rotate to find:

$$S \rightarrow S = \int dt \bar{\psi} \left[\begin{pmatrix} \hbar \hat{G}_{fo}^{-1} & 0 & v_1 & 0 \\ 0 & \hbar \hat{G}_{so}^{-1} & v_2 & v_b \\ v_1 & v_2 & i\hbar \partial_t & 0 \\ 0 & v_b^* & 0 & i\hbar \partial_t \end{pmatrix} \otimes \mathbb{1}_{2 \times 2} \right] \psi \quad (5.23)$$

where we introduced the eight component spinor

$$\bar{\psi} = (\bar{\psi}_{f1}, \bar{\psi}_{f2}, \bar{\psi}_{s1}, \bar{\psi}_{s2}, \bar{a}_1, \bar{a}_2, \bar{b}_1, \bar{b}_2) \quad (5.24)$$

and a similar one for the fields without the bar. Similarly a source action for the current in the new basis is:

$$S_W = - \int dt \bar{\psi} W_q(t) \left[\frac{-iev_1}{\hbar} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \otimes \gamma^q \right] \psi \quad (5.25)$$

where γ^q is the first Pauli matrix and $W_q(t)$ is a scalar source field. The reader is reminded that the minus sign in front of the integral just arises from the Legendre transformation $L(q, \dot{q}) = p\dot{q} - H(p, q)$. The generating functional is:

$$Z[W_q] = \mathcal{N} \int \mathcal{D}(\psi, \bar{\psi}) e^{\frac{i}{\hbar} S_W} e^{\frac{i}{\hbar} S} \quad (5.26)$$

where \mathcal{N} takes care of the fields we integrated out. To find the current we calculate:

$$I(t) \equiv \langle \hat{I}(t) \rangle = \frac{i\hbar}{2} \frac{\delta Z[W_q(t')]}{\delta W_q(t)} \Big|_{W_q=0} = \frac{1}{2} \left\langle \bar{\psi}(t) \left[\frac{-iev_1}{\hbar} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \otimes \gamma^q \right] \psi(t) \right\rangle \quad (5.27)$$

where the expectation signs $\langle (\dots) \rangle$ mean that the average is taken over the whole theory with weight $\mathcal{N} \exp(iS/\hbar)$. Employing the identity $x^\top A x = \text{Tr}(A x x^\top)$ for square matrices A and vectors x gives:

$$\begin{aligned} I(t) &= \frac{ev_1}{2\hbar} \text{Tr} \left\{ \left[\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \otimes \gamma^q \right] (-i \langle \psi(t) \bar{\psi}(t) \rangle) \right\} \\ &= \frac{ev_1}{2\hbar} \text{Tr}[\gamma^q G_{af} - \gamma^q G_{fa}] \\ &= \frac{ev_1}{2\hbar} (G_{af} - G_{fa})^K, \end{aligned} \quad (5.28)$$

where we used the (as-yet-unknown) 8×8 Green matrix:

$$G_{(t,t')} = -i\langle\psi(t)\bar{\psi}(t')\rangle = \begin{pmatrix} G_{ff} & G_{fs} & G_{fa} & G_{fb} \\ G_{sf} & G_{ss} & G_{sa} & G_{sb} \\ G_{af} & G_{as} & G_{aa} & G_{ab} \\ G_{bf} & G_{bs} & G_{ba} & G_{bb} \end{pmatrix}_{t,t'} \quad (5.29)$$

and the causality structure $G_{ij} = \begin{pmatrix} G_{ij}^r & G_{ij}^K \\ 0 & G_{ij}^a \end{pmatrix}$ where $i, j \in (f, s, a, b)$. Note that the superscript a denotes advanced functions and is unrelated to the Majorana a . We will stick to the ‘upstairs = character of Green function, downstairs = fermion channel’ choice so this will not be a problematic choice of notation.

5.4 General expression for the current

To proceed we can find the Green matrix using the block inversion formula:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}. \quad (5.30)$$

It is profitable to rearrange the basis first before the inversion:

$$\hat{G}^{-1} = \begin{pmatrix} \hat{G}_{fo}^{-1} & \frac{v_1}{\hbar} & 0 & 0 \\ \frac{v_1}{\hbar} & \hat{G}_{ao}^{-1} & \frac{v_2}{\hbar} & 0 \\ 0 & \frac{v_2}{\hbar} & \hat{G}_{so}^{-1} & \frac{v_b}{\hbar} \\ 0 & 0 & \frac{v_b^*}{\hbar} & \hat{G}_{bo}^{-1} \end{pmatrix} \quad (5.31)$$

such that the spinors in the action are $\bar{\psi} = (\bar{\psi}_{f1}, \bar{\psi}_{f2}, \bar{\psi}_{a1}, \bar{\psi}_{a2}, \bar{\psi}_{s1}, \bar{\psi}_{s2}, \bar{\psi}_{b1}, \bar{\psi}_{b2})$ and a similar one for the fields without the bar. As in the last chapter, note that the factor of $1/\hbar$ entering the inverse Green matrix is absorbed from the path integral, i.e. $Z = \int e^{iS/\hbar} = \int e^{i(\Psi|G^{-1}|\Psi)}$ schematically. The block inversion leads to a 4×4 matrix,

$$\begin{pmatrix} G_{ff} & G_{fa} \\ G_{af} & G_{aa} \end{pmatrix} = \begin{pmatrix} G_{ff} & -\frac{v_1}{\hbar}G_{fo}G_{aa} \\ -\frac{v_1}{\hbar}G_{aa}G_{fo} & G_{aa} \end{pmatrix}, \quad (5.32)$$

with components that are 2×2 matrices:

$$G_{ff} = \{G_{fo}^{-1} - \frac{v_1^2}{\hbar^2}[G_{ao}^{-1} - \frac{v_2^2}{\hbar^2}(G_{so}^{-1} - \frac{|v_b|^2}{\hbar^2}G_{bo})^{-1}]^{-1}\}^{-1} \quad (5.33)$$

and

$$G_{aa} = (G_{ao}^{-1} - \frac{v_2^2}{\hbar^2}(G_{so}^{-1} - \frac{|v_b|^2}{\hbar^2}G_{bo})^{-1} - \frac{v_1^2}{\hbar^2}G_{fo})^{-1}. \quad (5.34)$$

Substituting G_{af} and G_{fa} into (5.28) and using the causality structure gives:

$$I(t) = \frac{ev_1^2}{2\hbar^2} \int dt' (G_{fo(t,t')}^r G_{aa(t,t')}^K + G_{fo(t,t')}^K G_{aa(t',t)}^a - G_{aa(t,t')}^r G_{fo(t',t)}^K - G_{aa(t,t')}^K G_{fo(t',t)}^a) \quad (5.35)$$

in precise analogy to the resonant level toy model investigated in Chapter 4.

5.5 Outline for linear response calculations

As with the earlier RL model, an inability to exactly solve the integral equations for the fully time dependent dressed functions $G_{aa(t,t';V_0)}^{r,a}$, defined by (5.34), leads us to consider the linear response regime in the amplitude V_0 .

The retarded/advanced versions of the Green functions we need, \mathcal{G}_{fo} , \mathcal{G}_{so} , $G_{(a,b)o}$ and G_{aa} , must satisfy the inverse equations:

$$\hbar\delta(t-t') = \int ds\delta(t-s)(i\hbar\partial_s - \epsilon_k(s) \pm i0^+)\mathcal{G}_{fo}^{r,a}(s,t',k) \quad (5.36)$$

$$\hbar\delta(t-t') = \int ds\delta(t-s)(i\hbar\partial_s - \epsilon_k \pm i0^+)\mathcal{G}_{so}^{r,a}(s,t',k) \quad (5.37)$$

$$\hbar\delta(t-t') = \int ds\delta(t-s)(i\hbar\partial_s \pm i0^+)G_{(a,b)o}^{r,a}(s,t') \quad (5.38)$$

$$\delta(t-t') = \int ds[G_{ao}^{-1} - \frac{v_2^2}{\hbar^2}(G_{so}^{-1} - \frac{|v_b|^2}{\hbar^2}G_{bo})^{-1} - \frac{v_1^2}{\hbar^2}G_{fo}]_{t,s}^{r,a}G_{aa}^{r,a}(s,t'), \quad (5.39)$$

where $r(a)$ corresponds to the upper (lower) sign in $\pm i0^+$. Notation such as $G_{(a,b)o}$ indicates that there are two copies of the equation, one for G_{ao} and one for G_{bo} .

Solutions to the first three of these carry over directly from the last chapter. Equation (5.36) corresponds to the RL $\mathcal{G}_{co}^{r,a}$ function with $V_0 \neq 0$ and (5.37) corresponds to it $V_0 = 0$. The unmixed Majorana Green functions $G_{ao}^{r,a}$ and $G_{bo}^{r,a}$ are also special cases where $\epsilon_k = 0$. The equation for G_{aa} plays the same role as the one for the dressed impurity Green function G_{dd} in the resonant level model investigation.

The expansions for the Green functions are:

$$G_{fo(t,t';V_0)}^{r,a,K} = G_{fo(t,t';0)}^{r,a,K} \left(1 + \frac{ie}{\hbar} \int_t^{t'} ds V(s) \right) + \mathcal{O}(V_0^2) \quad (5.40)$$

$$G_{aa(t,t';V_0)}^{r,a} = G_{aa(t,t';0)}^{r,a} + \frac{iev_1^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) G_{aa(t,t_1;0)}^{r,a} G_{fo(t_1,t_2;0)}^{r,a} G_{aa(t_2,t';0)}^{r,a} + \mathcal{O}(V_0^2)$$

$$G_{aa(t,t';V_0)}^K = G_{aa(t,t';0)}^K + \frac{iev_1^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) \left[G_{aa(t,t_1;0)}^r G_{fo(t_1,t_2;0)}^r G_{aa(t_2,t';0)}^K \right. \\ \left. + G_{aa(t,t_1;0)}^r G_{fo(t_1,t_2;0)}^K G_{aa(t_2,t';0)}^a + G_{aa(t,t_1;0)}^K G_{fo(t_1,t_2;0)}^a G_{aa(t_2,t';0)}^a \right] + \mathcal{O}(V_0^2) \quad (5.41)$$

They follow the same form as before because only the full G_{fo} functions depend on V_0 . Consequently the same expansion for the current also follows:

$$I(t) = \underbrace{\mathcal{O}(V_0^0)}_{\sim v_1^2 \int dt(\dots)} + \underbrace{\mathcal{O}(V_0^1)}_{\sim v_1^4 \int dt(\dots)} + \mathcal{O}(V_0^2) \quad (5.42)$$

where

$$I_0(t) = \frac{ev_1^2}{2\hbar^2} \int dt' \left[G_{aa(t-t')}^r G_{fo(t'-t)}^K + G_{aa(t-t')}^K G_{fo(t'-t)}^a - G_{fo(t-t')}^r G_{aa(t'-t)}^K - G_{fo(t-t')}^K G_{aa(t'-t)}^a \right], \quad (5.43)$$

$$\begin{aligned}
 I_1(t) = & \frac{ie^2v_1^2}{2\hbar^3} \int dt' \left(\int_{t'}^t V(s) ds \right) \left[G_{aa(t-t')}^r G_{fo(t'-t)}^K + G_{aa(t-t')}^K G_{fo(t'-t)}^a + G_{fo(t-t')}^r G_{aa(t'-t)}^K \right. \\
 & \left. + G_{fo(t-t')}^K G_{aa(t'-t)}^a \right], \tag{5.44}
 \end{aligned}$$

$$\begin{aligned}
 I_2(t) = & \frac{ie^2v_1^4}{2\hbar^5} \int dt' \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) \left[G_{aa(t-t_1)}^r G_{fo(t_1-t_2)}^r G_{aa(t_2-t')}^r G_{fo(t'-t)}^K \right. \\
 & + G_{aa(t-t_1)}^r G_{fo(t_1-t_2)}^r G_{aa(t_2-t')}^K G_{fo(t'-t)}^a + G_{aa(t-t_1)}^r G_{fo(t_1-t_2)}^K G_{aa(t_2-t')}^a G_{fo(t'-t)}^a \\
 & + G_{aa(t-t_1)}^K G_{fo(t_1-t_2)}^a G_{aa(t_2-t')}^a G_{fo(t'-t)}^a - G_{fo(t-t')}^r G_{aa(t'-t_1)}^r G_{fo(t_1-t_2)}^r G_{aa(t_2-t)}^K \\
 & - G_{fo(t-t')}^r G_{aa(t'-t_1)}^K G_{fo(t_1-t_2)}^K G_{aa(t_2-t)}^a - G_{fo(t-t')}^r G_{aa(t'-t_1)}^K G_{fo(t_1-t_2)}^a G_{aa(t_2-t)}^a \\
 & \left. - G_{fo(t-t')}^K G_{aa(t'-t_1)}^a G_{fo(t_1-t_2)}^a G_{aa(t_2-t)}^a \right]. \tag{5.45}
 \end{aligned}$$

The distinguishing feature that makes this *not* identical to the resonant level model is that the dressed Majorana functions G_{aa} also depend on couplings v_2 and, in principle, v_b . By inspection of the integral equation (5.39) we note that if $v_2 = 0$ and $v_b = 0$ then we have precisely the same starting point as the linear response calculations for the resonant level model where $v_1^2 = g^2$. The results of the previous chapter therefore provide limiting cases of the present two-channel model.

5.6 Summary

In this chapter we saw how the linear response approach for the toy resonant level model develops for the two-channel model studied by Schiller and Hershfield. In a nutshell, the functional form of the perturbation theory in terms of Green functions is the same even down to the energy domain. Moreover we noticed from inspecting the defining equations for the Green functions that our earlier results for the RL model are a limiting case. This is not so surprising since, as we saw in Chapter 3, the anisotropic 2CK model at the Toulouse limit has a one-channel non-interacting limit as well as the more exotic Emery-Kivelson one with the NFL critical point.

While we stopped short of calculating the integrals we note here that the route forward is very similar. A next step would be to calculate the new 2×2 Majorana Green function $G_{aa}(\epsilon)$ which plays the role of $G_{dd}(\epsilon)$ in the resonant level investigation. By considering (5.39), we deduced that the Majorana Green function in principle should depend on all three couplings J^+ , J^- and J_{\perp}^{LR} of the Toulouse limit Hamiltonian (5.7).

In Ref. [9] the authors provide a solution to this very problem as an infinite series of integer Bessel functions depending on V_0 . On the basis of the investigation here, it remains unclear if this extraordinary solution is exact to all orders in the Kondo couplings. We provide an appendix (D.3) extracting the linear response results from that calculation for future comparison with the present investigation, including the $T = 0$ and low ω_0 limits where universal behaviour is expected.

Chapter 6

Discussion and outlook

Interest in the Kondo problem has continued to persist in theoretical physics ever since Jun Kondo's explanation in 1964 of the resistivity minimum in metals with a small number of magnetic impurities. It presented a perfect environment for the development of renormalisation group ideas, beginning with Anderson's 'scaling' and culminating with the fully nonperturbative NRG method which, for the first time, traced the full crossover from the high temperature phase with a free spin to the completely screened ground state.

From one point of view the continued interest is because it is a well defined many body problem with the dual elements of strong interactions and localisation, so it remains an ideal playground to develop new analytical and numerical tools. From another, it is due to the ever-increasing access to real strongly correlated electron systems given modern techniques in nanotechnology. With novel experiments reported as recently as last year, namely by the Pierre group [4], it is now possible to investigate fully tuneable multi-channel Kondo models *away* from equilibrium. While the research described in this thesis was theoretical in nature, and focusing on non-interacting limits, the findings have a direct relevance to such modern experiments due to the powerful idea of universality: the effective low energy Hamiltonian for the Kondo model constitutes a universality class that is accurate provided one tunes the experimental parameters correctly.

Chapter 2 opened with a description of how transport setups in semiconductor quantum dot devices may be broken down schematically into their different components with the Anderson model, followed by the basic physics of the local moment regime, followed by the Kondo regime which emerges below the Kondo temperature T_K . The techniques for setting up the exactly solvable limits of the Kondo models were then discussed and the main tool used for setting up our calculations in a non-equilibrium setting, the Keldysh functional integral, was thoroughly introduced. Chapter 3 showed the mappings of the Kondo models to their exactly solvable 'Toulouse' limits with the technique of bosonization. Chapter 4 investigated the charge current in a resonant level model away from equilibrium which maps onto the one-channel Kondo model at the Toulouse limit, and Chapter 5 showed how the same approach develops for a two-channel Kondo model at its Toulouse limit.

6.1 Results of this thesis and outlook

The main line of enquiry focused on the single lead resonant level (RL) model away from equilibrium where it may be loosely considered half of a tunnelling junction. We found the charge current in this set-up for a sinusoidal voltage bias to all orders in the tunnelling amplitudes, while staying within linear response in the strength of the bias. The main result was a prediction for this at all temperatures and driving frequencies ω_0 . We

also mapped to the Toulouse point Hamiltonian for the one-channel Kondo model away from equilibrium. In the dc limit this recovered the literature result (up to a numerical prefactor) describing the characteristic Kondo resonance that enhances the conductance to a peak around zero bias. This also reproduces experimental findings, agreeing quantitatively with the observation that the effect of increased temperature on the Kondo resonance is to smear and reduce the peak height.

In the final chapter we considered a two-channel Kondo (2CK) model at the Toulouse limit which was previously investigated thoroughly by A. Schiller and S. Hershfield [7–9]. We concluded that the linear response calculations follow an identical procedure to the RL investigation and that our earlier results should hold in a certain limit of the 2CK exchange couplings, *even* for the ac calculation at finite temperatures.

To conclude, the non-equilibrium 2CK problem is a particularly timely problem for several reasons. The most important is the aforementioned experimental progress with the ‘charge’ two channel Kondo effect which means this is now accessible at significantly higher scales for the Kondo temperature, specifically due to the ingenious experiment in Ref. [4], allowing for unprecedented access to the range of the Kondo couplings. Moreover, given excitement for experiments elsewhere which appear to contain signatures of Majorana fermions (e.g. coming in pairs at either end of a nanowire), the quantum critical point of the two-channel Kondo model provides an alternative route to Majorana-related physics due to the Emery-Kivelson solution for the exactly solvable Toulouse limit.

Appendix A

Detailed calculations - Chapter 2

A.1 Chiral fermion densities

In the text we defined operators $J_{\alpha_r}(p)$ which we claimed are chiral fermion *densities*. These really are just density operators as can be seen by taking the FT of $\psi^\dagger(x)\psi(x)$:

$$\int_0^L dx e^{-ipx} \psi_{\alpha_r}^\dagger(x) \psi_{\alpha_r}(x) = \frac{1}{L} \sum_{k,k'} c_{\alpha_r,k'}^\dagger c_{\alpha_r,k} \int_0^L dx e^{i(k-k'-p)x} = \sum_k c_{\alpha_r,k-p}^\dagger c_{\alpha_r,k} \equiv J_{\alpha_r}(-p) \quad (\text{A.1})$$

They are chiral because each J_{α_r} contains just one kind of fermion, R or L . We also claimed that they form an abelian Kac-Moody algebra. Consider,

$$\begin{aligned} [J_{\alpha_r}(p), J_{\alpha_{r'}}(-p')] &= \sum_{k_1 k_2} [c_{\alpha_r k_1+p}^\dagger c_{\alpha_r k_1}, c_{\alpha_{r'} k_2-p'}^\dagger c_{\alpha_{r'} k_2}] \\ &= \sum_{k_1 k_2} [c_{\alpha_r k_1+p}^\dagger (\delta_{r,r'} \delta_{k_2-p',k_1} - c_{\alpha_{r'},k_2-p'}^\dagger c_{r k_1}) c_{\alpha_{r'} k_2} \\ &\quad - c_{\alpha_{r'},k_2-p'}^\dagger (\delta_{r,r'} \delta_{k_1+p,k_2} - c_{\alpha_r,k_1+p}^\dagger c_{\alpha_{r'} k_2}) c_{\alpha_r k_1}] \\ &= \delta_{r,r'} \sum_{k_1 k_2} (\delta_{k_2-p',k_1} c_{\alpha_r k_1+p}^\dagger c_{\alpha_{r'} k_2} - \delta_{k_1+p,k_2} c_{\alpha_{r'} k_2-p'}^\dagger c_{\alpha_r k_1}) \end{aligned} \quad (\text{A.2})$$

At this point one might naively sum over k_2 in the rightmost terms and, after relabelling $k_2 \leftrightarrow k_1$ in the leftmost ones do the same there, so to find zero overall, but this would be incorrect. Any arbitrary result can be found by the subtraction of two infinities and this is the case here because k was extended to $\pm\infty$ in the Tomonaga-Luttinger model. Instead one needs to be more careful and use normal ordering:

$$: AB := AB - \langle AB \rangle_0. \quad (\text{A.3})$$

Only the finite normal ordered part can safely subtract to zero in such a manner.

$$\begin{aligned} [J_{\alpha_r}(p), J_{\alpha_{r'}}(-p')] &= \delta_{r,r'} \sum_{k_2} (c_{\alpha_r k_2-p'+p}^\dagger c_{\alpha_{r'} k_2} - c_{\alpha_{r'} k_2-p'}^\dagger c_{\alpha_r k_2-p}) \\ &= \delta_{r,r'} \sum_{k_2} (: c_{\alpha_r k_2-p'+p}^\dagger c_{\alpha_{r'} k_2} : - : c_{\alpha_{r'} k_2-p'}^\dagger c_{\alpha_r k_2-p} :) \\ &\quad + \delta_{r,r'} \sum_{k_2} (\langle c_{\alpha_r k_2-p'+p}^\dagger c_{\alpha_{r'} k_2} \rangle_0 - \langle c_{\alpha_{r'} k_2-p'}^\dagger c_{\alpha_r k_2-p} \rangle_0) \\ &= \delta_{r,r'} \sum_{k_2} (\langle c_{\alpha_r k_2-p'+p}^\dagger c_{\alpha_{r'} k_2} \rangle_0 - \langle c_{\alpha_{r'} k_2-p'}^\dagger c_{\alpha_r k_2-p} \rangle_0) \end{aligned}$$

$$\begin{aligned}
&= \delta_{r,r'} \delta_{p,p'} \sum_k (\langle c_{\alpha_r k}^\dagger c_{\alpha_r k} \rangle_0 - \langle c_{\alpha_r, k-p}^\dagger c_{\alpha_r, k-p} \rangle_0) \\
&\rightarrow \delta_{p,p'} \delta_{r,r'} L \int_{-\infty}^{\infty} \frac{dk}{2\pi} (\Theta(k_F - k) - \Theta(k_F - (k - p))) \\
&= -\delta_{p,p'} \delta_{r,r'} \frac{rLp}{2\pi}
\end{aligned} \tag{A.4}$$

where $0 < p < 2k_F$ and $\alpha_r \in (\alpha_1, \alpha_{-1}) = (R, L)$. So the commutator is equal to the particle number, thus forming the abelian Kac-Moody algebra. Importantly this is only true because we assumed the infinite number of occupied states coming from unphysical excitations below a cutoff $-\Lambda$.

A technical remark is that the non-zero commutator is a manifestation of the chiral anomaly associated with the screening effect of massless relativistic electrons: the massless Dirac theory is invariant under local U(1) gauge transformations of the fields $\psi_{R(L)}$ and yet the corresponding electric fields are paradoxically non-zero. This can be seen nicely on the level of the path integral, see e.g. Gogolin et al. Ch. 1 [10] for a discussion. In other words chiral symmetry is broken in (1+1) massless QED. The equivalent relation to (A.4) in real space is:

$$[J_{\alpha_r}(x), J_{\alpha_{r'}}(x')] = \frac{ir}{2\pi} \delta_{r,r'} \partial_x \delta(x - x') \tag{A.5}$$

It is possible to derive (A.5) by an analogous calculation to the one in momentum space. This requires considering the point-split correlation function $\langle \psi^\dagger(x) \psi(x + \epsilon) \rangle$ for a single Weyl fermion described by $H = v \int_0^L dx : \psi^\dagger(x) (-i\partial_x) \psi(x) :$. The correlator is singular in the following sense, using an alternative definition of normal ordering:

$$\langle \psi^\dagger(x) \psi(x + \epsilon) \rangle = \frac{1}{2\pi i \epsilon} + \mathcal{O}(1), \quad \epsilon \rightarrow 0 \tag{A.6}$$

$$J(x) =: \psi^\dagger(x) \psi(x + \epsilon) := \lim_{\epsilon \rightarrow 0} \left[\psi^\dagger(x) \psi(x) - \frac{1}{2\pi i \epsilon} \right]. \tag{A.7}$$

A.2 Fermion-boson correspondence

Here we establish the correspondence of the massless Dirac fermion in one dimension, described by the free Tomonaga-Luttinger model H_F , with a massless scalar field theory H_B . We adopt conventions for the fields from Gogolin et al. [10] and borrow parts of the discussion from the introduction to bosonization by Sénéchal [15].

Fermion side H_F

Using the chiral fermion densities $J_{\alpha_r}(p)$ we may rewrite the FTLM. To do this consider the commutator:

$$\begin{aligned}
[J_R(p), H_F] &= \sum_k v_F k [J_R(p), : (c_{Rk}^\dagger c_{Rk} - c_{Lk}^\dagger c_{Lk}) :] \\
&= \sum_{k, k_1} v_F k : (c_{R, k_1+p}^\dagger c_{R, k_1} c_{R, k}^\dagger c_{R, k} - c_{R, k}^\dagger c_{R, k} c_{R, k_1+p}^\dagger c_{R, k_1}) :
\end{aligned}$$

$$\begin{aligned}
 &= \sum_{k,k_1} v_F k : (c_{R,k_1+p}^\dagger \{c_{R,k_1}, c_{R,k}^\dagger\} c_{R,k} - c_{R,k}^\dagger \{c_{R,k}, c_{R,k_1+p}^\dagger\} c_{R,k_1}) : \\
 &= \sum_k v_F k : c_{R,k+p}^\dagger c_{R,k} : - \sum_k v_F (k+p) : c_{R,k+p}^\dagger c_{R,k} : \\
 &= -v_F p J_R(p)
 \end{aligned} \tag{A.8}$$

By a similar calculation,

$$[J_L(p), H_F] = v_F p J_L(p). \tag{A.9}$$

These two results and the J -algebra (A.4) are sufficient to determine the bosonic representation of H_F . This shall be done by constructing a mode expansion for a local scalar field $\phi(x)$ out of bosonic creation/annihilation operators (b^\dagger, b). First we will continue to rewrite H_F with the $J_{R/L}$ operators. Consider another commutator:

$$\begin{aligned}
 &\frac{\pi v_F}{L} \sum_q [: J_R(q) J_R(-q) :, J_R(p)] \\
 &= \frac{\pi v_F}{L} \sum_q : (J_R(q) J_R(-q) J_R(p) - J_R(p) J_R(q) J_R(-q)) : \\
 &= \frac{\pi v_F}{L} \sum_q : (J_R(q) [J_R(-q), J_R(p)] - [J_R(p), J_R(q)] J_R(-q)) : \\
 &= v_F p J_R(p),
 \end{aligned} \tag{A.10}$$

using (2.29). Similarly,

$$\frac{\pi v_F}{L} \sum_q [: J_L(q) J_L(-q) :, J_L(p)] = -v_F p J_L(p). \tag{A.11}$$

By comparing (A.8-A.11) we determine:

$$H_F = \frac{\pi v_F}{L} \sum_q (: J_R(q) J(-q) : + : J_L(q) J_L(-q) :) + \text{const.} \tag{A.12}$$

Now by using the Fourier pair,

$$J_{\alpha_r}(x) = \frac{1}{L} \sum_q e^{iqx} J_{\alpha_r}(q), \quad J_{\alpha_r}(q) = \int_{-L/2}^{L/2} dx e^{-iqx} J_{\alpha_r}(x), \tag{A.13}$$

we can recast the Hamiltonian in real space:

$$\begin{aligned}
 H_F &= \pi v_F \int_{-L/2}^{L/2} dx (J_R(x))^2 + (J_L(x))^2 \\
 &\rightarrow \pi v_F \int_{-\infty}^{\infty} dx (J_R(x))^2 + (J_L(x))^2, \quad \text{as } L \rightarrow \infty
 \end{aligned} \tag{A.14}$$

where we discarded the additive constant. For later convenience we include here the explicit real space commutation algebra of the currents $J_{L(R)}$ with the Weyl fermions $\psi_{L(R)}$, even though we didn't need them for the above:

$$\begin{aligned}
 [\psi_R(x), J_R(x')] &= \psi_R(x) \psi_R^\dagger(x') \psi_R(x') - \psi_R^\dagger(x') \psi_R(x') \psi_R(x) \\
 &= \{\psi_R(x), \psi_R^\dagger(x')\} \psi_R(x') \\
 &= \delta(x - x') \psi_R(x)
 \end{aligned} \tag{A.15}$$

This means a right mover $\psi_R(x)$ annihilates a fermion locally at position x and changes the density $J_R(x)$ at that point.

Boson side H_B

Now we pause and consider a Gaussian model:

$$H_B = \frac{v}{2} \int_{-\infty}^{\infty} dx [\Pi(x)^2 + (\partial_x \Phi(x))^2] \quad (\text{A.16})$$

where the scalar field $\Phi(x)$ and conjugate momentum $\Pi(x)$ are related by

$$[\Pi(x), \Phi(x')] = -i\delta(x - x'). \quad (\text{A.17})$$

This describes a set of coupled oscillators, familiar from quantum field theory. Time evolution shows that $\Pi(x, t) = \frac{1}{v} \partial_t \Phi(x, t)$ so Φ follows the wave equation:

$$v^{-2} \partial_t^2 \Phi(x, t) = \partial_x^2 \Phi(x, t) \quad (\text{A.18})$$

which has the general solution

$$\Phi(x, t) = \varphi(x + vt) + \varphi(x - vt). \quad (\text{A.19})$$

Equally, in imaginary time we may cast this as:

$$-v^{-2} \partial_\tau^2 \Phi(x, \tau) = \partial_x^2 \Phi(x, \tau), \quad (\text{A.20})$$

$$\Phi(x, \tau) = \phi(\tau - ix/v) + \phi(\tau + ix/v). \quad (\text{A.21})$$

We may also write this with the complex numbers z and \bar{z}

$$\Phi(z, \bar{z}) = \phi_L(\bar{z}) + \phi_R(z) \quad (\text{A.22})$$

where ϕ_L and ϕ_R are the left and right chiral components, chiral meaning that they each only move in one direction. The field Φ possesses a mode expansion:

$$\Phi(\tau, x) = \Phi_0 + \frac{i\sqrt{\pi}J\tau}{L} + \frac{\sqrt{\pi}Qx}{vL} + \sum_{q \neq 0} \frac{1}{\sqrt{2|q|L}} (b_q^\dagger e^{|q|\tau - iqx/v} + b_q e^{-|q|\tau + iqx/v}) \quad (\text{A.23})$$

where the creation and annihilation operators obey $[b_q, b_{q'}^\dagger] = \delta_{q, q'}$ and the wavevectors are quantised as $q = 2\pi n/L$ with $n = 0, \pm 1, \pm 2, \dots$. This is easily seen by substitution into the equation of motion (A.20). From this we may extract the chiral components:

$$\phi_R(z) = \frac{i\sqrt{\pi}}{2} (J - Q)z/L + \sum_{q > 0} \frac{1}{\sqrt{2qL}} (e^{-qz} b_{-q} + e^{qz} b_{-q}^\dagger) \quad (\text{A.24})$$

$$\phi_L(\bar{z}) = \frac{i\sqrt{\pi}}{2} (J + Q)\bar{z}/L + \sum_{q > 0} \frac{1}{\sqrt{2qL}} (e^{q\bar{z}} b_q^\dagger + e^{-q\bar{z}} b_q) \quad (\text{A.25})$$

(Φ_0 may be set to zero). As a side remark, it is also customary to define the dual field $\Theta(z, \bar{z}) = \phi_R(z) - \phi_L(\bar{z})$. Together with $\Phi(z, \bar{z})$, this provides a complete basis of bosonic exponents which may be used for expansions of any local periodic functional $F(\Phi, \Theta)$ and therefore for studying the scaling properties of its correlators.

Zero mode: The quantities Q and J are called the total charge and current through the system respectively.

Bringing both sides together ($H_F = H_B$)

As hinted at by the choice of notation, each Weyl fermion $\psi_{L(R)}$ is bosonized by its chiral boson $\phi_{L(R)}$:

$$\psi_R(z) = \frac{1}{\sqrt{2\pi a_0}} : e^{i\sqrt{4\pi}\phi_R(z)} :, \quad \psi_L(\bar{z}) = \frac{1}{\sqrt{2\pi a_0}} : e^{-i\sqrt{4\pi}\phi_L(\bar{z})} : \quad (\text{A.26})$$

The normal ordering signs $:(...):$ mean that all annihilation operators are commuted to the right and a_0 is a small distance cut-off assumed to be the smallest possible interval between two points in (τ, x) -space. Furthermore we also have expressions for the currents:

$$J_R(z) = -\frac{i}{\sqrt{\pi}} \partial_z \phi_R(z), \quad J_L(\bar{z}) = \frac{i}{\sqrt{\pi}} \partial_{\bar{z}} \phi_L(\bar{z}) \quad (\text{A.27})$$

Eqs. (A.26)-(A.27) are bosonization formulae. Using these we will show the equivalence $H_B = H_F$.

Upgrading to τ -dependent fields and decomposing the Gaussian model into the left and right movers with complex co-ordinates $z(x, \tau)$ gives:

$$H_B(\tau) = -\frac{1}{v} \int dx [(\partial_z \phi_R(z))^2 + (\partial_{\bar{z}} \phi_L(\bar{z}))^2]. \quad (\text{A.28})$$

The result follows by applying the $J_{L(R)}$ formulae:

$$H_B(\tau) = \frac{\pi}{v} \int dx [(J_R(z))^2 + (J_L(\bar{z}))^2] \equiv H_F(\tau), \quad \text{with} \quad v_F = \frac{1}{v}. \quad (\text{A.29})$$

We could alternatively have just parametrised z and \bar{z} differently as $z = v\tau - ix$ and $\bar{z} = v\tau + ix$ in order to find $v = v_F$, as done for example in the introduction by S en echal [15].

For a proof of the local operator algebra equivalence the reader is referred to the literature [10, 15]. The point split procedure is a nice way to show (A.27). One can also directly check that the commutators such as $\delta(x - x')\psi_R(x) = [\psi_R(x), J_R(x')]$ hold for the new Bose representation by using the Campbell-Baker-Hausdorff lemma. Equally, one could be satisfied by verifying that the massless theories produce equivalent correlation functions.

A.3 Kondo spin-flip scattering for the reduced dimension theory

As a starting point the full one-dimensional Hamiltonian reads

$$H = \hbar v_F \int \frac{dk}{2\pi} c_{k\lambda}^\dagger k c_{k\lambda} + \hbar v g \int \frac{dk}{2\pi} \int \frac{dp}{2\pi} c_{k\lambda}^\dagger c_{p\mu} \boldsymbol{\sigma}_{\lambda\mu} \cdot \mathbf{S} \quad (\text{A.30})$$

where repeated spin indices are summed and $g = J/\hbar v_F$ is a dimensionless parameter. In this reduced form the conduction electrons taken alone are Weyl fermions and there is only one Fermi point in the problem.

We may do perturbation theory in the weak coupling limit $g \ll 1$ and examine the spin flip scattering process which Kondo showed may account for the resistance minimum, Fig. A.1, but for the effective one-dimensional theory. Let the ingoing and outgoing states be

$$|\text{in}\rangle = \sqrt{\frac{L}{v_F \hbar}} |k \uparrow\rangle \otimes |\Downarrow\rangle, \quad |\text{out}\rangle = \sqrt{\frac{L}{v_F \hbar}} |k \downarrow\rangle \otimes |\Uparrow\rangle. \quad (\text{A.31})$$

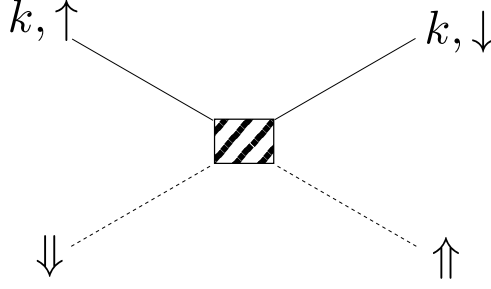


Figure A.1: For spin flip scattering all intermediate virtual processes are summed over.

where the outer ket denotes the spin-1/2 impurity moment. Using a discretised version of the Kondo coupling, the leading order scattering amplitude is

$$\begin{aligned}
\Gamma^{(1)} &= \langle \text{out} | \hat{V} | \text{in} \rangle = \langle \text{out} | \frac{gv\hbar}{L} \sum_{pr} c_{p\lambda}^\dagger \boldsymbol{\sigma}_{\lambda\mu} c_{r\mu} \cdot \mathbf{S} | \text{in} \rangle = g \langle \uparrow | \langle k \downarrow | \sum_{pr} c_{p\lambda}^\dagger \boldsymbol{\sigma}_{\lambda\mu} c_{r\mu} \cdot \mathbf{S}_d | k \uparrow \rangle | \downarrow \rangle \\
&= g \langle \uparrow | \langle 0 | \sum_{pr} \boldsymbol{\sigma}_{\lambda\mu} \cdot \mathbf{S} \delta_{k,r} \delta_{\mu\uparrow} \delta_{p,k} \delta_{\lambda,\downarrow} | 0 \rangle | \downarrow \rangle = g \langle \uparrow | \langle 0 | \begin{pmatrix} (\sigma^x)_{\downarrow\uparrow} \\ (\sigma^y)_{\downarrow\uparrow} \\ (\sigma^z)_{\downarrow\uparrow} \end{pmatrix} \cdot \begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix} | 0 \rangle | \downarrow \rangle \\
&= g \langle \uparrow | S^+ | \downarrow \rangle = g.
\end{aligned} \tag{A.32}$$

The second order amplitude calculation proceeds similarly.

$$\begin{aligned}
\Gamma^{(2)} &= \sum_{\nu} \langle \text{out} | \frac{\hat{V} |\nu\rangle \langle \nu| \hat{V}}{E_k - E_{\nu}} | \text{in} \rangle = \langle \text{out} | \sum_{\mu\lambda p} \frac{(\hbar v_F g)^2 \boldsymbol{\sigma}(0) \cdot \mathbf{S} c_{p\lambda}^\dagger | 0 \rangle \otimes |\mu\rangle \langle \mu| \otimes \langle 0 | c_{p\lambda} \boldsymbol{\sigma}(0) \cdot \mathbf{S}}{\hbar v_F (k - p)} | \text{in} \rangle \\
&\rightarrow 2g^2 \int_0^{\infty} \frac{dp}{2\pi} \frac{1}{k - p}
\end{aligned} \tag{A.33}$$

The scattering is restricted to positive momentum and we can see that the result logarithmically diverges. Introducing a UV-cutoff Λ and taking the principle value integral gives

$$\Gamma^{(2)} = 2g^2 \int_0^{\Lambda} \frac{dp}{2\pi} \frac{1}{k - p} = -2g^2 \log \left(\frac{\Lambda - k}{k} \right). \tag{A.34}$$

The spin flip scattering process, therefore, to second order is

$$\Gamma = \Gamma^{(1)} + \Gamma^{(2)} + \mathcal{O}(g^2) = g - 2g^2 \log \left(\frac{\Lambda - k}{k} \right) + \mathcal{O}(g^3) \tag{A.35}$$

Since scattering amplitudes like Γ are physical quantities, contributing to heat capacity and resistivity for example, but Λ and g are unphysical, the divergence from $\log(\Lambda)$ as $\Lambda \rightarrow \infty$ should be fixed. A natural next step is to make a second order correction to the Hamiltonian with a counterterm $H_k \rightarrow H_k + \# \log(\Lambda)$ and eliminate the troublesome area in the spectrum by choosing $\#$ appropriately. Proceeding in this direction is in the spirit of the Wilsonian renormalisation group. Kondo showed, however, with similar T-matrix calculations, that the higher order corrections diverge even more rapidly.

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A.4 Keldysh technique example: tunnelling conductance

Here we show the details of how to set up the Keldysh action for the example problem of the tunnelling conductance Hamiltonian, justifying the prescription in the text.

$$\begin{aligned}
 S &= \int_{\mathcal{C}} dt \sum_{k,k'} \begin{pmatrix} \bar{c}_k(t) \\ \bar{d}_k(t) \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hat{G}_{0k(c)}^{-1} & -t_{kk'} \\ -t_{kk'}^* & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} \end{pmatrix} \begin{pmatrix} c_{k'}(t) \\ d_{k'}(t) \end{pmatrix} \quad (\text{A.36}) \\
 &= \int_{-\infty}^{\infty} dt \sum_{k,k'} \left[\begin{pmatrix} \bar{c}_{k+} \\ \bar{d}_{k+} \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hat{G}_{0k(c)}^{-1} & -t_{kk'} \\ -t_{kk'}^* & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} \end{pmatrix} \begin{pmatrix} c_{k'+} \\ d_{k'+} \end{pmatrix} \right. \\
 &\quad \left. - \begin{pmatrix} \bar{c}_{k-} \\ \bar{d}_{k-} \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hat{G}_{0k(c)}^{-1} & -t_{kk'} \\ -t_{kk'}^* & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} \end{pmatrix} \begin{pmatrix} c_{k'-} \\ d_{k'-} \end{pmatrix} \right], \quad (\text{doubling the number of fields}) \\
 &= \int dt \sum_{k,k'} \begin{pmatrix} \bar{c}_{k+} \\ \bar{c}_{k-} \\ \bar{d}_{k+} \\ \bar{d}_{k-} \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hat{G}_{0k(c)}^{-1} & 0 & -t_{k,k'} & 0 \\ 0 & -\delta_{k,k'} \hat{G}_{0k(c)}^{-1} & 0 & t_{k,k'} \\ -t_{k,k'}^* & 0 & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} & 0 \\ 0 & t_{k,k'}^* & 0 & -\delta_{k,k'} \hat{G}_{0k(d)}^{-1} \end{pmatrix} \begin{pmatrix} c_{k'+} \\ c_{k'-} \\ d_{k'+} \\ d_{k'-} \end{pmatrix} \\
 &= \int dt \sum_{k,k'} \begin{pmatrix} \bar{c}_k(t) \\ \bar{d}_k(t) \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hat{G}_{0k(c)}^{-1} \sigma_3 & -t_{k,k'} \sigma_3 \\ -t_{k,k'}^* \sigma_3 & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} \sigma_3 \end{pmatrix} \begin{pmatrix} c_{k'}(t) \\ d_{k'}(t) \end{pmatrix}, \quad (\text{compressing notation}) \\
 &= \int dt \sum_{k,k'} \begin{pmatrix} \bar{\psi}_k^{(c)} \\ \bar{\psi}_k^{(d)} \end{pmatrix}^\top \begin{pmatrix} U \sigma_3 (\delta_{k,k'} \hat{G}_{0k(c)}^{-1} \sigma_3) U & U \sigma_3 (-t_{k,k'} \sigma_3) U \\ U \sigma_3 (-t_{k,k'}^* \sigma_3) U & U \sigma_3 (\delta_{k,k'} \hat{G}_{0k(d)}^{-1} \sigma_3) U \end{pmatrix} \begin{pmatrix} \psi_{k'}^{(c)} \\ \psi_{k'}^{(d)} \end{pmatrix}, \quad (\text{K rotation}) \\
 &= \int dt \sum_{k,k'} \begin{pmatrix} \bar{\psi}_{1k}^{(c)} \\ \bar{\psi}_{2k}^{(c)} \\ \bar{\psi}_{1k}^{(d)} \\ \bar{\psi}_{2k}^{(d)} \end{pmatrix}^\top \begin{pmatrix} \delta_{k,k'} \hat{G}_{0k(c)}^{-1} & 0 & -t_{k,k'} & 0 \\ 0 & \delta_{k,k'} \hat{G}_{0k(c)}^{-1} & 0 & -t_{k,k'} \\ -t_{k,k'}^* & 0 & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} & 0 \\ 0 & -t_{k,k'}^* & 0 & \delta_{k,k'} \hat{G}_{0k(d)}^{-1} \end{pmatrix} \begin{pmatrix} \psi_{1k'}^{(c)} \\ \psi_{2k'}^{(c)} \\ \psi_{1k'}^{(d)} \\ \psi_{2k'}^{(d)} \end{pmatrix} \quad (\text{A.37})
 \end{aligned}$$

Similarly for the source action used for finding the electric current:

$$\begin{aligned}
 S_W &= - \int_{-\infty}^{\infty} dt \sum_{k,k'} W(t) \hat{I}(t) \\
 &= - \frac{ie}{\hbar} \int_{\mathcal{C}} dt W_+ \sum_{k,k'} [t_{k,k'} c_{k+}^\dagger d_{k'+} - t_{k,k'}^* d_{k'+}^\dagger c_{k+}] - (\text{fields}_+ \rightarrow \text{fields}_-) \\
 &= - \frac{ie}{\hbar} \int_{-\infty}^{\infty} dt \sum_{k,k'} \begin{pmatrix} \bar{c}_{k+} \\ \bar{c}_{k-} \\ \bar{d}_{k+} \\ \bar{d}_{k-} \end{pmatrix}^\top \begin{pmatrix} 0 & 0 & W_+ t_{k,k'} & 0 \\ 0 & 0 & 0 & -W_- t_{k,k'} \\ -W_+ t_{k',k}^* & 0 & 0 & 0 \\ 0 & W_- t_{k',k}^* & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k+} \\ c_{k-} \\ d_{k+} \\ d_{k-} \end{pmatrix} \\
 &= - \frac{ie}{\hbar} \int_{-\infty}^{\infty} dt \sum_{k,k'} \bar{\Psi}_k (\mathbb{1} \otimes U \sigma_3) \left[\begin{pmatrix} 0 & t_{k,k'} \\ -t_{k',k}^* & 0 \end{pmatrix} \otimes (W_q \mathbb{1} + W_{cl} \sigma_3) \right] (\mathbb{1} \otimes U) \Psi_{k'} \\
 &= - \frac{ie}{\hbar} \int_{-\infty}^{\infty} dt \sum_{k,k'} \bar{\Psi}_k \left\{ \begin{pmatrix} 0 & t_{k,k'} \\ -t_{k',k}^* & 0 \end{pmatrix} \otimes [U \sigma_3 (W_q \mathbb{1} + W_{cl} \sigma_3) U] \right\} \Psi_k \\
 &= - \frac{ie}{\hbar} \int_{-\infty}^{\infty} dt \sum_{k,k'} \bar{\Psi}_k \left[\begin{pmatrix} 0 & t_{k,k'} \\ -t_{k',k}^* & 0 \end{pmatrix} \otimes W_\alpha \gamma^\alpha \right] \Psi_{k'} \quad (\text{A.38})
 \end{aligned}$$

as stated in the main text.

A useful linear algebra trick

In the main text we used the result $x^\top Ax = \text{Tr}(Axx^\top)$ for column vectors x and square matrices A . This is also used in the later chapters.

⌈ *Proof.* Consider that $(Ax)_{ij}$ is a column vector so $j = 1$ only:

$$(Ax)_{ij} = \sum_k A_{ik}x_{kj} \rightarrow (Ax)_i = \sum_k A_{ik}x_k \quad (\text{A.39})$$

Then consider:

$$\begin{aligned} x^\top Ax &= \sum_{ik} (x^\top)_i A_{ik} x_k = \sum_{ik} A_{ik} x_k (x^\top)_i = \sum_i (Ax)_i (x^\top)_i = \sum_i \sum_{\substack{k=1 \\ \text{only}}} (Ax)_{ik} (x^\top)_{ki} = \sum_i (Axx^\top)_{ii} \\ &= \text{Tr}(Axx^\top) \end{aligned} \quad (\text{A.40})$$

⌋

■

Appendix B

Detailed calculations - Chapter 3

B.1 1CK bosonization details, mapping to a resonant level Hamiltonian

Here we will fill in the steps outlined in the main text showing the mapping of the single-channel Kondo (1CK) model to the resonant level (RL) model.

Step 1: The spin densities $J^z(x)$ and $J^\pm(x)$ were expressed in terms of Bose fields in Eq. (3.6), as introduced in the previous chapter.

For the conduction electrons, the mapping to the bosonic description simply marks the return of the equivalence between the free boson and massless fermion theories (or half of it, loosely speaking). Just as the massless Dirac Hamiltonian is equivalent to the free boson Hamiltonian, which we showed in an earlier appendix, the Hamiltonian for the Weyl fermion is equivalent to the Hamiltonian for the chiral boson.

Step 2: A unitary transformation allowed for a redefinition of new Fermi fields

$$\psi(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\pi d^\dagger d} e^{i\sqrt{4\pi}\phi(x)}.$$

For the transformation of the transverse term, recalling the spin algebra result $[s_+, s_z] = -s_z$, consider

$$\begin{aligned} s_+ U &= s_+ \sum_{n=0}^{\infty} \frac{(i\sqrt{4\pi}\alpha s_z \phi(0))^n}{n!} \\ &= s_+ + s_+ i\sqrt{4\pi}\alpha s_z \phi(0) + s_+ \frac{1}{2} (i\sqrt{4\pi}\alpha s_z \phi(0))^2 + s_+ \frac{1}{3!} (i\sqrt{4\pi}\alpha s_z \phi(0))^3 + \dots \\ &= s_+ + i\sqrt{4\pi}\alpha \phi(0) (s_z - 1) s_+ + \frac{1}{2} (i\sqrt{4\pi}\alpha s_z \phi(0))^2 [(s_z - 1) s_+ s_z] + \dots \\ &= \sum_{n=0}^{\infty} \frac{(i\sqrt{4\pi}\alpha \phi(0) (s_z - 1))^n}{n!} s_+ \end{aligned} \tag{B.1}$$

Therefore

$$U^\dagger s_+ U = e^{-i\sqrt{4\pi}\alpha s_z \phi(0)} e^{-i\sqrt{4\pi}\alpha (s_z - 1) \phi(0)} s_+ = e^{-i\sqrt{4\pi}\alpha \phi(0)} s_+ \tag{B.2}$$

For the longitudinal exchange term and the H_0 contribution we must consider $U^\dagger \partial_x \phi(x) U$ and $U^\dagger [\partial_x \phi(x)]^2 U$. We have the convention for the Bose fields that

$$[\partial_x \phi(x), \phi(y)] = \frac{i}{2} \delta(x - y). \tag{B.3}$$

Using the Campbell-Baker-Hausdorff lemma:

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!} [X, [X, Y]] + \frac{1}{3!} [X, [X, [X, Y]]] + \dots \tag{B.4}$$

where $X = -i\sqrt{4\pi}\alpha s_z \phi(0)$ and $Y = \partial_x \phi(x)$, the first commutator is

$$[X, Y] = -\sqrt{\pi}\alpha s_z \delta(x). \quad (\text{B.5})$$

All of the successive nested commutators in the series vanish and we find

$$U^\dagger \partial_x \phi(x) U = \partial_x \phi(x) - \sqrt{\pi}\alpha s_z \delta(x). \quad (\text{B.6})$$

Using this, the transformation for H_0 is:

$$\begin{aligned} U^\dagger H_0[\phi] U &= v_F \int dx U^\dagger \phi'(x)^2 U = v_F \int dx U^\dagger \phi'(x) U [\phi'(x) - \sqrt{\pi}\alpha s_z \delta(x)] \\ &= -v_F \sqrt{\pi}\alpha s_z [U^\dagger \phi'(0) U] + v_F \int dx [U^\dagger \phi'(x) U] \phi'(x) \\ &= -v_F \sqrt{\pi}\alpha s_z [\phi'(0) - \sqrt{\pi}\alpha s_z \delta(0)] + v_F \int dx [\phi'(x) - \sqrt{\pi}\alpha s_z \delta(x)] \phi'(x) \\ &= H_0[\phi] - 2v_F \sqrt{\pi}\alpha s_z \partial_x \phi(0) + \frac{\pi v_F \alpha^2}{4} \delta(0) \end{aligned} \quad (\text{B.7})$$

where we used $s_z^2 = 1/4$ for spin-1/2 particles. Consider this together with the transformation for the longitudinal part. They combine to modify the longitudinal exchange coupling term:

$$\begin{aligned} &U^\dagger \left(H_0[\phi] + \frac{I_z}{\sqrt{2\pi}} s_z \partial_x \phi(0) \right) U \\ &= H_0 - 2v_F \sqrt{\pi}\alpha s_z \partial_x \phi(0) + \frac{\pi v_F \alpha^2}{4} \delta(0) + \frac{I_z}{\sqrt{2\pi}} s_z \phi'(0) - \frac{I_z}{\sqrt{2}} \alpha s_z^2 \delta(0) \\ &= H_0 + \frac{s_z}{\sqrt{\pi}} \left(\frac{I_z}{\sqrt{2}} - 2\pi v_F \alpha \right) \partial_x \phi(0) + \left(\alpha \pi v_F - \frac{I_z}{\sqrt{2}} \right) \frac{\alpha}{4} \delta(0) \end{aligned} \quad (\text{B.8})$$

The transformed Hamiltonian therefore reads

$$H = H_0[\phi] + \frac{I_\perp}{4\pi a_0} [s_+ e^{i\sqrt{4\pi}\phi(0)} + \text{h.c.}] + \frac{\lambda}{\sqrt{\pi}} s_z \partial_x \phi(0) + \delta H, \quad (\text{B.9})$$

where

$$\lambda = \frac{I_z}{\sqrt{2}} - 2\alpha \pi v_F = \frac{I_z}{\sqrt{2}} - 2(\sqrt{2} - 1)\pi v_F \quad (\text{B.10})$$

is the modified coupling, and

$$\delta H = \left(\alpha \pi v_F - \frac{I_z}{\sqrt{2}} \right) \frac{\alpha}{4} \delta(0) \quad (\text{B.11})$$

is an additive shift to the energies which may be discarded:

$$H = H_0[\phi] + \frac{I_\perp}{4\pi a_0} [s_+ e^{i\sqrt{4\pi}\phi(0)} + \text{h.c.}] + \frac{\lambda}{\sqrt{\pi}} s_z \partial_x \phi(0). \quad (\text{B.12})$$

Step 3: For the new Fermi fields,

$$\psi(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\pi d^\dagger d} e^{i\sqrt{4\pi}\phi(x)}, \quad (\text{B.13})$$

we have a fermionic representation (d, d^\dagger) for the spin-1/2 operators s_\pm of the Jordan-Wigner type:

$$s_+ = d^\dagger, \quad s_- = d, \quad s_z = d^\dagger d - \frac{1}{2} \quad (\text{B.14})$$

These should anticommute with the fields themselves, e.g.: $\{\psi(x), d\} = 0$, $\{\psi(x), d^\dagger\} = 0$. Taking the hermitian conjugates of these two relations gives all the different options, so only two need to be checked. Since a single fermionic number operator raised to any non-zero power $1, 2, 3, \dots$ is just the original number operator, we may write:

$$\begin{aligned} e^{i\pi d^\dagger d} &= \sum_{n=0}^{\infty} \frac{(i\pi d^\dagger d)^n}{n!} = 1 + \left(\sum_{n=0}^{\infty} \frac{(i\pi)^{n+1}}{(n+1)!} \right) d^\dagger d = 1 + \left[\left(\sum_{n=0}^{\infty} \frac{(i\pi)^n}{n!} \right) - 1 \right] d^\dagger d \\ &= 1 + (e^{i\pi} - 1)d^\dagger d = 1 - 2d^\dagger d \end{aligned} \quad (\text{B.15})$$

Making use of this, consider the first anticommutator

$$\begin{aligned} \{\psi(x), d\} &= \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi(x)} (e^{i\pi d^\dagger d} d + d e^{i\pi d^\dagger d}) \\ &= \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi(x)} [(1 - 2d^\dagger d)d + d(1 - 2d^\dagger d)] = \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi(x)} (2d^\dagger - 2dd^\dagger d) \\ &= \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi(x)} [2d^\dagger - 2(1 - d^\dagger d)d] = 0. \end{aligned} \quad (\text{B.16})$$

The second anticommutator proceeds similarly:

$$\{\psi(x), d^\dagger\} = \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{4\pi}\phi(x)} [(1 - 2d^\dagger d)d^\dagger + d^\dagger(1 - 2d^\dagger d)] = 0. \quad (\text{B.17})$$

For the refermionization mapping itself, noting that $d^\dagger e^{i\pi d^\dagger d} = d^\dagger$, the Hamiltonian straightforwardly becomes

$$H_{RL} = H_0[\psi] + \frac{I_\perp}{2\sqrt{2\pi a_0}} [d^\dagger \psi(0) + \text{h.c.}] + \lambda \left(d^\dagger d - \frac{1}{2} \right) : \psi^\dagger(0) \psi(0) : \quad (\text{B.18})$$

which is the resonant level type model we set out to show.

Appendix C

Detailed calculations - Chapter 4

C.1 Equations of motion for the RL action

Setting $\hbar = 1$ and $g/\sqrt{L} = v$ for convenience, the Heisenberg equations of motion for the RL toy model are:

$$\begin{aligned}
 \dot{c}_k(t) &= -i[c_k(t), H(t)] = -iU^\dagger(t, 0)[c_k, H(t)]U(t, 0) \\
 &= -iU^\dagger(t, 0) \sum_{k'} \left[\epsilon_k(t)[c_k, c_{k'}^\dagger c_{k'}] + v([c_k, d^\dagger c_{k'}] + [c_k, c_{k'}^\dagger d]) \right] U(t, 0) \\
 &= -iU^\dagger(t, 0) \left(\epsilon_k(t)c_k + vd \right) U(t, 0) \\
 &= -i\epsilon_k(t)c_k(t) - ivd(t)
 \end{aligned} \tag{C.1}$$

and

$$\begin{aligned}
 \dot{d}(t) &= -i[d(t), H(t)] = -iU^\dagger(t, 0) \left(v \sum_k [d, d^\dagger c_k] + \epsilon_d[d, d^\dagger d] \right) U(t, 0) \\
 &= -iU^\dagger(t, 0) \left(v \sum_k c_k + \epsilon_d d \right) U(t, 0) \\
 &= -iv \sum_k c_k(t) - i\epsilon_d d(t).
 \end{aligned} \tag{C.2}$$

The Euler-Lagrange equation for $c(x, t)$ is:

$$\begin{aligned}
 0 &= \partial_t \left(\frac{\partial \mathcal{L}}{\partial (\partial_t c(x, t))} \right) + \partial_x \left(\frac{\partial \mathcal{L}}{\partial (\partial_x c(x, t))} \right) - \frac{\partial \mathcal{L}}{\partial c(x, t)} \\
 &= i\partial_t c^\dagger(x, t) + iv_F \partial_x c^\dagger(x, t) + eV(t)c^\dagger(x, t) + \sqrt{L}vd^\dagger \delta(x) \\
 \implies 0 &= -i\partial_t c(x, t) - iv_F \partial_x c(x, t) + eV(t)c(x, t) + \sqrt{L}vd \delta(x) \\
 &= -\frac{1}{\sqrt{L}} \sum_k \{ i\dot{c}_k(t) - [v_F k + eV(t)]c_k(t) \} e^{ikx} + \sqrt{L}vd(t)\delta(x) \\
 \sum_k \frac{i}{L} \left(\int_0^L dx e^{i(k-k')x} \right) \dot{c}_k(t) &= \frac{1}{L} \sum_k c_k(t) \int_0^L dx e^{i(k-k')x} \epsilon_k(t) + vd(t) \int_0^L dx e^{-ik'x} \delta(x) \\
 \sum_k i\delta_{k,k'} \dot{c}_k(t) &= \sum_k c_k(t) \delta_{k,k'} \epsilon_k(t) + vd(t) \\
 \implies \dot{c}_k &= -i\epsilon_k(t)c_k(t) - ivd(t)
 \end{aligned} \tag{C.3}$$

Similarly, the Euler-Lagrange equation for d is:

$$\begin{aligned}
 0 &= \partial_t \left(\frac{\partial \mathcal{L}}{\partial (\partial_t d(t))} \right) - \frac{\partial \mathcal{L}}{\partial d(t)} \\
 &= i\dot{d}(t)^\dagger \delta(x) + \sqrt{L}vc^\dagger(x, t)\delta(x) + \epsilon_d d^\dagger(t)\delta(x) \\
 \implies 0 &= i\dot{d}(t) + \sqrt{L}vc(0, t) + \epsilon_d d(t) \\
 \dot{d}(t) &= -iv \sum_k c_k(t) - i\epsilon_d d(t).
 \end{aligned} \tag{C.4}$$

By comparing Eqs. (C.1)-(C.4) the action we quoted in the main text is justified.

C.2 Local Green functions and Fourier transformations

Throughout this thesis we used the following definition for the Fourier expansion of the field operator $c(x, t)$ into its creation/annihilation coefficients $c_k(t)$:

$$c(x, t) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} c_k(t), \quad c_k(t) = \frac{1}{\sqrt{L}} \int_0^L dx e^{-ikx} \psi(x, t). \tag{C.5}$$

Consequently the Fourier expansion for the real space Green function contains a $1/L$:

$$\begin{aligned}
 G(x, t; x', t') &= -i \langle \psi(x, t) \bar{\psi}(x', t') \rangle = -\frac{i}{L} \sum_{k, k'} e^{i(kx - k'x')} \langle c_k(t) \bar{c}_{k'}(t') \rangle \\
 &= \frac{1}{L} \sum_{k, k'} e^{i(kx - k'x')} G_{(k, t; k', t')}
 \end{aligned} \tag{C.6}$$

In addition, for translationally invariant systems we have:

$$G(x, x'; t, t') = G(x - x'; t, t') \tag{C.7}$$

Explicitly, we find for the Fourier transform with respect to the difference $x - x'$, where we may set x' to zero, that:

$$G(x; t, t') = \frac{1}{L} \sum_{k, k'} e^{ikx} G_{(k, t; k', t')} \tag{C.8}$$

The translational invariance implies that $G_{(k, t; k', t')}$ is diagonal in momentum space:

$$G_{(k, t; k', t')} = \delta_{k, k'} G_{(k; t, t')} \tag{C.9}$$

Thus,

$$G(x; t, t') = \frac{1}{L} \sum_k e^{ikx} G_{(k; t, t')}. \tag{C.10}$$

In the two research chapters we often use local Green functions for the conduction electrons at the impurity location $x = 0$. These follow from (C.10), e.g. for the toy resonant level model:

$$G_{co}(t, t') = \frac{1}{L} \sum_k G_{(k; t, t')}, \quad \text{where} \quad G_{co}(t, t') \equiv G_c(x = 0; t, t'). \tag{C.11}$$

Example for (C.9)

Green functions are defined by

$$\int dx_1 \int dt_1 \hat{G}^{-1}(x, t; x_1, t_1) G(x_1, t_1; x', t') = \delta(x - x') \delta(t - t') \quad (\text{C.12})$$

where \hat{G}^{-1} may be read off from the action $S = (\psi | \hbar \hat{G}^{-1} | \psi)$. The operator \hat{G}^{-1} is diagonal:

$$\hat{G}^{-1}(x, t; x_1, t_1) = \delta(t - t_1) \delta(x - x_1) \hat{G}^{-1}(x_1; t_1) \quad (\text{C.13})$$

Plugging into (C.12):

$$\implies \hat{G}^{-1}(x, t) G(x, t; x', t') = \delta(x - x') \delta(t - t'). \quad (\text{C.14})$$

For the non-interacting one-dimensional theories we study in this thesis, the bare \hat{G}^{-1} have a general form:

$$\hat{G}^{-1}(x, t) = \frac{1}{\hbar} \left[i\hbar \frac{\partial}{\partial t} + i\hbar v_F \frac{\partial}{\partial x} + f(t) \right] \quad (\text{C.15})$$

where $f(t)$ is just a time-dependent function. Thus:

$$\hbar \delta(x - x') \delta(t - t') = \left[i\hbar \frac{\partial}{\partial t} + i\hbar v_F \frac{\partial}{\partial x} + f(t) \right] G(x, t; x', t'), \quad (\text{C.16})$$

which shows that G is mathematically a Green function. A solution can be constructed:

$$G(x, t; x', t') = \frac{1}{L} \sum_k i\theta(t' - t) e^{ik(x-x')} e^{-iv_F k(t-t')} e^{\frac{-i}{\hbar} \int_t^{t'} f(s) ds}, \quad (\text{C.17})$$

which holds for the continuum limit $\frac{1}{L} \sum_k(\dots) \rightarrow \int \frac{dk}{2\pi}(\dots)$ given that the sum over k converges absolutely. Therefore, by comparing (C.17) to (C.8), we may confirm $G(x, t; x', t') = G(x - x'; t, t')$ by inspection and also that $G_{(k,t;k',t')} = \delta_{k,k'} G_{(k;t,t')}$:

$$G_{(k,t;k',t')} = \delta_{k,k'} \left[i\theta(t' - t) e^{-iv_F k(t-t')} e^{\frac{-i}{\hbar} \int_t^{t'} f(s) ds} \right]. \quad (\text{C.18})$$

C.3 Linear response details

C.3.1 Derivations of the Green functions

Here we show derivations for the Green functions we quoted in the text.

Time domain Green functions

For convenience the defining equations a second time are:

$$\hbar \delta(t - t') = \int ds \delta(t - s) (i\hbar \partial_s - \epsilon_k(s) \pm i0^+) \mathcal{G}_{co(k;s,t')}^{r,a} \quad (\text{C.19})$$

$$\hbar \delta(t - t') = \int ds \delta(t - s) (i\hbar \partial_s - \epsilon_d \pm i0^+) G_{do(s,t')}^{r,a} \quad (\text{C.20})$$

$$\hbar \delta(t - t') = \int ds [\delta(t - s) (i\hbar \partial_s - \epsilon_d \pm i0^+) - \frac{g^2}{\hbar} G_{co(t,s)}^{r,a}] G_{dd(s,t')}^{r,a}, \quad (\text{C.21})$$

The retarded/advanced Green functions for the electrons of momentum k subject to the harmonic potential are:

$$\mathcal{G}_{co(t,t',k)}^{r,a} = \mp i\theta[\pm(t - t')] e^{-\frac{i\epsilon_k}{\hbar}(t-t')} e^{\frac{-ie}{\hbar} \int_t^{t'} V(s) ds}. \quad (\text{C.22})$$

⌈ *Proof.*

$$\begin{aligned}
 & [i\hbar\partial_t - \epsilon_k(t) \pm i0^+] \mathcal{G}_{co}^{r,a}(t, t') \\
 &= \hbar\delta(t-t')e^{(\dots)} \mp i^2\theta[\pm(t-t')] \left(-i\epsilon_k - ie \frac{d}{dt} \int_t^{t'} V(s) ds \right) e^{-i\epsilon_k(t-t')/\hbar} e^{\frac{-ie}{\hbar} \int_t^{t'} ds V(s)} \\
 &- \epsilon_k(t) \mathcal{G}_{co}^{r,a}(t, t') \\
 &= \hbar\delta(t-t') e^{-i\epsilon_k(t-t')/\hbar} e^{\frac{-ie}{\hbar} \int_t^{t'} V(s) ds} + (\epsilon_k - eV(t)) \mathcal{G}_{co}^{r,a}(t, t') - \epsilon_k(t) \mathcal{G}_{co}^{r,a}(t, t') \\
 &= \hbar\delta(t-t') e^{-i\epsilon_k(t-t')/\hbar} e^{\frac{-ie}{\hbar} \int_t^{t'} V(s) ds} \\
 &= \hbar\delta(t-t')
 \end{aligned}$$

⌋ The last step is true because both expressions equal one when integrated over all t . ■

The local version comes by integrating over k :

$$G_{co}^{r,a}(t, t', V_0) = \mp i\theta[\pm(t-t')] \int \frac{dk}{2\pi} e^{-i\epsilon_k(t-t')/\hbar} e^{\frac{-ie}{\hbar} \int_t^{t'} V(s) ds} \quad (C.23)$$

For the Keldysh component, taking the lead to be in equilibrium, applying $\mathcal{G}_{co(k;t,t')}^K = (\mathcal{G}_{co(k;t,t')}^r - \mathcal{G}_{co(k;t,t')}^a)(1 - 2n_F(\epsilon_k))$ straightforwardly leads to:

$$G_{co}^K(t, t') = -i \int \frac{dk}{2\pi} (1 - 2n_F(\epsilon_k)) e^{-i\epsilon_k(t-t')/\hbar} e^{\frac{-ie}{\hbar} \int_t^{t'} ds V(s)}. \quad (C.24)$$

Similarly, G_{do} is a bare Green function for the single d -fermion with energy ϵ_d , just like the case in chapter II where we introduced the Keldysh technique:

$$G_{do}^{r,a}(t-t') = \mp i\theta[\pm(t-t')] e^{-i\epsilon_d(t-t')/\hbar}, \quad (C.25)$$

$$G_{do}^K(t-t') = -i(1 - 2n_F(\epsilon_d)) e^{-i\epsilon_d(t-t')/\hbar}. \quad (C.26)$$

We may group the results into their associated matrices.

$$G_{co(t,t';V_0)} = -i \int \frac{dk}{2\pi} e^{-i\epsilon_k(t-t')/\hbar} e^{\frac{-ie}{\hbar} \int_t^{t'} ds V(s)} \begin{pmatrix} \theta(t-t') & 1 - 2n_F(\epsilon_k) \\ 0 & -\theta(t'-t) \end{pmatrix}, \quad (C.27)$$

$$G_{do(t-t')} = -ie^{-i\epsilon_d(t-t')/\hbar} \begin{pmatrix} \theta(t-t') & 1 - 2n_F(\epsilon_d) \\ 0 & -\theta(t'-t) \end{pmatrix}. \quad (C.28)$$

C.3.2 Expansions for the Green functions G_{co} and G_{dd}

The fully time dependent solutions $G_{co}^{r,a,K}$ share a common functional form in V_0 . Expanding around $V_0 = 0$ gives:

$$\begin{aligned}
 G_{co(t,t';V_0)}^{r,a,K} &= G_{co(t,t';0)}^{r,a,K} + \left. \frac{\partial G_{co(t,t';V_0)}^{r,a,K}}{\partial V_0} \right|_{V_0=0} V_0 + \mathcal{O}(V_0^2) \\
 &= G_{co(t,t';0)}^{r,a,K} \left(1 - ie \int_t^{t'} ds V(s) \right) + \mathcal{O}(V_0^2)
 \end{aligned} \quad (C.29)$$

For G_{dd} we recall the 2×2 matrix $\left[(G_{do})^{-1} - \frac{g^2}{\hbar^2} G_{co} \right]^{-1}$ from the block matrix inversion:

$$G_{dd(t,t';V_0)} = G_{dd(t,t';0)} + \frac{\partial \left[(G_{do})^{-1} - \frac{g^2}{\hbar^2} G_{co} \right]^{-1}_{(t,t';V_0)}}{\partial V_0} \Bigg|_{V_0=0} V_0 + \mathcal{O}(V_0^2). \quad (\text{C.30})$$

Applying the rule¹ for derivatives of the inverse of a matrix,

$$\frac{\partial A^{-1}(x)}{\partial x} = -A^{-1}(x) \frac{\partial A(x)}{\partial x} A^{-1}(x),$$

we find an expansion in 2×2 matrices:

$$\begin{aligned} G_{dd(t,t';V_0)} &= G_{dd(t,t';0)} + \frac{g^2}{\hbar^2} \left[G_{dd}|_{V_0=0} \frac{\partial G_{co}}{\partial V_0} \Big|_{V_0=0} G_{dd}|_{V_0=0} \right]_{t,t'} V_0 + \mathcal{O}(V_0^2) \\ &= G_{dd(t-t')} - \frac{ieg^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) [G_{dd(t-t_1)} G_{co(t_1-t_2)} G_{dd(t_2-t')}] + \mathcal{O}(V_0^2) \end{aligned} \quad (\text{C.31})$$

where the multiplication included integration over the intermediate times. By straightforward matrix multiplication using the form $G_{dd} = \begin{pmatrix} G_{dd}^r & G_{dd}^K \\ 0 & G_{dd}^a \end{pmatrix}$, the various components we quoted follow:

$$\begin{aligned} G_{dd(t,t';V_0)}^{r,a} &= G_{dd(t,t';0)}^{r,a} - \frac{ieg^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) G_{dd(t-t_1)}^{r,a} G_{co(t_1-t_2)}^{r,a} G_{dd(t_2-t')}^{r,a} \\ &\quad + \mathcal{O}(V_0^2) \\ G_{dd(t,t';V_0)}^{K} &= G_{dd(t,t';0)}^{K} - \frac{ieg^2}{\hbar^3} \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) \left[G_{dd(t-t_1)}^r G_{co(t_1-t_2)}^r G_{dd(t_2-t')}^K \right. \\ &\quad \left. + G_{dd(t-t_1)}^r G_{co(t_1-t_2)}^K G_{dd(t_2-t')}^a + G_{dd(t-t_1)}^K G_{co(t_1-t_2)}^a G_{dd(t_2-t')}^a \right] + \mathcal{O}(V_0^2) \end{aligned} \quad (\text{C.32})$$

Energy domain Green functions

Following this were the equilibrium versions,

$$G_{co,dd}^{r,a,K}(t, t', V_0 = 0) \equiv G_{co,dd}^{r,a,K}(t - t'), \quad (\text{C.33})$$

written in the energy domain. For the Fourier transformation of the $\mathcal{G}_{co}^{r,a}$ and $G_{do}^{r,a}$ functions we use the integral representation of the step function:

$$\theta(t) = \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi i} \int_{-\infty}^{\infty} ds \frac{e^{its}}{s - i\delta} \quad (\text{C.34})$$

which leads to

$$G_{do}^{r,a}(\epsilon) = \hbar(\epsilon - \epsilon_d \pm i0^+)^{-1}, \quad (\text{C.35})$$

$$\mathcal{G}_{co}^{r,a}(\epsilon, k) = \hbar(\epsilon - \epsilon_k \pm i0^+)^{-1}. \quad (\text{C.36})$$

¹Consider expanding: $0 = \frac{\partial[A^{-1}(x)A(x)]}{\partial x}$.

⌈ *Proof.* Consider $G_{do}^{r,a}(\epsilon)$ since the derivation is identical for $\mathcal{G}_{co}^{r,a}(\epsilon, k)$. By Fourier transformation:

$$\begin{aligned}
 G_{do}^{r,a}(\epsilon) &= \int dt_1 e^{i\epsilon t_1/\hbar} G_{do}^{r,a}(t_1) \\
 &= \int dt_1 e^{i\epsilon t_1/\hbar} (\mp i) \left(\lim_{\delta \rightarrow 0^+} \frac{1}{2\pi i} \int d\left(\frac{s}{\hbar}\right) \frac{e^{\pm i t_1 s/\hbar}}{\frac{s}{\hbar} - i\delta} \right) e^{-i\epsilon t_1/\hbar} \\
 &= \mp \lim_{\delta \rightarrow 0^+} \int ds \frac{\hbar \delta (\epsilon - \epsilon_d \pm s)}{s - i\delta} \\
 &= \lim_{\delta \rightarrow 0^+} \frac{\mp \hbar}{\mp (\epsilon - \epsilon_d) - i\delta} \\
 &= \hbar (\epsilon - \epsilon_d \pm i0^+)^{-1}.
 \end{aligned}$$

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The local version of $\mathcal{G}_{co}^{r,a}$ is:

$$G_{co}^{r,a}(\epsilon) = \frac{1}{2\pi v_F} \ln \left| \frac{\hbar v_F \Lambda + \epsilon}{\hbar v_F \Lambda - \epsilon} \right| \mp \frac{i}{2v_F} (-1 + \theta(\epsilon + \hbar v_F \Lambda) + \theta(\hbar v_F \Lambda - \epsilon)) \quad (\text{C.37})$$

$$\approx \frac{\epsilon}{\pi \hbar v_F^2 \Lambda} \mp \frac{i}{2v_F} \quad (\text{C.38})$$

where we introduced a UV cutoff Λ , with SI units m^{-1} , and $v_F > 0$.

⌈ *Proof.*

$$\begin{aligned}
 G_{co}^{r,a}(\epsilon) &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\hbar}{\epsilon - \epsilon_k \pm i0^+} \\
 &\rightarrow \mathcal{P} \int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} \frac{\hbar}{\epsilon - \epsilon_k} \mp i\pi \hbar \int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} \delta(\epsilon - \epsilon_k) \\
 &= \lim_{\delta \rightarrow 0^+} \int_{-\Lambda}^{(\epsilon/\hbar v_F) - \delta} \frac{dk}{2\pi} \frac{\hbar}{\epsilon - \hbar v_F k} + \lim_{\delta \rightarrow 0^+} \int_{(\epsilon/\hbar v_F) + \delta}^{\Lambda} \frac{dk}{2\pi} \frac{\hbar}{\epsilon - \hbar v_F k} \\
 &\mp \frac{i}{2|v_F|} \int_{-\Lambda}^{\Lambda} dk \delta(k - (\epsilon/\hbar v_F)), \quad \text{set } v_F > 0 \text{ from now on.} \\
 &= -\frac{\lim_{\delta \rightarrow 0^+}}{2\pi v_F} \left(\ln |\epsilon - \hbar v_F k| \Big|_{-\Lambda}^{\frac{\epsilon}{\hbar v_F} - \delta} + \ln |\epsilon - \hbar v_F k| \Big|_{\frac{\epsilon}{\hbar v_F} + \delta}^{\Lambda} \right) \\
 &\mp \frac{i}{2v_F} (-1 + \theta(\epsilon + \hbar v_F \Lambda) - \theta(\epsilon - \hbar v_F \Lambda)) \\
 &= \frac{1}{2\pi v_F} \ln \left| \frac{\hbar v_F \Lambda + \epsilon}{\hbar v_F \Lambda - \epsilon} \right| \mp \frac{i}{2v_F} (-1 + \theta(\epsilon + \hbar v_F \Lambda) + \theta(\hbar v_F \Lambda - \epsilon))
 \end{aligned}$$

where the θ -functions here are defined with $\theta(x) = 1$ if $x \geq 0$ and zero otherwise to ensure the δ -function integral equals one if $-\Lambda \leq \epsilon/\hbar v_F \leq \Lambda$ and zero otherwise. For $\Lambda \rightarrow \infty$ we may treat $|\epsilon/\hbar v_F \Lambda| \ll 1$ as a small parameter:

$$\ln \left| \frac{1 + (\epsilon/\hbar v_F \Lambda)}{1 - (\epsilon/\hbar v_F \Lambda)} \right|$$

$$\begin{aligned}
 &= \left[\frac{\epsilon}{\hbar v_F \Lambda} - \frac{1}{2} \left(\frac{\epsilon}{\hbar v_F \Lambda} \right)^2 + \frac{1}{3} \left(\frac{\epsilon}{\hbar v_F \Lambda} \right)^3 - \dots \right] + \left[\frac{\epsilon}{\hbar v_F \Lambda} + \frac{1}{2} \left(\frac{\epsilon}{\hbar v_F \Lambda} \right)^2 + \frac{1}{3} \left(\frac{\epsilon}{\hbar v_F \Lambda} \right)^3 + \dots \right] \\
 &= 2 \sum_{n=0}^{\infty} \left(\frac{\epsilon}{\hbar v_F \Lambda} \right)^{2n+1} \\
 &= \frac{2\epsilon}{\hbar v_F \Lambda} + O[(\epsilon/\hbar v_F \Lambda)^3]
 \end{aligned}$$

which gives the lowest order approximation:

$$G_{co}^{r,a}(\epsilon) \approx \frac{\epsilon}{\pi \hbar v_F^2 \Lambda} \mp \frac{i}{2v_F}$$

⌊ Discarding the real part with $1/\Lambda$ is the wide-band limit. ■

The equilibrium Keldysh function $G_{co}^K(\epsilon)$ is:

$$G_{co}^K(\epsilon) = \frac{-i}{v_F} (1 - 2n_F(\epsilon)), \quad v_F > 0 \quad (\text{C.39})$$

⌈ *Proof.* Taking the Fourier transform of $G_{co(t,t';0)}^K = G_{co(t-t')}^K$ where we may set t' to zero, we find:

$$\begin{aligned}
 G_{co}^K(\epsilon) &= -i \int \frac{dk}{2\pi} (1 - 2n_F(\epsilon_k)) \int dt e^{i(\epsilon - \epsilon_k)t/\hbar} \\
 &= -i \int dk (1 - 2n_F(\hbar v_F k)) \frac{1}{|v_F|} \delta[k - (\epsilon/\hbar v_F)] \\
 &= -\frac{i}{v_F} (1 - 2n_F(\epsilon)), \quad v_F > 0,
 \end{aligned}$$

⌊ in agreement with the FDT: $G_{co(\epsilon)}^K = (G_{co(\epsilon)}^r - G_{co(\epsilon)}^a)(1 - 2n_F(\epsilon))$. ■

The retarded/advanced energy-domain version of $G_{dd}^{r,a}(t - t')$ is:

$$G_{dd}^{r,a}(\epsilon) = \frac{G_{do}^{r,a}(\epsilon)}{1 - \frac{g^2}{\hbar^2} G_{do}^{r,a}(\epsilon) G_{co}^{r,a}(\epsilon)} \quad (\text{C.40})$$

which reduces to the bare $G_{do}^{r,a}(\epsilon)$ function as $g \rightarrow 0$.

⌈ *Proof.*

$$\begin{aligned}
 &\int ds \hat{G}_{dd}^{r,a}(t, s)^{-1} G_{dd}^{r,a}(s, t') \\
 &= \int ds \left[\frac{1}{\hbar} \delta(t - s) (i\hbar \partial_s - \epsilon_d \pm i0^+) - \frac{g^2}{\hbar^2} G_{co}^{r,a}(t - s) \right] G_{dd}^{r,a}(s - t') \\
 &= \int \frac{d\epsilon}{2\pi\hbar} \left[\frac{1}{\hbar} (\epsilon - \epsilon_d \pm i0^+) G_{dd}^{r,a}(\epsilon) e^{-i\epsilon(t-t')/\hbar} \right. \\
 &\quad \left. - \frac{g^2}{\hbar^2} \int \frac{d\omega}{2\pi\hbar} G_{co}^{r,a}(\omega) G_{dd}^{r,a}(\epsilon) e^{-i(\omega t - \epsilon t')/\hbar} \int ds e^{-is(\epsilon - \omega)/\hbar} \right]
 \end{aligned}$$

$$\begin{aligned}
 &= \int \frac{d\epsilon}{2\pi\hbar} e^{-i\epsilon(t-t')/\hbar} (G_{do}^{r,a}(\epsilon)^{-1} - \frac{g^2}{\hbar^2} G_{co}^{r,a}(\epsilon)) G_{dd}^{r,a}(\epsilon) \\
 &= \int \frac{d\epsilon}{2\pi} e^{-i\epsilon(t-t')/\hbar} (G_{do}^{r,a}(\epsilon)^{-1} - \frac{g^2}{\hbar^2} G_{co}^{r,a}(\epsilon)) \frac{G_{do}^{r,a}(\epsilon)}{1 - \frac{g^2}{\hbar^2} G_{do}^{r,a}(\epsilon) G_{co}^{r,a}(\epsilon)} \\
 &= \delta(t-t')
 \end{aligned}$$

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The expression for $G_{dd}^{r,a}(\epsilon)$ is:

$$G_{dd}^{r,a}(\epsilon) \approx \frac{\hbar}{\epsilon - \epsilon_d \pm \frac{ig^2}{2\hbar v_F}}. \quad (\text{C.41})$$

┌ *Proof.*

$$\begin{aligned}
 &G_{dd}^{r,a}(\epsilon) \\
 &= \left(\frac{1}{\hbar} (\epsilon - \epsilon_d \pm i0^+) - \frac{g^2}{\hbar^2} G_{co}^{r,a}(\epsilon) \right)^{-1} \\
 &= \left\{ \frac{1}{\hbar} (\epsilon - \epsilon_d \pm i0^+) - \frac{g^2}{\hbar^2} \left[\frac{1}{2\pi v_F} \ln \left| \frac{\hbar v_F \Lambda + \epsilon}{\hbar v_F \Lambda - \epsilon} \right| \mp \frac{i}{2v_F} (-1 + \theta(\epsilon + \hbar v_F \Lambda) + \theta(\hbar v_F \Lambda - \epsilon)) \right] \right\}^{-1} \\
 &\approx \left[\frac{1}{\hbar} (\epsilon - \epsilon_d \pm i0^+) - \frac{g^2}{\hbar^2} \left(\frac{\epsilon}{\pi \hbar v_F^2 \Lambda} \mp \frac{i}{2v_F} \right) \right]^{-1} \\
 &\approx \hbar \left(\epsilon - \epsilon_d \pm \frac{ig^2}{2\hbar v_F} \right)^{-1}
 \end{aligned}$$

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The Keldysh function for the bare impurity is zero:

$$G_{do}^K(\epsilon) = 0. \quad (\text{C.42})$$

┌ *Proof.* Consider:

$$\begin{aligned}
 &\int_{-\infty}^{\infty} d\epsilon (G_{do}^r(\epsilon) - G_{do}^a(\epsilon)) = \int d\epsilon \lim_{\delta \rightarrow 0^+} \left[\frac{\hbar}{\epsilon - \epsilon_d + i\delta} - \frac{\hbar}{\epsilon - \epsilon_d - i\delta} \right] \\
 &= \lim_{\delta \rightarrow 0^+} \int d\epsilon \frac{-2i\hbar\delta}{(\epsilon - \epsilon_d)^2 + \delta^2}
 \end{aligned}$$

The integrand, call it $f(\epsilon)$, has two simple poles at $\epsilon_{\pm} = \epsilon_d \pm i\delta$. Integrating this anticlockwise around a semicircular contour with radius R over the upper-half complex plane, the semicircular arc contribution vanishes as $R \rightarrow \infty$ because $|f(z)| \leq a/|z|^2$ for sufficiently large $|z|$ where $a > 0 \in \mathbb{R}$. By the residue theorem the integration of $f(z)$ around the path therefore becomes

$$\int_{-\infty}^{\infty} d\epsilon \frac{-2i\hbar\delta}{(\epsilon - \epsilon_+)(\epsilon - \epsilon_-)} = 2\pi i \text{Res}_{\epsilon_+} f(z) = 2\pi i \lim_{z \rightarrow \epsilon_+} (z - \epsilon_+) \frac{-2i\hbar\delta}{(z - \epsilon_+)(z - \epsilon_-)} = 2\pi i \hbar \frac{-2i\delta}{2i\delta}$$

i.e. $\int_{-\infty}^{\infty} d\epsilon (G_{do}^r(\epsilon) - G_{do}^a(\epsilon)) = -2\pi i\hbar$ which suggests the identity:

$$G_{do}^r(\epsilon) - G_{do}^a(\epsilon) = -2\pi i\hbar\delta(\epsilon - \epsilon_d). \quad (\text{C.43})$$

In other words we have found the nascent δ -function:

$$\lim_{\delta \rightarrow 0^+} \frac{1}{\pi} \frac{\delta}{x^2 + \delta^2} = \delta(x).$$

Applying the fluctuation dissipation theorem therefore gives a dependence on the spectral function which is a δ -spike:

$$\begin{aligned} G_{do}^K(\epsilon) &= \tanh\left(\frac{\epsilon - \mu}{2k_B T}\right) (G_{do}^r(\epsilon) - G_{do}^a(\epsilon)) \\ &= -2\pi i\hbar \tanh\left(\frac{\epsilon - \mu}{2k_B T}\right) \delta(\epsilon - \epsilon_d) \end{aligned} \quad (\text{C.44})$$

⌊ Since the chemical potential for the quantum dot is ϵ_d , however, this is actually zero. ■

The Keldysh function for the dressed impurity, by contrast, is broadened:

$$G_{dd}^K(\epsilon) = \frac{-i\left(\frac{g^2}{v_F}\right)}{(\epsilon - \epsilon_d)^2 + \left(\frac{g^2}{2\hbar v_F}\right)^2} \tanh\left(\frac{\epsilon - \mu}{2k_B T}\right). \quad (\text{C.45})$$

⌈ *Proof.* Multiplying out the Dyson equation,

$$\left[\begin{pmatrix} (G_{do}^r)^{-1} & 2i0^+ F \\ 0 & (G_{do}^a)^{-1} \end{pmatrix} - \begin{pmatrix} \Sigma_d^r & \Sigma_d^K \\ 0 & \Sigma_d^a \end{pmatrix} \right] \circ \begin{pmatrix} G_{dd}^r & G_{dd}^K \\ 0 & G_{dd}^a \end{pmatrix} = \mathbb{1} \quad (\text{C.46})$$

gives

$$G_{dd}^K = G_{dd}^r \Sigma_d^K G_{dd}^a. \quad (\text{C.47})$$

By explicitly integrating out all lead electrons from the partition function, a similar but simpler calculation to the one shown in the section ‘Conversion to a local theory’, we can find the full self energy matrix. The reader is referred to that calculation for details of the procedure. The result is

$$Z = \mathcal{N} \int \mathcal{D}(d) e^{\frac{i}{\hbar} \int dt \int dt' \bar{d} \left[i\hbar \partial_t - \epsilon_d - \frac{g^2}{\hbar^2} \left(\frac{1}{L} \sum_k \frac{1}{i\hbar \partial_t - \epsilon_k(t)} \right) \right] d} \quad (\text{C.48})$$

We therefore determine that $\Sigma_d = \frac{g^2}{\hbar^2} G_{co}$, and so the Keldysh component is proportional to the Keldysh component for the lead. Simple multiplication gives the final result:

$$G_{dd}^K = \frac{g^2}{\hbar^2} G_{dd}^r G_{co}^K G_{dd}^a = \frac{-i\left(\frac{g^2}{v_F}\right)}{(\epsilon - \epsilon_d)^2 + \left(\frac{g^2}{2\hbar v_F}\right)^2} \tanh\left(\frac{\epsilon - \mu}{2k_B T}\right) \quad (\text{C.49})$$

⌋ ■

A note on SI units for the Green functions

In energy-space the units for the Green functions are $[G_{dd(\epsilon)}^{r,a,K}] = s$ and $[G_{co(\epsilon)}^{r,a,K}] = \frac{s}{m}$ by inspection of our results. The FT to move back to the time-domain is:

$$G_{dd,co}^{r,a,K}(t-t') = \int \frac{d\epsilon}{2\pi\hbar} e^{-i\frac{\epsilon}{\hbar}(t-t')} G_{dd,co}^{r,a,K}(\epsilon).$$

Consequently we find $[G_{dd}^{r,a,K}(t-t')] = \frac{J}{J_s} s = 1$ and $[G_{co}^{r,a,K}(t-t')] = \frac{J}{J_s} \frac{s}{m} = \frac{1}{m}$. This provides an easy way to check that each contribution in the perturbation series for the current has the correct units of Cs^{-1} .

C.3.3 Useful identities

Useful FT identity for I_0 and I_1 : The useful FT identity we referred to in the text for grinding down the integrals I_0 and I_1 is:

$$G_{dd,co(t-t')}^X G_{co,dd(t'-t)}^Y = \int \frac{d\omega}{2\pi\hbar} \int \frac{d\nu}{2\pi\hbar} G_{dd,co}^X(\nu) G_{co,dd}^Y(\nu - \omega) e^{-i\omega(t-t')/\hbar} \quad (\text{C.50})$$

┌ *Proof.*

$$\begin{aligned} & G_{dd,co(t-t')}^X G_{co,dd(t'-t)}^Y \\ &= \int dt_1 G_{dd,co}^X(-t_1) G_{co,dd}^Y(t_1) \delta(t_1 - t' + t) \\ &= \int dt_2 \int dt_1 G_{dd,co}^X(t_2) G_{co,dd}^Y(t_1) \delta(t_2 + t_1) \delta(t_1 - t' + t) \\ &= \int \frac{d(\omega/\hbar)}{2\pi} \int \frac{d(\nu/\hbar)}{2\pi} \int dt_2 \int dt_1 G_{dd,co}^X(t_2) G_{co,dd}^Y(t_1) e^{i(\nu/\hbar)(t_2+t_1)} e^{-i(\omega/\hbar)(t_1-t'+t)} \\ &= \int \frac{d\omega}{2\pi\hbar} \int \frac{d\nu}{2\pi\hbar} \left(\int dt_2 G_{dd,co}^X(t_2) e^{i\nu t_2/\hbar} \right) \left(\int dt_1 G_{co,dd}^Y(t_1) e^{i(\nu-\omega)t_1/\hbar} \right) e^{-i\omega(t-t')/\hbar} \\ &= \int \frac{d\omega}{2\pi\hbar} \int \frac{d\nu}{2\pi\hbar} G_{dd,co}^X(\nu) G_{co,dd}^Y(\nu - \omega) e^{-i\omega(t-t')/\hbar} \end{aligned}$$

└

■

Useful identities for I_2 : For the $I_2(t)$ integrals we went a step further and stated formulae for just immediately converting four time integrals to a single energy integral.

$$\begin{aligned} & \int dt' \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) a_{1(t-t_1)} a_{2(t_1-t_2)} a_{3(t_2-t')} a_{4(t'-t)} \\ &= \frac{-iV_0}{4\pi\hbar\omega_0} \int d\epsilon a_{1(\epsilon)} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} (a_{2(\epsilon-\zeta\hbar\omega_0)} - a_{2(\epsilon)}) a_{3(\epsilon-\zeta\hbar\omega_0)} a_{4(\epsilon-\zeta\hbar\omega_0)}, \quad (\text{C.51}) \end{aligned}$$

and

$$\begin{aligned} & \int dt' \int dt_1 \int dt_2 \left(\int_{t_1}^{t_2} ds V(s) \right) a_{1(t-t')} a_{2(t'-t_1)} a_{3(t_1-t_2)} a_{4(t_2-t)} \\ &= \frac{-iV_0}{4\pi\hbar\omega_0} \int d\epsilon a_{1(\epsilon)} a_{2(\epsilon)} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} (a_{3(\epsilon-\zeta\hbar\omega_0)} - a_{3(\epsilon)}) a_{4(\epsilon-\zeta\hbar\omega_0)}, \quad (\text{C.52}) \end{aligned}$$

We will only show a sketch proof for (C.51) as the proof for (C.52) is very similar.

□ *Proof.* Let the LHS of (C.51) be called A. The s -integral is

$$\int_{t_1}^{t_2} ds V(s) = \frac{V_0}{2i\omega_0} (e^{i\omega_0 t_2} - e^{-i\omega_0 t_2} - e^{i\omega_0 t_1} + e^{-i\omega_0 t_1}) \quad (\text{C.53})$$

and therefore all of the remaining time integrals reduce to δ -functions by using the Fourier transforms for each $a_{\{i\}}$.

$$\begin{aligned} A = & \frac{-iV_0}{4\pi\hbar\omega_0} \int d\epsilon_1 \int d\epsilon_2 \int d\epsilon_3 \int d\epsilon_4 \int d\epsilon_1 \int d\epsilon_4 a_1(\epsilon_1) a_2(\epsilon_2) a_3(\epsilon_3) a_4(\epsilon_4) e^{-it(\epsilon_1 - \epsilon_4)} \{ \\ & \delta(\epsilon_4 - \epsilon_3) [\delta(\epsilon_2 - \epsilon_1) (\delta(\epsilon_3 - \epsilon_2 - \hbar\omega_0) - \delta(\epsilon_3 - \epsilon_2 + \hbar\omega_0)) \\ & - \delta(\epsilon_3 - \epsilon_2) (\delta(\epsilon_2 - \epsilon_1 - \hbar - \omega_0) - \delta(\epsilon_2 - \epsilon_1 + \hbar\omega_0))] \} \end{aligned} \quad (\text{C.54})$$

From this point it is just a process of using up the δ -functions and noticing a symmetry with $\omega_0 \rightarrow -\omega_0$ in the expression in order to write the sum over ζ . ■

C.4 The $I_1(t)$ calculation

For the integral $I_1(t)$, consider the Fourier transform $\tilde{I}_1(\omega)$:

$$\tilde{I}_1(\omega) = \frac{-ie^2 g^2}{2\hbar^3} \int dt \int dt' \left(\int_{t'}^t ds V(s) \right) e^{i\omega t/\hbar} \int \frac{d\epsilon_1}{2\pi\hbar} \int \frac{d\epsilon_2}{2\pi\hbar} e^{-i\epsilon_2(t-t')/\hbar} f(\epsilon_1, \epsilon_2) \quad (\text{C.55})$$

where we have defined a new function f :

$$f(\epsilon_1, \epsilon_2) = G_{dd(\epsilon_1)}^r G_{co(\epsilon_1 - \epsilon_2)}^K + G_{dd(\epsilon_1)}^K G_{co(\epsilon_1 - \epsilon_2)}^a + G_{co(\epsilon_1)}^r G_{dd(\epsilon_1 - \epsilon_2)}^K + G_{co(\epsilon_1)}^K G_{dd(\epsilon_1 - \epsilon_2)}^a. \quad (\text{C.56})$$

Focusing on the temporal integrals, the integral over s is

$$\int_{t'}^t ds V(s) = \frac{V_0}{2i\omega_0} (e^{i\omega_0 t} - e^{-i\omega_0 t} - e^{i\omega_0 t'} + e^{-i\omega_0 t'}) \quad (\text{C.57})$$

and therefore all of the time integrals in (C.55) reduce to δ -functions:

$$\begin{aligned} & \int \frac{dt}{2\pi\hbar} \int \frac{dt'}{2\pi\hbar} \left(\int_{t'}^t ds V(s) \right) e^{i\omega t/\hbar} e^{-i\epsilon_2(t-t')/\hbar} \\ &= \frac{V_0}{2i\omega_0} \int \frac{dt}{2\pi\hbar} \int \frac{dt'}{2\pi\hbar} (e^{i(\omega + \hbar\omega_0 - \epsilon_2)t/\hbar} e^{i\epsilon_2 t'/\hbar} - e^{i(\omega - \hbar\omega_0 - \epsilon_2)t/\hbar} e^{i\epsilon_2 t'/\hbar} - e^{i(\omega - \epsilon_2)t/\hbar} e^{i(\hbar\omega_0 + \epsilon_2)t'/\hbar} \\ &+ e^{i(\omega - \epsilon_2)t/\hbar} e^{i(\epsilon_2 - \hbar\omega_0)t'/\hbar}) \\ &= \frac{V_0}{2i\omega_0} (\delta(\omega - \epsilon_2 + \hbar\omega_0)\delta(\epsilon_2) - \delta(\omega - \epsilon_2 - \hbar\omega_0)\delta(\epsilon_2) - \delta(\epsilon_2 + \hbar\omega_0)\delta(\omega - \epsilon_2) \\ &+ \delta(\epsilon_2 - \hbar\omega_0)\delta(\omega - \epsilon_2)) \end{aligned} \quad (\text{C.58})$$

So far we have

$$\begin{aligned} \tilde{I}_1(\omega) = & \frac{-V_0 e^2 g^2}{4\hbar^3 \omega_0} \int d\epsilon_1 \int d\epsilon_2 (\delta(\hbar\omega_0 + \omega - \epsilon_2)\delta(\epsilon_2) - \delta(\omega - \hbar\omega_0 - \epsilon_2)\delta(\epsilon_2) \\ & - \delta(\epsilon_2 + \hbar\omega_0)\delta(\omega - \epsilon_2) + \delta(\epsilon_2 - \hbar\omega_0)\delta(\omega - \epsilon_2)) f(\epsilon_1, \epsilon_2) \end{aligned} \quad (\text{C.59})$$

Next we can complete the ω -integral and the ϵ_2 -integral via the δ -functions:

$$\begin{aligned}
 I_1(t) &= \int \frac{d\omega}{2\pi\hbar} e^{-i\omega t/\hbar} \tilde{I}_1(\omega) \\
 &= \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \int d\epsilon_1 \int d\epsilon_2 [(e^{-i(\epsilon_2 - \hbar\omega_0)t/\hbar} - e^{-i(\epsilon_2 + \hbar\omega_0)t/\hbar}) \delta(\epsilon_2) - e^{-i\epsilon_2 t/\hbar} \delta(\epsilon_2 + \hbar\omega_0) \\
 &\quad + e^{-i\epsilon_2 t/\hbar} \delta(\epsilon_2 - \hbar\omega_0)] f(\epsilon_1, \epsilon_2) \\
 &= \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \left[e^{i\omega_0 t} \int d\epsilon (f(\epsilon, 0) - f(\epsilon, -\hbar\omega_0)) - e^{-i\omega_0 t} \int d\epsilon (f(\epsilon, 0) - f(\epsilon, \hbar\omega_0)) \right] \\
 &= \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \sum_{\zeta \in (-1, 1)} \zeta e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon (f(\epsilon, \zeta\hbar\omega_0) - f(\epsilon, 0)) \tag{C.60}
 \end{aligned}$$

The reorganisation of the ϵ -integral into the pieces h_1 and h_2 is:

$$\begin{aligned}
 &\int d\epsilon (f(\epsilon, \zeta\hbar\omega_0) - f(\epsilon, 0)) \\
 &= \int d\epsilon \left[G_{dd}^r(\epsilon) G_{co(\epsilon - \zeta\hbar\omega_0)}^K + G_{dd}^K(\epsilon) G_{co(\epsilon - \zeta\hbar\omega_0)}^a + G_{co(\epsilon)}^r G_{dd(\epsilon - \zeta\hbar\omega_0)}^K + G_{co(\epsilon)}^K G_{dd(\epsilon - \zeta\hbar\omega_0)}^a \right. \\
 &\quad \left. - (G_{dd}^r(\epsilon) G_{co(\epsilon)}^K + G_{dd}^K(\epsilon) G_{co(\epsilon)}^a + G_{co(\epsilon)}^r G_{dd(\epsilon)}^K + G_{co(\epsilon)}^K G_{dd(\epsilon)}^a) \right] \\
 &= \int d\epsilon G_{dd}^K(\epsilon) (G_{co(\epsilon + \zeta\hbar\omega_0)}^r + G_{co(\epsilon - \zeta\hbar\omega_0)}^a - G_{co(\epsilon)}^r - G_{co(\epsilon)}^a) \\
 &\quad + \int d\epsilon G_{co(\epsilon)}^K (G_{dd(\epsilon + \zeta\hbar\omega_0)}^r - G_{dd(\epsilon)}^r + G_{dd(\epsilon - \zeta\hbar\omega_0)}^a - G_{dd(\epsilon)}^a) \\
 &= \int d\epsilon (h_1(\epsilon, \zeta\hbar\omega_0) + \int d\epsilon h_2(\epsilon, \zeta\hbar\omega_0)) \tag{C.61}
 \end{aligned}$$

where along the way we made constant shifts to the integration variables in order to factor out the $G_{co,dd}^K(\epsilon)$ in front. So far the integral for $I_1(t)$ has been reduced to:

$$I_1(t) = \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \sum_{\zeta \in (-1, 1)} \zeta e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon (h_1(\epsilon, \zeta\hbar\omega_0) + h_2(\epsilon, \zeta\hbar\omega_0)). \tag{C.62}$$

For the first piece the integrand is vanishingly small with the UV cutoff Λ .

$$\begin{aligned}
 &h_1(\epsilon, \zeta\hbar\omega_0) \\
 &= G_{dd}^K(\epsilon) \left\{ \frac{1}{2\pi v_F} \ln \left[\frac{(\hbar v_F \Lambda + \epsilon + \zeta\hbar\omega_0)(\hbar v_F \Lambda + \epsilon - \zeta\hbar\omega_0)}{(\hbar v_F \Lambda - \epsilon - \zeta\hbar\omega_0)(\hbar v_F \Lambda - \epsilon + \zeta\hbar\omega_0)} \right] - \frac{1}{\pi v_F} \ln \left(\frac{\hbar v_F \Lambda + \epsilon}{\hbar v_F \Lambda - \epsilon} \right) \right\} \\
 &= \frac{-i(\frac{g^2}{v_F})}{(\epsilon - \epsilon_d)^2 + (\frac{g^2}{2\hbar v_F})^2} \tanh \left(\frac{\epsilon - \mu}{2k_B T} \right) \sum_{\zeta} \zeta e^{-i\zeta\omega_0 t} \\
 &\quad \cdot \ln \left[\frac{(\hbar v_F \Lambda + \epsilon + \zeta\hbar\omega_0)(\hbar v_F \Lambda + \epsilon - \zeta\hbar\omega_0)}{(\hbar v_F \Lambda - \epsilon - \zeta\hbar\omega_0)(\hbar v_F \Lambda - \epsilon + \zeta\hbar\omega_0)} \left(\frac{\hbar v_F \Lambda + \epsilon}{\hbar v_F \Lambda - \epsilon} \right)^2 \right] \\
 &\propto -2 \sin(\omega_0 t) \ln \left[\frac{(\hbar v_F \Lambda + \epsilon + \hbar\omega_0)(\hbar v_F \Lambda + \epsilon - \hbar\omega_0)}{(\hbar v_F \Lambda - \epsilon - \hbar\omega_0)(\hbar v_F \Lambda - \epsilon + \hbar\omega_0)} \left(\frac{\hbar v_F \Lambda + \epsilon}{\hbar v_F \Lambda - \epsilon} \right)^2 \right] \\
 &\propto \frac{-10 \sin(\omega_0 t)}{v_F} \frac{\epsilon}{\hbar v_F \Lambda} + O[(\epsilon/\hbar v_F \Lambda)^3] \rightarrow 0 \quad \text{as } \Lambda \rightarrow \infty. \tag{C.63}
 \end{aligned}$$

C.4. The $I_1(t)$ calculation

Alternatively, by keeping just the lowest order approximation in $(\epsilon/\hbar v_F \Lambda)$ for the functions $G_{co(\epsilon)}^{r,a}$ one immediately finds:

$$G_{co(\epsilon+\zeta\hbar\omega_0)}^r + G_{co(\epsilon-\zeta\hbar\omega_0)}^a - G_{co(\epsilon)}^r - G_{co(\epsilon)}^a \approx \frac{\epsilon + \zeta\hbar\omega_0}{\pi\hbar v_F^2 \Lambda} + \frac{\epsilon - \zeta\hbar\omega_0}{\pi\hbar v_F^2 \Lambda} - \frac{\epsilon}{\pi\hbar v_F^2 \Lambda} - \frac{\epsilon}{\pi\hbar v_F^2 \Lambda} = 0 \quad (\text{C.64})$$

so we can be convinced that there is no contribution from h_1 . We are therefore left with:

$$\begin{aligned} I_1(t) &= \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \sum_{\zeta \in (-1,1)} \zeta e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon h_2(\epsilon, \zeta\hbar\omega_0) \\ &= \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \sum_{\zeta \in (-1,1)} \zeta e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon G_{co(\epsilon)}^K (G_{dd(\epsilon+\zeta\hbar\omega_0)}^r - G_{dd(\epsilon)}^r + G_{dd(\epsilon-\zeta\hbar\omega_0)}^a - G_{dd(\epsilon)}^a) \end{aligned} \quad (\text{C.65})$$

Consider:

$$\begin{aligned} G_{dd(\epsilon+\alpha\zeta\hbar\omega_0)}^{\xi_\alpha} - G_{dd(\epsilon)}^{\xi_\alpha} &= \frac{\hbar}{\epsilon - \epsilon_d + i\alpha\frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0} - \frac{\hbar}{\epsilon - \epsilon_d + i\alpha\frac{g^2}{2\hbar v_F}} \\ &= \frac{-\alpha\zeta\hbar^2\omega_0}{(\epsilon - \epsilon_d + i\alpha\frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon - \epsilon_d + i\alpha\frac{g^2}{2\hbar v_F})} \end{aligned} \quad (\text{C.66})$$

where $\xi_\alpha \in (\xi_{-1}, \xi_1) = (a, r)$, so α takes values ± 1 correspondingly. Plugging in the Green functions, $I_1(t)$ becomes:

$$\begin{aligned} I_1(t) &= \frac{-V_0 e^2 g^2}{8\pi\hbar^4 \omega_0} \sum_{\zeta, \alpha = -1,1} \zeta e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon \frac{(1 - 2n_F(\epsilon + \epsilon_d))}{iv_F} \frac{-\alpha\zeta\hbar^2\omega_0}{(\epsilon + i\alpha\frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\alpha\frac{g^2}{2\hbar v_F})} \\ &= \frac{iV_0 e^2 g^2}{4\pi\hbar^2 v_F} \sum_{\zeta, \alpha = -1,1} \alpha e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} d\epsilon \frac{n_F(\epsilon + \epsilon_d)}{(\epsilon + i\alpha\frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\alpha\frac{g^2}{2\hbar v_F})} \end{aligned} \quad (\text{C.67})$$

$$= \frac{iV_0 e^2 g^2}{4\pi\hbar^2 v_F} \sum_{\zeta = -1,1} e^{-i\zeta\omega_0 t} X_\zeta, \quad (\text{C.68})$$

where

$$X_\zeta = \sum_{\alpha = -1,1} \alpha \int_{-\infty}^{\infty} d\epsilon \frac{n_F(\epsilon + \epsilon_d)}{(\epsilon + i\frac{\alpha g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\frac{\alpha g^2}{2\hbar v_F})} \quad (\text{C.69})$$

One integral has been immediately discarded because all poles lie in one half of the complex plane (so we can enclose the other half with a semi-circular contour in the usual manner to give zero by Cauchy-Goursat). By transferring to a Matsubara sum we can trade the coefficient named X_ζ for infinite sums by further treatment with the residue theorem. The Matsubara form of the Fermi function is

$$n_F(\epsilon) = \frac{k_B T}{\hbar} \sum_n \frac{1}{i\omega_n - (\epsilon - \mu)/\hbar}, \quad \omega_n = \pi(2n + 1)k_B T/\hbar, \quad n = 0, \pm 1, \pm 2, \dots, \quad (\text{C.70})$$

This gives:

$$\begin{aligned}
 X_\zeta &= \sum_{\alpha=-1,1} \alpha \int_{-\infty}^{\infty} d\epsilon \frac{n_F(\epsilon + \epsilon_d)}{(\epsilon + i\frac{\alpha g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\frac{\alpha g^2}{2\hbar v_F})} \\
 &= k_B T \sum_{\alpha=-1,1} \alpha \sum_{n=-\infty}^{\infty} \int d\epsilon \frac{-1}{\epsilon - (i\hbar\omega_n - \epsilon_d + \mu)} \frac{1}{(\epsilon + i\frac{\alpha g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\frac{\alpha g^2}{2\hbar v_F})} \\
 &= -k_B T \sum_{\alpha=-1,1} \alpha \left(\sum_{n \geq 0} + \sum_{n < 0} \right) \int d\epsilon \frac{1}{[\epsilon - (i\hbar\omega_n - \epsilon_d + \mu)](\epsilon + i\frac{\alpha g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\frac{\alpha g^2}{2\hbar v_F})} \tag{C.71}
 \end{aligned}$$

Using $\sum_{n < 0} g(i\omega_n) = \sum_{n \geq 0} g(-i\omega_n)$ for fermionic Matsubara frequencies gives:

$$\begin{aligned}
 X_\zeta &= -k_B T \sum_{\alpha=-1,1} \alpha \sum_{n \geq 0} \int d\epsilon \left[\frac{1}{[\epsilon - (i\hbar\omega_n - \epsilon_d + \mu)](\epsilon + i\frac{\alpha g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\frac{\alpha g^2}{2\hbar v_F})} \right. \\
 &\quad \left. + \frac{1}{[\epsilon - (-i\hbar\omega_n - \epsilon_d + \mu)](\epsilon + i\frac{\alpha g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\frac{\alpha g^2}{2\hbar v_F})} \right] \tag{C.72}
 \end{aligned}$$

The integral for the first line has poles only in the upper-half plane for $\alpha = -1$, for any given n , so in this case it vanishes by taking the semi-circular contour in the lower-half plane. The integral for the second line vanishes by a similar reasoning for $\alpha = 1$. So we can sum over α at this point. This leaves:

$$\begin{aligned}
 X_\zeta &= -k_B T \sum_{n \geq 0} \int d\epsilon \left[\frac{1}{[\epsilon - i\hbar\omega_n + \epsilon_d - \mu](\epsilon + i\frac{g^2}{2\hbar v_F} + \zeta\hbar\omega_0)(\epsilon + i\frac{g^2}{2\hbar v_F})} \right. \\
 &\quad \left. - \frac{1}{[\epsilon + i\hbar\omega_n + \epsilon_d - \mu](\epsilon - i\frac{g^2}{2\hbar v_F} - \zeta\hbar\omega_0)(\epsilon - i\frac{g^2}{2\hbar v_F})} \right] \tag{C.73}
 \end{aligned}$$

By further application of the residue theorem we may show:

$$\begin{aligned}
 &\int_{-\infty}^{\infty} d\epsilon \frac{1}{[\epsilon + \epsilon_d - \mu - i\pi k_B T(2n + 1)](\epsilon + i\frac{g^2}{2\hbar v_F} + \zeta\hbar\omega_0)(\epsilon + i\frac{g^2}{2\hbar v_F})} \\
 &= \frac{-2\pi i}{(\frac{g^2}{2\hbar v_F} + \pi k_B T(2n + 1) + i(\epsilon - \mu))(\frac{g^2}{2\hbar v_F} + \pi k_B T(2n + 1) + i(\epsilon - \mu - \zeta\hbar\omega_0))} \tag{C.74}
 \end{aligned}$$

and

$$\begin{aligned}
 &\int_{-\infty}^{\infty} d\epsilon \frac{1}{[\epsilon + \epsilon_d - \mu + i\pi k_B T(2n + 1)](\epsilon - i\frac{g^2}{2\hbar v_F} - \zeta\hbar\omega_0)(\epsilon - i\frac{g^2}{2\hbar v_F})} \\
 &= \frac{2\pi i}{(\frac{g^2}{2\hbar v_F} + \pi k_B T(2n + 1) - i(\epsilon - \mu))(\frac{g^2}{2\hbar v_F} + \pi k_B T(2n + 1) - i(\epsilon - \mu + \zeta\hbar\omega_0))}. \tag{C.75}
 \end{aligned}$$

After substituting these last two results into (C.73) the sum over n can be converted into digamma functions Ψ by using the relation:

$$\sum_{n=0}^{\infty} \frac{1}{(n+a)(n+b)} = \frac{1}{a-b} [\Psi(a) - \Psi(b)]. \tag{C.76}$$

This gives:

$$I_1(t) = \frac{V_0 e^2 g^2}{4\pi \hbar^2 v_F} \sum_{\zeta=-1,1} i e^{-i\zeta\omega_0 t} X_\zeta \quad (\text{C.77})$$

where:

$$X_\zeta = \frac{-\zeta}{\hbar\omega_0} \left\{ \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu - \zeta\hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] + \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} - i(\epsilon_d - \mu + \zeta\hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} - i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \right\} \quad (\text{C.78})$$

For brevity let us use a shorthand notation:

$$\psi(x, y) = \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + ix(\epsilon_d - \mu + y)}{2\pi k_B T} \right) \quad (\text{C.79})$$

The conjugation property for polygamma functions $\Psi^{(n)}(z^*) = [\Psi^{(n)}(z)]^*$ implies that the following holds:

$$\psi^{(n)}(+, y) = [\psi^{(n)}(-, y)]^* \quad (\text{C.80})$$

where $+$ ($-$) in the arguments alone indicates 1 (-1). Consider taking the conjugate for the $\zeta = 1$ term in the sum over ζ :

$$\begin{aligned} & \left\{ i e^{-i\omega_0 t} \left(\frac{-1}{\hbar\omega_0} \right) [(\psi(+, -\hbar\omega_0) - \psi(+, 0)) + (\psi(-, \hbar\omega_0) - \psi(-, 0))] \right\}^* \\ &= i e^{i\omega_0 t} \left(\frac{1}{\hbar\omega_0} \right) [(\psi(-, -\hbar\omega_0) - \psi(-, 0)) + (\psi(+, \hbar\omega_0) - \psi(+, 0))]. \end{aligned} \quad (\text{C.81})$$

But this is exactly the $\zeta = -1$ term so we are adding a function to its complex conjugate in (C.65). With some further algebra we arrive at:

$$\begin{aligned} I_1(t) &= \frac{eV_0}{\hbar\omega_0} \frac{e \cdot \left(\frac{g^2}{2\hbar v_F} \right)}{\pi \hbar} \text{Im} \left\{ e^{-i\omega_0 t} [\psi(+, -\hbar\omega_0) - \psi(+, 0) + \psi(-, \hbar\omega_0) - \psi(-, 0)] \right\} \\ &= \frac{eV_0}{\hbar\omega_0} \frac{e \cdot \left(\frac{g^2}{2\hbar v_F} \right)}{\pi \hbar} \text{Im} \left\{ e^{-i\omega_0 t} \sum_{\alpha=1,-1} [\psi(\alpha, -\alpha\hbar\omega_0) - \psi(\alpha, 0)] \right\} \end{aligned} \quad (\text{C.82})$$

In hindsight we could have rewritten the integral before integration to arrive at this result with less effort. Picking up from (C.65) we rewrite it as:

$$I_1(t) = \frac{-V_0 e^2 g^2}{4\pi \hbar^4 \omega_0} \text{Re} \left[e^{-i\omega_0 t} \int_{-\infty}^{\infty} d\epsilon G_{co(\epsilon)}^K (G_{dd(\epsilon+\hbar\omega_0)}^r - G_{dd(\epsilon)}^r + G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a) \right] \quad (\text{C.83})$$

by using the properties $G^r = (G^a)^*$ and $G^K = -(G^K)^*$.

C.4.1 $I_1(t)$ dc limit

For the dc limit we may continue from (C.77)-(C.78). By grouping terms appropriately we notice that the limit $\omega_0 \rightarrow 0$ just gives the definition of the derivative, e.g.:

$$\begin{aligned} & \lim_{\omega_0 \rightarrow 0} \frac{1}{\omega_0} \left[\Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu - \hbar\omega_0)}{2\pi k_B T} \right) - \Psi \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \\ &= \frac{-i\hbar}{2\pi k_B T} \Psi^{(1)} \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu)}{2\pi k_B T} \right). \end{aligned} \quad (\text{C.84})$$

where $\Psi^{(n)}$ is the n^{th} derivative of the digamma function ($\Psi^{(1)}$ is the ‘trigamma’), along with one for each $e^{\pm i\omega_0 t}$ factor. In general, using the shorthand ψ , we have:

$$\lim_{\omega_0 \rightarrow 0} \frac{\psi(\alpha, \beta\hbar\omega_0) - \psi(\alpha, 0)}{\omega_0} = i \frac{\alpha\beta\hbar}{2\pi k_B T} \psi^{(1)}(\alpha, 0) \quad (\text{C.85})$$

Repeated reapplication of this leads to:

$$I_{1,\text{dc}} = -V_0 \frac{2e^2}{\pi\hbar} \frac{g^2}{2\pi k_B T} \text{Re} \left[\Psi^{(1)} \left(\frac{1}{2} + \frac{\frac{g^2}{2\hbar v_F} + i(\epsilon_d - \mu)}{2\pi k_B T} \right) \right] \quad (\text{C.86})$$

C.4.2 $I_1(t)$ zero temperature limit:

Picking up from (C.67) we can find the zero temperature limit $I_1(t, T) \rightarrow I_1(t, 0)$.

$$\begin{aligned} I_1(t, 0) &= \frac{iV_0 e^2 g^2}{4\pi\hbar^2 v_F} \sum_{\zeta, \alpha=-1,1} \alpha e^{-i\zeta\omega_0 t} \int_{-\infty}^{\mu-\epsilon_d} d\epsilon \frac{1}{(\epsilon + i\alpha \frac{g^2}{2\hbar v_F} + \alpha\zeta\hbar\omega_0)(\epsilon + i\alpha \frac{g^2}{2\hbar v_F})} \\ &= \frac{ie^2 g^2 V_0}{4\pi\hbar^2 v_F} \sum_{\zeta} e^{-i\zeta\omega_0 t} \int_{-\infty}^{\mu-\epsilon_d} d\epsilon \frac{-2\epsilon(\epsilon_1 + \epsilon_2)}{(\epsilon^2 - \epsilon_1^2)(\epsilon^2 - \epsilon_2^2)}, \quad \text{where } \epsilon_1 = \frac{ig^2}{2\hbar v_F} + \zeta\hbar\omega_0, \quad \epsilon_2 = \frac{ig^2}{2\hbar v_F} \\ &= \frac{ie^2 g^2 V_0}{4\pi\hbar^2 v_F} \sum_{\zeta} e^{-i\zeta\omega_0 t} \left[\frac{\ln(\epsilon^2 - \epsilon_1^2) - \ln(\epsilon^2 - \epsilon_2^2)}{\epsilon_1 - \epsilon_2} \right] \Big|_{-\infty}^{\mu-\epsilon_d}, \quad \text{for } \omega_0 \neq 0 \\ &= \frac{ie^2 g^2 V_0}{4\pi\hbar^3 v_F \omega_0} \sum_{\zeta} \zeta e^{-i\zeta\omega_0 t} \ln \left(\frac{\epsilon^2 - [(ig^2/2\hbar v_F) + \zeta\hbar\omega_0]^2}{\epsilon^2 - (\frac{ig^2}{2\hbar v_F})^2} \right) \Big|_{-\infty}^{\mu-\epsilon_d} \\ &= \frac{ie^2 g^2 V_0}{4\pi\hbar^3 v_F \omega_0} \left[e^{-i\omega_0 t} \ln \left(\frac{\epsilon^2 - (\frac{ig^2}{2\hbar v_F} + \hbar\omega_0)^2}{\epsilon^2 - (\frac{ig^2}{2\hbar v_F})^2} \right) - e^{i\omega_0 t} \ln \left(\frac{\epsilon^2 - (\frac{ig^2}{2\hbar v_F} - \hbar\omega_0)^2}{\epsilon^2 - (\frac{ig^2}{2\hbar v_F})^2} \right) \right] \Big|_{-\infty}^{\mu-\epsilon_d} \\ &= \frac{ie^2 g^2 V_0}{4\pi\hbar^3 v_F \omega_0} \left\{ e^{-i\omega_0 t} \ln \left[\frac{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F} + \hbar\omega_0)^2}{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F})^2} \right] - e^{i\omega_0 t} \ln \left[\frac{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F} - \hbar\omega_0)^2}{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F})^2} \right] \right. \\ &\quad \left. - \lim_{D \rightarrow \infty} \left[e^{-i\omega_0 t} \ln \left(\frac{D^2 - (\frac{ig^2}{2\hbar v_F} + \hbar\omega_0)^2}{D^2 - (\frac{ig^2}{2\hbar v_F})^2} \right) - e^{i\omega_0 t} \ln \left(\frac{D^2 - (\frac{ig^2}{2\hbar v_F} - \hbar\omega_0)^2}{D^2 - (\frac{ig^2}{2\hbar v_F})^2} \right) \right] \right\} \\ &= \frac{ie^2 g^2 V_0}{4\pi\hbar^3 v_F \omega_0} \left\{ e^{-i\omega_0 t} \ln \left[\frac{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F} + \hbar\omega_0)^2}{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F})^2} \right] - e^{i\omega_0 t} \ln \left[\frac{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F} - \hbar\omega_0)^2}{(\epsilon_d - \mu)^2 - (\frac{ig^2}{2\hbar v_F})^2} \right] \right\} \end{aligned} \quad (\text{C.87})$$

1CK mapping at $T = 0$

To map onto the single channel Kondo model at the Toulouse limit we can set $\mu = \epsilon_d$.

$$\begin{aligned} I_1^{\text{1CK}}(t) &= \frac{ie^2 g^2 V_0}{4\pi \hbar^3 v_F \omega_0} \left[e^{-i\omega_0 t} \ln \left(\frac{(\frac{ig^2}{2\hbar v_F} + \hbar\omega_0)^2}{(\frac{ig^2}{2\hbar v_F})^2} \right) - e^{i\omega_0 t} \ln \left(\frac{(\frac{ig^2}{2\hbar v_F} - \hbar\omega_0)^2}{(\frac{ig^2}{2\hbar v_F})^2} \right) \right] \\ &= \frac{ie^2 g^2 V_0}{2\pi \hbar^3 v_F \omega_0} \left[e^{-i\omega_0 t} \ln \left(1 - \frac{2i\hbar^2 v_F \omega_0}{g^2} \right) - e^{i\omega_0 t} \ln \left(1 + \frac{2i\hbar^2 v_F \omega_0}{g^2} \right) \right] \end{aligned} \quad (\text{C.88})$$

For the dc limit ($\omega_0 \rightarrow 0$) we may use standard Taylor expansions for the logarithms since we satisfy the condition $\left| \frac{2i\hbar^2 \omega_0 v_F}{g^2} \right| < 1$.

$$\begin{aligned} I_{1, \text{dc}}^{\text{1CK}}(T \rightarrow 0) &= \lim_{\omega_0 \rightarrow 0} \frac{ie^2 g^2 V_0}{2\pi \hbar^3 v_F \omega_0} \left[(1 - i\omega_0 t + \dots) \left(-\frac{2i\hbar^2 \omega_0 v_F}{g^2} - \frac{1}{2} \left(\frac{2i\hbar^2 \omega_0 v_F}{g^2} \right)^2 + \dots \right) - (\omega_0 \rightarrow -\omega_0) \right] \\ &= \lim_{\omega_0 \rightarrow 0} \frac{ie^2 g^2 V_0}{2\pi \hbar^3 v_F \omega_0} \left[-\frac{4i\hbar^2 \omega_0 v_F}{g^2} + \mathcal{O}(\omega_0^2) \right] \\ &= \frac{4e^2 V_0}{h} \end{aligned} \quad (\text{C.89})$$

C.5 The $I_2(t)$ calculation

Resuming from the integral in energy space, derived by the ‘useful identities’ described earlier in this appendix, we isolated a non-vanishing part called h_3 leading to the expression:

$$I_2(t) = \frac{-e^2 g^4 V_0}{8\pi \hbar^6 \omega_0} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} \int dh_3(\epsilon, \zeta\hbar\omega_0) \quad (\text{C.90})$$

with:

$$h_3(\epsilon_1, \epsilon_2) = \sum_{\alpha=1,-1} G_{co(\epsilon_1)}^K G_{dd(\epsilon_1)}^{\xi\alpha} (G_{co(\epsilon_1)}^{\xi\alpha} - G_{co(\epsilon_1-\alpha\epsilon_2)}^{\xi-\alpha}) G_{dd(\epsilon_1-\alpha\epsilon_2)}^{\xi-\alpha} \quad (\text{C.91})$$

Consider the fragment $S(\epsilon) = \sum_{\zeta, \alpha=-1,1} \zeta e^{-i\zeta\omega_0 t} h_3(\epsilon, \alpha\zeta\hbar\omega_0)$:

$$\begin{aligned} S(\epsilon) &= \sum_{\zeta, \alpha=-1,1} \zeta e^{-i\zeta\omega_0 t} G_{co(\epsilon)}^K G_{dd(\epsilon)}^{\xi\alpha} (G_{co(\epsilon)}^{\xi\alpha} - G_{co(\epsilon-\alpha\zeta\hbar\omega_0)}^{\xi-\alpha}) G_{dd(\epsilon-\alpha\zeta\hbar\omega_0)}^{\xi-\alpha} \\ &= e^{-i\omega_0 t} [G_{dd(\epsilon)}^r (G_{co(\epsilon)}^r - G_{co(\epsilon-\hbar\omega_0)}^a) G_{dd(\epsilon-\hbar\omega_0)}^a + G_{dd(\epsilon)}^a (G_{co(\epsilon)}^a - G_{co(\epsilon+\hbar\omega_0)}^r) G_{dd(\epsilon+\hbar\omega_0)}^r] G_{co(\epsilon)}^K \\ &\quad - e^{i\omega_0 t} [G_{dd(\epsilon)}^r (G_{co(\epsilon)}^r - G_{co(\epsilon+\hbar\omega_0)}^a) G_{dd(\epsilon+\hbar\omega_0)}^a + G_{dd(\epsilon)}^a (G_{co(\epsilon)}^a - G_{co(\epsilon-\hbar\omega_0)}^r) G_{dd(\epsilon-\hbar\omega_0)}^r] G_{co(\epsilon)}^K \end{aligned} \quad (\text{C.92})$$

Using the identities $(G_{dd(\epsilon)}^r)^* = G_{dd(\epsilon)}^a$ and $G_{dd(\epsilon)}^K = -(G_{dd(\epsilon)}^K)^*$, consider

$$\begin{aligned} &[e^{-i\omega_0 t} G_{dd(\epsilon)}^r (G_{co(\epsilon)}^r - G_{co(\epsilon-\hbar\omega_0)}^a) G_{dd(\epsilon-\hbar\omega_0)}^a G_{co(\epsilon)}^K]^* \\ &= -e^{i\omega_0 t} G_{dd(\epsilon)}^a (G_{co(\epsilon)}^a - G_{co(\epsilon-\hbar\omega_0)}^r) G_{dd(\epsilon-\hbar\omega_0)}^r G_{co(\epsilon)}^K \end{aligned} \quad (\text{C.93})$$

and

$$\begin{aligned} & [-e^{i\omega_0 t} G_{dd(\epsilon)}^r (G_{co(\epsilon)}^r - G_{co(\epsilon+\hbar\omega_0)}^a) G_{dd(\epsilon+\hbar\omega_0)}^a]^* \\ &= e^{-i\omega_0 t} G_{co(\epsilon)}^a (G_{co(\epsilon)}^a - G_{co(\epsilon+\hbar\omega_0)}^r) G_{dd(\epsilon+\hbar\omega_0)}^r G_{co(\epsilon)}^K, \end{aligned} \quad (\text{C.94})$$

This allows us to write

$$\begin{aligned} S(\epsilon) &= 2 \operatorname{Re}\{e^{-i\omega_0 t} [G_{dd(\epsilon)}^r (G_{co(\epsilon)}^r - G_{co(\epsilon-\hbar\omega_0)}^a) G_{dd(\epsilon-\hbar\omega_0)}^a G_{co(\epsilon)}^K \\ &\quad + G_{co(\epsilon)}^a (G_{co(\epsilon)}^a - G_{co(\epsilon+\hbar\omega_0)}^r) G_{dd(\epsilon+\hbar\omega_0)}^r G_{co(\epsilon)}^K]\} \end{aligned} \quad (\text{C.95})$$

Using $G_{co(\epsilon_1)}^{r,a} - G_{co(\epsilon_2)}^{a,r} = \mp \frac{i}{v_F}$ for all ϵ_1, ϵ_2 , we find:

$$S(\epsilon) = \frac{2}{v_F} \operatorname{Im}[e^{-i\omega_0 t} (G_{dd(\epsilon)}^r G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a G_{dd(\epsilon+\hbar\omega_0)}^r) G_{co(\epsilon)}^K] \quad (\text{C.96})$$

which, when reinserted into the $I_2(t)$ integral, gives the form quoted in the text:

$$I_2(t) = \frac{-e^2 g^4 V_0}{4\pi \hbar^6 v_F \omega_0} \operatorname{Im} \left\{ e^{-i\omega_0 t} \int_{-\infty}^{\infty} d\epsilon (G_{dd(\epsilon)}^r G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a G_{dd(\epsilon+\hbar\omega_0)}^r) G_{co(\epsilon)}^K \right\} \quad (\text{C.97})$$

We can complete the integrals in a similar manner to those for $I_1(t)$. Immediately we can write for the integral:

$$\begin{aligned} & \int_{-\infty}^{\infty} d\epsilon (G_{dd(\epsilon)}^r G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a G_{dd(\epsilon+\hbar\omega_0)}^r) G_{co(\epsilon)}^K \\ &= \frac{2i}{v_F} \int_{-\infty}^{\infty} d\epsilon (G_{dd(\epsilon)}^r G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a G_{dd(\epsilon+\hbar\omega_0)}^r) n_F^{(c)}(\epsilon) \end{aligned} \quad (\text{C.98})$$

by integration shifts, and then for the Fermi function we use the Matsubara form again.

In an identical manner to the I_1 calculation above, where we were reasonably explicit, the integral may be computed to give infinite sums by appropriate use of the residue theorem with semi-circular contours. Then we sum to infinity to find:

$$\begin{aligned} & \frac{2i}{v_F} \int_{-\infty}^{\infty} d\epsilon (G_{dd(\epsilon)}^r G_{dd(\epsilon-\hbar\omega_0)}^a - G_{dd(\epsilon)}^a G_{dd(\epsilon+\hbar\omega_0)}^r) n_F^{(c)}(\epsilon) \\ &= \frac{2\hbar^2}{v_F} \frac{(\frac{g^2}{\hbar v_F} + i\hbar\omega_0)}{(\frac{g^2}{\hbar v_F})^2 + (\hbar\omega_0)^2} \sum_{\alpha=1,-1} [\psi(\alpha, -\alpha\hbar\omega_0) - \psi(\alpha, 0)] \end{aligned} \quad (\text{C.99})$$

where ψ was defined in (C.79). The final result is:

$$I_2(t) = \frac{-eV_0}{\hbar\omega_0} \frac{e}{2\pi\hbar} \frac{(\frac{g^2}{\hbar v_F})^2}{(\frac{g^2}{\hbar v_F})^2 + (\hbar\omega_0)^2} \operatorname{Im} \left\{ e^{-i\omega_0 t} (\frac{g^2}{\hbar v_F} + i\hbar\omega_0) \sum_{\alpha=1,-1} [\psi(\alpha, -\alpha\hbar\omega_0) - \psi(\alpha, 0)] \right\} \quad (\text{C.100})$$

where $\psi(x, y)$ was defined earlier in Eq. (C.79).

Appendix D

Detailed calculations - Chapter 5

Here we include some calculations specific to Chapter 5. The details for the set-up of the linear response and most of the information for the Green functions directly carries over from Chapter 4 and may be found in the previous Appendix.

D.1 Keldysh set-up

To keep the notation compact we can introduce the eight-component spinor

$$\bar{A}_k = (\bar{\psi}_{fk+}, \bar{\psi}_{fk-}, \bar{\psi}_{sfk+}, \bar{\psi}_{sfk-}, a_+, a_-, b_+, b_-)$$

and a similar one for fields without the bar so that the action becomes:

$$S = \sum_k \int dt \bar{A}_k \left[\begin{pmatrix} i\hbar\partial_t - \epsilon_k(t) & 0 & v_1/\sqrt{L} & 0 \\ 0 & i\hbar\partial_t - \epsilon_k & v_2/\sqrt{L} & v_b/\sqrt{L} \\ v_1/\sqrt{L} & v_2/\sqrt{L} & \delta_{k,0}i\hbar\partial_t & 0 \\ 0 & v_b^*/\sqrt{L} & 0 & \delta_{k,0}i\hbar\partial_t \end{pmatrix} \otimes \sigma_3 \right] A_k \quad (\text{D.1})$$

The generalisation of the Keldysh rotation for a $2N$ -component spinor may be written as:

$$((\bar{A}_+^{(1)}, \bar{A}_-^{(1)}), \dots, (\bar{A}_+^{(N)}, \bar{A}_-^{(N)})) = ((\bar{\psi}_1^{(1)}, \bar{\psi}_2^{(2)}), \dots, (\bar{\psi}_1^{(N)}, \bar{\psi}_2^{(N)})) \cdot (\mathbb{1}_{N \times N} \otimes U \sigma_3) = \bar{\psi} [\mathbb{1}_{N \times N} \otimes U \sigma_3] \quad (\text{D.2})$$

$$((A_+^{(1)}, A_-^{(1)}), \dots, (A_+^{(N)}, A_-^{(N)}))^\top = (\mathbb{1}_{N \times N} \otimes U) \cdot ((\psi_1^{(1)}, \psi_2^{(2)}), \dots, (\psi_1^{(N)}, \psi_2^{(N)}))^\top = [\mathbb{1}_{N \times N} \otimes U] \psi \quad (\text{D.3})$$

Using this, where $\mathbb{1}_{N \times N}$ is the $N \times N$ identity matrix, we rotate to find:

$$\begin{aligned} S &= \sum_k \int dt \bar{\psi}_k (\mathbb{1}_{4 \times 4} \otimes U \sigma_3) \left[\begin{pmatrix} i\hbar\partial_t - \epsilon_k(t) & 0 & v_1/\sqrt{L} & 0 \\ 0 & i\hbar\partial_t - \epsilon_k & v_2/\sqrt{L} & v_b/\sqrt{L} \\ v_1/\sqrt{L} & v_2/\sqrt{L} & \delta_{k,0}i\hbar\partial_t & 0 \\ 0 & v_b^*/\sqrt{L} & 0 & \delta_{k,0}i\hbar\partial_t \end{pmatrix} \otimes \sigma_3 \right] (\mathbb{1}_{4 \times 4} \otimes U) \psi_k \\ &= \sum_k \int dt \bar{\psi}_k \left[\begin{pmatrix} i\hbar\partial_t - \epsilon_k(t) & 0 & v_1/\sqrt{L} & 0 \\ 0 & i\hbar\partial_t - \epsilon_k & v_2/\sqrt{L} & v_b/\sqrt{L} \\ v_1/\sqrt{L} & v_2/\sqrt{L} & \delta_{k,0}i\hbar\partial_t & 0 \\ 0 & v_b^*/\sqrt{L} & 0 & \delta_{k,0}i\hbar\partial_t \end{pmatrix} \otimes \mathbb{1}_{2 \times 2} \right] \psi_k \end{aligned} \quad (\text{D.4})$$

by using the mixed product property $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$ twice. Converting this to a local problem by integrating out all fermions other than those at site zero from the partition function amounts to discarding the sum and kronecker deltas:

$$S \rightarrow S = \int dt \bar{\psi} \left[\begin{pmatrix} i\hbar\partial_t - \epsilon_0(t) & 0 & v_1 & 0 \\ 0 & i\hbar\partial_t - \epsilon_0 & v_2 & v_b \\ v_1 & v_2 & i\hbar\partial_t & 0 \\ 0 & v_b^* & 0 & i\hbar\partial_t \end{pmatrix} \otimes \mathbb{1}_{2 \times 2} \right] \psi \quad (\text{D.5})$$

D.2 Summary of Green functions inherited from Chapter 4

For convenience we list here the equilibrium Green functions that carry over from Chapter 4 for the 2CK model studied in Chapter 5.

$$G_{(a,b)o}(\epsilon) = \begin{pmatrix} \frac{\hbar}{\epsilon+i0^+} & 0 \\ 0 & \frac{\hbar}{\epsilon-i0^+} \end{pmatrix} \quad (\text{D.6})$$

$$G_{(s,f)o}(\epsilon) = \begin{pmatrix} \frac{i}{2v_F} & -\frac{i}{v_F}(1-2n_F(\epsilon)) \\ 0 & -\frac{i}{2v_F} \end{pmatrix} + \mathcal{O}(\Lambda^{-1}) \quad (\text{D.7})$$

D.3 Linear response result extracted from S&H '96

From ‘‘Solution of an ac Kondo Model’’ [9] by S&H we adapt the following expression for the charge current to match our study in Ch. 5:

$$I_c(t) = \frac{e}{\hbar} \Gamma_1 \text{Im} \left\{ e^{i(eV_0/\hbar\omega) \sin(\omega_0 t)} \sum_{k=-\infty}^{\infty} e^{-i\omega_0 k t} J_k\left(\frac{eV_0}{\hbar\omega_0}\right) g(k\hbar\omega_0) \right\} \quad (\text{D.8})$$

for the harmonic potential $V(t) = V_0 \cos(\omega_0 t)$, where

$$g(x) = \int \frac{d\epsilon}{\pi} G_{aa}(\epsilon + i\eta) [n_F(\epsilon) - n_F(\epsilon - x)] \quad (\text{D.9})$$

where the retarded Majorana Green function is:

$$G_{aa}(\epsilon + i\eta) = \frac{1}{\epsilon + i\Gamma_a} \quad (\text{D.10})$$

and J_k are Bessel functions of the first kind. For the linear response regime in V_0 one has:

$$I_c(t) = I_c(V_0 = 0) + \left. \frac{\partial I_c(t)}{\partial V_0} \right|_{V_0=0} V_0 + \mathcal{O}(V_0^2) \quad (\text{D.11})$$

The zeroth order term in V_0 is zero. It is easily shown with the integral representation of the Bessel functions,

$$J_k(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(k\tau - x \sin(\tau))} d\tau, \quad (\text{D.12})$$

that only the $k = 0$ mode for $J_k(x = 0)$ is non-zero (it is 1). From this point $g(k\hbar\omega = 0)$ is straightforwardly zero due to the vanishing integrand in (D.9). For the first order contribution to the current in V_0 , by a similar line of reasoning we immediately write:

$$\left. \frac{\partial I_c(t)}{\partial V_0} \right|_{V_0=0} V_0 = \frac{eV_0}{\hbar} \Gamma_1 \text{Im} \left\{ \sum_{k=-\infty}^{\infty} e^{-i\omega_0 k t} \left[\left. \frac{\partial J_k\left(\frac{eV_0}{\hbar\omega_0}\right)}{\partial V_0} \right] \right|_{V_0=0} g(k\hbar\omega_0) \right\}. \quad (\text{D.13})$$

Differentiating the same integral representation of the Bessel function gives:

$$\left. \frac{\partial J_k\left(\frac{eV_0}{\hbar\omega_0}\right)}{\partial V_0} \right|_{V_0=0} = \frac{e}{2\hbar\omega_0} (\delta_{k,1} - \delta_{k,-1}) \quad (\text{D.14})$$

This leads to,

$$\begin{aligned} \left. \frac{\partial I_c(t)}{\partial V_0} \right|_{V_0=0} V_0 &= \frac{e^2 V_0}{2\hbar^2 \omega_0} \Gamma_1 \operatorname{Im}[e^{-i\omega_0 t} g(\hbar\omega_0) - (\omega_0 \rightarrow -\omega_0)] \\ &= \frac{e^2 V_0}{2\hbar^2 \omega_0} \Gamma_1 \operatorname{Im} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} g(\zeta\hbar\omega_0) \end{aligned} \quad (\text{D.15})$$

In conclusion, the linear response result for the charge current according to the paper [9] by S&H is:

$$I_c(t) = \frac{e^2 V_0}{2\hbar^2 \omega_0} \Gamma_1 \operatorname{Im} \sum_{\zeta=-1,1} \zeta e^{-i\zeta\omega_0 t} g(\zeta\hbar\omega_0) \quad (\text{D.16})$$

Zero temperature limit

The zero temperature limit is easily expressed in terms of just elementary functions because the Fermi functions become step functions so the energy integrals can be completed by hand.

From (D.16) we extract:

$$\begin{aligned} \operatorname{Im}[e^{-i\zeta\omega_0 t} g(\zeta\hbar\omega_0)] &= \operatorname{Im} \left\{ e^{-i\zeta\omega_0 t} \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} \left(\frac{\epsilon - i\Gamma_a}{\epsilon^2 + \Gamma_a^2} \right) [n_F(\epsilon) - n_F(\epsilon - \zeta\hbar\omega_0)] \right\} \\ &= - \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} \left(\frac{\Gamma_a \cos(\omega_0 t) + \sin(\zeta\omega_0 t)\epsilon}{\epsilon^2 + \Gamma_a^2} \right) [n_F(\epsilon) - n_F(\epsilon - \zeta\hbar\omega_0)] \end{aligned} \quad (\text{D.17})$$

At temperature tends to zero one has the following limits for the integrals:

$$\int_{-\infty}^{\infty} d\epsilon \frac{n_F(\epsilon) - n_F(\epsilon - \zeta\hbar\omega_0)}{\epsilon^2 + \Gamma_a^2} \rightarrow \frac{1}{\Gamma_a} \left[\arctan \left(\frac{\mu}{\Gamma_a} \right) - \arctan \left(\frac{\mu + \zeta\hbar\omega_0}{\Gamma_a} \right) \right] \quad (\text{D.18})$$

$$\int_{-\infty}^{\infty} d\epsilon \frac{\epsilon [n_F(\epsilon) - n_F(\epsilon - \zeta\hbar\omega_0)]}{\epsilon^2 + \Gamma_a^2} \rightarrow \frac{1}{2} \ln \left(\frac{\mu^2 + \Gamma_a^2}{(\mu + \zeta\hbar\omega_0)^2 + \Gamma_a^2} \right) \quad (\text{D.19})$$

The resulting current in the $T = 0$ limit is:

$$\begin{aligned} I_c(t, T \rightarrow 0) &= \frac{e^2 V_0}{2\hbar^2 \omega_0} \Gamma_1 \left\{ \left[\arctan \left(\frac{\mu + \hbar\omega_0}{\Gamma_a} \right) - \arctan \left(\frac{\mu - \hbar\omega_0}{\Gamma_a} \right) \right] \cos(\omega_0 t) \right. \\ &\quad \left. - \ln \left(\frac{(\mu^2 + \Gamma_a^2)^2}{[(\mu + \hbar\omega_0)^2 + \Gamma_a^2][(\mu - \hbar\omega_0)^2 + \Gamma_a^2]} \right) \frac{\sin(\omega_0 t)}{2} \right\} \end{aligned} \quad (\text{D.20})$$

We get the ac conductance by the chain rule

$$G(\omega_0) \equiv \frac{dI_c(t)}{dV(t)} = \frac{1}{\cos(\omega_0 t)} \frac{dI_c(t)}{dV_0} \quad (\text{D.21})$$

$$\begin{aligned} &= \frac{e^2}{2\hbar^2 \omega_0} \Gamma_1 \left\{ \left[\arctan \left(\frac{\mu + \hbar\omega_0}{\Gamma_a} \right) - \arctan \left(\frac{\mu - \hbar\omega_0}{\Gamma_a} \right) \right] \right. \\ &\quad \left. - \ln \left(\frac{(\mu^2 + \Gamma_a^2)^2}{[(\mu + \hbar\omega_0)^2 + \Gamma_a^2][(\mu - \hbar\omega_0)^2 + \Gamma_a^2]} \right) \frac{\tan(\omega_0 t)}{2} \right\}. \end{aligned} \quad (\text{D.22})$$

Setting μ to zero gives:

$$G(\omega) = \frac{e^2 \Gamma_1}{2\hbar^2 \omega} \left[2 \arctan \left(\frac{\hbar \omega}{\Gamma_a} \right) - \log \left(\frac{\Gamma_a^2}{(\hbar \omega)^2 + \Gamma_a^2} \right) \tan(\omega t) \right] \quad (\text{D.23})$$

We can extract the leading low- ω term in a power series around 0 and compare to the low- ω asymptote from the NRG calculation. This means using $\Gamma_a \rightarrow \Gamma_1 \sim \frac{J_\perp^2}{\hbar v_F} \equiv \Gamma$, due to the emergent spin isotropy at the low energy crossover, and considering time $t = 0$. This gives:

$$G(\omega) = \frac{e^2}{h} \left(1 - \frac{(\hbar \omega)^2}{3\Gamma^2} + \mathcal{O}(\omega^4) \right) \quad (\text{D.24})$$

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