

# Zeeman splitting of the Kondo resonance in high magnetic fields

Zeemanaufspaltung der Kondo-Resonanz in starken Magnetfeldern

## Diplomarbeit

von

### Mathias Cabrera Cano

an der Fakultät für Physik Institut für Theorie der Kondensierten Materie (TKM) am Karlsruher Institut für Technologie

und

am Institut Néel – Département Nano CNRS Grenoble

### 28.02.2011

Referent:

Koreferent und Betreuer:

Prof. Dr. Alexander Shnirman Karlsruhe Institut für Technologie Institut für Theorie der Kondensierten Materie Dr. Serge Florens Insitut Néel (CNRS und UJF) in Grenoble Theory for Nanosciences

# Contents

1.	Intro	oductio	n	1
2.	The	Kondo	effect in quantum dots	6
	2.1.	Transp	port theory and the $\mathcal{T}$ -Matrix	6
		2.1.1.	Coulomb blockade	7
		2.1.2.	Beyond the classical Coulomb blockade	8
	2.2.	Condu	ctance in the Kondo regime	9
		2.2.1.	Anderson model	10
		2.2.2.	Kondo model	12
		2.2.3.	Relation between the conductance and the $\mathcal{T}$ -matrix	13
	2.3.	The K	ondo problem	15
		2.3.1.	Kondo effect in metals	16
		2.3.2.	Weak-coupling regime	16
		2.3.3.	Numerical renormalization group (NRG)	18
		2.3.4.	Strong-coupling regime	24
		2.3.5.	The Kondo effect in quantum dots	25
	2.4.	Summ	ary	27
3.	Maio	orana f	ermion diagrammatics	29
-	3.1.	Matsu	bara Green's functions	29
	0.2.	3.1.1.	Properties of Matsubara Green's functions	30
	3.2.	Kondo	interaction and Majorana fermions	33
	0.2.	3.2.1.	Majorana fermions	34
		3.2.2.	The magnetic susceptibility	40
		323	The $\mathcal{T}$ -matrix	41
	3.3.	Summ	ary	42
л	Ran	dom ph	as a approximation (RPA) for the $\tau_{-}$ matrix	13
4.		BPA f	as approximation (((A) for the )-matrix or $B = 0$ with free propagators	43 /3
	т.1.	<i>A</i> 1 1	Wick's theorem for the response functions	-10 
		4.1.2	Geometric series	
		4.1.2.	Result	50
	4.9	4.1.J. DDA f.	$R \neq 0 \text{ with free propagators}$	51
	4.2.	101 A 10	$D \neq 0$ with new propagators	51
		4.2.1. 4.9.9	The Kondo interaction in the presence of a magnetic field	51 51
		4.2.2.	The Kondo Interaction in the presence of a magnetic field	02 52
		4.2.3. 4.9.4	DDA result with free propagators	00 E0
		4.2.4.	<b>RFA-result with free propagators</b>	99

	4.2.5. The limits of the RPA	. 62
	4.3. Ferromagnetic Kondo coupling and the RPA	. 62
	4.3.1. The underscreened Kondo effect	. 62
	4.3.2. RPA and experiments	. 63
	4.4. Summary	. 64
5.	The spin-relaxation-time	67
	5.1. Derivation of the self-energies $\Sigma_f$ and $\Sigma_\eta$ for $B \neq 0$	. 67
	5.1.1. Self energy $\Sigma_f$	. 68
	5.1.2. Self energy $\Sigma_{\eta}$	. 70
	5.1.3. Dyson's equation $\ldots$	. 71
	5.2. Discussion of the magnetic susceptibility	. 73
	5.3. Spin relaxation time for the $\mathcal{T}$ -matrix $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	. 74
	5.4. Summary	. 75
6.	Conclusion	76
	6.1. Summary	. 76
	6.2. Outlook	. 78
Α.	. Zero temperature Green's functions and Fermi liquid theory	79
	A.1. Schrödinger, Heisenberg and Interaction picture	. 79
	A.1.1. Schrödinger picture	. 79
	A.1.2. Heisenberg picture	. 79
	A.1.3. Interaction picture	. 80
	A.2. Green's functions	. 80
	A.3. Perturbation theory for the Green's function	. 82
	A.3.1. Adiabatic principle	. 82
	A.3.2. Feynman diagrams	. 82
	A.3.3. Dyson's equation and Fermi liquid theory	. 84
В.	. Equations of motion technique and the ${\mathcal T}$ -matrix	87
C.	. Polarization diagrams and self-energies	91
	C.1. Polarization diagrams	. 91
	C.1.1. Polarization diagram for $B = 0$	01
	0	. 91
	C.1.2. Polarization diagram for $B \neq 0$	. 91 . 92
	C.1.2. Polarization diagram for $B \neq 0$	. 91 . 92 . 93
	C.1.2. Polarization diagram for $B \neq 0$	. 91 . 92 . 93 . 94
	C.1.2. Polarization diagram for $B \neq 0$	. 91 . 92 . 93 . 94 . 95

## Deutsche Zusammenfassung

Die Leitfähigkeit<sup>1</sup>  $\mathcal{G}$  beziehungsweise der Widerstand  $\rho = \mathcal{G}^{-1}$  ist schon immer eine wichtige Messgröße in der Festkörperphysik gewesen. In vielen Experimenten ist die Leitfähigkeit durch das Ohmsche Gesetz  $I = \mathcal{G} \cdot V$ , das einen linearen Zusammenhang zwischen dem gemessenen Strom I und der angelegten Spannung V angibt. Die Leitfähigkeit lässt Rückschlüsse über die im Festkörper stattfindenden Prozesse zu. Zum Beispiel hat sich in der klassischen Festkörperphysik das Drude-Modell durchgesetzt, bei dem angenommen wird, dass Elektronen, die im elektrischen Feld beschleunigt werden, an Störstellen im Festkörper gestreut werden, was zu einer endlichen Leitfähigkeit führt, die sich von Material zu Material unterscheidet [1]. Mit der technischen Entwicklung der Tieftemperaturphysik ist es Anfang des letzten Jahrhunderts zusätzlich möglich geworden, die Leitfähigkeit bei Temperaturen weit unter der Raumtemperatur zu messen. Das hat zu vielen neuen, interessanten Erkenntnissen geführt. Ein sehr bekanntes und heute populäres Beispiel ist die Supraleitung: Unterhalb einer bestimmten kritischen Temperatur gehen Metalle in einen neuen thermodynamischen Zustand über, bei dem der Widerstand plötzlich auf null abfällt. Dieses Phänomen wurde 1911 von H. K. Onnes in Quecksilber entdeckt, dessen kritische Temperatur etwa 4.2 K beträgt. Ein weiteres, für die vorliegende Diplomarbeit wichtiges, aber weniger bekanntes Beispiel ist der Kondo-Effekt. Er wurde in den 1930er Jahren in Legierungen mit magnetischen Störstellen ebenfalls bei niedrigen Temperaturen um die 10K beobachtet und führt zu einem unerwarteten, anomalen, logarithmischen Anstieg des Widerstandes (siehe Abbildung 0.1). Dies widerspricht der Annahme, dass der Widerstand eines Festkörpers für tiefe Temperaturen polynomiell monoton fallend gegen einen konstanten Wert strebt [1, 2]. Eine Erklärung für beide Effekte hat Physiker mehrere Jahrzehnte lang beschäftigt und trug dazu bei, dass die Quantentheorie der Festkörper entwickelt wurde. In dieser Theorie wird der Festkörper durch Phononen und Elektronen beschrieben und der Transport von Elektronen durch den Festkörper im Wesentlichen durch die Elektron-Phonon-, Elektron- und Elektron-Störstellen-Wechselwirkung bestimmt [3].

Die Supraleitung wurde 1957 mit der BCS-Theorie erklärt, welche zeigt, dass es eine unerwartete, effektive attraktive Wechselwirkung zwischen Elektronen im Festkörper geben kann, was zur Cooper-Instabilität führt [4]. Der Kondo-Effekt wurde schließlich 1964 von J. Kondo erklärt. Er benutzt eine durch das Anderson-Modell [5, 6] herleitbare effektive Spin-Spin-Wechselwirkung (siehe auch Kapitel 2). Dabei wechselwirkt der Spin S der magnetischen Störstelle mit den Spins s der Leitungselektronen, was zum Kondo-Modell mit der Wechselwirkung  $JS \cdot s$  führt. Diese wird in dem üblichen Formalismus der semi-klassischen Transport-Theorie verwendet, welcher die Boltzmann-

<sup>&</sup>lt;sup>1</sup>In dieser Diplomarbeit wird durchgehend  $\hbar = 1$  (Plancksche Konstante) und  $k_B = 1$  (Boltzmann Konstante) verwendet

gleichung benutzt. Der Einfluss dieser Wechselwirkung auf die Streurate wird in dritter Ordnung Störungstheorie in J ausgerechnet. Das ergibt den logarithmischen Anstieg des Widerstandes. Durch weitere Anwendung störungstheoretischer Methoden (siehe Kapitel 2) erhält man schließlich für den Widerstand [7, 8]

$$\rho(T) \propto \log^{-2}(T/T_K). \tag{0.1}$$

Dabei wird die für das Kondo-Modell typische Energieskala  $T_K$  – die Kondo-Temperatur - definiert, welche für Metalle bei etwa 8K liegt. Ist die Temperatur im Bereich der Kondo-Temperatur, divergiert der für den Widerstand erhaltene Ausdruck in Gleichung (0.1), was zum Zusammenbruch der Störungstheorie führt und Kondo-Problem genannt wird. Ein Ausweg aus diesem Dilemma wurde letztlich durch K. G. Wilson 1975 mit der numerischen Renormierungsgruppe (NRG) gefunden [9] (siehe auch Kaptitel 2). Mit dieser ist es auch möglich, den Widerstand für beliebig tiefe Temperaturen zu berechnen. Dabei stimmen die Ergebnisse qualitativ mit den Experimenten überein.



Abbildung 0.1.: In dieser Abbildung wird der Kondo-Effekt im Widerstand von verschiedenen MoNb Legierungen gezeigt, welche als Störstellen 1% Eisen (Fe) enthalten [7].

Der Widerstand wird korrekt berechnet, der für tiefe Temperaturen konstant wird. Etwa 20 Jahre später wurde der Kondo-Effekt in Quantenpunkten wieder entdeckt [10].

Die heutige, populäre Nanotechnologie wurde in den späten 1960er Jahren durch die Entdeckung der Molekularstrahlepitaxie in den Bell-Phone-Laboratorien eingeleitet. Diese erlaubt es, künstliche Halbleiterkristalle herzustellen, die mit verschiedenen Halbleitermaterialien Schicht für Schicht zu einem Kristall gezüchtet werden [11, 12]. Die wurde zunächst vor Allem dazu verwendet, wichtige Bauelemente wie Dioden und Transistoren herzustellen. Die verschiedenen Eigenschaften der Halbleitermaterialen, wie zum Beispiel unterschiedliche Energielücken, führen dazu, dass die Elektronen sich nach dem Zusammensetzen der verschiedenen Halbleiter in einem modulierten Potential befinden. In bestimmen halbleitenden Heterostrukturen entsteht dabei durch das Zusammensetzen an der Grenze zwischen zwei Halbleitern, die unterschiedliche Bandlücken besitzen, ein Dreieckspotential im Leitungsband, in dem sich die Leitungselektronen ansammeln. Dies friert einen Freiheitsgrad ein und führt zur Bildung eines sogenannten zwei-dimensionalen Elektronengases (2DEG) [13]. Durch die Entwicklung der Elektronenstrahllithographie in den 1980er Jahren ist es möglich, zusätzliche Elektroden (Top-Gates) auf dem Kristall aufzubringen. An den Elektroden wird eine Spannung angelegt, mit der man das 2DEG einsperren kann. Dabei entsteht ein Quantenpunkt. Um diesen befinden zwei Elektronenreservoire. Zwischen diesen beiden Elektronenreservoiren liegt die Spannung  $V_b$  an ("bias voltage"), die einen Elektronenfluss durch den



Abbildung 0.2.: In Abbildung 0.2(a) (http://marcuslab.harvard.edu/research.shtml) ist eine Halbleiterstruktur zu sehen, auf welcher Top-Gates aufgebracht wurden, wodurch es möglich ist das 2DEG, das sich in der Grenzschicht zwischen den beiden verschiedenen Halbleitermaterialien befindet, zu manipulieren. In Abbildung 0.2(b) ist erklärt, wie es zur Bildung des 2DEG kommt. Durch das Angleichen der Fermienergie und der Bänder  $E_v$  und  $E_c$  in beiden Halbleitern wird das Potential für das Leitungsband  $E_c$  derart modifiziert, dass sich Elektronen in einem Dreieckspotential ansammeln, was zu einem Einfrieren eines Freiheitsgrades führt. Mit den Top-Gates lassen sich weitere Freiheitsgrade der Elektronen einfrieren, was zur Bildung des Quantenpunktes führt.

Quantenpunkt ermöglicht (siehe Abbildung 0.5(a)). Diese Geometrie bietet nun die Möglichkeit, die Leitfähigkeit dieser kleinen Region zu messen. Dabei kann man experimentell überprüfen, welchen Einfluss die Stärke der Barrieren auf die Leitfähigkeit hat. Der Quantenpunkt hat dabei diskrete Energieniveaus wie ein Atom, was zu massiven Modifikationen der Leitfähigkeit führt [14] (siehe Abbildung 0.5(a)). Unter anderem kann man in diesen Geometrien den Kondo-Effekt in der Leitfähigkeit messen.

Die Grundlage dafür ist der Ein-Elektron-Transistor, in dem ein einzelnes Elektron durch den Quantenpunkt transmittiert wird und die Barrieren stark eingestellt werden. Dieses Phänomen der Coulomb-Blockade wurde von M. A. Kastner 1992 [13] entdeckt und führt zu Peaks in der Leitfähigkeit des Quantenpunkts in Abhängigkeit von der Gate-Spannung (siehe Abbildung 0.3(a)). Es lässt sich folgendermaßen klassisch erklären: Man braucht eine bestimmte Energie um ein Elektron dem Quantenpunkt hinzuzufügen, welche durch die Kapazität des Quantenpunkts bestimmt ist. Zum Beispiel kostet es die Energie  $E_C(N)$ , um N Elektronen auf den Quantenpunkt zu bringen. Mit der Gate-Spannung kann diese Energie modifiziert werden. Durch Ändern der Gate-Spannung  $V_g$  kann die Energie  $E_C(N+1)$  so modifiziert werden, dass man eine Ladungsenergieentartung  $E_C(N) = E_C(N+1)$  erzeugt, was dazu führt, dass ein Elektron ohne zusätzliche Energie den Quantenpunkt betreten und wieder verlassen kann. An diesen Entartungspunkten beobachtet man einen Peak in der Leitfähigkeit. Außerdem wird durch weiteres Erhöhen der Gate-Spannung  $V_g$  die Besetzungszahl N des Quantenpunkts nach N + 1 geändert [13, 15, 16]. Wird neben der Gate-Spannung  $V_g$  die am Quantenpunkt anliegende Spannung  $V_b$  verändert, erhält man schließlich die sogenannten Coulomb Diamanten für die Leitfähigkeit (Abbildung 0.3(b)). Die Coulomb



Abbildung 0.3.: In Abbildung 0.3(a) sind die Coulomb Peaks der Leitfähigkeit des Quantenpunktes in Abhängigkeit von der Gate-Spannung  $V_g$  dargestellt. Die Peaks sind dabei quasiperiodisch mit einer Periode proportional zu  $E_C$  angeordnet. Verändert man zusätzlich die angelegte Spannung  $V_b$  am Quantenpunkt, ergibt sich die 2-dimensionale Diamantstruktur für die Leitfähigkeit. Dabei kennzeichen die schwarzen Regionen eine Leitfähigkeit  $\mathcal{G} = 0$  und die weiß-grauen Ränder einen Peak in der Leitfähigkeit [17, 18].

Diamanten kennzeichnen dabei Regionen, mit konstanter Elektronenanzahl N auf dem Quantenpunkt und mit einer Leifähigkeit  $\mathcal{G} = 0$ . An den Grenzen der Diamanten ändert sich die Elektronenanzahl entweder nach N-1 oder N+1 und führt zu einem Peak in der Leitfähigkeit, da nun die Energie<br/>entartungspunkte von beiden Spannungen  $V_g$  und  $V_b$  abhängen (Abbildung 0.3). Der Ein-Elektron-Transistor bietet also die Möglichkeit die Anzahl an Elektronen auf dem Quantenpunkt zu kontrollieren. An diesem Punkt kommt der Kondo-Effekt wieder ins Spiel, welcher die Leitfähigkeit des Quantenpunkts stark beeinflussen kann. Um diesen messen zu können, müssen zunächst die Barrieren geschwächt werden, was dazu führt, dass Elektronen durch den Quantenpunkt tunneln können. Außerdem muss die Ladungsenergie, die man benötigt um ein Elektron auf den Quantenpunkt zu bringen, groß sein im Vergleich zur Kondo-Temperatur [19] (siehe Kapitel 2). Dabei werden die Energieniveaus als virtuelle Zwischenzustände genutzt. Das führt dazu, dass man in Regionen, in denen der Quantenpunkt mit einer ungeraden Anzahl an Elektronen besetzt ist, einen effektiven Spin beobachtet, der wie in einem Metall mit den Leitungselektronen wechselwirkt. Während aber in einem Metall das Erhöhen der Streurate zu einem Anstieg des Widerstandes führt, wird in einem Quantenpunkt die Leitfähigkeit durch den Kondo-Effekt erhöht, da hier eine erhöhte Streurate eine erhöhte Transmission von Elektronen durch den Quantenpunkt bedeutet. Diese erhöhte Transmissionsrate wird Kondo-Resonanz genannt. Tatsächlich konnte D. Goldhaber-Gordon 1998 [19] (Abbildung 0.4) am MIT den Kondo-Effekt in einem halbleitenden Ein-Elektron-Transistor messen. In solchen Transistoren ist die Ladungsenergie  $E_C \approx 1 \text{K} - 10 \text{K}$  und die Kondo-Temperatur liegt bei etwa  $T_K \approx 0.5 \text{K}$ . Die Entdeckung hat dazu geführt, dass der Kondo-Effekt wieder verstärkt sowohl theoretisch als auch experimentell untersucht wurde [16, 18, 20–23]. In Kapitel 2 wird erläutert, wie der Transport von Elektronen durch den Quantenpunkt mit Hilfe der Transmissionsmatrix ( $\mathcal{T}$ -Matrix) beschrieben werden kann (siehe Abbildung 0.5(a)). Unter anderem



Abbildung 0.4.: In dieser Abbildung ist der Kondo-Effekt in einem Ein-Elektron-Transistor zu sehen. Durch die Coulomb-Blockade wird dieser abwechselnd mit einer geraden und ungeraden Elektronenanzahl besetzt. Für ungerade Anzahl bleibt ein Nettospin übrig, mit dem Leitungselektronen wechselwirken können, was zum Kondo-Effekt führt, wenn die Temperatur gesenkt wird. Ein Absenken der Temperatur führt außerdem zu schärferen Peaks der Coulomb-Blockade, da thermische Anregungen unwahrscheinlicher werden [17, 19].

wird für das Kondo-Modell die Relation zwischen Leitfähigkeit und  $\mathcal{T}$ -Matrix erklärt.

Mit den heutigen Methoden der Nanotechnologie kann man eine Vielzahl derartiger Experimente realisieren. Dabei kann man Quantenpunkte aus Carbon-Nanotubes (CNTs) herstellen und diese miteinander koppeln (siehe Abbildung 0.5). Die Ladungsenergie der Quantenpunkte hat dabei mit immer kleiner werdenden Quantenpunktgeometrien weiter zugenommen. So betragen typische Ladungsenergien in Quantenpunkten aus CNTs etwa  $E_C \approx 10 \text{K} - 100 \text{K}$  und die Kondo-Temperatur beträgt  $T_K \approx 4 \text{K}$ . Dies führt das dazu, dass man den Kondo-Effekt immer besser beobachten kann und zeigt, dass die Elektronen immer stärker korreliert sind, je kleiner die Quantenpunktgeometrien werden. Dies bietet den Anlass, das Wissen, welches man in den 1980er Jahren über den Kondo-Effekt gewonnen hat, heute zu nutzen, um die Physik in Quantenpunkten zu verstehen. Dabei kann man neue theoretische Methoden entwickeln und direkt mit Experimenten vergleichen und testen. In dieser Diplomarbeit werden in Kapitel 3 Majorana Fermionen als Hilfsteilchen genutzt, um eine diagrammatische Störungstheorie zu definieren, welche die Wechselwirkung des Spins des Quantenpunkts mit den Spins der Leitungselektronen beschreibt. In Anhang A ist eine allgemeine Kurzeinführung in die diagrammatische Störungstheorie zu finden. In den Kapiteln 3 und 4 wird schließlich gezeigt, wie man die Diagrammtik für die  $\mathcal{T}$ -Matrix verwenden kann. Dabei wird die  $\mathcal{T}$ -Matrix in eine Random Phase Approximation (RPA) entwickelt, wo nur die führenden, logarithmischen Beiträge aufsummiert werden und die Kondo-Wechselwirkung J renormieren. Desweiteren wird gezeigt, wie man die RPA für die  $\mathcal{T}$ -Matrix im Magnetfeld anwendet. Dabei erzeugt das Magnetfeld einen zusätzlichen Zeemanterm im Hamiltonoperator, welcher die Kopplung eines Spins an das angelegte Magnetfeld beschreibt. Der Zeemanterm führt schließlich zur Zeemanaufspaltung der Kondo-Resonanz. Die Ergebnisse der RPA ohne und mit Magnetfeld werden schließlich mit DM-NRG (Density-Matrix Numerical Renormalization Group) und NRG (Numerical Renormalization Group) Rechnungen für die  $\mathcal{T}$ -Matrix im Kapitel 4 verglichen. Für den Fall ohne Magnetfeld wird gezeigt, dass die RPA äquivalent zum "poor man's scaling" ist [7, 24]. Für ein angelegtes Magnetfeld wird die DM-NRG angewandt, welche eine Verallgemeinerung der NRG ist. Die DM-NRG Rechnungen werden dabei mit "Flexible DM-NRG"durchgeführt (http://www.phy.bme.hu/ dmnrg/, [25]). Die Zeeman Ener-



Abbildung 0.5.: In Abbildung 0.5(a) ist schematisch dargestellt, wie man den Elektronentransport durch den Quantenpunkt in einem Modell beschreiben kann. Der Elektronentransport wird durch die Potentialdifferenz  $V_b$  zwischen den beiden Elektronreservoiren links und rechts getrieben. Die Energieniveaus des Quantenpunkts werden dabei als virtuelle Zwischenzustände genutzt und können durch die Gate-Spannung  $V_g$  geändert werden. In Abbildung 0.5(b) ist eine Rasterkraftmikroskopaufnahme http://marcuslab.harvard.edu/research.shtml von zwei gekoppelten Quantenpunkten in einem CNT zu sehen. Mit Hilfe der Top-Gate Spannungen an  $TG_R$ ,  $TG_L$  und  $TG_M$  werden die Barrieren und mit  $SG_L$  und  $SG_R$  wird die Anzahl der Elektronen auf dem jeweiligen Quantenpunkt kontrolliert, was den Elektronenfluss durch den Quantenpunkt beeinflusst.

gie des Zeemanterms definiert eine zusätzliche Energieskala, welche die NRG in Frage stellt [26]. Um das zu überprüfen, wird das RPA Resulat für die *T*-Matrix mit den DM-NRG Rechnungen und mit schon durchgeführten Rechnungen [27, 28] für verschiedene Verhältnisse  $B/T_K$  verglichen. Als letztes wird in Kapitel 4 auch das ferromagnetische Kondo-Modell im endlichen Magnetfeld diskutiert, welches Relationen zum S = 1 Kondo-Effekt hat [29–31], welcher erst vor kurzem in einem molekularen Ein-Elektron-Transistor entdeckt wurde [18, 32]. Am Ende dieser Diplomarbeit wird dann in Kapitel 5 noch die Rolle der **Spinrelaxationsrate** diskutiert, welche mit Hilfe der Dyson-Gleichung (siehe Anhang A) zu den Majorana-Propagatoren hinzufügt wird. Die Spinrelaxationsrate hilft dabei, Divergenzen in der RPA zu beseitigen.

## 1. Introduction

In solid-state physics the electrical conductance  $\mathcal{G}$  and resistivity  $\rho = \mathcal{G}^{-1}$  have always been an important properties and are usually well described by Ohm's law  $I = \mathcal{G} \cdot V$ . This law relates the current I linearly to the applied voltage V. In classical physics, the transport of electrons is described by the Drude model, where electrons are scattered by impurities embedded in the crystal. These scattering events are described phenomenologically by a mean scattering time  $\tau$ . With the advent of low temperature physics in the beginning of the 20th century unexpected behaviour of the conductance of macroscopic samples was observed, i.e. superconductivity and the Kondo effect. For some metals, called superconductors, the electrical conductance becomes infinite if they are cooled down below a certain critical temperature (typically 4.2K-16K). It was H. K. Onnes who discovered this behaviour for the first time in 1911 at the university Leiden in mercury. A second important effect is the so-called Kondo effect which was observed in the early 1930s. It describes an unexpected logarithmic decrease of the conductance below a certain temperature (5K-10K) [1, 2]. The explanation of these two effects required a further development of quantum mechanics and statistical physical [3] and after a few decades the two phenomena were understood. In 1957 the BCS-theory explains the superconductivity using an attractive electron-electron interaction which leads to the Cooper instability. [4]. Furthermore, the semi-classical Boltzmann equation explains different distributions to the conductance, i.e. electron-phonon interaction, electron-electron interaction and impurity-scattering [1]. J. Kondo was able to explain the Kondo effect using the Boltzmann equation and assuming a phenomenological spinspin interaction between the conduction electrons and an impurity in 1964 [7, 8]. This interaction has been explained later when the formation of magnetic moments in metals was studied. The so-called Anderson model [5] describes the interaction of electrons and magnetic impurities embedded in a Fermi sea. This term is given by  $JS \cdot s$  which describes interaction between the spin S of the impurity with the spin s of the conduction electrons being spin dependent. Perturbation theory in second order for the relaxation time explains finally the logarithmic decrease of the conductance of metals. This logarithmic anomaly is only observed for a certain range of temperatures described by the Kondo temperature  $T_K$ . The Kondo temperature occurs in the resistivity  $\rho(T) = \propto \log^{-2} T/T_K$ . For a metal it is typically 5K-10K. If the temperature is lowered further, the measured conductance saturates while the result obtained by applying perturbation theory does not describe this observation. It is even worse because the result diverges which indicates that the perturbation theory breaks down. This is called the Kondo problem and it is one of the first real many-body effects in solid-state physics. Due to the spin-spin scattering the electrons can not anymore be treated independently from each other – they are correlated by the impurity spin dynamics. The Kondo temperature separates the model into the regime  $T \gg T_K$  where the electrons are weakly correlated and the regime  $T \ll T_K$  where the electrons are strongly correlated and where perturbation theory breaks down. The Kondo problem was finally solved by K. Wilson 1975 who developed the powerful numerical renormalization group (NRG) [7, 9]. Using this technique allows one to calculate the conductance for all temperatures and the results agree quantitatively with experimental results. About 20 years later **the Kondo effect in quantum dots** was detected leading to its revival [10, 16].

The advent of molecular-beam epitaxy in the late 1960s (developed at the Bell Telephone laboratories) was the starting point for the realization of quantum dots. It became possible to grow artificial semiconductor crystals and the nanotechnology began [11, 12], because using this technique these crystals are formed atomic layer by atomic layer. The ability to switch abruptly between different semiconductor materials allows to create manifold sandwich structures, i.e. semiconducting diodes and transistors. Since each material has different energy bands and Fermi energies the sandwich structure produces a modulated one-dimensional potential for the electrons (see Figure 1.1(b)) where one degree of freedom is frozen. The electrons can only move in a plane. Within this plane, the electrons can move freely with different in-plane momenta, giving the electrons a continuous energy dispersion. This gives rise to the so-called two dimensional electron gas (2DEG) [1, 14]. Another important experimental technique of the ongoing miniaturization is electron beam lithography which allows to define electric gates with a precision of several hundreds of nanometers on the top of the crystal. The 2DEG can now be modified with the help electric top-gates so that the electrons can be confined to a small region within the plane. This small region has discrete energy levels like an atom. Due to this property, a confined 2DEG is also called artificial atom or quantum dot. The size and form of the quantum dot can be controlled by the fabrication techniques. Additionally, a voltage  $V_b$  is directly applied to the 2DEG which defines a potential difference between the two electron reservoirs, so that a current can flow through the quantum dot (see Figure 1.2(a)). With the help of the top-gates the current through the quantum dots can be modified (Figure 1.1(a)). Tuning the top-gate voltages leads to a variety of different experimental set-ups, i. e. the strength of the barriers between the 2DEG and the quantum dot can be controlled [14].

The Kondo effect was finally detected in the **single electron transistor** which is one amongst many applications of quantum dots [14]. In this configuration the quantum dot is weakly coupled to the leads and for sufficient low temperatures Coulomb blockade peaks in the conductance occur [13]. This phenomenon allows to control the number of electrons on the quantum dot. The Coulomb blockade can be understood classically because the number N of electrons on the dot is a good quantum number. It is assumed that it costs the electrostatic energy E(N) to add N electrons to the dot. If E(N+1) = E(N) - a situation which is called a charge degeneracy point (obtained by shifting the energy levels of the dot by tuning the gate voltage  $V_g$  (Figure 1.2(a))) – one electron can hop on and off the dot without paying any energy so that at each degeneracy point a peak in the conductance is observed. However, these peaks are broadened by tunneling



Figure 1.1.: Figure 1.1(a) shows a semiconducting heterostructure where a 2DEG is formed between two different semiconducting layers. The diagram in Figure 1.1(b) illustrates the formation of a 2DEG. Putting two semiconductors with different energy gaps together leads to a small triangle in the conduction band where electrons are accumulated. This freezes one degree of freedom of the electrons and they are confined in a plane – the 2DEG. On the top of the created heterostructure electric gates are defined using electron beam lithography (see Figure 1.1(a)). The bias voltage defines a potential difference between the two electron reservoirs so that a current can flow through the dot (http://marcuslab.harvard.edu/research.shtml).

and thermal effects [13, 15]. These tunable properties of the quantum dots can be used to recover certain effects that are observed in solids. For example, one can bring the dot into a configuration where an odd number of electrons is on the dot, which leads to an unpaired spin. It turns out that if the dot is strongly coupled to the leads the results can be understood in the context of Kondo physics. In this configuration the quantum dot geometry corresponds to an embedded artificial magnetic impurity in a Fermi sea – as it was shown before in metals. The quantum dot geometry allows to measure electrons tunneling through the dot leading to the conductance. Thus the higher scattering rate which stems from the Kondo effect increases the conductance, while the higher scattering rate increases the resistivity of metals for low temperatures. The rise in the scattering rate due to the Kondo effect is called Kondo resonance. The Kondo resonance in the low temperature conductance of a single electron transistor was detected for the first time in 1998 by Goldhaber-Gordon at the MIT [19] where he used a semiconducting heterostructure (see Figure 1.1(a)). In such structures the Kondo temperature is usually  $T_K \approx 0.5$ K and the charging energy is  $E_C \approx 1$ K – 10K. Recently, carbon-nanotubes (CNTs), which are rolled-up sheets of graphene have been become very popular to form quantum dots where top gates are also used to confine electrons (see Figure 1.2). The typical size of a CNT is around 100nm. Typically the Kondo temperature is  $T_K \approx 4$ K and the charging energy is  $E_C \approx 10$ K - 100K. This allows to observe the Kondo effect more clearly in a CNT [18].

The Kondo effect is one of the best understood many-body models in condensed matter physics and there are a variety of techniques to treat the Kondo problem, even



Figure 1.2.: Figure 1.2(a) illustrates how electrons tunnel from the left to the right lead by using the energy levels of the quantum dot as intermediate states. The black solid lines separate the quantum dot from the leads and the strength of these barriers can be controlled by top-gates. The gate voltage  $V_g$  controls the number of electrons on the dot and the bias voltage  $V_b$  defines a potential difference between the two leads so that current can flow. In Figure 1.2(b) an atomic force microscopy picture (www.spie.org/x8587.xml?ArticleID=x8587) of a CNT quantum dot is shown. This geometry is called a double quantum dot. With the gates  $SG_L$ ,  $SG_R$  the number of electrons on the two dots can be controlled and with the three top-gates  $TG_L$ ,  $TG_R$  and  $TG_M$  the coupling between the dots and the coupling to the electron reservoirs is controlled. With these top-gates a lot of different quantum dot geometries can be realized with different conductances.

exact solutions. In the ongoing miniaturization, correlations between the electrons become more and more important. This can be understood from the increasing charging energies due to the higher capacity for decreasing size of the quantum dot. The Kondo model is a prototype model for strongly correlated electrons which helps to understand and test newly developed techniques [14, 16, 18, 20–23]. In this thesis the magnetoconductance in the Kondo regime with a ferromagnetic and anti-ferromagnetic Kondo coupling J will be discussed in a theoretical framework and the results will be compared to corresponding experimental set-ups where an additional magnetic field is applied to the impurity [27, 28, 33, 34]. The magnetic field involves a Zeeman term in the Hamiltonian which describes the coupling of the spin and the magnetic field. The consequences for the applied methods such as the NRG and the experiments will be discussed.

In chapter 2 a review of the Kondo effect in quantum dots is given. We will explain how to describe the electron transport through the quantum dot using perturbation theory. We will further review how the NRG works. In addition, typical experimental results will be compared with NRG and perturbation theory results so that the Kondo problem becomes clearer. The Kondo problem will be further discussed in the presence of a magnetic field. This leads to the Zeeman term in the Kondo Hamiltonian which has to be treated by using the density matrix renormalization group (DM-NRG). This method is a generalization of the NRG for the Kondo model at finite magnetic field [26].

In chapter 3 the **Majorana fermion formalism** will be explained. The spin S of the impurity will be represented by Majorana fermion propagators which will enable us to include the spin relaxation time by Dyson's equation. This involves an intro-

duction on how the Majorana fermion can be used in many-body perturbation theory where the most important details are summarized. This introduction will also show the advantages of using this technique, i.e. how to apply Wick's theorem (see appendix A).

Then, in chapter 4 it will be shown how the  $\mathcal{T}$ -matrix can be expanded into a Random Phase Approximation (RPA). It will be illustrated how the RPA for  $\mathcal{T}$ -matrix can be carried out for the both the cases, with and without magnetic field. The result at finite magnetic field will lead to the discussion of the **Zeeman splitting of the Kondo resonance**. Additionally, the RPA result of the  $\mathcal{T}$ -matrix is compared to DM-NRG calculations of the  $\mathcal{T}$ -matrix which will evoke a thorough discussion of the two applied methods. The DM-NRG results were calculated by using the "Flexible DM-NRG" code (http://www.phy.bme.hu/ dmnrg/, [25]). In the end of chapter 4 the  $\mathcal{T}$ -matrix will be discussed for ferromagnetic Kondo coupling J where the perturbation theory does not break down. The result of the DM-NRG and the RPA for this case will be compared to experimental results where the underscreened S = 1 Kondo effect in a molecular transistor has been observed [32]. We will show that there is a connection between the underscreened S = 1 Kondo effect and the ferromagnetic  $S = \frac{1}{2}$  Kondo effect which was already found in the 1980s by P. Nozières [30].

The **spin relaxation rate** will finally be included into the discussed in chapter 5 where it will be calculated to lowest non-vanishing order using Dyson's equation. The spin relaxation rate will be used to discuss the magnetic susceptibility for the Kondo model at finite magnetic field which will complete the discussion of the benchmark of the RPA and the DM-NRG. It will be eventually seen that the spin relaxation rate helps to cut divergences in the RPA.

In the last chapter 6, the results of this diploma thesis will be summarized and an outlook will be given.

In order to increase the readability of the thesis technicals details can be found in the appendices. In appendix A one can find a short introduction to zero-temperature Green's functions where concepts like Feynman diagrams, Dyson's equation and Wick's theorem are summarized. This appendix shows the importance of Wick's theorem for many-body techniques. For more details we refer to Ref. [35–40]. Then, in appendix B the expression of the  $\mathcal{T}$ -matrix for the Kondo model is derived. This expression is then calculated in this diploma thesis using Majorana fermions and DM-NRG. The calculation of the polarization diagram (see chapter 4) and the self-energies (see chapter 5) is done in appendix C. We also refer to the list of the most important symbols and abbreviations given in appendix D.

## 2. The Kondo effect in quantum dots

In this chapter the conductance of quantum dots in the Kondo regime will be discussed. In the first part of this chapter we will illustrate how perturbation theory can be used to describe the electron transport through the quantum dot. A quantum dot has several energy levels which are coupled to two electron reservoirs with a continuous density of states. Furthermore, there are interactions between the electrons on the quantum dot. The number of energy levels and the strength of the interactions can dramatically change the conductance. In the second part of this chapter we will introduce the Anderson model, where a single energy level is coupled to the electron reservoirs. The interactions in this model are described by the Coulomb repulsion U for a double occupied energy level. The low energy physics of the Anderson model opens a tunneling channel for the electrons which increases the conductance logarithmically. This enhancement of the conductance is the Kondo resonance and leads to the Kondo problem. The Kondo problem has been solved by K. G. Wilson's NRG. The NRG is a non-perturbative method to describe the electron transport through the dot. In the last part of this chapter the steps of the NRG will be explained.

### 2.1. Transport theory and the T-Matrix

In this section we are going to show how perturbation theory can be used to describe the electron transport. In Figure 2.1 it is illustrated how the quantum dot geometry can be formalized. The coupling of the quantum dot to the two electron reservoirs is described by tunneling amplitudes which are determined by the strength of the barriers. The energy levels and interactions in the quantum dot are described by the Hamiltonian  $H_D$  and the reservoirs electrons in the right or left by the Hamiltonians



Figure 2.1.: This Figure shows the quantum dot which is coupled to two leads.  $H_D$  describes the energy levels of the quantum dot and  $H_R$  ( $H_L$ ) describes the free electrons on the left (right) lead, respectively. The quantum dot is coupled to the two leads by tunneling terms  $t_R$  and  $t_L$  which describe the tunneling amplitudes between the dot and the leads. The energy levels of the dot can be shifted by applying a gate voltage  $V_g$ . This allows to change the number of electrons residing on the dot.

 $H_R$  or  $H_L$  respectively. Electrons which tunnel from one lead through the dot to the other lead will contribute to the conductance. We want to describe these processes in the following using perturbation theory. Therefore, we separate first of all them into sequential tunneling and co-tunneling. The former describes a direct tunneling of the electrons and thus corresponds to a classical description. Co-tunneling events are processes where the energy levels of the quantum dots are used as intermediate states when the electrons tunnel from the right to the left lead. The number of co-tunneling events increases for a stronger coupling of the quantum dot to the leads. We want to use perturbation theory to describe the rate of electrons tunneling through the quantum dot. This rate finally determines the conductance. The probability for a transition from an initial state  $|i\rangle$  to a final state  $|f\rangle$  is expanded into a perturbation series in the tunneling Hamiltonian  $H_t$  which is switched on adiabatically. For more details about perturbation theory in quantum mechanics we refer to different introductions, i.e. Ref. [41–43]. Since the strength of the coupling is adiabatically increased the eigenstates of the Hamiltonian  $H_0 = H_L + H_R + H_D$  are the unperturbed eigenstates used in the perturbation series. The corresponding eigenvalues are given by  $H_0|i\rangle = E_i|i\rangle$ . In the interaction representation (see appendix A) the probability P for a transition is given by[37]

$$P = |\langle f|i(t)\rangle|^2 = 2\pi |\langle f|\mathcal{T}|i\rangle|^2 \,\delta\left(E_f - E_i\right)t,\tag{2.1}$$

where the  $\mathcal{T}$ -matrix is given by

$$\mathcal{T} = V + \frac{1}{E_f - H_0 + i0^+} \mathcal{T}.$$
 (2.2)

The positive damping rate  $0^+$  represents the causality of the adiabatically switched-on coupling. Calculating this rate leads to the conductance of the quantum dot where the  $\mathcal{T}$ -matrix describes all orders of tunneling processes. This allows to describe many-body transport phenomena. Equation (2.1) can also be seen as a generalization of Fermi's golden rule [37]. The quantum dot is coupled to leads which consist of free electrons. Thus, the quantum numbers of the matrix elements in equation (2.1) are given by the spin  $\sigma$  and the momentum  $\mathbf{k}$  of the initial and final states.

#### 2.1.1. Coulomb blockade

The Coulomb blockade phenomenon occurs when the quantum dot is weakly coupled to the two leads. This can be realized experimentally by tuning the top-gates between the leads and the quantum dot to very high potentials. (Figure 2.2(b)). In this limit the transport can be described classically by an electrostatic energy E(q) which depends on the charge q [13, 15, 16]. The quantum dot which is weakly coupled to the two leads can be mapped on to an equivalent circuit with capacitors  $C_R$ ,  $C_L$  and  $C_g$  (see Figure 2.2(a)). The electrostatic energy E(q) in this circuit reads

$$E(q) = \frac{q^2}{2C} - q\frac{C_g}{C}V_g,$$
(2.3)



Figure 2.2.: Figure 2.2(a) shows the classical circuit with the total capacitance  $C = C_R + C_L + C_g$  of the system.  $V_g$  is the gate voltage which allows modify to the charging energy. In Figure 2.2(b) it is shown how the top-gates deplete the 2DEG into the finite region in the middle which is called the dot. One can control the coupling to the leads via the voltages  $V_R$  and  $V_L$ .

where  $C = C_R + C_L + C_g$  is the total capacitance of the quantum dot. This classical expression for the energy can be used to find the Hamiltonian for the model. Using the correspondence principle of quantum mechanics [16, 42] leads to

$$H_D = \sum_{n\sigma} \epsilon_n d_{n\sigma}^{\dagger} d_{n\sigma} + E_C (N - N_0)^2, \qquad (2.4)$$

where  $\epsilon_n$  labels the eigen-energies of the single particle states of the quantum dot,  $E_C$ the charging energy,  $N = \sum_{n\sigma} d_{n\sigma}$  the number of electrons on the quantum dot and  $N_0 = \frac{C_g V_g}{e}$  the occupancy of the quantum dot which depends on the gate voltage  $V_q$ . The operator  $d_{n\sigma}^{\dagger}$   $(d_{n\sigma})$  creates (destroy) an electron on the energy level n with spin  $\sigma$  and follows usual fermionic anti-commutation rules. The eigenenergies of the Hamiltonian  $H_D$  in equation 2.4 depend on the number of electrons N on the dot and are given by E(N). This eigenenergy defines the needed energy to add N electrons on the dot. The energy for adding one electron can be changed with the gate voltage. If the energies E(N) and E(N+1) are equal, it costs no energy to add an electron. This situation is called a charge degeneracy point which explains the single electron transistor [13, 15]. If the mean spacing  $\delta E$  between the single particle energies  $\epsilon_n$  is small compared to the electrostatic  $E_C$ , quasi-periodic peaks in the conductance  $\mathcal{G}$  are measured by changing the gate voltage  $V_q$  with a period which is proportional to  $E_C$ . The resulting Coulomb blockade peaks are broadened by thermal effects and tunneling events. Changing additionally the bias voltage  $V_b$  leads to the typical diamond structure of the conductance  $\mathcal{G}$ . Each diamond contains a different number of electrons residing on the quantum dot. The Coulomb peaks and diamonds are shown in Figure 2.3.

#### 2.1.2. Beyond the classical Coulomb blockade

If the voltages of the top-gates are tuned in such a way that the quantum dot is strongly coupled to the two leads (see Figure 2.2(b)), co-tunneling events become important. In



Figure 2.3.: This Figure shows the typical Coulomb blockade peaks (Figure 2.3(a)) and diamonds (Figure 2.3(b)). The dark areas of the diamonds describe a constant number of electrons on the quantum dot and the conductance is zero. The bright areas of the diamonds indicate the change of the number of electrons on the quantum dot with a finite conductance.

this regime higher-orders terms in perturbation theory have to be taken into account. For instance, in second order there are two different possibilities for tunneling events: either 1.) an electron can tunnel from the left lead on the dot and then an electron tunnels from the dot to the right lead or 2.) an electron firstly tunnels from the dot to the right lead and then an electron tunnels from the left lead on the dot. During these tunneling processes spin-flip processes can occur which lead to the Kondo effect. Furthermore, the tunneling processes can be classified into elastic and inelastic processes. Inelastic second order tunneling events change the energy of the dot, i.e. the result is created electron-hole pair on the dot. In such a process are sketched. The contribution to the conductance for low temperatures of inelastic second order processes is proportional to  $T^2$  (temperature) while the contribution of elastic processes is a constant. In general these contributions modify only weakly the conductance and we will see later how the latter modifies the conductance strongly for low temperatures.

This section is finished with an example. The conductance  $\mathcal{G}$  of a single non-interacting energy level  $\epsilon_d$  symmetrically coupled to two reservoirs is given by [44]

$$\mathcal{G}(V_b, T) \propto \frac{4}{T} \frac{1}{\cosh^2((\epsilon_d - V_b)/2T)},\tag{2.5}$$

The result is a peak broadened with increasing temperature T and centered around  $\epsilon_d$ . In the following we want to discuss co-tunneling contributions to the conductance. This peak has the same form as the Coulomb blockade peaks in Figure 2.3(a).

### 2.2. Conductance in the Kondo regime

In this section we show how the Anderson model leads to the Kondo model and how this model modifies the conductance. The example of a single non-interacting level has



Figure 2.4.: In 2.4(a) an inelastic co-tunneling process is shown where an electron tunnels from the left lead onto a vacant energy level of the quantum dot while another electron tunnels out of the quantum dot leaving behind an electron-hole pair on the quantum dot. In 2.4(b) an elastic co-tunneling process is sketched where the initial and final states are the same and finally in 2.4(c) an elastic co-tunneling process with spin-flip is shown which gives rise to the Kondo effect.

been discussed with equation (2.5) and as we have seen it results in a Coulomb blockade behaviour. The Anderson model assumes that the quantum dot has one energy level coupled to the two leads. The interaction is described by a constant Coulomb repulsion U for double occupancy of the dot. The aim is to derive the relation between the conductance and the  $\mathcal{T}$ -matrix [22, 45] for such geometries. The discussion will show that the conductance is strongly modified by the Kondo effect.

#### 2.2.1. Anderson model

The Hamiltonian consists of three different terms (2.6)-(2.9)). The right and the left lead contain free electrons given by

$$H_{R;L} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{R;L \ \boldsymbol{k}\sigma} c_{R;L \ \boldsymbol{k}\sigma}, \qquad (2.6)$$

where R (L) labels the right (left) lead respectively. The operator  $c_{Rk\sigma}^{\dagger}$  creates one electron in the right lead with momentum  $\mathbf{k}$  and spin  $\sigma$ . The operators  $c_{Rk\sigma}^{\dagger}$  and  $c_{Rk\sigma}$ follow usual anti-commutation rules for  $i, j \in \{R, L\}$  given by

$$\begin{cases} c_{j\boldsymbol{k}_{1}\sigma_{1}}, c_{i\boldsymbol{k}_{2}\sigma_{2}}^{\dagger} \end{cases} = \delta_{i,j}\delta_{\sigma_{1},\sigma_{2}}\delta_{\boldsymbol{k}_{1},\boldsymbol{k}_{2}} \\ \\ \left\{ c_{j\boldsymbol{k}_{1}\sigma_{1}}, c_{i\boldsymbol{k}_{2}\sigma_{2}} \right\} = \left\{ c_{j\boldsymbol{k}_{1}\sigma_{1}}^{\dagger}, c_{i\boldsymbol{k}_{2}\sigma_{2}}^{\dagger} \right\} = 0.$$

$$(2.7)$$

We use the Anderson model to describe the quantum dot [5, 6, 37]:

$$H_D = \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow}, \qquad (2.8)$$

where  $d_{\sigma}^{\dagger}$  is a fermionic operator obeying anti-commutation rules. The operator  $d_{\sigma}^{\dagger}$  creates an electron on the quantum dot with spin  $\sigma$ ,  $n_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$  is the number of electrons with spin  $\sigma$ , and U is the Coulomb repulsion when the dot is occupied by two electrons. The tunneling terms are described by a tunneling Hamiltonian with the

tunneling amplitudes  $t_{R,L}$ . As already mentioned they do not depend on energy and the tunneling Hamiltonian is given by

$$H_T = \sum_{k\sigma} \left( t_R c^{\dagger}_{Rk\sigma} d_{\sigma} + t_L c^{\dagger}_{Lk\sigma} d_{\sigma} + \text{h. c.} \right).$$
(2.9)

The coupling between the leads and the dot broadens the energy level  $\epsilon_d v$  and is called hybridization  $\Gamma_{R;L} = \pi \rho_0 |t_{R;L}|^2$ .

The historical Anderson model with particle-hole symmetry where one energy level is coupled to the left electron reservoir is sketched in Figure 2.5. When the Fermi level  $\epsilon_F$  and the energy level  $\epsilon_d$  are defined as  $\epsilon_F = 0$  and  $\epsilon_d = -\frac{U}{2}$  the model is particle-hole symmetric. Before we discuss this it is shown how the energy level coupled to two leads can be mapped on to the historical Anderson model. This can be achieved by applying a unitary transformation in the *R-L*-space. The unitary transformation is defined through [22, 37]

$$\begin{pmatrix} c_{\boldsymbol{k}\sigma} \\ \psi_{\boldsymbol{k}\sigma} \end{pmatrix} = \frac{1}{\sqrt{|t_L|^2 + |t_R|^2}} \begin{pmatrix} t_L^* & t_R^* \\ -t_R & t_L \end{pmatrix} \begin{pmatrix} c_{L\boldsymbol{k}\sigma} \\ c_{R\boldsymbol{k}\sigma} \end{pmatrix},$$
(2.10)

leading to the transformed tunneling Hamiltonian  $H_T$ 

$$H_T = \sum_{k\sigma} \sqrt{|t_L|^2 + |t_R|^2} \left( c_{k\sigma}^{\dagger} d_{\sigma} + \text{h. c.} \right).$$
(2.11)

If we compare the tunneling term with a model where only one reservoir is coupled to the quantum dot we conclude that this term leads only to a modified hybridization. This equation shows that electrons which are created by  $\psi_{k\sigma}^{\dagger}$  can not tunnel onto the dot and stay free. Electrons created by  $c_{k\sigma}^{\dagger}$  can tunnel onto the dot and only the spectral function of these electrons is changed by the interaction. Thus, the transformation separates the quantum dot coupled to two leads into two different channels. One of them describes free electrons and the other describes a single electron reservoir coupled to the quantum dot. This justifies to drop the index R or L of the operators describing the free electrons. The transformation has shown that it suffices to discuss the historical Anderson model where only the left lead is coupled to the impurity as shown in Figure 2.5. We use a flat-band density of states for the conduction electrons:

$$\rho(\omega) = \frac{1}{2D}\Theta(D^2 - \omega^2) = \rho_0\Theta(D^2 - \omega^2).$$
 (2.12)

It can be seen in Figure 2.5 that the energy level is occupied by one electron for a sufficient strong Coulomb repulsion U compared to the broadening  $\Gamma_L$  of the energy level  $\epsilon_d$ . This is the magnetic phase of the Anderson model<sup>1</sup>. The critical value where a magnetic moment with spin  $\mathbf{S} = \frac{1}{2}$  is formed is given by  $U_c \approx \pi \Gamma_L$ . This can be understood as a competition between the hybridization and the Coulomb repulsion.

<sup>&</sup>lt;sup>1</sup>The energy level  $\epsilon_d$  has to be below the Fermi level.



Figure 2.5.: In this Figure an energy level  $\epsilon_d$  is coupled to an electron reservoir. The density of states of the conductions electrons is  $\rho(\omega) = \frac{1}{2D} := \rho_0$ . The energy level can be occupied by zero, one or two electrons. Charging the energy level with two electrons costs the Coulomb energy U. The tunneling t broadens the energy level  $\epsilon_d$  with width  $\Gamma_L$ . The situation where one electron occupies the energy level corresponds to a magnetic impurity interacting with the conduction electrons. If the Coulomb repulsion U is big compared to  $\Gamma_L$  the energy level is occupied in average by one electron which gives rise to the Kondo model.

For values  $U \ll U_c$  the resonance is centered around the Fermi energy and for  $U \gg U_c$  the resonance splits into two resonances centered around  $\epsilon_d$  and  $\epsilon_d + U$  which are called Hubbard bands [44]. In the next step we are going to sketch how the Anderson model can be projected into the low energy sub-space. This will lead to an effective spin-spin interaction in the low energy limit.

#### 2.2.2. Kondo model

The Kondo model turns out to be an effective Hamiltonian which describes the low energy physics of the Anderson model. In 1966 J. R. Schrieffer and P. A. Wolff [46] cancelled out the high energy states where the energy levels are occupied by two or zero electrons by projecting the Hamiltonian  $H_D$  into the low energy subspace, where only one electron is residing on the energy level. For the original Anderson model where one electron reservoir is coupled to the impurity one obtains the effective Hamiltonian [7, 46]

$$H_{\rm eff} = -\sum_{\mathbf{k}_1 \mathbf{k}_2 \sigma_1 \sigma_2} \left| t \right|^2 \left( \frac{(c_{\mathbf{k}_1 \sigma_1}^{\dagger} d_{\sigma_1})(d_{\sigma_2}^{\dagger} c_{\mathbf{k}_2 \sigma_2})}{\epsilon_d + U} + \frac{(d_{\sigma_2}^{\dagger} c_{\mathbf{k}_2 \sigma_2})(c_{\mathbf{k}_1 \sigma_1}^{\dagger} d_{\sigma_1})}{-\epsilon_d} \right), \qquad (2.13)$$

where the high energy levels are only occupied virtually and the excitation energies are given in the denominator. The first term describes the process between the double occupied and the single occupied subspace. The second term describes the process between the non-occupied and the single occupied subspace. In the language of the  $\mathcal{T}$ -matrix these are transmission processes in second order. Rewriting the effective Hamiltonian leads to the Kondo model, where the interactions are described by the effective Hamiltonian. Regarding the free electrons described by  $H_0$  leads to

$$H_{\text{Kondo}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} + \frac{J}{2} \mathbf{S}_{d} \cdot \sum_{\mathbf{k}_{1}\mathbf{k}_{2}\sigma_{1}\sigma_{2}} c_{\boldsymbol{k}_{1}\sigma_{1}}^{\dagger} \boldsymbol{\tau}_{\sigma_{1}\sigma_{2}} c_{\boldsymbol{k}_{2}\sigma_{2}}, \qquad (2.14)$$

where  $\boldsymbol{\tau}$  denotes the vector  $\boldsymbol{\tau} = (\tau^x, \tau^y, \tau^z)^T$  formed by the three Pauli matrices and  $\boldsymbol{\tau}_{\sigma_1\sigma_2}$  labels the matrix elements of the Pauli matrices [41, 43]:

$$\tau^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
 (2.15)

Usually, the abbreviation  $c_{0\sigma}^{\dagger} = \sum_{k} c_{k\sigma}^{\dagger}$  and the local spin-density s

$$\boldsymbol{s} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} c^{\dagger}_{0\sigma_1} \boldsymbol{\tau}_{\sigma_1 \sigma_2} c_{0\sigma_2}$$
(2.16)

of the conduction electrons are introduced. The interaction term in the Kondo Hamiltonian  $H_{\text{Kondo}}$  can thus be rewritten as  $H_{\text{eff}} = J \boldsymbol{S} \cdot \boldsymbol{s}$ . The interaction constant J in this derivation is given by

$$J = 2|t|^2 \left(\frac{1}{|\epsilon_d|} + \frac{1}{\epsilon_d + U}\right) = 8\frac{|t|^2}{U},$$
(2.17)

which is always positive in the Anderson model, i.e. the coupling between the two spins is always anti-ferromagnetic. The effective Hamiltonian describes the interactions  $H_{\rm I}$  of the Kondo model. The Kondo Hamiltonian will be written from now on as  $H_K = H_0 + H_{\rm I}$ . The consequences of this interaction for the conductance is the subject of the remaining parts in this chapter. We mention that the Kondo Hamiltonian is a simplification of the Anderson model and that it describes its low energy limit.

#### 2.2.3. Relation between the conductance and the T-matrix

The conductance is a physical property which can be measured in an experiment. In the next step we are going to show how the conductance is related to the  $\mathcal{T}$ -matrix which describes the transmission processes. This relation justifies to discuss only the  $\mathcal{T}$ -matrix. The conductance can be evaluated in a linear response regime which will be done in the following by using the Kubo formula [37, 39]

$$\mathcal{G} = \lim_{\omega \to 0} \frac{1}{\omega} \int_0^\infty e^{i\omega t} \left\langle [I(t), I(0)] \right\rangle dt, \qquad (2.18)$$

with the current operator:

$$I = \frac{e}{2} \frac{d}{dt} \left( N_R - N_L \right). \tag{2.19}$$

It describes the number of electrons which flow from the right to the left reservoir per time unit. If one uses the unitary transformation defined in equation (2.10) for

the current operator in the Kubo formula, two particle correlation functions will occur such as [21, 22]

$$\left\langle c_{\boldsymbol{k}\sigma}^{\dagger}(t)\Psi_{\boldsymbol{k}\sigma}(t)\Psi_{\boldsymbol{k}\sigma}^{\dagger}(0)c_{\boldsymbol{k}\sigma}(0)\right\rangle.$$
 (2.20)

With the help of Wick's theorem (see appendix A), the correlation function can be expressed as a product of free retarded Green's functions

$$G^{R}_{\Psi \boldsymbol{k}\sigma}(\omega) = \frac{1}{\omega - \epsilon_{\boldsymbol{k}} + i0^{+}}$$
(2.21)

and full Green's functions

$$G^{R}_{\boldsymbol{k}\boldsymbol{k}'\sigma}(t-t') = -i\Theta(t)\left\langle \left\{ c_{\boldsymbol{k}\sigma}(t), c^{\dagger}_{\boldsymbol{k}\sigma}(0) \right\} \right\rangle.$$
(2.22)

The conductance  $\mathcal{G}$  of the quantum dot is given by a convolution of Fermi distribution functions  $n_F(\epsilon_k) = 1/(e^{\beta(\epsilon_k - \mu)} + 1)$  and the Green's functions [21]:

$$\mathcal{G} \propto \lim_{\omega \to 0} \omega \int d\epsilon_{\mathbf{k}} \left( n_F(\epsilon_{\mathbf{k}} + \omega) - n_F(\epsilon_{\mathbf{k}}) \right) G_{\Psi \mathbf{k} \sigma}^{'' R}(\epsilon_{\mathbf{k}}) G_{\mathbf{k} \mathbf{k}' \sigma}^{'' R}(\epsilon_{\mathbf{k}})$$
(2.23)

where  $G_{\Psi \boldsymbol{k}\sigma}^{''R}(\omega_1)$  and  $G_{\boldsymbol{k}\boldsymbol{k}'\sigma}^{''R}(\omega_1)$  are the imaginary parts of the corresponding retarded Green's function, respectively. This definition is convenient and will be used from now on in this work for all functions, i.e. the  $\mathcal{T}$ -matrix. The full Green's function is usually written as [45]

$$G^{R}_{\boldsymbol{k}\boldsymbol{k}'\sigma}(\omega) = G^{R}_{0\boldsymbol{k}\sigma}(\omega)\delta_{\boldsymbol{k},\boldsymbol{k}'} + G^{R}_{0\boldsymbol{k}\sigma}(\omega)\mathcal{T}^{R}_{\boldsymbol{k}\boldsymbol{k}'\sigma}(\omega)G^{R}_{0\boldsymbol{k}'\sigma}(\omega), \qquad (2.24)$$

where  $\mathcal{T}_{\boldsymbol{k}\boldsymbol{k}'\sigma}^{R}(\omega)$  denotes the matrix elements of the retarded  $\mathcal{T}$ -matrix. The Green's function  $G_{0\boldsymbol{k}\sigma}^{R}(\omega)$  indicates free propagation of the conduction electrons. For a local interaction such as the Kondo interaction, the matrix elements of  $\mathcal{T}$ -matrix do not depend on  $\boldsymbol{k}$ . The interpretation of this equation is the following: A Green's function describes the probability amplitude that a particle which is created with momentum  $\boldsymbol{k}$  and spin  $\sigma$  at time 0 can be removed at time t with momentum  $\boldsymbol{k}'$  and spin  $\sigma$ . If there are no interactions the momentum  $\boldsymbol{k}$  is conserved. The first term describes thus no scattered particles. The second term describes in principle all possible scattering processes by the  $\mathcal{T}$ -matrix, i.e. multiple scattering. Equation (2.24) is therefore a generalization of equation (2.2), where Green's functions are used for perturbation theory. This equation for the  $\mathcal{T}$ -matrix can also be used to describe inelastic scattering [45, 47]. With the optical theorem [43] it is possible to calculate the total and the elastic cross section. The generalized equation can be used to evaluate the conductance  $\mathcal{G}$ . The first term does not contribute to the conductance and the second term gives the important relation between the  $\mathcal{T}$ -matrix and the conductance which is given by

$$\mathcal{G} = \frac{2e^2}{h} \frac{4|t_L|^2 |t_R|^2}{(|t_L|^2 + |t_R|^2)^2} \int_{-\infty}^{\infty} d\epsilon_k \left(-\frac{dn_F(\epsilon_k)}{d\epsilon_k}\right) \frac{1}{2} \sum_{\sigma} \left[-\pi \rho_0 \mathcal{T}_{\sigma}^{''R}(\epsilon_k)\right].$$
(2.25)

The  $\mathcal{T}$ -matrix of the Kondo model is derived in appendix B and will be discussed in the next chapter. Alternatively, the conductance for the Anderson model is given by [37]

$$\mathcal{G} = e^2 \sum_{\sigma} \int_{-\infty}^{\infty} \frac{d\epsilon_{\boldsymbol{k}}}{2\pi} \frac{\Gamma^L \Gamma^R}{\Gamma^L + \Gamma^R} A(d\sigma, \epsilon_{\boldsymbol{k}}) \left( -\frac{dn_F(\epsilon_{\boldsymbol{k}})}{d\epsilon_{\boldsymbol{k}}} \right), \qquad (2.26)$$

where  $\Gamma^{R;L} = 2\pi |t_{R;L}|^2 \rho_0$  is the hybridization and  $A(d\sigma, \epsilon_k)$  is the spectral function of the quantum dot. It is quite remarkable that the conductance of the quantum dot is determined by the spectral function. The spectral function can be derived from the retarded Green's function  $G_{d\sigma}^R$  which describes the propagation of electrons on the dot. The conductance of the quantum dot thus is determined by local properties. The retarded Green's function of the electrons residing on the dot is given by

$$G_{d\sigma}^{R} = -i\Theta(t) \left\langle \left\{ d_{\sigma}(t), d_{\sigma}^{\dagger}(0) \right\} \right\rangle, \qquad (2.27)$$

which is related to the spectral function  $A(d\sigma, \epsilon_k)$  by (see also appendix A)

$$A(d\sigma, \epsilon_{\boldsymbol{k}}) = -2G_{d\sigma}^{''R}(\epsilon_{\boldsymbol{k}}).$$
(2.28)

Y. Meier and N. S. Wingreen [37, 48] calculated the current through a quantum dot for finite bias voltages using Keldysh Green's functions [49, 50] and obtained

$$I = e^2 \sum_{\sigma} \int_{-\infty}^{\infty} \frac{d\epsilon_{\mathbf{k}}}{2\pi} \frac{\Gamma^L \Gamma^R}{\Gamma^L + \Gamma^R} A(d\sigma, \epsilon_{\mathbf{k}}) \left( n_F(\epsilon_{\mathbf{k}} - \mu_L) - n_F(\epsilon_{\mathbf{k}} - \mu_R) \right), \qquad (2.29)$$

from which the differential conductance  $\frac{dI}{dV}$  can be calculated. Further, it can be seen that in the limit of small voltages V the result in equation (2.26) is obtained. All these result have in common that they are limited by the unitary limit  $\frac{2e^2}{h}$ .

### 2.3. The Kondo problem

The Kondo resonance is one of the most important hallmarks of the Kondo effect and leads to the Kondo problem [7] which will be discussed in this section. The Kondo resonance is centered around the Fermi level and is broadened by  $T_K$  – the Kondo temperature. The Kondo temperature separates the physics in different regimes. In the weak-coupling regime where the temperature  $T \gg T_K$  the Kondo coupling J remains small and perturbation theory is valid. When  $T \ll T_K$  the coupling J becomes very big and perturbation theory is not valid anymore which is known as the Kondo problem. The two regimes are connected by the cross-over regime where perturbation theory begins to break down. It will be shown how the numerical renormalization group (NRG) [7, 9] solves the Kondo problem. Before we discuss this in detail the Kondo effect in metals is discussed.

#### 2.3.1. Kondo effect in metals

We want to begin this section with a short review of the Kondo effect in metals where it was observed the first time in the 1930s [7]. The Kondo effect can be observed in diluted magnetic alloys such as Fe in Au or MoNb which is shown in Figure 2.6. The logarithmic increase of the resistivity for low temperatures in called Kondo effect. We have seen that the Anderson model describes how magnetic moments are formed in those alloys. The spin of the conduction electrons interacts with the spin of the magnetic moment. This interaction leads to an additional scat-



Figure 2.6.: This Figure shows the Kondo effect in the resistivity  $\rho(T)$  as a function of the temperature T of different kinds of MoNb-alloys containing 1% Fe [7].

tering. In metals scattering events raise the resistivity which can be calculated with the help of the Boltzmann equation [1]. The inverse of the momentum relaxation time

$$\frac{1}{\tau(\boldsymbol{k})} = \frac{c_{\rm imp}}{(2\pi)^2} \int d\boldsymbol{k}' \delta(\boldsymbol{k} - \boldsymbol{k}') |\mathcal{T}_{\boldsymbol{k}\boldsymbol{k}'\sigma}|^2 (1 - \cos(\Theta'))$$
(2.30)

describes the effect of scattering events on the conduction electrons, where  $c_{imp}$  is the impurity concentration. This allows to calculate the resistivity. In first oder perturbation a constant momentum relaxation is obtained. This leads to an additional term for the residual resistivity of the metal. Second order perturbation theory of the  $\mathcal{T}$ -matrix leads to the resistivity

$$\rho(T) \propto -\log \left| \frac{T}{D} \right|.$$
(2.31)

J. Kondo was the first who calculated the relaxation time in second order perturbation theory and by doing so he managed to explain the Kondo effect [8]. The calculated resistivity in equation (2.31) diverges for temperature  $T \rightarrow 0$ . This indicates that the perturbation theory is not valid for all temperatures leading to the Kondo problem.

#### 2.3.2. Weak-coupling regime

In this subsection we further discuss the Kondo problem. The  $\mathcal{T}$ -matrix of the Kondo Hamiltonian describes spin-flip processes of all orders. We expand the imaginary part  $\mathcal{T}''^{R}(\omega)$  of the retarded  $\mathcal{T}$ -matrix into a perturbation series. Each term can be used for equation (2.25) to calculate the conductance of the quantum dot in the Kondo regime.

The first contribution in the perturbation series of  $\mathcal{T}^{(1)''R}$  is given by  $\mathcal{T}^{(1)''R}_{\sigma}(\omega) \propto J$ and the more interesting second order  $\mathcal{T}^{(2)''R}$  contribution is given by

$$\mathcal{T}_{\sigma}^{(2)''R}(\omega) \propto J^2 \log \left| \frac{D}{\omega} \right|.$$
 (2.32)

If one looks carefully at each order of the perturbation one asserts that the logarithmic divergence appears in every order n > 2 as

$$\mathcal{T}_{\sigma}^{(n)''R}(\omega) \propto J^n \log^{n-1} \left| \frac{D}{\omega} \right| + J^n \log^{n-p} \left| \frac{D}{\omega} \right| \text{ with } p < n-1.$$
 (2.33)

The leading logarithmic contributions of each order can be summed up which results in a geometric series

$$\mathcal{T}_{\sigma}^{''R}(\omega) = J \sum_{n} \left[ \rho_0 J \log \left| \frac{D}{\omega} \right| \right]^n = \frac{J}{1 - \rho_0 J \log \left| \frac{D}{\omega} \right|}.$$
 (2.34)

In this procedure (the leading logarithmic approximation) the Kondo interaction J is renormalized and which is equivalent to the renormalization group (RG) or poor man's scaling [24]. The renormalization starts with a Hamiltonian describing the high energy physics. Since we are interested in the low energy physics the idea is to find a transformation for the Hamiltonian which removes the high energy states and absorbs it into a Hamiltonian with the same form but different parameters. In the poor man's scaling approach the high energy states are integrated out step by step. This is done by reducing the half-band width D by  $\delta D$  and absorbing it into the Kondo coupling J. In both cases the Kondo coupling J is renormalized in the following way:

$$\rho_0 J_{\rm R} = \frac{\rho_0 J}{1 - J \log \left|\frac{D}{\omega}\right|} = \frac{1}{\log \left|\frac{\omega}{T_K}\right|}; \quad T_K = D e^{-\frac{1}{\rho_0 J}}, \tag{2.35}$$

where the Kondo temperature  $T_K$  has been defined and where the Boltzmann constant is  $k_B = 1$ . The remarkable point which kept physicists busy is the divergence of the renormalized Kondo coupling J when the energy reaches the range defined by the Kondo temperature. Since perturbation theory works only for small interactions J the divergence indicates firstly the breakdown of the perturbative calculation and defines secondly a range where the perturbation theory is valid. This is called weak-coupling regime.

The summation of leading logarithms corresponds to an accumulation of spin-flip processes which leads to the Kondo resonance which is a narrow peak centered at the Fermi level  $\epsilon_F$  and broadened by  $T_K$  in the spectral function of the single energy level. In the weak-coupling regime the conductance  $\mathcal{G}(T)$  is given by

$$\frac{\mathcal{G}(T)}{\mathcal{G}(0)} = \frac{3\pi^2}{16} \frac{1}{\log^2 \left|\frac{T}{T_K}\right|},$$
(2.36)

where it is normalized. The result is valid for  $T \gg T_K$  in accordance with discussion given above. The divergence describes only qualitatively the Kondo resonance in the conductance. In reality the conductance saturates for very low temperatures (the strongcoupling regime) and tends to the unitary limit  $\frac{2e^2}{h}$ . The increasing Kondo coupling Jindicates a new physics for low temperatures which is called the strong-coupling regime. K. G. Wilson found a solution to describe the cross-over regime (1975) by developing the numerical renormalization group (NRG) [9]. Using this method leads to results which agree qualitatively with experiments! In the following we will briefly explain the NRG and then we will turn to the discussion of the strong-coupling regime.

#### 2.3.3. Numerical renormalization group (NRG)

Today, the non-perturbative NRG method is used for a wide range of systems. Since the basic idea in 1975 it has been developed and improved so that it can be applied to systems where a bath of non-interacting fermions or bosons is coupled to a quantum dot with arbitrary interactions. We are using the above introduced Anderson model (see equation (2.8)) to illustrate how the NRG method can be used and follow the introduction given by R. Bulla et al. in [51]. Furthermore, the above used flat-band approach is not crucial for the NRG, i.e. the spectral function  $\rho(\omega)$  can depend on  $\omega$ . However, the flat-band approach is again used to keep the introduction clearer and thus the spectral function is given by  $\rho(\omega) = \rho_0 \Theta(D^2 - \omega)$ . The method consists of five steps:

- 1. Logarithmic division of the continuous density of states
- 2. Logarithmic discretization of the continuous density of states
- 3. Mapping of the discrete model on to a semi-infinite chain
- 4. Iterative diagonalization
- 5. Discussion of fixed points and dynamical properties

#### From the logarithmic division to the semi-infinite chain (steps 1 -3)

The spectral function of the reservoir electrons where the half-band width is D = 1 is separated logarithmically by

$$x_n = \pm \Lambda^{-n}, \quad n = 0, 1, 2, \dots$$
 (2.37)

into intervals with a width  $d_n$  which is given by

$$d_n = \Lambda^{-n} - \Lambda^{-n-1} = \Lambda^{-n} \left( 1 - \Lambda^{-1} \right).$$
 (2.38)

The width decreases for energies around the Fermi level and thus the resolution for low energies increases. The spectral function  $\rho_0$  of the electrons can be discretized by introducing a complete set of orthonormal functions  $\Psi_{np}^{\pm}(\epsilon)$  within each interval

$$\Psi_{np}^{\pm}(\epsilon) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm \omega_n p\epsilon} & \text{if } x_{n-1} < \pm \epsilon < x_n \\ 0 & \text{else} \end{cases}$$
(2.39)

where  $\omega_n = 2\pi/d_n$  and p can take all integer values between  $-\infty$  and  $\infty$ . This corresponds to a Fourier transformation of the states which describe electrons in the lead. The states as defined in equation (2.39) are the so-called Wannier-states and are the basis for the logarithmic discretization. It turns out that the  $p \neq 0$  states couple only to the p = 0 states with a prefactor  $(1 - \Lambda^{-1})$  and not at all to the impurity. In the limit  $\Lambda \to 1$  this coupling between the  $p \neq 0$  and p = 0 vanishes. Here, the first approximation of the NRG is done where the  $p \neq 0$  modes are neglected which is valid for  $\Lambda \to 1$ . But this limit violates the separation of scales. As a compromise the discretization parameter  $\Lambda \approx 2$  is chosen which often produces very good results. The resulting Hamiltonian consists of discrete energy states which couple to the impurity. This Hamiltonian can further be mapped on to a semi-infinite chain by using a standard tridiagonalization procedure. The chain is given by

$$H = H_D + t \sum_{\sigma} \left( c_{0\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{0\sigma} \right) + \sum_{n\sigma} t_n \left( c_{n\sigma}^{\dagger} c_{n+1\sigma} + c_{n+1\sigma}^{\dagger} c_{n\sigma} \right), \qquad (2.40)$$

where  $H_D$  is the dot described by the Anderson model (equation (2.8)),  $d_{\sigma}^{\dagger}(d_{\sigma})$  creates (destroys) an electron on the quantum dot, and  $c_{n\sigma}^{\dagger}(c_{n\sigma})$  creates (destroys) an electron on the *n*-site of the chain with spin  $\sigma$ . The parameter *t* is the tunneling coupling of equation (2.9) describing the coupling between the impurity and the first site of the chain. The parameters  $t_n \approx \frac{1}{2}(1 + \Lambda^{-1})\Lambda^{-\frac{n}{2}}$  for  $n \gg 1$  are the tunneling terms between the different sites of the chain which describes the conduction electrons. It is very important to remark that the tunneling amplitudes obtained during the tridiagonalization procedure decrease exponentially with *n*. This ensures the scale separation and allows the iterative diagonalization of the Hamiltonian to work. These steps are sketched in Figure 2.7 on page 20.

#### Iterative diagonalization (step 4)

The semi-infinite chain can be used for an iterative renormalization group where the usual renormalization scheme  $H_{N+1} = R(H_N)$  is used. The transformation R transforms the chain consisting of N + 1 sites into one which consists of N + 2 sites:

$$H_{N+1} = \sqrt{\Lambda}H_N + \Lambda^{\frac{N}{2}} \sum_{\sigma} t_N \left( c_{N\sigma}^{\dagger} c_{N+1\sigma} + c_{N+1\sigma}^{\dagger} c_{N\sigma} \right)$$
(2.41)



Figure 2.7.: This Figure shows the initial steps of the NRG method exemplified for a flat-band density of states. In Figure 2.7(a) the density of states is divided into logarithmic intervals. After a Fourier transformation one can show that only discrete energies couple to the impurity. This logarithmic discretization of  $\rho_0$  is shown in Figure 2.7(b). In the last step the semi-infinite chain is visualized. Only the first site of the chain couples to the impurity (Figure 2.7(c)) and the tunneling elements  $t_n$  decrease exponentially with increasing N.

where  $H_N$  can be obtained equation (2.40),

$$H_N = \Lambda^{\frac{(N-1)}{2}} \left[ H_D + t \sum_{\sigma} \left( c_{0\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{0\sigma} \right) + \sum_{n=0,\sigma}^{N-1} t_n \left( c_{n\sigma}^{\dagger} c_{n+1\sigma} + c_{n+1\sigma}^{\dagger} c_{n\sigma} \right) \right], \tag{2.42}$$

with the starting Hamiltonian

$$H_0 = \Lambda^{-\frac{1}{2}} \left[ H_D + t \sum_{\sigma} \left( c_{0\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{0\sigma} \right) \right].$$
(2.43)

for the renormalization scheme. From these equations one can see that adding one site corresponds to a Hamiltonian which describes lower energies. Furthermore, it is important that the scales of the Hamiltonian are well separated which is ensured by  $t_n \approx \frac{1}{2}(1 + \Lambda^{-1})\Lambda^{-\frac{n}{2}}$  for  $\Lambda \gg 1$ . The idea is to diagonalize the Hamiltonian  $H_N$  after each step N

$$H_N |r\rangle_N = E_N(r) |r\rangle_N, \qquad (2.44)$$

where  $|r\rangle_N$  is the eigenstate and  $r \in \{1, 2, ..., N_s\}$  where  $N_s$  is the dimension of the corresponding Hilbert space of the N-th iteration. With the help of this basis the new basis for the N + 1 step can be constructed

$$|r;s\rangle_{N+1} = |r\rangle_N \otimes |s(N+1)\rangle, \qquad (2.45)$$

where  $|s(N+1)\rangle$  is the basis of the added site defined as

$$|s(N+1)\rangle = |0,0\rangle, |\uparrow,0\rangle, |0,\downarrow\rangle, |\uparrow,\downarrow\rangle.$$
(2.46)

The matrix elements of the Hamiltonian  $H_{N+1}$  in the basis are given by

$$H_{N+1}(rs; r's') =_{N+1} \langle r; s | H_{N+1} | r'; s' \rangle_{N+1}$$
(2.47)

and have to be diagonalized by a unitary matrix. The eigenvalues and eigenstates are obtained from the Schrödinger equation

$$H_{N+1}|\omega\rangle_{N+1} = E_{N+1}(\omega)|\omega\rangle_{N+1}.$$
(2.48)

During the iterative diagonalization the dimension of the Hilbert space increases exponentially. The second approximation in the NRG procedure is to truncate the dimension of the Hilbert space where the lowest eigenvalues  $N_{s'}$  (s' < s) are kept and the other eigenvalues are discarded which limits the maximum size of the Hilbert space to  $N_{s'}$ . The idea is that higher eigenvalues than  $N_{s'}$  describe the high energy physics which can be neglected if one is interested in the low energy physics. In practice the truncation value is varied in order to test how it affects the result of the NRG. If it does not vary the result too much the truncation scheme is a suitable approximation which eventually makes the numerical diagonalization possible. In the case of a fermion reservoir which is coupled to the quantum dot the reliability of NRG result depends only on the two parameters  $N_{s'}$  and  $\Lambda$ . If  $\Lambda$  is too big there is a very good separation of the energy scales but the resolution is very poor leading to wrong results because the first approximation is not valid. In the limit  $\Lambda \to 1$  the discretization is exact but the separation of the energy scales is very bad and makes NRG instable because the truncation tends to  $N_{s'} \to \infty$ . Thus,  $\Lambda \approx 2$  is a compromise. Using symmetries in the Hamiltonian which separates the full matrix into block-diagonal sub-matrices make the diagonalization more efficient.

#### Renormalization group flow (step 5a)

The renormalization group flow describes the behaviour of the eigenvalues  $E_N(r)$  as a function of the iteration number N and involves a discussion of fixed points. The renormalization group flow for the Anderson model is given in Figure 2.8 and shows how the eigenvalues are changed from high energies to low energies. The case where the spectrum only remains unchanged for several iterations is called an unstable fixed point. The case where the spectrum stays the same for all higher iterations is called stable fixed point. (For more details about fixed points see [52]). The physics changes from a free orbital (FO) to a local moment (LM) behaviour and eventually to the strongcoupling (SC) regime. One can use the fixed points to obtain an effective Hamiltonian. Doing so one finds for the LM behaviour that the effective Hamiltonian is indeed given by equation (2.14). The entropy S is also given in the flow diagram. While for the FO there are 4 possible states, there are only two possible states for the LM because the high energy states are only occupied virtually. The ground-state is achieved in the SC regime where the conduction-electrons and the spin of the impurity are in a complex singlet state. From this point it can be seen that high entropy states tend to be unstable for low energies. It turns out that behaviour of the ground-state of the Anderson model matches the one of a Fermi liquid.

#### Spectral functions (step 5b)

In the last step the NRG results are used to calculate physical properties. This will be exemplified for the normalized spectral function of the impurity  $\rho_{d\sigma}(\omega, T) = -\frac{1}{\pi}G_{d\sigma}^{''R}(\omega, T)$  where the retarded Green's function of the impurity is given by

$$G^{R}_{d\sigma}(\omega,T) = -i \int dt \Theta(t) \left\langle \left\{ d_{\sigma}(t), d^{\dagger}_{\sigma}(0) \right\} \right\rangle.$$
(2.49)

In statistical physics all interesting physical properties can be calculated using the density matrix  $\rho(T)$  [53] if one knows all eigenvalues  $E_r$  as well as all eigenstates  $|r\rangle$  of the full system

$$\varrho(T) = \frac{1}{Z(T)} \sum_{r} e^{-\beta E_r} |r\rangle \langle r|, \quad Z(T) = \sum_{r} e^{-\beta E_r}, \quad (2.50)$$



Figure 2.8.: This Figure shows the flow of the lowest energy levels for even iteration numbers N. The eigenvalues are scaled with  $\Lambda$  to make them visible in this plot for higher iteration numbers N. The physics can be separated into three different regimes: The free orbital regime (FO), the local moment regime (LM) and the strong-coupling regime (SC). The LM regime is achieved after  $N \approx 18$  iterations and the SC regime after  $N \approx 65$  iterations which can be seen from the change of the spectrum. If the energy levels remain constant in a certain range one has a fixed point. The fixed points of the FO- and the LM-regime are unstable, the one of the SC-regime is stable. This means that the energy levels have the same value after 140 iterations as they have after about 65 iterations.

where Z(T) is the partition function. This can be used to write down the Lehmann representation of the normalized spectral function  $\rho_{d\sigma}$ 

$$\rho_{d\sigma}(\omega,T) = \frac{1}{Z(T)} \sum_{r,r'} |M_{r,r'}|^2 \left( e^{-\beta E_r} + e^{-\beta E_{r'}} \right) \delta(\omega - (E_{r'} - E_r)), \quad (2.51)$$

with the many-body matrix elements  $M_{r,r'} = \langle r | d_{\sigma} | r' \rangle$ . The Lehmann representation can be used for any other operator, i.e. the  $\mathcal{T}$ -matrix which will be discussed in the next chapters of this work. The iterative diagonalization of the Hamiltonians  $H_N$  in the NRG method give eigenvalues  $E_r^N$  and eigenstates  $|r\rangle_N$  on a characteristic energy scale  $\omega_N$ 

$$\omega_N = \frac{1}{2} (1 + \Lambda^{-1}) \Lambda^{-\frac{(N-1)}{2}}.$$
(2.52)

In the Lehman representation two different competing energy scales appear – the temperature T and the frequency  $\omega$ . This makes the calculation of dynamic properties more complicated because the NRG only works for one energy scale. The limit of  $T \to 0$  or  $\omega \to 0$  neutralizes this competition of energy scales and the eigenvalues and eigenstates can be used to calculate the relevant matrix elements. In the case of T = 0 the normalized spectral function  $\rho_{d\sigma}(\omega)$  is given by

$$\rho_{d\sigma}^{N}(\omega) \approx \frac{1}{Z_{N}} \left( \sum_{r} |M_{r,0}^{N}|^{2} \delta(\omega + E_{r}^{N}) + \sum_{r'} |M_{0,r'}^{N}|^{2} \delta(\omega - E_{r'}^{N}) \right),$$
(2.53)

for each characteristic energy scale  $\omega_N$  with the ground state energy  $E_0 = 0$ . In other words, the spectral function is calculated from high energies (N = 0) to low energies

 $(N \approx 80)$ . The matrix elements for each step are obtained recursively during the NRG run so that only the initial matrix has to be known. In order to get a smooth curve of the spectral function one performs a broadening of the given discrete points which has to be done carefully. Typical broadening methods are the Gaussian broadening

$$P_G(\omega \pm E_r^N) = \frac{1}{\eta_N \sqrt{\pi}} e^{-\left[\frac{\omega \pm E_r^N}{\eta_N}\right]^2}$$
(2.54)

and the logarithmic Gaussian broadening  $P_{LG}$  which will be used in this work

$$P_{LG}(\omega \pm E_r^N) = \frac{e^{-\frac{b^2}{4}}}{bE_r^N \sqrt{\pi}} e^{-\left[\frac{\log(|\omega|/E_r^N)}{b}\right]^2}.$$
 (2.55)

The Gaussian broadening is characterized by the broadening parameter  $\eta_N$ . Typical values are  $\eta = 0.3\omega_N - 0.7\omega_N$ . The logarithmic Gaussian broadening is characterized by the broadening parameter b where typical values are b = 0.3 - 0.7. The broadening is a rather technical process and there are further techniques which can improve the results. With the z-averaging a lot more NRG data are obtained because data are mixed together from different discretization intervals given by  $x_n = \pm \Lambda^{-n+z}$  [54]. Another problem occurs if there are sharp peaks in spectral functions. The z-averaging can help to to improve the resolution of these peaks. Adjusting further the broadening parameter depending on the behaviour of the curve leads to better resolved peaks. There is an algorithm finding the optimal and smallest broadening parameter b [55] for each region of the spectral function by using a superposition of the obtained peaks [56]. The broadening will be discussed again in more detail later when the spin-resolved  $\mathcal{T}$ -matrix has been calculated. This closes the explanation of the NRG and for more details and other possible applications of it the many papers and introductions which exists such as in Ref. [57, 58] are recommended.

For the Kondo interaction it turns out that the low-temperature behaviour of the entropy  $S_{imp}(T)$ , specific heat  $C_{imp}(T)$  and magnetic susceptibility  $\chi_{imp}(T)$  (the subscript imp indicates the local property) behave like the ones of a Fermi liquid thus the fixed point is a local Fermi liquid which is the subject of the next subsection.

#### 2.3.4. Strong-coupling regime

The physical picture of the strong-coupling regime is the screening of the local spin by the surrounding conduction electrons [44]. The effective interaction between the conduction electrons and the spin of the impurity is given by  $JS \cdot s$  with J > 0. In the low energy limit where J becomes dominant the spin S of the impurity and the spindensity s of the conduction electrons create a complicated many-body singlet which also is the ground state. The first excited state is a triplet. The Kondo temperature can also be interpreted as the energy gap between the ground state and the first excited state (see Figure 2.9). The screening of the local spin can also be seen from the obtained semi-infinite chain which was obtained in equation (2.40): As the coupling J becomes stronger the electrons in the chain will avoid to hop onto the impurity. The physics


Figure 2.9.: In this Figure the weak and the strong coupling regime are sketched. In the weak coupling regime the impurity can be treated as a weak spin-dependent scattering center. For the strong-coupling regime the spin of the electrons and the spin of the impurity are highly correlated and form a complex singlet ground state.  $T_K$  is the energy gap between this ground-state and the first excited state.

is thus dominated by free electrons on a chain and the effect of the impurity becomes a weak interaction thus the effect of the scattering can be expressed as a phase shift  $\delta_s$ . In the zero-temperature limit the unitary limit  $\frac{2e}{h}$  for the conductance is obtained. Finally, the conductance for  $T \ll T_K$  is given by

$$\frac{\mathcal{G}(T)}{\mathcal{G}(0)} = 1 - \frac{\pi^4}{16} \left(\frac{T}{T_K}\right)^2 \tag{2.56}$$

and the static spin susceptibility reads as follows

$$\chi_{\rm imp}(T=0) = \frac{1}{4T_K},$$
(2.57)

which defines the Kondo temperature  $T_K$ . The  $T^2$ -behaviour of the conductance represents the life-time of the quasi-particles which occur in the Fermi liquid picture (see also appendix A). The Kondo resonance can be destroyed for sufficiently strong magnetic fields B or applied bias voltages  $V_b$  (see Figure 2.10). The energy which is defined by these fields has to be larger than the energy defined by the Kondo temperature. In this case the Kondo singlet can be destroyed. The temperature T smears out the Fermidistribution function in each lead, avoiding the formation of the Kondo resonance. The differential conductance in the perturbative regime follows

$$\left| \frac{dI}{dV} \propto \log^2 \left| \frac{\max(V_b, B, T)}{T_K} \right| \right|. \tag{2.58}$$

If one of the given energies exceeds the energy scale defined by the Kondo temperature the calculation remains perturbative.

## 2.3.5. The Kondo effect in quantum dots

The Kondo effect in quantum dots has been detected the first time in 1998 by Goldhaber-Gordon<sup>2</sup> at the MIT [19, 59] in a single In the single electron transistor the discussed

<sup>&</sup>lt;sup>2</sup>http://www.stanford.edu/group/GGG/kondo.html for Figure 2.11



Figure 2.10.: Figure 2.10(a) shows the Kondo resonance centered at the Fermi level  $\epsilon_F$  with the broadened energy levels at  $\pm U/2$ . The Kondo resonance can be destroyed by applying an magnetic field *B* if the magnetic field is strong enough which is shown in Figure 2.10(b). Sufficient strong voltages  $V_b$  suppress the formation of the Kondo resonance as well (Figure 2.10(c)) because resonant tunneling is suppressed.

Coulomb blockade and the Kondo effect occur at the same time. When the number of electrons on the dot is odd there is an unpaired spin. This can be mapped on to the Anderson model and the Kondo model. With decreasing temperature one can observe an unusual behaviour of the measured conductance G of the quantum dot. With decreasing temperature the Coulomb blockade peaks become narrower but otherwise the conductance for an odd number of electrons increases due to the Kondo effect. This experiment shows that quantum dots are indeed tunable objects where different theoretical models (i.e. the Kondo effect) can be tested (see Figure 2.12 where also the conductance is plotted in dependence of the gate and bias voltage leading to Coulomb diamonds and the Kondo resonance for zero bias.) electron transistor. The possibility to tune quantum dots into the Kondo regime gave rise to other experiments [18, 23, 60, 61]. For example it is possible to measure the influence of a magnetic field on the Kondo resonance and compare it theoretical predictions. In this work we want to calculate the  $\mathcal{T}$ -matrix with an applied magnetic field.



Figure 2.11.: This Figure shows the Kondo effect and the Coulomb blockade in quantum dots. For  $V_g \approx -145$ mV and  $V_g \approx -115$ mV there is an an even number of electrons on the quantum dot and the conductance decreases with decreasing temperature – the Coulomb blockade. For  $V_g \approx -130$ mV an odd number of electrons resides on the dot is odd and the conductance increases with decreasing temperature – the Kondo effect [17, 19].



Figure 2.12.: In the plot on the right hand side the NRG is compared to the weak-coupling and strong-coupling regime. On the left hand side the differential conductance is given and again the Coulomb diamonds can be seen. For odd occupancy of the quantum dot the Kondo resonance appears at zero bias. The NRG fits very well with the experimental data (N. Roch 2009 [17, 18]).

# 2.4. Summary

In this section we have seen how the Kondo effect can strongly modify the Coulomb blockade peaks of a quantum dot. These peaks are broadened by thermal effects and tunneling. The Coulomb blockade can be understood classically and can be observed in an isolated quantum dot and allows to control the number of electrons via the gate voltage. For strongly coupled dots, higher order tunneling events become important which are described by the  $\mathcal{T}$ -matrix. Second order tunneling events contribute only weakly to the conductance in the limit of low temperatures. In the case of an odd occupancy the quantum dot is described by the Anderson model where only a single interacting energy level is coupled to the leads. The low energy physics of the Anderson model is determined by the effective Kondo model which describes conduction electrons interacting with a magnetic impurity. This opens a new channel for electrons to tunnel from one lead to the other one leading to a strong increase of the conductance in the limit of low temperatures. Thus, the Kondo effect can only be detected in a quantum dot occupied by an odd number of electrons. For both the Anderson and Kondo model the  $\mathcal{T}$ -matrix plays a major role because it is related to the conductance  $\mathcal{G}$  by

$$\mathcal{G} = \frac{2e^2}{h} \frac{4|t_L|^2|t_R|^2}{(|t_L|^2 + |t_R|^2)^2} \int d\epsilon_{\mathbf{k}} \left(-\frac{dn_F(\epsilon_{\mathbf{k}})}{d\epsilon_{\mathbf{k}}}\right) \frac{1}{2} \sum_{\sigma} \left[-\pi\rho_0 T_{\sigma}^{''R}(\epsilon_{\mathbf{k}})\right].$$
(2.59)

Further, the Kondo temperature  $T_K$  can be interpreted as the binding energy of the singlet between the spin of the conduction electrons and the local moment. The Kondo temperature separates the conductance into the weak-coupling regime  $(T \gg T_K)$  where the perturbation theory is valid and the strong-coupling regime  $(T \ll T_K)$  where a local Fermi liquid behaviour is detected. In the weak coupling regime the conductance and

the differential can be described by

$$\mathcal{G}(T,B) \propto \frac{1}{\log^2 \left| \frac{\max(T,B)}{T_k} \right|} \quad \text{and} \quad \frac{dI}{dV} \propto \frac{1}{\log^2 \left| \frac{\max(T,B,V)}{T_k} \right|}$$
(2.60)

where *B* correspond to the energy scale which is defined by the Zeeman splitting. It should be mentioned that the reliability of the NRG is in question when a Zeeman term occurs in the impurity Hamiltonian thus we are going to use the DM-NRG which is a generalized NRG for dynamical quantities [26]. The DM-NRG runs were carried out with "Flexible DM-NRG<sup>3</sup>" which uses the idea of A.I. Toth et al. [25]. In this work we will come back to the discussion of the role of the magnetic field in chapter 4.

In this chapter we used an single energy level Anderson model but quantum dots can also be described by multi-level Anderson models where the Hamiltonian of the dot is given by [51]

$$H_D = \sum_{i\sigma} \epsilon_{i\sigma} d^{\dagger}_{i\sigma} d_{i\sigma} + E_C (N - \langle N \rangle)^2 - J_H S^2, \qquad (2.61)$$

where N is the operator of the total number of electrons,  $\langle N \rangle$  is the mean value of that number and  $J_H$  is the Hund's exchange. In the case of a two-level quantum dot the measured transport properties show new physics. The relevant energies for this dot are the level spacing  $\delta = \epsilon_2 - \epsilon_1$ , the Hund exchange  $J_H$  and the charging energy  $E_C$ . The S = 1 can be observed on quantum dots with an even number of electrons when the energy level spacing  $\delta < 2J_H$ . This makes the triplet of the two electrons on the dot the ground-state. By changing the gate voltage the quantum dot can be tuned to S = 0(ground-state is the singlet of the two electrons on the dot) [61] and the Kondo effect vanishes. This has been done in a recent work, leading to the underscreened Kondo effect [32], and will be discussed later in chapter 4.

<sup>&</sup>lt;sup>3</sup>http://www.phy.bme.hu/ dmnrg/

# 3. Majorana fermion diagrammatics

In this chapter we are going to introduce the Majorana fermion diagrammatics. It will be particularly exemplified how the diagrammatics works for the Kondo Hamiltonian. The aim is to expand the  $\mathcal{T}$ -matrix of the Kondo model into a perturbation series. The problem is that the  $\mathcal{T}$ -matrix consists of spin operators following more complicated commutation rules than usual fermionic operators and Wick's theorem can not be applied for spin operators. Wick's theorem is very central for many-body perturbation theory. It allows to rewrite the Green's functions of the interacting system in terms of free single particle Green's functions [36]. Using the Majorana fermions for spin  $S = \frac{1}{2}$  operators will circumvent this problem and will finally allow to use Wick's theorem. We will introduce Matsubara Green's functions which can be used to calculate properties of the many-body quantum system at finite temperature [37]. The full Matsubara Green's function can be expressed in terms of free Matsubara Green's functions. This defines a perturbation theory for the spin-dynamics.

# 3.1. Matsubara Green's functions

For the evaluation of correlation functions at finite temperature the zero-temperature formalism has to be modified. A finite temperature leads to excitations out of the ground-system of the system. An average for two given operators A and B at finite temperature in statistical quantum physics is given by [37]

$$C_{AB}(t,t_0) = -\frac{1}{Z} \operatorname{Tr} \left[ \exp\left(-\beta H\right) A(t) B(t_0) \right], \qquad (3.1)$$

where Z is the partition function given by  $Z = \text{Tr}[\exp(-\beta H)]$ .  $\text{Tr}[\cdots]$  denotes the trace of the operator between the brackets. The correlation is calculated between the times t and  $t_0$ . It is very complicated to expand the expression in equation (3.1) directly in a perturbation series as it is done for zero-temperature Green's functions. The solution is to introduce a imaginary-time [36, 37]. This modifies the Schrödinger equation for the time-evolution operator  $U(t, t_0)$ . Replacing the time t by  $t \to -i\tau$  leads to the following equation for the imaginary-time evolution operator

$$\partial_{\tau} U_I(\tau, \tau_0) = -V_I(\tau) U_I(\tau, \tau_0). \tag{3.2}$$

The transformation for the operators in the interaction picture with imaginary times is given by  $V_I(\tau) = \exp(\tau H_0)V \exp(-\tau H_0)$  and solving equation (3.2) leads to

$$U_{I}(\tau,\tau_{0}) = T_{\tau} \exp\left(-\int_{\tau_{0}}^{\tau} d\tau_{1} V_{I}(\tau_{1})\right).$$
(3.3)

Using the properties of the imaginary-time ordering operator  $T_{\tau}$  and transforming equation (3.1) to imaginary times, one obtains the Matsubara Green's function

$$G_{AB}(\tau,\tau_0) = -\langle T_\tau \left[ A(\tau) B(\tau_0) \right] \rangle, \qquad (3.4)$$

which can be expanded into a series of terms, averaged over the free system. This expansion is the basis for the next section, and it is given by

$$G_{AB}(\tau,\tau_0) = -\frac{\langle T_\tau \left[ U_I(\beta,0) A_I(\tau) B_I(\tau_0) \right] \rangle_0}{\langle U_I(\beta,0) \rangle_0}$$
(3.5)

This equation allows us to use similar Feynman-diagrams as introduced in appendix A. How the are used for the Kondo Hamiltonian is discussed below. The denominator of equation (3.5) cancels the non-linked diagrams of the numerator leading to the linked-cluster theorem [37].

# 3.1.1. Properties of Matsubara Green's functions

In this subsection the most important properties of the Matsubara Green's function in equation (3.4) are summarized and the Feynman rules are explained. The Matsubara Green's function depends only on time differences

$$G_{AB}(\tau, \tau_0) = G_{AB}(\tau - \tau_0),$$
 (3.6)

where  $\tau > \tau_0$  and  $-\beta < \tau - \tau_0 < \beta$ . The periodicity of the Matsubara Green's function

$$G_{AB}(\tau + \beta) = \pm G_{AB}(\tau) \tag{3.7}$$

enables one to develop the Green's function into a discrete Fourier series with the following notation:

$$G_{AB}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} G_{AB}(i\omega_n)$$

$$G_{AB}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} G_{AB}(\tau)$$
(3.8)

where  $\omega_n = \frac{2n\pi}{\beta}$  are called bosonic and  $\omega_n = \frac{\pi(2n+1)}{\beta}$  fermionic Matsubara frequencies. In this work we will use  $i\omega_b$  as bosonic,  $i\omega_n$  and  $i\nu_j$  as fermionic Matsubara frequencies. In the real-time formalism we are dealing with a Fourier-transformation in the timedomain while in the imaginary-time formalism the coefficients of the Fourier series in equation (3.8) have to be calculated. A typical expression in this work will be a product of two Green's functions

$$G_1(\tau)G_2(-\tau) = \frac{1}{\tau} \underbrace{0}_2^2,$$
 (3.9)

where  $G_1$  and  $G_2$  are fermion Matsubara Green's function. Such expressions occur when a local interaction is given such as the interaction in the Kondo Hamiltonian. This expression can be expanded into a discrete Fourier series

$$\int_{0}^{\beta} d\tau e^{i\omega_{b}\tau} G_{1}(\tau) G_{2}(-\tau) = \frac{1}{\beta^{2}} \sum_{\nu_{1},\nu_{2}} \int_{0}^{\beta} e^{i(\omega_{b}-\nu_{1}+\nu_{2})\tau} G_{1}(i\nu_{1}) G_{2}(i\nu_{2})$$

$$= \frac{1}{\beta} \sum_{\nu_{2}} G_{1}(i\nu_{2}+i\omega_{b}) G_{2}(i\nu_{2}) e^{i\nu_{2}0^{+}},$$
(3.10)

This example shows the conservation of energies at each vertex but in the language of Matsubara frequencies [37]. The incoming Matsubara frequencies have to be the same as the outgoing ones. Is the interaction non-local the momentum  $\mathbf{k}$  is also conserved at each vertex. This sum over frequencies in equation (3.10) can be evaluated using the theory of analytic functions. If a contour is defined, which encloses all fermion frequencies  $z = i\nu_2$  and the analytic region of the two Green's functions in the example, the sum can be rewritten

$$\frac{1}{\beta} \sum_{\nu_2} G_1(i\nu_2 + i\omega_n) G_2(i\nu_2) e^{i\nu_2 0^+} = -\frac{1}{2\pi i} \int_C dz n_F(z) G_1(z + i\omega_n) G_2(z) e^{z0^+}, \quad (3.11)$$

where  $0^+$  regularizes the integral. The Fermi distribution  $n_F(x)$  has poles at each fermion Matsubara frequency and the residue is  $\frac{1}{\beta}$ . In the case of free fermion Green's functions the summation has to be done over simple poles  $z_j$  with  $z = i\nu_2$ .

$$G_{1,2} = \prod_{j} \frac{1}{z - z_j}.$$
(3.12)

In this case the contour is a circle which covers the entire complex plane (see Figure 3.1). The contour integral has a value of zero due to the regularization of the integral and it follows that the sum over the frequencies  $i\omega_n$  is given by [37]

$$\frac{1}{\beta} \sum_{\nu_2} G_1(i\nu_2 + i\omega_n) G_2(i\nu_2) e^{i\nu_2 0^+} = \sum_j \operatorname{Res}_{z=z_j} \left[ G_1(z + i\omega_n) G_2(z) \right] n_F(z_j) e^{z_j 0^+} ,$$
(3.13)

where  $\text{Res} [\cdots]$  indicates the residue of the functions between the brackets. For bosonic frequencies similar steps with the Bose-Einstein-distribution function  $n_B(x)$  can be carried out. Next, we will discuss the connection between the retarded (advanced) Green's function and the Matsubara Green's function with the analytical continuation.

# Lehmann representation of Matsubara Green's function and the analytical continuation

The Matsubara Green's function can be expanded into the eigenstates of the Hamilton operator. Since the Hamiltonian is given in second quantization, the grand-canonical



Figure 3.1.: This Figure shows how the sum over simple poles of free imaginary time Green's functions can be evaluated. The red circle encloses all poles and due to the infinite small exponential factor this contour integral gives zero.

ensemble is appropriate for the thermal average. The Matsubara Green's function is given in this representation by

$$G_{AB}(\tau) = -\frac{1}{Z} \sum_{n,m} e^{-\beta E_n} \langle n | A | m \rangle \langle m | B | n \rangle e^{\tau(E_n - E_m)}.$$
(3.14)

Performing a Fourier transformation leads to the Lehmann representation. Assuming that A and B are fermion operators and replacing  $i\omega_n$  by z gives the Green's function which in the entire complex plane is defined by

$$G_{AB}(z) = \frac{1}{Z} \sum_{n,m} \frac{\langle n|A|m\rangle\langle m|B|n\rangle}{z + E_n - E_m} \left(e^{-\beta E_n} - e^{-\beta E_m}\right).$$
(3.15)

This result states that the Matsubara Green's function and the zero-temperature Green's function are not independent. The Matsubara Green's function is an extension of the Green's function to the entire complex plane from which the retarded Green's function can be obtained by replacing  $i\omega_n \rightarrow \omega + i0^+$  and vice versa. This follows if one compares the Lehmann representation of the real-time Green's function and the imaginary time Green's function. Further, the advanced Green's function can be obtained by replacing  $i\omega_n \rightarrow \omega + i0^+$  in the Matsubara Green's function and vice versa (see Figure 3.2). Another important concept is the Kramers-Kronig relation, which relates the real part and the imaginary-part of a function, given by

$$\operatorname{Re}(G^{R}(\omega)) = \frac{1}{\pi} \operatorname{P} \int \frac{\operatorname{Im}(G^{R}(\epsilon))}{\epsilon - \omega},$$
(3.16)



Figure 3.2.: This Figure summarizes how the analytic continuation works. The Matsubara Green's function is defined in the entire complex plane except for the real-axis. If the Lehmann representation of the retarded (advanced) Green's function is compared with that of the Matsubara Green's function, one can conclude that the retarded (advanced) Green's function can be obtained by replacing  $i\omega_n \rightarrow \omega + i0^+$  ( $i\omega_n \rightarrow \omega + i0^+$ ) in the Matsubara Green's function.

Another important property for all the discussed Green's function is

$$G_{AB}^{R,A}(\omega) = \operatorname{Re}(G_{AB}(\omega)) \pm i \operatorname{coth}\left(\frac{\beta\omega}{2}\right) \operatorname{Im}(G_{AB}(\omega)), \qquad (3.17)$$

which is an indication of the fluctuation-dissipation-theorem. The property relates the retarded (advanced) Green's functions  $G_{AB}^R$  ( $G_{AB}^A$ ) to the Green's function  $G_{AB}$ . If the temperature goes to zero  $T \to 0$ ,  $\operatorname{coth}(\beta x)$  is given by  $\operatorname{sign}(x)$ .

# 3.2. Kondo interaction and Majorana fermions

In this section a diagram technique for the Kondo problem is introduced using Majorana fermions. First of all we make the problem of spin operators clearer. We want to show what happens if the usual perturbation theory is applied to a simple spin-spin-correlation function  $\chi_z(\tau) = \langle S^z(\tau) S^z(0) \rangle$  or to the more complicated  $\mathcal{T}$ -matrix

$$\mathcal{T}_{\sigma}(\tau) = -\frac{J}{2} \left\langle S^{z} \right\rangle - \frac{J^{2}}{4} \left\langle T_{\tau} \left[ c_{0\sigma_{1}}(\tau) \boldsymbol{\tau}_{\sigma\sigma_{1}} \cdot \boldsymbol{S}(\tau); c_{0\sigma_{2}}^{\dagger}(0) \boldsymbol{\tau}_{\sigma_{2}\sigma} \cdot \boldsymbol{S}(0) \right] \right\rangle.$$
(3.18)

The interaction term of the Kondo Hamiltonian is given by  $JS \cdot s$  where S is the spin of the impurity and s the local spin-density of the conduction electrons. We expand the spin-spin correlation function into a perturbation series

$$\chi_z(\tau) = -\frac{\langle T_\tau \left[ U_I(\beta, 0) S^z(\tau) S^z(0) \right] \rangle_0}{\langle U_I(\beta, 0) \rangle_0},\tag{3.19}$$

where the imaginary time evolution operator is given by

$$U_I(\beta,0) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n T_\tau \left[ J^n \boldsymbol{S} \tau_1 \boldsymbol{s}(\tau_1) \cdots \boldsymbol{S}(\tau_n) \boldsymbol{s}(\tau_n) \right].$$
(3.20)

The averages which occur in the perturbation series are very cumbersome to evaluate since Wick's theorem can not be applied due to the complicated algebra [41]

$$\left[S^i, S^j\right] = i\epsilon_{i,j,k}S^k,\tag{3.21}$$

where  $\epsilon_{i,j,k}$  is the Levi-Civita symbol. The idea is to rewrite the spin as an operator of two fermionic operators. One example are Abrikosov's pseudo-fermions [62] where the spin S is rewritten by

$$\boldsymbol{S} = \frac{1}{2} f_{\sigma_1}^{\dagger} \boldsymbol{\tau}_{\sigma_1, \sigma_2} f_{\sigma_2}, \qquad (3.22)$$

where  $\tau$  denotes the three Pauli matrices. A very hard restriction is the condition  $n_f = 1$ , which means that there is only one particle in one state and this necessary that the formalism works. This can be used for the spin S for the interaction-term of the Kondo Hamiltonian and in the spin-spin-correlation function which becomes a usual two particle interaction. The problem occurs for the  $\mathcal{T}$ -matrix if the pseudo-fermions are used. If the spin is here rewritten using equation (3.22), it is very hard to do perturbation theory for the  $\mathcal{T}$ -matrix because it consists of six fermion operators or in other words a three particle Green's functions. In the following we want to introduce Majorana fermions and to show how these fermions can be used to express the spin-spin correlation function in terms of a Majorana fermion propagator and the  $\mathcal{T}$ -matrix in terms of a two particle Green's functions. The calculation of a two particle Green's functions.

### 3.2.1. Majorana fermions

Majorana fermions are well known in particle physics. The starting point for particle physics and relativistic quantum theory is very often Dirac's equation from which the usual fermions, also called Dirac fermions, can be derived using the usual Pauli matrices. This derivation also leads to the first picture of particles and holes, i.e. electrons and positrons. In a more thorough study of Dirac's equation, one will find, that there is also the possibility to use the Majorana representation. In this representation one ends up with real fermionic fields i.e. particles are their own anti-particles [63]! This property will be encountered in the following beside other properties, which will eventually allow to rewrite the  $\mathcal{T}$ -matrix as a two particle Green's function. Spin-operators are rewritten by

$$\boldsymbol{S} = -\frac{i}{2}\boldsymbol{\eta} \times \boldsymbol{\eta}, \qquad (3.23)$$

where  $\boldsymbol{\eta} = (\eta_1, \eta_2, \eta_3)$  is a triplet of Majorana fermions which satisfy  $\{\eta_a, \eta_b\} = \delta_{ab}$ . One advantage is for instance that the Hilbert space has not to be restricted because  $S^2 = \frac{3}{4}$  is fulfilled following from the given definitions [64, 65]. In the case where a Hamiltonian H describes the dynamics of the spin operator S we introduce a single Dirac fermion  $\Phi$  which is defined in a completely different Hilbert space and commutes with H and  $\eta$ . This means that the single Majorana fermion  $\Phi$  is a constant of motion with a fixed magnitude  $\Phi^2 = \frac{1}{2}$  and it anti-commutes with all other fermions. The following two identities are important and can be verified quickly

$$\boldsymbol{\eta} = 2\Phi \boldsymbol{S}, \qquad \boldsymbol{S} = \Phi \boldsymbol{\eta} \ . \tag{3.24}$$

One can choose for example  $\Phi = -2i\eta_1\eta_2\eta_3$  and verify the demanded properties. One can think that  $\mathbf{S} = \Phi \boldsymbol{\eta}$  is of limited use for the interaction term in the Kondo Hamiltonian because  $\Phi$  depends on  $\boldsymbol{\eta}$  but we can rewrite the spin operators in terms of a Majorana fermion multiplied with a constant fermionic field  $\Phi$  in the spin-spin-correlation function. The constant fermionic field  $\Phi$  commutes with all operators in the Kondo Hamiltonian and so it can be pulled out of the average. The Majorana fermions can be used to define Majorana fermion propagators which are given by

$$G_{ij}(\tau) = -\langle T_{\tau} \left[ \eta_i(\tau) \eta_j^{\dagger}(0) \right] \rangle.$$
(3.25)

and the resulting matrix can also have non-diagonal elements depending on the interaction. The fermionic field  $\Phi$  can be used to define the free propagator  $G_{\Phi}$  which is given by

$$G_{\Phi}(\tau) = -\langle T_{\tau} \left[ \Phi(\tau) \Phi^{\dagger}(0) \right] \rangle.$$
(3.26)

These two propagators can be used for the spin-spin correlation function where Wick's theorem can be applied

$$\chi_{z}(\tau,0) = -\left\langle T_{\tau} \left[ S^{z}(\tau) S^{z}(0) \right] \right\rangle = -\left\langle T_{\tau} \left[ \Phi(\tau) \eta_{3}(\tau) \Phi^{\dagger}(0) \eta_{3}^{\dagger}(0) \right] \right\rangle = G_{\Phi}(\tau) G_{\eta_{3}}(\tau).$$
(3.27)

This equation shows that the spin-dynamics can be expressed by a Majora fermion propagator [64, 66, 67]!

In the next step the interaction in the Kondo Hamiltonian is rewritten and it shown how the diagrammatics works using Majorana fermion propagators. We remember that the Kondo Hamiltonian is given by

$$H_K = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \frac{J}{2} \sum_{\sigma_1 \sigma_2} c^{\dagger}_{0\sigma_1} \boldsymbol{\tau}_{\sigma_1 \sigma_2} c_{0\sigma_2} \cdot \boldsymbol{S}.$$

The spin S of the quantum dot is rewritten using Majorana fermions. This is firstly illustrated for the interaction term  $c_{0\uparrow}^{\dagger}c_{0\downarrow}S^x$  and the illustration is secondly used to generalize the procedure for the other terms. The spin  $S^x$  reads in terms of Majorana fermions  $S^x = -i\eta_2\eta_3$ . The correlation-function  $C_{23}$  is defined to find the vertex after the transformation

$$C_{23} = -\left\langle T_{\tau} \left[ c_{0\downarrow}(\tau) \eta_2(\tau) c_{0\uparrow}^{\dagger}(0) \eta_3^{\dagger}(0) \right] \right\rangle.$$
(3.28)

Although Majorana fermions are real we distinguish formally  $\eta^{\dagger}$  and  $\eta$ . This step makes the diagrammatics clearer because it is expressed in terms of particle and holes [68]. But it is important to regard this choice in all the following calculations. The vertex can be found if the correlation function  $C_{23}$  is expanded into first order perturbation theory where the rewritten interaction-term  $-ic_{\uparrow}^{\dagger}c_{\downarrow}\eta_{2}\eta_{3}$  is used as

$$C_{23}^{(1)}(\tau) = -i \int_{0}^{\beta} d\tau_1 \left\langle T_{\tau} \left[ c_{0\downarrow}(\tau) \eta_2(\tau) c_{0\uparrow}^{\dagger}(0) \eta_3^{\dagger}(0) c_{0\uparrow}^{\dagger}(\tau_1) \eta_2^{\dagger}(\tau_1) \eta_3(\tau_1) c_{0\downarrow}(\tau_1) \right] \right\rangle.$$
(3.29)

At this stage it can be seen that Wick's theorem can be applied. The contractions are given by

$$C_{23}^{(1)}(\tau) = -i \int_0^\beta d\tau_1 \left\langle T_\tau \left[ c_{0\downarrow}(\tau) \eta_2(\tau) c_{0\uparrow}^\dagger(0) \eta_3^\dagger(0) c_{0\uparrow}^\dagger(\tau_1) \eta_2^\dagger(\tau_1) \eta_3(\tau_1) c_{0\downarrow}(\tau_1) \right] \right\rangle_{\substack{0 \\ (3.30)}},$$

and can be expressed according to the introduced perturbation theory as a convolution of free propagators

$$C_{23}^{(1)}(\tau) = -i \int_0^\beta d\tau_1 G_{0c\uparrow}(\tau - \tau_1) G_{0c\downarrow}(\tau_1) G_{02}(\tau - \tau_1) G_{03}(\tau_1).$$
(3.31)

Furthermore, we mention that the interaction term of this example can be written as  $-ic_{\uparrow}^{\dagger}c_{\downarrow}\eta_{2}^{\dagger}\eta_{3}$  or  $-ic_{\uparrow}^{\dagger}\eta_{2}^{\dagger}\eta_{2}c_{\downarrow}$  and that the Kondo coupling J/2 has to be multiplied to both the terms.

The result can be used to define the vertex where the spin of the conduction electrons is changed from  $\downarrow$  to  $\uparrow$  and Majorana fermion 3 is destroyed and 2 is created and can be represented diagrammatically

$$C_{23} = \begin{array}{c} \uparrow & \downarrow \\ \hline & -\frac{iJ}{2} \\ \hline & 2 \\ \hline & 3 \\ \hline \end{array}$$
(3.32)

where the imaginary time evolves from the right to the left. This can be used for all the other terms in the Kondo Hamiltonian by rewriting the spin S of the impurity, where  $S^x = -i\eta_2\eta_3$ ,  $S^y = -i\eta_3\eta_1$  and  $S^z = -i\eta_1\eta_2$  which causes the given different vertices

$$H_{K_{1}} = \left(\frac{-iJ}{2}\right) \left(c_{0\uparrow}^{\dagger}c_{0\downarrow} + c_{0\downarrow}^{\dagger}c_{0\uparrow}\right) \eta_{2}^{\dagger}\eta_{3} + \left(\frac{-J}{2}\right) \left(c_{0\uparrow}^{\dagger}c_{0\downarrow} - c_{0\downarrow}^{\dagger}c_{0\uparrow}\right) \eta_{1}^{\dagger}\eta_{3} + \left(\frac{-iJ}{2}\right) \left(c_{0\uparrow}^{\dagger}c_{0\uparrow} - c_{0\downarrow}^{\dagger}c_{0\downarrow}\right) \eta_{1}^{\dagger}\eta_{2}.$$

$$(3.33)$$



Figure 3.3.: In this Figure all possible vertices defined by the interaction Hamiltonians  $H_{K1}$  and  $H_{K2}$  are shown. Dashed lines represent the entering or leaving Majorana fermion and solid lines the entering or leaving electrons. In a given Feynman diagram, one has to check the value of the vertex.

But there is also another possibility to write the co-tunneling spin-flip processes due to the anti-commutation rule in equation (3.23) which changes the sign of the Majorana fermions when they are commuted and it is given by

$$H_{K_{2}} = \left(\frac{iJ}{2}\right) \left(c_{0\uparrow}^{\dagger}c_{0\downarrow} + c_{0\downarrow}^{\dagger}c_{0\uparrow}\right) \eta_{3}^{\dagger}\eta_{2} + \left(\frac{J}{2}\right) \left(c_{0\uparrow}^{\dagger}c_{0\downarrow} - c_{0\downarrow}^{\dagger}c_{0\uparrow}\right) \eta_{3}^{\dagger}\eta_{1} + \left(\frac{iJ}{2}\right) \left(c_{0\uparrow}^{\dagger}c_{0\uparrow} - c_{0\downarrow}^{\dagger}c_{0\downarrow}\right) \eta_{2}^{\dagger}\eta_{1}.$$

$$(3.34)$$

These free vertices are represented diagrammatically Figure 3.3 and will be used for the following perturbation theory.

Majorana fermions do not have an energy dispersion law in the given Hamiltonian. The free Majorana fermion propagators are given by

$$G_{0j}(i\omega_n) = -\int_0^\beta d\tau e^{i\omega\tau} \langle T_\tau \left[ \eta_1(\tau) \eta_1^\dagger(0) \right] \rangle_0 = \frac{1}{i\omega_n}.$$
(3.35)

The full propagator can be expanded for example up to second order as

$$G_{01}(\tau) = \cdots + \frac{\tau_{2}}{1} + \frac{\tau_{2}}{1} + \frac{\tau_{1}}{1} + \cdots$$
(3.36)

where  $i \in \{2, 3\}$ . In the next step the analytical expression is derived for that diagram. The second order correction is given by

$$G_{\eta}^{(2)}(\tau) = -\frac{1}{2} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \left\langle T_{\tau} \left[ H_{\mathrm{I}}(\tau_{1}) H_{\mathrm{I}}(\tau_{2}) \eta(\tau) \eta^{\dagger}(0) \right] \right\rangle_{0}, \qquad (3.37)$$

where the linked cluster theorem [37] has to be considered (see appendix A). It reduces the number of possible contraction. We remember: The contraction  $\langle \eta(\tau)\eta^{\dagger}(0)\rangle_0$  is cancelled by the denominator in the definition of the perturbation series of the Green's functions. The derivation is again illustrated for the Majorana fermion i = 1 using the vertex  $1 \rightarrow 2$  is used. This leads to

$$\begin{aligned} G_{\eta}^{(2)}(\tau) &= -\frac{1}{2} \frac{J^{2}}{4} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \\ &\times \left\langle T_{\tau} \left[ c_{0\sigma}^{\dagger}(\tau_{1}) \eta_{2}^{\dagger}(\tau_{1}) \eta_{1}(\tau_{1}) c_{0\sigma}(\tau_{1}) c_{0\sigma}^{\dagger}(\tau_{2}) \eta_{1}^{\dagger}(\tau_{2}) \eta_{2}(\tau_{2}) c_{0\sigma}(\tau_{2}) \eta_{1}(\tau) \eta_{1}^{\dagger}(0) \right] \right\rangle_{0} \\ &= \frac{J^{2}}{8} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} G_{0c}(\tau_{2} - \tau_{1}) G_{0c}(\tau_{1} - \tau_{2}) \\ &\times \left\langle T_{\tau} \left[ \eta_{2}^{\dagger}(\tau_{1}) \eta_{1}(\tau_{1}) \eta_{1}^{\dagger}(\tau_{2}) \eta_{2}(\tau_{2}) \eta_{1}(\tau) \eta_{1}^{\dagger}(0) \right] \right\rangle_{0} \\ &= -\frac{J^{2}}{8} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} G_{01}(\tau_{1}) G_{01}(\tau - \tau_{2}) \\ &\times \underbrace{G_{0c}(\tau_{2} - \tau_{1}) G_{0c}(\tau_{1} - \tau_{2}) G_{02}(\tau_{2} - \tau_{1})}_{\Sigma_{\eta}(\tau_{2} - \tau_{1})} \end{aligned}$$
(3.38)

The conjugated process gives the same contribution thus a factor 2 has to be multiplied. We conclude that the second order Feynman diagram in equation (3.36) can be translated into an analytical expression using i = 2 for the internal Majorana fermion propagator which is given by

$$G_{\eta}^{(2)}(\tau) = -\frac{J^2}{4} G_{01}(\tau - \tau_2) G_{01}(\tau_1) \times \sum_{\sigma} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_{c0\sigma}(\tau_1 - \tau_2) G_{c0\sigma}(\tau_2 - \tau_1) G_{02}(\tau_2 - \tau_1),$$
(3.39)

where the label 0 indicates free propagators. Further, the free local conduction electron propagator  $G_{c0\sigma}$  is given by

$$G_{0c\sigma}(i\omega_n) = \int_{-\infty}^{\infty} \frac{\rho(\epsilon)d\epsilon}{i\omega_n - \epsilon} := G_{0c}(i\omega_n), \qquad (3.40)$$

where  $\rho(\epsilon)$  is the density of states of the conduction electrons and the spin-label is dropped because the given propagator does not depend on the spin. In this work we are using a flat-band spectral density

$$\rho(\omega) = \frac{1}{2D} \Theta(D^2 - \omega^2),$$

thus the imaginary part of the retarded conduction electron Green's function is given by

$$G_{0c}^{''R}(\omega) = -\rho_0 \pi \Theta (D^2 - \omega^2).$$
(3.41)

In agreement with the introduced Green's functions formalism, the retarded Green's function can be obtained by analytical continuation. The diagram given in equation (3.36) can be summed up in Dyson's equation leading to the relaxation time of the spin of the impurity. Dyson's equation is given by



where the double dashed line represents the full and the single dashed line the free Majorana fermion propagator. The self-energy diagram  $\Sigma_{\eta}(\tau)$  can be used for all the Majorana fermion propagators because all the free Majorana fermions propagators are equal. The resulting self-energy is given by

$$\Sigma_{\eta}(\tau) = -4 \frac{J^2}{4} G_{c0}(-\tau) \underbrace{G_{0c}(\tau) G_{0\eta}(\tau)}_{\Pi_{0\eta}(\tau)}$$

$$= -J^2 G_{0c}(-\tau) \Pi_{0\eta}(\tau),$$
(3.43)

where the factor 4 indicates that there are 4 different self-energy diagrams in second order. The external free Majorana fermion propagators of the self-energy are given for instance by  $G_{0\eta_1}(\tau)$  so that only  $i = \{2, 3\}$  are allowed and further, two different spins for the conduction electron can be taken into account, thus there are four selfenergy diagrams. Using the vertices of the rewritten Kondo interaction leads to the same vertex for all of them giving the factor 4 in equation (3.43). Additionally, the polarization diagram  $\Pi_{0\eta}(\tau)$  was defined which is calculated in appendix C.1 and can be used for the calculation of the self-energy at finite temperatures. The retarded



Figure 3.4.: In this Figure, the real- and the imaginary part of the self-energy for the Majorana fermion is shown. The functions are calculated using J = 0.145 for the Kondo coupling and D = 1 for the half-band width. The imaginary part part consists only of linear functions and therefore the real part has a logarithmic behaviour see Appendix C.2. Such a term is called Korringa-term [64].

self-energy  $\Sigma_{\eta}^{R}$  is then obtained by analytical continuation and the self-energy can be included to the retarded Majorana fermion propagator via Dyson's equation

$$G_{\eta}^{R}(\omega) = \frac{1}{\omega - \Sigma_{\eta}^{R}(\omega)}.$$
(3.44)

The self-energy is given in lowest non-vanishing order by

$$\Sigma_{\eta}(\tau) = \underbrace{\tau}_{\tau} \underbrace{\tau}_{\eta} \underbrace{\tau}_{\sigma_2} \underbrace{\tau}_{\sigma}_{\sigma_2} \underbrace{\tau}_{\sigma_2} \underbrace{\tau}_{\sigma_2$$

which is the same diagram as in equation (3.36).

## 3.2.2. The magnetic susceptibility

The self-energy can now be used to derive the magnetic susceptibility

$$\chi_1(\tau) = G_{\Phi}(\tau) G_{\eta_1}(\tau). \tag{3.46}$$

The derivation of that diagram can be see as an further example how Matsubara sums are evaluated. The diagram is given in Fourier-space by

$$\chi_{1}(i\omega_{n}) = \frac{1}{\beta\pi^{2}} \sum_{i\nu_{1}} \int_{-\infty}^{\infty} d\omega_{1} \int_{-\infty}^{\infty} d\omega_{2} G_{\Phi}^{''R}(\omega_{1}) G_{\eta_{1}}^{''R}(\omega_{2}) \frac{1}{i\omega_{n} - \omega_{1}} \frac{1}{i\omega_{n} - i\nu_{1} - \omega_{2}}$$

$$= \frac{1}{\pi} \int d\omega_{2} G_{\eta_{1}}^{''R}(\omega_{2}) \frac{\frac{1}{2} - n_{F}(-\omega_{2})}{i\omega_{n} - \omega_{2}}.$$
(3.47)

The retarded imaginary part of the susceptibility is obtained by analytical continuation. Using

$$\frac{1}{2} - n_F(-x) = -\frac{1}{2} \tanh\left(\frac{\beta x}{2}\right),$$
 (3.48)

the imaginary part of the susceptibility is given by

$$\chi_1^{''R}(\omega) = -\frac{1}{2} \tanh\left(\frac{\beta\omega}{2}\right) G_{\eta_1}^{''R}(\omega)$$
(3.49)

The self-energy above can be included in the imaginary part of the retarded Majorana fermion Green's function

$$G_{\eta_1}^{''R}(\omega) = \frac{\Sigma_{\eta}^{R''}(\omega)}{\left(\omega - \Sigma_{\eta}^{R'}(\omega)\right)^2 + \left(\Sigma_{\eta}^{R''}(\omega)\right)^2}.$$
(3.50)

# 3.2.3. The T-matrix

In this subsection we are going to show how the  $\mathcal{T}$ -matrix can be rewritten using Majorana fermions. It was shown that there are two possibilities to rewrite the spin S in the  $\mathcal{T}$ -matrix given in the second term of equation (3.18). The first possibility is  $S = -\frac{i}{2}\boldsymbol{\eta} \times \boldsymbol{\eta}$  which was used also for the interaction term in the Kondo Hamiltonian and the  $\mathcal{T}$ -matrix<sup>1</sup> is given then by

$$\mathcal{T}_{\sigma}(\tau) = -\frac{J^2}{8} \left\langle T_{\tau} \left[ c_{0\sigma_1}(\tau) \tau_{i\sigma\sigma_1} \epsilon^{i,j,k} \eta_j(\tau) \eta_k(\tau); c^{\dagger}_{0\sigma_2}(0) \tau_{l\sigma_2\sigma} \epsilon^{l,o,p} \eta^{\dagger}_o(0) \eta^{\dagger}_p(0) \right] \right\rangle, \quad (3.51)$$

but this is again a three particle Green's function and it is very complicated to expand this into a perturbation series and calculate diagrams. The second possibility  $S = \Phi \eta$ leads to

$$\mathcal{T}_{\sigma}(\tau) = -\frac{J^2}{4} \left\langle \mathcal{T}_{\tau} \left[ c_{0\sigma_1}(\tau) \tau_{i\sigma\sigma_1} \Phi(\tau) \eta_i(\tau); c_{0\sigma_2}^{\dagger}(0) \tau_{l\sigma_2\sigma} \Phi^{\dagger}(0) \eta_l^{\dagger}(0) \right] \right\rangle \\ = \boxed{-\frac{J^2}{4} G_{\Phi}(\tau) \underbrace{\left\langle T_{\tau} \left[ c_{0\sigma_1}(\tau) \tau_{i\sigma\sigma_1} \eta_i(\tau); c_{0\sigma_2}^{\dagger}(0) \tau_{l\sigma_2\sigma} \eta_l^{\dagger}(0) \right] \right\rangle}_{\text{two particle Green's function!}},$$
(3.52)

where only for the two particle Green's functions a perturbation theory has to be applied which will be done in the next chapter. The two particle Green's function is multiplied by the free fermionic propagator  $G_{\Phi}$ .

<sup>&</sup>lt;sup>1</sup>We neglect for the discussion the average  $\langle S^z \rangle$  of the  $\mathcal{T}$ -matrix because the average is only a number and we want to describe the dynamics of  $\mathcal{T}$ - matrix.

# 3.3. Summary

In this chapter it was explained how Matsubara Green's functions containing spin operators can be expanded into a perturbation series with the help of Majorana fermions where Wick's theorem can be applied. In this work we are using Majorana fermions for the Kondo Hamiltonian were the spin S of the quantum dot is rewritten by  $S = -\frac{i}{2}\eta \times \eta$ . This leads to usual vertices in the diagrammatics, where a Majorana fermion and a conduction electron are destroyed and created (see Figure 3.3). The spin in correlation functions such as the  $\mathcal{T}$ -matrix is rewritten by  $S = \Phi \eta$  which has the advantage that the  $\mathcal{T}$ -matrix becomes a two particle Green's function. It was shown that for pseudo fermions the  $\mathcal{T}$ -matrix remains a three particle Green's function. Further, the usage of Majorana fermions ensures the property  $S^2 = \frac{3}{4}$  which is not the case when pseudo-fermions are used where a restriction of the Hilbert space is needed. This restriction makes the calculation of diagrams harder to calculate. The motivation is thus for using Majorana fermions that a visible diagrammatics is tested where the spin relaxation can be included properly.

# 4. Random phase approximation (RPA) for the $\mathcal{T}$ -matrix

In this chapter the  $\mathcal{T}$ -matrix is expanded into a perturbation series using Majorana fermions. We will be inspired by the Random Phase Approximation (RPA) for the interacting electron-gas, where the density-density correlation function of electrons is calculated by summing up the polarization diagram. This leads to a screening of the Coulomb interaction potential. For the interacting electron-gas the RPA is valid for the high-density limit, where the polarization diagram is the leading diagram in each order [4, 37]. In this chapter we are going to use only free propagators and will discuss the  $\mathcal{T}$ -matrix in both the cases without and with magnetic field B. The latter will evoke a thourough discussion of the magneto-conductance of the quantum dot where the RPA will be compared to DM-NRG calculations.

# 4.1. RPA for B = 0 with free propagators

The  $\mathcal{T}$ -matrix is given according to chapter 3 by

$$\mathcal{T}_{\sigma}(\tau) = -\frac{J^2}{4} G_{\Phi}(\tau) \left\langle T_{\tau} \left[ c_{0\sigma_1}(\tau) \tau^i_{\sigma_1 \sigma} \eta_i(\tau); c^{\dagger}_{0\sigma_2}(0) \tau^j_{\sigma\sigma_2} \eta^{\dagger}_j(0) \right] \right\rangle, \tag{4.1}$$

where Wick's theorem and the definition for the propagator of the independent Majorana fermion is used. The  $\mathcal{T}$ -matrix separates into the independent Majorana fermion propagator  $G_{\Phi}(\tau)$  and a usual response function. In the following the perturbation theory is applied for the response function function while  $G_{\Phi}$  stays a constant of motion and is omitted in all diagrams. The response function in the  $\mathcal{T}$ -matrix is given diagrammatically by

$$\left\langle T_{\tau} \left[ c_{0\sigma_{1}}(\tau) \tau_{\sigma_{1}\sigma}^{i} \eta_{i}(\tau); c_{0\sigma_{2}}^{\dagger}(0) \tau_{\sigma\sigma_{2}}^{j} \eta_{j}^{\dagger}(0) \right] \right\rangle = \left\langle \begin{array}{c} \sigma_{1} \\ \sigma_{1} \\ \eta_{i} \\ \eta_{i} \\ \eta_{j} \\ \eta_{$$

where the box represents all the interactions. We are going to carry out the RPA for these interactions. Since there are three different Majorana fermions, in principle nine different expansions have to be carried out. For each of this response functions a leadinglog summation is performed. Here it is assumed that the polarization diagram (bubble



Figure 4.1.: In this Figure, the RPA-expansion of the response function of the  $\mathcal{T}$ -matrix is shown. It is assumed that the polarization diagram in each order has the main contribution to the series and other diagrams are sub-leading. The polarization diagram is the product of a Majorana fermion propagator  $G_{\eta}$  and a conduction electron propagator.

diagram) has the main contribution to the perturbation series, because diagrams with crossing lines produce sub-leading diagrams in each order. In Figure 4.1 the expansion of one response function is shown. The polarization diagrams are summed up to infinity while the other diagrams with crossing lines are neglected. It is expected that a similar result like the usual leading-log summation is obtained (see chapter 2).

In the following the derivation of the RPA for the response functions is done in three steps. First of all, Wick's theorem is applied so that one gets sure about the signs and vertices-values in the series. Then, in the second step the Fourier transformation of the response functions is derived and it is shown that the convolutions in each order of the perturbation series separate into products. In the last step, all diagrams are summed up and a geometric series will be found. The section ends with a discussion of the RPA-result.

### 4.1.1. Wick's theorem for the response functions

In this chapter Wick's theorem is applied for the response function and it is shown how the vertices can be used to find the pre-factors and the signs of the diagrams. For the first contribution to the series Wick's theorem has to be applied for the four operators in the response function. Since the Majorana fermions and the conduction electrons are defined in different Hilbert spaces, there is only one possible contraction given by

$$\Pi_{\sigma_{1},i}^{(0)}(\tau) = \left\langle T_{\tau} \left( c_{0\sigma_{1}}^{\dagger}(\tau) \tau_{\sigma_{1}\sigma}^{i} \eta_{i}(\tau) c_{0\sigma_{2}}^{\dagger}(0) \tau_{\sigma\sigma_{2}}^{j} \eta_{j}^{\dagger}(0) \right) \right\rangle_{0}$$

$$= -\tau_{\sigma_{1}\sigma}^{i} \tau_{\sigma\sigma_{1}}^{i} G_{0c\sigma_{1}}(\tau) G_{0\eta_{i}}(\tau).$$

$$(4.3)$$

Although the free conduction electron propagator does not depend on the spin we keep it here to find the correct pre-factors for the polarization diagrams. For the following discussion the response functions are rewritten as a matrix so that the prefactor of the product of the two matrix-elements of the Pauli-matrices can be read off faster. The product is given by  $\tau^i_{\sigma_1\sigma}\tau^i_{\sigma\sigma_1i}$  and is determined by the spin of the conduction electron propagator. Using the following abbreviation for the response functions introduced in equation (4.2) for the matrix allows to write  $\mathcal{T}_{\uparrow}(\tau)$  more compactly

$$M(\tau) = \begin{pmatrix} \langle \downarrow \eta_1 \downarrow \eta_1 \rangle & i \langle \downarrow \eta_1 \downarrow \eta_2 \rangle & \langle \downarrow \eta_1 \uparrow \eta_3 \rangle \\ -i \langle \downarrow \eta_2 \downarrow \eta_1 \rangle & \langle \downarrow \eta_2 \downarrow \eta_2 \rangle & -i \langle \downarrow \eta_2 \uparrow \eta_3 \rangle \\ \langle \uparrow \eta_3 \downarrow \eta_1 \rangle & i \langle \uparrow \eta_3 \downarrow \eta_2 \rangle & \langle \uparrow \eta_3 \uparrow \eta_3 \rangle \end{pmatrix},$$
(4.4)

leading to the following form of the  $\mathcal{T}$ -matrix

$$T_{\uparrow}(\tau) = -\frac{J^2}{4} G_{\Phi}(\tau) \begin{pmatrix} 1, & 1, & 1 \end{pmatrix} \cdot M(\tau) \cdot \begin{pmatrix} 1\\ 1\\ 1 \end{pmatrix}.$$
 (4.5)

We want to carry out the RPA for the matrix M and discuss the first two orders. The zeroth order matrix  $M^{(0)}$  is given by

$$M^{(0)} = \begin{pmatrix} -G_{0c\downarrow}(\tau)G_{0\eta_1}(\tau) & 0 & 0\\ 0 & -G_{0c\downarrow}(\tau)G_{0\eta_2}(\tau) & 0\\ 0 & 0 & -G_{0c\uparrow}(\tau)G_{0\eta_3}(\tau) \end{pmatrix}.$$
 (4.6)

For the first order perturbation theory in the Kondo coupling we can use the vertices defined in chapter 3. This is exemplified with the same example as before where the vertex

$$C_{23} = \underbrace{-\frac{iJ}{2}}_{2} \qquad (4.7)$$

is defined. This vertex can be used for the response function  $-i\langle \downarrow \eta_2 \uparrow \eta_3 \rangle$ . The corresponding first order diagram is given by

where the vertex occurs in the middle of the diagram over which is integrated. The corresponding analytical expression is given by

$$\Pi_{2,3,\uparrow,\downarrow}^{(1)}(\tau) = -\frac{J}{2} \int_{0}^{\beta} d\tau_{1} \left\langle c_{0\uparrow}(\tau)\eta_{2}(\tau)c_{0\downarrow}^{\dagger}(0)\eta_{3}^{\dagger}(0)c_{0\uparrow}^{\dagger}(\tau_{1})\eta_{2}^{\dagger}(\tau_{1})\eta_{3}(\tau_{1})c_{0\downarrow}(\tau_{1})\right\rangle_{0}$$

$$= -\frac{J}{2} \int_{0}^{\beta} d\tau G_{0c\downarrow}(\tau_{1})G_{0c\uparrow}(\tau-\tau_{1})G_{02}(\tau-\tau_{1})G_{03}(\tau_{1}).$$

$$(4.9)$$

The values of the vertices for the other diagrams are obtained in the same way and are all given by  $-\frac{J}{2}$ , thus the matrix M is given in first order by

$$M^{(1)} = \begin{pmatrix} 0 & \Pi^{(1)}_{1,2,\downarrow,\downarrow}(\tau) & \Pi^{(1)}_{1,3,\downarrow,\uparrow}(\tau) \\ \Pi^{(1)}_{2,1,\downarrow,\downarrow}(\tau) & 0 & \Pi^{(1)}_{2,3,\downarrow,\uparrow}(\tau) \\ \Pi^{(1)}_{3,1,\uparrow,\downarrow}(\tau) & \Pi^{(1)}_{3,2,\uparrow,\downarrow}(\tau) & 0 \end{pmatrix}.$$
 (4.10)

This expression looks more scary than it is, because the conduction electron propagators do not depend on the spin. The free Majorana fermion propagators are further all equal giving one bubble diagram

$$\Pi_{0\eta}(\tau) = G_{0c}(\tau)G_{0\eta}(\tau).$$
(4.11)

The first correction can be written as a convolution

$$\Pi^{(1)}(\tau) = -\frac{J}{2} \int_0^\beta d\tau_1 \Pi_0(\tau - \tau_1) \Pi_0(\tau_1) := -\frac{J}{2} \left[ \Pi_0 * \Pi_0 \right](\tau), \tag{4.12}$$

where the convolution is defined as  $[\cdot * \cdot * \cdot * \dots](\tau)$ . This can be used to write down the RPA-expansion of the  $\mathcal{T}_{\uparrow}$ -matrix up to first order

$$\mathcal{T}_{\uparrow}(\tau) = \frac{J^2}{4} G_{\Phi}(\tau) \left[ 3\Pi_{0\eta} + \frac{J}{2} 6\Pi_{0\eta} * \Pi_{0\eta} + \dots \right] (\tau).$$
(4.13)

The factors 3 and 6 stem from equation (4.5) where the zeroth and first order of the matrix M are used. The Fourier transformation of the first convolutions are given by

$$\Pi^{(0)}(i\omega_b) = \frac{1}{\beta} \sum_{\nu_1} G_{0\eta}(-i\nu_1 + i\omega_b) G_{0c}(i\nu_1)$$

and

$$\Pi^{(1)}(i\omega_b) = \frac{1}{\beta} \sum_{\nu_1} G_{0\eta}(-i\nu_1 + i\omega_b) G_{0c}(i\nu_1) \frac{1}{\beta} \sum_{\nu_2} G_{0\eta}(-i\nu_2 + i\omega_b) G_{0c}(i\nu_1)$$
$$= \left(\Pi^{(0)}(i\omega_b)\right)^2,$$
(4.14)

where  $i\omega_b$  is a bosonic Matsubara frequency. Higher order convolutions also separate into a product of bubble diagrams which can be shown by induction. In the next section the pre-factors are found by using recursive relations between the coefficients. In the end of the section a more systematic way is presented how these pre-factors can be derived.

## 4.1.2. Geometric series

In this paragraph we show how the RPA can be carried out systematically. Therefore, the structure of the diagrams has to be further discussed and it is shown how the coefficients in the sum can be obtained via a recursion. This recursion can be found by using the following rules:

• In principle, there are only two different response-functions. The first type is a response-function where the same Majorana fermion or conduction electron enters and leaves the interacting region (gray box of the  $\mathcal{T}$ -matrix). These are

			n	$a_n$	$b_n$	$3a_n + 6b_n$
$(1)(2) \cdots (1)$			0	1	0	$3 \cdot 2^0$
$a_n = \underbrace{(1)}_{(3)} \cdots \underbrace{(1)}_{(1)}$		$a_n = 2b_{n-1}$	1	0	1	$3\cdot 2^1$
	$\rightarrow$	$\rightarrow$	2	1	2	$3 \cdot 2^2$
$b_n = \underbrace{\begin{pmatrix} 1 \\ 2 \end{pmatrix}}_{n} \cdots \underbrace{\begin{pmatrix} 2 \\ 2 \end{pmatrix}}_{n}$		$b_n = a_{n-1} + b_{n-1}$	3	3	2	$3 \cdot 2^3$
$(1)(3) \cdots (2)$			4	5	6	$3 \cdot 2^4$

Figure 4.2.: On the left hand side, the recursion is represented diagrammatically. The  $a_n$  represent according to the definition in this work the diagonal response-functions and it suffices to analyze one of this type, where the Majorana fermion, labeled by 1 enters and leaves. The same can be done for  $b_n$ , where the Majorana fermion 1 enters and 2 leaves. For each of these types, there are two possible processes for the next diagram which is calculated before. These relations are given in the middle of the Figure and together with the initial conditions given in equation (4.15) the coefficients for each order can be calculated and are given up to fourth order on the right hand side.

the diagonal terms of the matrix given in equation (4.4) and are labeled with  $a_n$ . The 3 diagonal terms lead to  $3a_n$ . The second type is a response-function where different Majorana fermions and conduction electron with flipped spin enter and leave the interacting region. These processes are labeled with  $b_n$ . These terms are given by the non-diagonal terms of the matrix in equation (4.4) thus  $6b_n$ .

• For the spin-flip processes exists the following rule which simplifies the diagrammatics. The spin of the conduction electron is always related to a certain Majorana fermion. If the index i, j, k, ... of the Majorana fermions is 1 or 2 the spin  $\sigma_1, \sigma_2, \sigma_3, ...$  of the electron can only be spin-down in the expansion of the response-function. If the index number of the Majorana fermion is 3, the spin has to be spin-up. This rule reduces the number of possible diagrams and it suffices only to keep the Majorana fermion indices for the recursion (see Figure 4.2).

Following these rules the  $\mathcal{T}_{\uparrow}$ -matrix up to first order perturbation theory reads

$$\mathcal{T}_{\uparrow}(\tau) = \frac{J^2}{4} G_{\Phi}(\tau) \left[ (3a_0 + 6b_0) \Pi_{0\eta} + \frac{J}{2} (3a_1 + 6b_1) \Pi_{0\eta} * \Pi_{0\eta} + \dots \right] (\tau) = \frac{J^2}{4} G_{\Phi}(\tau) \sum_{n=0}^{\infty} (3a_n + 6b_n) \left(\frac{J}{2}\right)^n \underbrace{[\Pi_{0\eta} * \dots * \Pi_{0\eta}]}_{(n+1) \text{ times}} (\tau),$$

$$(4.15)$$

where  $a_0 = 1$ ,  $b_0 = 0$ ,  $a_1 = 0$  and  $b_1 = 1$ . Figure 4.2 leads to the assumption that the coefficients in the series are given by

$$3a_n + 6b_n = 3 \cdot 2^n, \tag{4.16}$$

which can be verified by induction using the discovered recursion rules. This is quite remarkable and leads to a usual geometric series. Using this result the  $\mathcal{T}$ -matrix is

given by

$$\mathcal{T}_{\uparrow}(\tau) = \frac{3J^2}{4} G_{\Phi}(\tau) \Pi_{\eta}(\tau), \qquad (4.17)$$

where  $\Pi_{\eta}(\tau)$  is determined by the geometric series obtained above

$$\Pi_{\eta}(\tau) = \sum_{n=0}^{\infty} J^n \underbrace{[\Pi_{0\eta} * \dots * \Pi_{0\eta}]}_{(n+1) \text{ times}}(\tau).$$
(4.18)

For each order there is a convolution of n + 1 polarization diagrams. In the last paragraph it was illustrated that the first two orders separate into products after expanding the convolution into a Fourier series. This can be used to show that higher order convolutions also separate into products so that the geometric series can be finally carried out leading to

$$\Pi_{\eta}(i\omega_b) = \frac{\Pi_{0\eta}(i\omega_b)}{1 - J\Pi_{0\eta}(i\omega_b)}$$
(4.19)

where bosonic Matsubara frequencies occur in the polarization diagrams.

Before the polarization diagram is discussed in detail a more systematic way is given to obtain the geometric series in the last equation. The relation between the coefficients in Figure 4.2 can also be written as a matrix equation given by

$$\begin{pmatrix} a_n \\ b_n \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 1 & 1 \end{pmatrix}^n \cdot \begin{pmatrix} a_0 \\ b_0 \end{pmatrix}.$$
 (4.20)

This can be used to rewrite the series in Fourier space

$$3\Pi_{\eta}(i\omega_{b}) = \Pi_{0\eta} \begin{pmatrix} 3, & 6 \end{pmatrix} \cdot \sum_{n=0}^{\infty} \begin{pmatrix} a_{n} \\ b_{n} \end{pmatrix} \left( \frac{J\Pi_{0\eta}}{2} \right)^{n} \\ = \Pi_{0\eta} \begin{pmatrix} 3, & 6 \end{pmatrix} \cdot \sum_{n=0}^{\infty} \begin{pmatrix} 0 & 2 \\ 1 & 1 \end{pmatrix}^{n} \cdot \begin{pmatrix} a_{0} \\ b_{0} \end{pmatrix} \left( \frac{J\Pi_{0\eta}}{2} \right)^{n} \\ = \Pi_{0\eta} \begin{pmatrix} 3, & 6 \end{pmatrix} \cdot \left( 1 - \frac{J\Pi_{0\eta}}{2} \begin{pmatrix} 0 & 2 \\ 1 & 1 \end{pmatrix} \right)^{-1} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
(4.21)
$$= \left[ \frac{\Pi_{0\eta}}{(1 - J\Pi_{0\eta}) \left( 1 + \frac{J\Pi_{0\eta}}{2} \right)} \right] \begin{pmatrix} 3, & 6 \end{pmatrix} \cdot \left( \frac{1 - \frac{J\Pi_{0\eta}}{2}}{\frac{J\Pi_{0\eta}}{2}} \right) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ = \frac{3\Pi_{0\eta}}{1 - J\Pi_{0\eta}},$$

where  $\Pi_{0\eta} := \Pi_{0\eta}(i\omega_b)$ . This is the same result as obtained before. In the first step, the term  $3a_n + 6b_n$  were rewritten as a scalar product of two vectors. Then, we used the recursion relation written as a matrix. This led to expression where only the first coefficients  $a_0$  and  $b_0$  are needed. The final result can be found using

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{ad - cb} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$
 (4.22)

In the last step, the Fourier transformation  $\mathcal{T}_{\uparrow}(i\omega_n)$  is calculated and it is given by

$$\mathcal{T}_{\uparrow}(i\omega_{n}) = \frac{3J^{2}}{4} \frac{1}{\beta} \sum_{i\nu_{1}} G_{\Phi}(i\nu_{1})\Pi(i\omega_{n} - i\nu_{1})$$

$$= \frac{3J^{2}}{4\pi^{2}} \int_{-\infty}^{\infty} d\omega_{1} \int_{-\infty}^{\infty} d\omega_{2} \underbrace{G_{\Phi}^{''R}(\omega_{1})}_{=-\pi\delta(\omega_{1})} \Pi^{''R}(\omega_{2}) \frac{1}{\beta} \sum_{i\nu_{1}} \underbrace{\frac{1}{i\nu_{1} - \omega_{1}} \frac{1}{i\omega_{n} - i\nu_{1} - \omega_{2}}}_{=-\frac{n_{F}(\omega_{1}) + n_{B}(-\omega_{2})}{\omega_{2} - i\omega_{n}}}$$

$$= \frac{3J^{2}}{8\pi} \int_{-\infty}^{\infty} d\omega_{2} \Pi_{\eta}^{''R}(\omega_{2}) \frac{1 + 2n_{B}(-\omega_{2})}{\omega_{2} - i\omega_{n}}, \qquad (4.23)$$

where  $i\omega_n$  of the Fourier transformation is a fermionic Matsubara frequency. Since one is interested in the imaginary part of the retarded  $\mathcal{T}$ -matrix the analytic continuation  $i\omega_n \to \omega + i0^+$  is carried out and the result is given by

$$\mathcal{T}^{''R}_{\uparrow}(\omega) = -\frac{3J^2}{8} \coth\left(\frac{\beta\omega}{2}\right) \Pi^{''R}_{\eta}(\omega)$$

$$= -\frac{3J^2}{8} \coth\left(\frac{\beta\omega}{2}\right) \operatorname{Im}\left(\frac{\Pi^R_{0\eta}(\omega)}{1 + J\Pi^R_{0\eta}(\omega)}\right).$$

$$(4.24)$$

This result is valid for any  $\Pi(i\omega_b)$  and this can be understood in the context of the dissipation-fluctuation theorem which is in agreement with the given analytic properties of Green's functions in chapter 3. In this case  $\Pi_{\eta}^{"R}(\omega)$  can be derived from

$$\tau$$
 $\eta$ 
 $\eta$ 
 $= \Pi_{0\eta}(\tau) = G_{0\eta}(\tau)G_{0c}(\tau).$ 
(4.25)

If the limit temperature  $T \to 0$  is taken, the functions  $\operatorname{coth}(\beta x)$  and  $\tanh(\beta x)$  become  $\operatorname{sign}(x)$ . The polarization diagram which provides the main contribution to the perturbation series is calculated in appendix C.1 and given by

$$\Pi_{0\eta}^{R}(\omega) = \frac{\rho_{0}}{2} \log\left(\left|\frac{\omega^{2} - D^{2}}{\omega^{2}}\right|\right) + i\pi \frac{\rho_{0}}{2} \operatorname{sign}(\omega)\Theta(\omega^{2} - D^{2})$$
(4.26)

This leads to the final result for  $\mathcal{T}$ -matrix which is given by

$$\mathcal{T}_{\uparrow}^{''R}(\omega) = -\frac{3J^2}{16} \frac{\pi\rho_0}{\left(1 - \frac{J}{2}\rho_0 \log\left|\frac{D^2 - \omega^2}{\omega^2}\right|\right)^2 + \frac{J^2}{4}\pi^2\rho_0^2}$$
(4.27)

This subsection ends with a short summary of the most important steps of the evaluation of the RPA result, which will be adapted to the  $\mathcal{T}$ -matrix at finite magnetic field in the next section:

- 1. The  $\mathcal{T}$ -matrix was rewritten by using Majorana fermions for spin operators. This separates the  $\mathcal{T}$ -matrix into a free Majorana fermion propagator  $G_{\Phi}$  and different response functions which consist of conduction electron  $G_c$  and Majorana fermion propagators  $G_{\eta}$
- 2. We used the conservation of the total spin which relates the spin of the conduction electron with certain Majorana fermions. This simplified the diagrammatics and enabled us finally to find the recursion rule between the coefficients in the RPA-series (see Figure 4.1).
- 3. The  $\mathcal{T}$ -matrix consists of two different types of response functions. The first type corresponds to processes where the same Majorana fermions enter and leave the interacting region and the second type to processes where different Majorana fermions enter and leave the interacting region.
- 4. The summation of the two different response-functions can be done systematically using recursion-relation between the pre-factors of the different orders in the perturbation series. In fact, in this case here, the summation led to a typical geometric series when a RPA is carried out.
- 5.  $\mathcal{T}_{\downarrow}$  can be obtained by using  $\mathcal{T}_{\uparrow}(\omega) = \mathcal{T}_{\downarrow}(\omega)$  which follows from Kramers degeneracy.

### 4.1.3. Result

In this section we discuss the result which is obtained by performing a RPA for the  $\mathcal{T}$ -matrix. In the weak-coupling regime, which is given by  $D \gg \omega \gg T_K$ , this result can be rewritten using the Kondo temperature  $T_K$  leading to

$$-\pi\rho_0 \mathcal{T}^{''R}_{\uparrow}(\omega) \approx \frac{3\pi^2}{16} \frac{1}{\log^2 \left|\frac{\omega}{T_K}\right| + \frac{\pi^2}{4}}.$$
(4.28)

This result confirms that the RPA and using Majorana fermions for the  $\mathcal{T}$ -matrix is equal to poor man's scaling (renormalization of the Kondo coupling) in the weakcoupling regime where the small constant term in the denominator in equation (4.28) is negligible. But the this term helps us to cut the divergence for  $\omega \approx T_K$ . This difference between the two derivations (RPA and poor man's scaling) stems from the fact, that in the RPA the imaginary part of the polarization diagram is not neglected for the renormalization of  $J_R(\omega)$ . However, as a hallmark of the Kondo problem the strong-coupling regime can not be achieved with the RPA for the  $\mathcal{T}$ -matrix, even with the small constant term in the denominator of equation (4.28). This can be seen from the large deviations from the NRG-calculation for low energies where the NRG describes the cross-over and the strong-coupling regime well. The  $\mathcal{T}$ -matrix is given in Figure 4.3 where it is compared with a NRG-run for the  $\mathcal{T}$ -matrix. Additionally, we gave the result of the local Fermi liquid and it can be clearly seen that the RPA does not match it.



Figure 4.3.: RPA compared to leading log summation, Fermi liquid and NRG. It can be seen that the RPA agrees with the poor man's scaling result.

# 4.2. RPA for $B \neq 0$ with free propagators

In this section we want to discuss the RPA for the  $\mathcal{T}$ -matrix in the presence of a magnetic field and compare it with DM-NRG calculations. This serves as benchmark for the Majorana fermion diagrammatics and the DM-NRG calculations. As already mentioned in chapter 2 the reliability of the NRG is in question. Since the  $\mathcal{T}$ -matrix is related to the conductance of the quantum dot the  $\mathcal{T}$ -matrix at finite magnetic field describes the magneto-conductance. We will begin therefore this section with a short review of experiments on the magneto-conductance.

### 4.2.1. Experimental set-up

When the effect of an applied magnetic field is studied in an experiment, quantum dots formed from carbon nanotubes have advantages relative to quantum dots formed from semiconducting heterostructures. Beside the already discussed higher Kondo temperatures in these dots they have also a large Landé-factor  $g \approx 2$ . The coupling of a spin S to a magnetic field B is given by the Pauli-equation which can be derived from the Dirac equation and the coupling reads

$$H_z \propto -g\boldsymbol{S} \cdot \boldsymbol{B},\tag{4.29}$$

where the energy is lowered when the magnetic field B is parallel to the spin S. This energy is the Zeeman energy and has to be bigger than  $T_K$ .  $T_K$  is the binding energy



Figure 4.4.: The experimental data for this graph are obtained by N. Roch [17, 18, 61] where the differential magneto-conductance in the Kondo regime was measured. It shows the critical field for the splitting at  $B \approx 5T$ .

of the ground-state of the anti-ferromagnetic Kondo model [33, 34] which has to be exceeded by the Zeeman energy. This leads to two experimental boundary conditions:

- Kondo temperature has to be larger than the accessible temperature so that one can observe the Kondo resonance
- A large g leads to a Zeeman energy that is larger than the energy-scale defined through the Kondo temperature

For the theoretical discussion we put the Zeeman energy in the definition of the magnetic field  $||\boldsymbol{B}||$ . There is a disagreement between the measured critical magnetic field and the predicted theoretical one [28, 33].

# 4.2.2. The Kondo interaction in the presence of a magnetic field

The applied magnetic field affects the spin of the conduction electrons and of the impurity. Since the Fermi energy is defined as zero and the magnetic field is applied in the negative direction of the z-axis  $\mathbf{B} = -B\hat{e}_z$  leads to the Zeeman term [41]

$$H_Z = BS^z + \frac{B}{2} \sum_{k\sigma} \sigma c^{\dagger}_{k\sigma} c_{k\sigma}, \qquad (4.30)$$

The focus is on the regime where  $T_K \ll B \ll D$  so that the Zeeman splitting can be observed. The magnetic field leads to a renormalized half-band width which is given by  $D_R = D - B \approx D$ . This effect can be neglected since  $B \ll D$  and the old half-band width can be used and the second term in equation (4.30) drops out. The magnetic field thus only affects the spin **S** of the quantum dot.

# 4.2.3. Transformation of the Majorana fermions and RPA

The additional Zeeman term in the Kondo Hamiltonian is given by

$$H_Z = BS^z = -iB\eta_1\eta_2, \tag{4.31}$$

where B is measured in units of the Zeeman splitting. If the spin is rewritten using Majorana fermions the Majorana fermion propagator  $G_{ij}(\tau)$  has non-diagonal elements which makes it more difficult to carry out the RPA for the  $\mathcal{T}$ -matrix. The idea is to transform the Majorana fermions so that the propagator becomes diagonal. The Kondo Hamiltonian can be rewritten by using the ladder-operators  $S^+$ ,  $S^-$ , and the zcomponent of the total spin operator  $S^z$  with  $S^{\pm} = S^x \pm iS^y$ . The Kondo Hamiltonian is given using the ladder-operators by

$$H_K = \frac{J}{2} \left( c^{\dagger}_{0\downarrow} c_{0\uparrow} S^+ + c^{\dagger}_{0\uparrow} c_{0\downarrow} S^- \right) + \frac{J}{2} \left( c^{\dagger}_{0\uparrow} c_{0\uparrow} - c^{\dagger}_{0\downarrow} c_{0\downarrow} \right) S^z.$$
(4.32)

The Majorana fermion propagator becomes diagonal by introducing

$$f^{\dagger} = \frac{1}{\sqrt{2}}(\eta_1 + i\eta_2), \quad \left\{f^{\dagger}, f\right\} = 1.$$
 (4.33)

The ladder-operators are given after this transformation by

$$S^{+} = S^{x} + iS^{y} = \eta_{3}(\eta_{1} + i\eta_{2}) = \sqrt{2\eta_{3}}f^{\dagger},$$
  

$$S^{-} = S^{x} - iS^{y} = (\eta_{1} - i\eta_{2})\eta_{3} = \sqrt{2}f\eta_{3},$$
(4.34)

and the z-component of the total spin operator by

$$S^{z} = -ff^{\dagger} + \frac{1}{2}, \tag{4.35}$$

where terms  $f^{\dagger}f^{\dagger}$  and ff give zero, because the Pauli-principle which forbids more than one fermion in one state. The Kondo Hamiltonian is given after this transformation<sup>1</sup> by

$$H_K = -\frac{J}{2}\sqrt{2}\left(c^{\dagger}_{0\downarrow}c_{0\uparrow}f^{\dagger}\eta_3 + c^{\dagger}_{0\uparrow}c_{0\downarrow}\eta^{\dagger}_3f\right) + \frac{J}{2}\left(c^{\dagger}_{0\uparrow}f^{\dagger}fc_{0\uparrow} - c^{\dagger}_{0\downarrow}f^{\dagger}fc_{0\downarrow}\right)$$
(4.36)

and the Zeeman term is given by

$$H_z = Bf^{\dagger}f - \frac{1}{2}B, \qquad (4.37)$$

where the last term of the Zeeman term is only a constant and is thus dropped from now on. Further, the transformation leads to two different fermionic propagators which are given by

$$G_f(i\omega_n) = \frac{1}{i\omega_n - B}, \quad G_{\eta_3}(i\omega_n) = \frac{1}{i\omega_n}, \tag{4.38}$$

<sup>&</sup>lt;sup>1</sup>The term  $\propto \frac{J}{4}c_{0\sigma}^{\dagger}c_{0\sigma}$  was dropped since it corresponds to a weak external potential scattering term. This term becomes important for the self-energy in second order (see chapter 5).

where  $G_f$  is a Dirac fermion and  $G_{\eta_3}$  is the unchanged part of the original Majorana fermion propagator and the label 3 can be dropped and we will use  $G_{\eta}$  as Majorana fermion propagator. Next, the  $\mathcal{T}$ -matrix is transformed using f and  $\eta$ . As an intermediate step the matrix  $M(\tau)$  which was defined above in equation (4.5) is rewritten by

$$\begin{array}{ll} (1, \quad 1, \quad 1) \cdot M(\tau) \cdot \begin{pmatrix} 1\\1\\1 \end{pmatrix} \\ &= (1, \quad 1, \quad 1) \cdot \begin{pmatrix} \langle \downarrow \eta_1 \downarrow \eta_1 \rangle & i \langle \downarrow \eta_1 \downarrow \eta_2 \rangle & \langle \downarrow \eta_1 \uparrow \eta_3 \rangle \\ -i \langle \downarrow \eta_2 \downarrow \eta_1 \rangle & \langle \downarrow \eta_2 \downarrow \eta_2 \rangle & -i \langle \downarrow \eta_2 \uparrow \eta_3 \rangle \\ \langle \uparrow \eta_3 \downarrow \eta_1 \rangle & i \langle \uparrow \eta_3 \downarrow \eta_2 \rangle & \langle \uparrow \eta_3 \uparrow \eta_3 \rangle \end{pmatrix} \cdot \begin{pmatrix} 1\\1\\1 \end{pmatrix} \\ &= (1, \quad 1) \cdot \begin{pmatrix} \langle \downarrow (\eta_1 - i\eta_2) \downarrow (\eta_1 + i\eta_2) \rangle & \langle \downarrow (\eta_1 - i\eta_2) \uparrow \eta_3 \rangle \\ \langle \uparrow \eta_3 \downarrow (\eta_1 + i\eta_2) \rangle & \langle \uparrow \eta_3 \uparrow \eta_3 \rangle \end{pmatrix} \cdot \begin{pmatrix} 1\\1 \end{pmatrix},$$

$$(4.39)$$

where the colors show which terms were combined. The new form allows to apply the given transformation-rules and the  $\mathcal{T}$ -matrix transforms to

$$\mathcal{T}_{\uparrow}(\tau) = -\frac{J^2}{4} G_{\Phi}(\tau) \left( 2 \langle \downarrow f \downarrow f^{\dagger} \rangle + \sqrt{2} \langle \downarrow f \uparrow \eta \rangle + \sqrt{2} \left\langle \uparrow \eta \downarrow f^{\dagger} \rangle + \langle \uparrow \eta \uparrow \eta \rangle \right), \quad (4.40)$$

For those 4 response functions the RPA is carried out in the following. To clarify the procedure of the RPA in the case of the magnetic field we want to take a look at the first two orders of perturbation theory. In zeroth order there are two different polarization diagrams given by

Thus, the zeroth order is given by

$$\mathcal{T}^{(0)}_{\uparrow}(\tau) = -\frac{J^2}{4} G_{\Phi}(\tau) \left(-2\Pi_{0f}(\tau) - \Pi_{0\eta}(\tau)\right), \qquad (4.42)$$

The second order diagrams can be obtained by using the vertices defined in equation (4.32). They correspond to the vertex where a f-fermion is destroyed and the  $\eta$ -Majorana fermion is created or vice versa, and are given by  $-\sqrt{2}\frac{J}{2}$  in both the cases. The first order perturbation theory contributions to the  $\mathcal{T}$ -matrix are thus given by

$$\mathcal{T}^{(1)}_{\uparrow}(\tau) = -\frac{J^2}{4} G_{\Phi}(\tau)(-2) J \int_0^\beta d\tau_1 \Pi_{0\eta}(\tau - \tau_1) \Pi_{0f}(\tau_1), \qquad (4.43)$$



Figure 4.5.: This Figure shows the four response-functions in the RPA up to second order. It can be seen, that the off-diagonal elements do not contribute in zeroth order. In each order the diagrams represent a convolution or in Fourier space a product of the two different polarization diagrams  $\Pi_{0f}$  and  $\Pi_0$ . The recursion allows to sum them up systematically.

which also separates into in product in Fourier space. The two different diagrams which contribute to the series are shown up to second order in Figure 4.5. In the next step it is demonstrated that again a recursion can be found which allows to carry out the RPA. The response-function contributing to the  $\mathcal{T}$ -matrix in equation (4.40) can be classified into two groups. The coefficients of the first group are defined as  $a_n$  and correspond to a response-function where the Dirac fermion f enters and leaves. The coefficients of the second group are defined as  $b_n$  where the fermion which enters the interacting region is different from the leaving fermion. As before there is an important relation between the spin of the conduction electrons which occurs in the polarization diagram and the corresponding fermion propagator and this relation states that the f Dirac fermion propagator occurs with the spin-down and the  $\eta$  with the spin-up conduction electron propagator in the polarization diagram. This relation helps us again to use only f and  $\eta$  to find the recursion relation between the coefficients. These definitions

$$\begin{array}{cccc} a_n = \overbrace{f \ f} & \cdots & \overbrace{f} & & & \\ f \ \eta & \cdots & f & & \\ b_n = \overbrace{\eta \ f} & \cdots & \overbrace{f} & & & \\ b_n = \overbrace{\eta \ f} & \cdots & \overbrace{f} & & & \\ b_n = \sqrt{2}\Pi_0 a_{n-1} & & \\ \end{array}$$

Figure 4.6.: This Figure shows graphically the recursion-relation between the coefficients which enter the RPA for the response-function. The coefficients for the first response-function in (4.40) are labeled with  $a_n$ , the two in the middle are composed to  $b_n$  and the last term can be rewritten, so that  $a_n$  can be used for it. The Figure shows the coefficient n and which transitions are allowed, so that one can find the recursion relation. For  $a_n$  there are two possible vertices, one where f stays f and the other where  $\eta$  is created. On the other hand, for  $b_n$  there is only one allowed process because there is no vertex where  $\eta$  is destructed and created.

are used in Figure 4.6 which makes the role of the coefficients clearer. The coefficients are used to define the sum of the different response functions.

The RPA-summation for the third response-function can be rewritten as

$$\langle \uparrow \eta \uparrow \eta \rangle = -\Pi_{0\eta} - 2\Pi_{0\eta}^2 \sum_{n=2}^{\infty} a_{n-2} \left(\frac{J}{2}\right)^n$$
  
$$= -\Pi_{0\eta} - 2 \left(\frac{J\Pi_{0\eta}}{2}\right)^2 \sum_{n=0}^{\infty} a_n \left(\frac{J}{2}\right)^n,$$
 (4.44)

which allows to use to the coefficients  $a_n$  in the summation and avoids to define a third coefficient where the Majorana fermion  $\eta$  would enter and leave the interacting region of the response function.

The blue terms of the  $\mathcal{T}$ -matrix (see Figure 4.5) represent a response functions where the fermion which enters the interaction region differs from the leaving fermion thus they can be summed up using the coefficients  $b_n$ 

$$\sqrt{2}\left(\langle \uparrow \eta \downarrow f^{\dagger} \rangle + \langle \downarrow f \uparrow \eta \rangle\right) = -2\sqrt{2}\sum_{n=0}^{\infty} b_n \left(\frac{J}{2}\right)^n.$$
(4.45)

Since the blue terms provide the same contribution to the series they can be written as sum with factor 2.

The green term of the  $\mathcal{T}$ -matrix corresponds to a response function where the f Dirac fermion enters and the leaves the interacting region and therefore the coefficients  $a_n$  are used for the RPA

$$2\langle \downarrow f \downarrow f^{\dagger} \rangle = 2 \sum_{n=0}^{\infty} a_n \left(\frac{J}{2}\right)^n.$$
(4.46)

Using these rewritten contributions the four response functions in the  $\mathcal{T}$ -matrix are summed up by

$$\Pi(i\omega_n) = -\Pi_{0\eta} - 2\sum_{n=0}^{\infty} \left(\frac{J}{2}\right)^n \left(1 + \left(\frac{J\Pi_{0\eta}}{2}\right)^2, \quad \sqrt{2}\right) \cdot \begin{pmatrix}a_n\\b_n\end{pmatrix}.$$
 (4.47)

The recurrence relation between the coefficients can be read-off from Figure 4.6 and is given by

$$\begin{pmatrix} a_n \\ b_n \end{pmatrix} = \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix} \cdot \begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix} = \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix}^n \cdot \begin{pmatrix} a_0 \\ b_0 \end{pmatrix}$$
(4.48)

The initial values are given by  $a_0 = \Pi_{0f}$ ,  $b_0 = 0$ , which can be seen from Figure 4.5. Applying the systematic summation of the polarization diagrams gives

$$\Pi = -\Pi_{0\eta} - \begin{pmatrix} A, & 2\sqrt{2} \end{pmatrix} \sum_{n=0}^{\infty} \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix}^n \begin{pmatrix} \Pi_{0f} \\ 0 \end{pmatrix} \begin{pmatrix} J \\ 2 \end{pmatrix}^n$$

$$= -\Pi_{0\eta} - \begin{pmatrix} A, & 2\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 - \frac{J}{2} \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix} \end{pmatrix}^{-1} \begin{pmatrix} \Pi_{0f} \\ 0 \end{pmatrix}.$$
(4.49)

Inverting the matrix, where 1 is the  $2 \times 2$  identity matrix gives

$$\begin{pmatrix} 1 - \frac{J}{2} \begin{pmatrix} \Pi_{0f} & \sqrt{2}\Pi_{0f} \\ \sqrt{2}\Pi_{0\eta} & 0 \end{pmatrix} \end{pmatrix}^{-1} = \\ \frac{1}{1 + \frac{J}{2}\Pi_{0f} - \frac{J^2}{2}\Pi_{0\eta}\Pi_{0f}} \cdot \begin{pmatrix} 1 & \Pi_{0f} \frac{J}{2}\sqrt{2} \\ \Pi_{0\eta} \frac{J}{2} & 1 - \frac{J}{2}\Pi_{0f} \end{pmatrix}.$$

$$(4.50)$$

Calculating the matrix-vector product by using the relation between the  $\mathcal{T}^{''R}(\omega)$ -matrix and the function  $\Pi^{''R}(\omega)$  leads to

$$\mathcal{T}_{\uparrow}^{''R}(\omega) = -\frac{J^2}{4} \frac{1}{2} \coth\left(\frac{\beta\omega}{2}\right) \operatorname{Im}\left(\frac{\Pi_{0\eta} + 2\Pi_{0f} + \frac{3}{2}J\Pi_{0f}\Pi_{0\eta}}{1 - \frac{J}{2}\Pi_{0f} - \frac{J^2}{2}\Pi_{0\eta}\Pi_{0f}}\right),\tag{4.51}$$

which gives is limit B = 0 (where  $\Pi_{0\eta} = \Pi_{0f}$ ) the same result as before

$$\mathcal{T}^{''R}_{\uparrow}(\omega) = -\frac{J^2}{4} \frac{1}{2} \operatorname{coth}\left(\frac{\beta\omega}{2}\right) \operatorname{Im}\left(\frac{3\Pi_{0\eta}\left(1+\frac{J}{2}\Pi_{0\eta}\right)}{\left(1-J\Pi_{0\eta}\right)\left(1+\frac{J}{2}\Pi_{0\eta}\right)}\right)$$
$$= -\frac{J^2}{4} \frac{1}{2} \operatorname{coth}\left(\frac{\beta\omega}{2}\right) \operatorname{Im}\left(\frac{3\Pi_{0\eta}}{1-J\Pi_{0\eta}}\right).$$
(4.52)

The polarization diagrams  $\Pi_{0\eta}$  and  $\Pi_{0f}$  are given by the following two expressions with a magnetic field B > 0 (see appendix C.1)

$$\Pi_{0\eta}(\omega) = \frac{\rho_0}{2} \log \left| \frac{D^2 - \omega^2}{\omega^2} \right| + i \frac{1}{2} \pi \rho_0 \operatorname{sign}(\omega)$$

$$\Pi_{0f}(\omega) = \rho_0 \log \left| \frac{D + B - \omega}{B - \omega} \right| + i \pi \rho_0 \theta(\omega - B).$$
(4.53)

The final result which will be discussed in the next paragraph is shown in Figure 4.7.



Figure 4.7.: This graph shows equation (4.51) and the corresponding asymptotes which are obtained in equation (4.57). It can be seen that the spin-resolved  $\mathcal{T}$ -matrix is antisymmetric due to the different polarization diagrams and the peak is centered at B which is related to the Zeeman splitting of the Kondo resonance.

### 4.2.4. RPA-result with free propagators

In this section the result of the derived formula is discussed and compared with DM-NRG-calculations of the  $\mathcal{T}$ -matrix. First of all we want to discuss the asymmetric asymptotes from Figure 4.7 in the high energy limit which is given by  $D \gg \omega \gg B$  or  $D \ll -\omega \ll B$ . Since in the analytic result for  $\Pi_{0f}(\omega)$  only has an imaginary part for  $\omega > B$  we obtain according to the sign of  $\omega$ 

$$\Pi_{0f}(\omega) \approx \rho_0 \left( \log(x) + i\pi \right) \quad D \gg \omega \gg B$$
  
$$\Pi_{0f}(\omega) \approx \rho_0 \log(x) \qquad -D \ll \omega \ll B.$$
(4.54)

 $\Pi_{0\eta}(\omega)$  is given by

$$\Pi_{0\eta}(\omega) \approx \rho_0 \left( \log(x) + i\frac{\pi}{2} \right) \qquad D \gg \omega \gg B$$
  
$$\Pi_{0\eta}(\omega) \approx \rho_0 \left( \log(x) - i\frac{\pi}{2} \right) \qquad -D \ll \omega \ll B,$$
(4.55)

where  $\operatorname{sign}(\omega)$  changes the sign of the imaginary part and for all four expressions the abbreviation  $x = \frac{D}{\omega}$  is used. These limits are taken for the derived formula for the  $\Pi^{R}(\omega)$ -matrix. Then, the imaginary part  $\Pi^{''R}(\omega)$ -matrix is developed for  $\frac{1}{\log(x)} \to 0$  which gives only in leading order

$$\Pi^{''R}(\omega) \approx -\pi \frac{5}{2J^2 \rho_0 \log^2(x)} \qquad D \gg \omega \gg B$$
  
$$\Pi^{''R}(\omega) \approx \pi \frac{1}{2J^2 \rho_0 \log^2(x)} \qquad -D \ll \omega \ll B.$$
(4.56)

Taking these limits for the evaluated formula for the  $\mathcal{T}$ -matrix agrees with the result which has been found by A. Rosch, T. A. Costi, J. Paaske and P. Wölfle in 2003 by

applying the functional renormalization group (fRG) [27, 69]:

$$-\pi\rho_0 \mathcal{T}^{\prime\prime R}_{\uparrow}(\omega) \approx \pi^2 \frac{5}{16\log^2\left(\left|\frac{\omega}{T_K}\right|\right)} \qquad D \gg \omega \gg B$$
  
$$-\pi\rho_0 \mathcal{T}^{\prime\prime R}_{\uparrow}(\omega) \approx \pi^2 \frac{1}{16\log^2\left(\left|\frac{\omega}{T_K}\right|\right)} \qquad -D \ll \omega \ll B.$$
 (4.57)

The result is an asymmetric behaviour far away from the shifted resonance. Without a magnetic field the resonance is around  $\omega = 0$  and with a magnetic field it is shifted in this case to  $\omega = B$  which can be only observed when the quantum dot is in the Kondo regime. The suppression of the Kondo resonance is also present because the maximum of the curve is far away from the unitary limit (see Figure 4.7).

In the following the calculated formula for the  $\mathcal{T}$ -matrix is compared with DM-NRG-calculations. For all the DM-NRG-calculations the half-band width D = 1 and the Kondo coupling J = 0.145 were chosen so that the Kondo temperature  $T_K =$  $1.0 \cdot 10^{-6}$ . Further, we kept only the first 320 states. The spectral functions obtained by the DM-NRG are compared to the one evaluated with the RPA and free propagators. The DM-NRG spectral functions are broadened with different parameters b = 0.55, 0.65, 0.75, 0.85 (for the explanation of the broadening see chapter 2). The DM-NRG and RPA results are benchmarked for different ratios of  $\frac{B}{T_K}$ . We begin the discussion for sufficient high magnetic fields where the ratio  $B/T_K = 5 \cdot 10^4$  and  $B/T_K = 4 \cdot 10^3$ . In this case it can be seen that the RPA agrees well with the DM-NRG for energies  $\omega \neq B$ . For  $\omega = B$  we observe a disagreement between the RPA and the DM-NRG. The peak of the RPA is very sharp and diverges. In contrast the peak of the DM-NRG is large (see Figure 4.8). In chapter 5 we will clarify the discussion of the deviations at the peak. We mention that the DM-NRG calculation has an insufficient resolution at the peak which leads to a too large peak and the RPA result is too narrow since the spin relaxation time has not been included. However, the divergence at  $\omega = B$ is very slow which is in agreement with Ref. [27] and we conclude that the result should be between the two.

For smaller ratios  $\frac{B}{T_K}$  one can observe an artefact in the RPA result for small energies For decreasing magnetic field the range, where the RPA result is valid, becomes more and more smaller and we observe big deviations from the DM-NRG result and the unitary limit (see Figure 4.9). The origin of this artefact is discussed in the next subsection. In Figure 4.10 the  $\mathcal{T}$ -matrix is plotted 2-dimensional as  $\mathcal{T}(\omega, B)$ . It can be seen clearly that there is a linear Zeeman splitting of the Kondo resonance for high magnetic fields. Due to the divergence in the resonance in RPA-result of the  $\mathcal{T}$ -matrix values exceeding 0.03 are set to 0.03. In the limit of weak magnetic fields this result is not valid any more and the RPA does not match the experiment where a critical magnetic field is observed for the splitting (compare Figure 4.10 with Figure 4.11).

The conclusion of this intermediate discussion is that the Zeeman splitting energy has to be sufficiently big where the RPA-evaluation is valid. If it is too small the perturbation theory breaks down which is related to the Kondo problem. Furthermore,



Figure 4.8.: In the graph we see that the RPA agrees well with the DM-NRG except at  $\omega \approx B$ . If  $B/T_K$  is sufficiently high the RPA works well.



Figure 4.9.: These graphs show more clearly what happens for the RPA result when  $\max(B, \omega) \gg T_K$  is not true. This indicates the break-down of the perturbation theory and is related to the Kondo problem.


Figure 4.10.: This Figure shows a 2-dimensional plot of the imaginary part of the retarded  $\mathcal{T}$ -matrix. One can see very well the expected Zeeman splitting of the Kondo resonance in high magnetic fields. For too small values of the magnetic field the evaluation of the  $\mathcal{T}$ -matrix is not any more valid so one has to treat the plot very carefully.



Figure 4.11.: In this Figure two different experiments where the differential magneto-conductance is measured are shown. In both the experiments it can be seen that a certain energy is needed to break the Kondo singlet which explains the critical magnetic field.

the effect of the spin relaxation time has to be discussed in order to get sure about the behaviour of the  $\mathcal{T}$ -matrix in the neighbourhood of the Zeeman shifted resonance.

#### 4.2.5. The limits of the RPA

In this section we want to discuss the artefact for small  $\omega$  in the RPA which can be observed in the last section. In the absence of a magnetic field it was shown that the RPA it equivalent to poor man's scaling. The poor man's scaling approach can be interpreted as a one loop renormalization group scheme given diagrammatically by [69]

$$\mathbf{M} = \mathbf{M} + \mathbf{M} +$$

which renormalizes the Kondo coupling J. The second-order diagrams give rise to the logarithms. If this scheme is compared with the RPA for the  $\mathcal{T}$ -matrix it can be seen that the RPA does not include the particle-hole channel of the one-loop scheme. The neglected particle-hole diagram in the RPA is given by

and becomes important for low energies. The leading contribution of that diagram is given approximately by  $\Pi_{0\eta}(\omega)^2 \Pi_{0f}(0)$ . The approximation uses a decoupling of the crossing lines from which the given expression can be obtained. This expression can be used for the RPA result and this shows that the diagram is in fact important for small energies and the artefact vanishes. We mention that this correction shows only qualitatively that this diagram becomes important. Figure 4.12 further shows that the approximation is too rough.

## 4.3. Ferromagnetic Kondo coupling and the RPA

In the last section we want to discuss the RPA-result with a ferromagnetic coupling. The motivation is that the ferromagnetic  $S = \frac{1}{2}$  Kondo effect can help to understand to the underscreened S = 1 Kondo effect with anti-ferromagnetic coupling. In this section the relation between these two different Kondo effects is explained and verified by comparing the RPA-result with the underscreened Kondo effect which has been observed recently in a molecular single electron transistor [32, 61].

#### 4.3.1. The underscreened Kondo effect

In 1980 P. Nozières and A. Blandin discussed the underscreened Kondo effect in real metals [30] and earlier in 1978 D. M. Cragg and P. Lloyd [31]. The physical interpretation is that the spin  $s = \frac{1}{2}$  of the conduction electron can not screen the spin S = 1



Figure 4.12.: This result shows the corrected RPA with an approximated particle hole channel(p. h. c. diagram) and without correction.

of the embedded magnetic impurity as it is the case where spin of the electrons is anti-ferromagnetically coupled to the spin  $S = \frac{1}{2}$  of the magnetic impurity. This leads to an uncompensated spin  $S = \frac{1}{2}$  of the impurity which is ferromagnetically coupled to the spin  $s = \frac{1}{2}$  of the conduction electrons in the low-temperature limit. Thus, in the low-temperature limit the physics of the underscreened anti-ferromagnetic S = 1Kondo effect show the same behaviour as the ferromagnetic  $S = \frac{1}{2}$  Kondo effect. In the ferromagnetic case the spin S of the impurity can be polarized with any B and thus we expect that there is no critical magnetic field for the Zeeman splitting.

#### 4.3.2. RPA and experiments

We compare again the RPA result with DM-NRG runs where the Kondo coupling is changed to J = -0.138. This change of the sign changes dramatically the renor-



Figure 4.13.: The two graphs show the RPA-result for **ferromagnetic** Kondo coupling for two different magnetic fields. It is compared to DM-NRG calculations of the  $\mathcal{T}$ -matrix with different broadening parameters.



Figure 4.14.: On the left hand side the RPA-result is compared to DM-NRG calculations and on the right hand side the total matrix is shown from which it can be seen that the splitting persists for  $B \rightarrow 0$ .

malization equation of the Kondo coupling and for low energies the Kondo coupling remains small and tends even to zero which allows to apply perturbation theory for the whole range of energies. From Figure 4.13 and Figure 4.14 it can be seen that indeed the curves do not change with B and have the same behaviour. Further, as expected the splitting is present when B tends to zero where we arrive at the RPA-result in the absence of a magnetic field. The plot of the total  $\mathcal{T}$ -matrix (see Figure 4.14) shows again that there is the artefact for small  $\omega$  which can be explained with the neglected particle-hole channel diagram which completes the one-loop renormalization group scheme. When the energy  $\omega$  is in the vicinity of B a step in the  $\mathcal{T}$ -matrix is observed and it can be seen in the RPA result that there is a singularity which is related to the neglected spin relaxation time discussed in the next chapter. If we compare a 2 dimensional plot of the  $\mathcal{T}$ -matrix with the recent experiment carried out by W. Wernsdorfer et al. [32] it can be seen that the Zeeman splitting is also present for  $B \to 0$  (see Figures 4.15 and 4.16) The resolution of the NRG is again insufficient in the vicinity of the magnetic field because there are not enough points. In the next section where the role of the spin relaxation time is discussed this statement will be clarified.

### 4.4. Summary

In this chapter we have seen that the RPA for the  $\mathcal{T}$ -matrix works well in the absence of a magnetic field when the energy is in the weak-coupling regime  $\omega \gg T_K$ . It was shown how the RPA can be performed systematically by introducing a recursive scheme which renormalizes J in the same way as it does poor man's scaling. For low energies the RPA approach breaks clearly down because in the Kondo problem the strong-coupling regime can not be matched with perturbation theory. Further, in the present of a magnetic field the RPA became more complex because after the transformation we had to deal with two different propagators in the diagrammatics. We adapted the recursive



Figure 4.15.: A 2 dimensional plot of the total  $\mathcal{T}$ -matrix obtained with the RPA.



Figure 4.16.: On the left hand side the Zeeman splitting of the differential conductance is shown (experiment W. Wernsdorfer et al. ) and on the right hand side a NRG evaluation of the spectral function of the S = 1 anti-ferromagnetic Kondo effect is shown. In both the graphs the Zeeman splitting is present for  $B \rightarrow 0$  [17, 32].

scheme for the  $\mathcal{T}$ -matrix and obtained

$$\mathcal{T}_{\uparrow}^{''R}(\omega) = -\frac{J^2}{4} \frac{1}{2} \coth\left(\frac{\beta\omega}{2}\right) \operatorname{Im}\left(\frac{\Pi_{0\eta} + 2\Pi_{0f} + \frac{3}{2}J\Pi_{0f}\Pi_{0\eta}}{1 - \frac{J}{2}\Pi_{0f} - \frac{J^2}{2}\Pi_{0\eta}\Pi_{0f}}\right),$$
(4.60)

which was compared in detail for anti-ferromagnetic and ferromagnetic coupling with DM-NRG calculations of the  $\mathcal{T}$ -matrix. We stated that for  $\max(B, \omega) \gg T_K$  the RPA matches well the DM-NRG result but there is a problem for energies in the proximity of B where the peak in the RPA result is too sharp and diverges slowly. This stems from the neglected spin relaxation time which is discussed in the next chapter. It has also been shown that the RPA at a finite magnetic field is not fully equivalent to a one-loop renormalization scheme because the particle-hole diagram is neglected in the RPA. This diagram is important to get rid of the artefact in the RPA for low energies. Looking at the DM-NRG calculation we asserted that there are not enough points for energies  $\omega$  in the neighbourhood of B and the broadening of these points leads to a too broad Zeeman peak. The assumption is thus that the real curve for the resonance in the vicinity of B is between the two curves. The quality of the DM-NRG calculations might be improved by using z-averaging where the NRG is carried for different discretization parameters  $\Lambda^{n+z}$  which shifts the energy shells and more points are obtained [54].

# 5. The spin-relaxation-time

The self-energy  $\Sigma_{\eta}$  was discussed in chapter 3 and calculated in appendix C.2. In this chapter we are going to discuss the self-energy at finite magnetic field. Thus, we have to include the two different self-energies  $\Sigma_{\eta}$  and  $\Sigma_{f}$  to the two propagators  $G_{f}$  and  $G_{\eta}$ . Using Wick's theorem will give the analytic expressions for both the self-energies. Then, they will be used to discuss the magnetic susceptibility at finite magnetic field and the analytic result is going to be compared to DM-NRG calculations which clarifies the benchmark of the two methods. In the end, the spin elaxation time will be discussed for the  $\mathcal{T}$ -matrix.

# 5.1. Derivation of the self-energies $\Sigma_f$ and $\Sigma_\eta$ for $B \neq 0$

We use the Kondo interaction from equation (4.36) to evaluate the second-order order contribution of the expansion of the full propagators

$$G_{f}(\tau) = -\left\langle T_{\tau} \left[ f(\tau) f^{\dagger}(0) \right] \right\rangle$$
  

$$G_{\eta}(\tau) = -\left\langle T_{\tau} \left[ \eta(\tau) \eta^{\dagger}(0) \right] \right\rangle$$
(5.1)

According to the introduced concept of Green's functions these corrections will be given in terms of free propagators. For this purpose the imaginary-time evolution operator is used in second order (see chapter 3) leading to the second-order contributions given by

$$G_{f}^{(2)}(\tau) = -\frac{1}{2} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \left\langle T_{\tau} \left[ H_{\mathrm{I}}(\tau_{1}) H_{\mathrm{I}}(\tau_{2}) f(\tau) f^{\dagger}(0) \right] \right\rangle_{0}$$

$$G_{\eta}^{(2)}(\tau) = -\frac{1}{2} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \left\langle T_{\tau} \left[ H_{\mathrm{I}}(\tau_{1}) H_{\mathrm{I}}(\tau_{2}) \eta(\tau) \eta^{\dagger}(0) \right] \right\rangle_{0},$$
(5.2)

where the interaction in the Kondo Hamiltonian is given by

$$H_{\rm I} = -\frac{J}{2}\sqrt{2} \left( c^{\dagger}_{0\downarrow} f^{\dagger} \eta c_{0\uparrow} + c^{\dagger}_{0\uparrow} \eta^{\dagger} f c_{0\downarrow} \right) + \frac{J}{2} \left[ \sum_{\sigma} \sigma c^{\dagger}_{0\sigma} f^{\dagger} f c_{0\sigma} - \sigma \frac{1}{2} c^{\dagger}_{0\sigma} c_{0\sigma} \right].$$
(5.3)

In the next two subsections the different possibilities for the self-energy-diagrams are calculated.

# 5.1.1. Self energy $\Sigma_f$

We want to begin with the self-energy diagrams for the propagator  $G_f$ . The first possibility with interactions in second order is given by

$$\begin{aligned} G_{f}^{(2.1)}(\tau) &= -\frac{1}{2} \frac{J^{2}}{4} \sum_{\sigma} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \\ & \times \left\langle T_{\tau} \left[ c_{0\sigma}^{\dagger}(\tau_{1}) f^{\dagger}(\tau_{1}) f(\tau_{1}) c_{0\sigma}(\tau_{1}) c_{0\sigma}^{\dagger}(\tau_{2}) f^{\dagger}(\tau_{2}) f(\tau_{2}) c_{0\sigma}(\tau_{2}) f(\tau) f^{\dagger}(0) \right] \right\rangle_{0} \\ &= \frac{1}{2} \frac{J^{2}}{4} \sum_{\sigma} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} G_{0c}(\tau_{1} - \tau_{2}) G_{0c}(\tau_{2} - \tau_{1}) \\ & \times \left\langle T_{\tau} \left[ f^{\dagger}(\tau_{1}) f(\tau_{1}) f^{\dagger}(\tau_{2}) f(\tau_{2}) f(\tau) f^{\dagger}(0) \right] \right\rangle_{0}. \end{aligned}$$
(5.4)

There are two possible contractions. The average over the six fermionic operators f separates into

$$\left\langle T_{\tau} \left[ f^{\dagger}(\tau_1) f(\tau_1) f^{\dagger}(\tau_2) f(\tau_2) f(\tau) f^{\dagger}(0) \right] \right\rangle_0 = -G_{0f}(\tau_2 - \tau_1) G_{0f}(\tau_2) G_{0f}(\tau_1 - \tau)$$
(5.5)

and

$$\left\langle T_{\tau} \left[ f^{\dagger}(\tau_{1}) f(\tau_{1}) f^{\dagger}(\tau_{2}) f(\tau_{2}) f(\tau) f^{\dagger}(0) \right] \right\rangle_{0} = -G_{0f}(\tau_{1} - \tau_{2}) G_{0f}(\tau_{2} - \tau) G_{0f}(\tau_{1}) \quad (5.6)$$

which give the same contribution to the integral in equation (5.4) and thus give a factor 2. Since the propagators do not depend on the spin, the sum over the spins  $\sum_{\sigma}$  gives another factor 2 and the first integral in second order is given by

$$G_{f}^{(2.1)}(\tau) = -\frac{J^{2}}{2} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \underbrace{G_{0c}(\tau_{1} - \tau_{2})G_{0c}(\tau_{2} - \tau_{1})G_{0f}(\tau_{1} - \tau_{2})}_{=\Sigma_{f}^{(2.1)}(\tau_{2} - \tau_{1})} G_{0f}(\tau_{2} - \tau)G_{0f}(\tau_{1}),$$
(5.7)

where the first contribution to the self-energy  $\Sigma_f$  is given  $\Sigma_f^{(2.1)}(\tau_2 - \tau_1)$ .

The second possibility with interactions in second order is given by

$$\begin{aligned} G_{f}^{(2.2)}(\tau) &= -\frac{1}{2} \frac{J^{2}}{2} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \\ &\times \left\langle T_{\tau} \left[ c_{0\downarrow}^{\dagger}(\tau_{1}) f^{\dagger}(\tau_{1}) \eta(\tau_{1}) c_{0\uparrow}(\tau_{1}) c_{0\uparrow}^{\dagger}(\tau_{2}) \eta^{\dagger}(\tau_{2}) f(\tau_{2}) c_{0\downarrow}(\tau_{2}) f(\tau) f^{\dagger}(0) \right] \right\rangle_{0} \\ &= \frac{1}{2} \frac{J^{2}}{2} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} G_{0c}(\tau_{1} - \tau_{2}) G_{0c}(\tau_{2} - \tau_{1}) \\ &\times \left\langle T_{\tau} \left[ f^{\dagger}(\tau_{1}) \eta(\tau_{1}) \eta^{\dagger}(\tau_{2}) f(\tau_{2}) f(\tau) f^{\dagger}(0) \right] \right\rangle_{0} \\ &= - \frac{J^{2}}{4} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} G_{0f}(\tau_{2}) G_{0f}(\tau - \tau_{1}) \\ &\times \underbrace{G_{0c}(\tau_{1} - \tau_{2}) G_{0\eta}(\tau_{2} - \tau_{1}) G_{0c}(\tau_{2} - \tau_{1})}_{=\Sigma_{f}^{(2.2)}(\tau_{2} - \tau_{1})} \end{aligned}$$
(5.8)

leading to the second contribution to the self-energy  $\Sigma_f$ . The third and last contribution can be calculated from the second contribution. It is given by the conjugated process leading to the same expression. This gives another factor 2. From this discussion we conclude that the self-energy  $\Sigma_f$  consists of two different contributions is given by

$$\Sigma_{f}(\tau) = -\frac{J^{2}}{2}G_{0c}(-\tau)\left[G_{0f}(\tau)G_{0c}(\tau) + G_{0\eta}(\tau)G_{0c}(\tau)\right]$$
  
$$= -\frac{J^{2}}{2}G_{0c}(-\tau)\left[\Pi_{0f}(\tau) + \Pi_{0\eta}(\tau)\right].$$
(5.9)

If we look more carefully at the Hamiltonian in equation (5.3) there is a last contribution to the self-energy whose diagram is given by

$$\sum_{\sigma \in f} \sum_{cf} (5.10)$$

which describes the interaction of conduction electrons with an external potential. The external potential occurs because of the transformation  $f^{\dagger} = \frac{1}{\sqrt{2}}(\eta_1 + i\eta_2)$  (see chapter 4). Until now, we omitted the interaction

$$-\frac{J}{4}\sum_{\sigma}\sigma c_{0\sigma}^{\dagger}c_{0\sigma}$$

in the transformed Kondo Hamiltonian. This terms represents an external potential scattering term and gives a constant contribution to the self-energy in second order.

The diagram is given by the analytical expression

$$\Sigma_{cf} = -\frac{J^2}{4} \int_0^\beta d\tau G_{0c}(\tau) G_{0c}(-\tau).$$
(5.11)

## 5.1.2. Self energy $\Sigma_{\eta}$

In this subsection we perform the same procedure as before for the second propagator  $G_{\eta}$ . The first expression with interactions in second order is given by

$$\begin{aligned} G_{\eta}^{(2.1)}(\tau) &= -\frac{J^2}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \\ &\times \left\langle T_{\tau} \left[ c_{0\downarrow}^{\dagger}(\tau_1) f^{\dagger}(\tau_1) \eta(\tau_1) c_{0\uparrow}(\tau_1) c_{0\uparrow}^{\dagger}(\tau_2) \eta^{\dagger}(\tau_2) f(\tau_2) c_{0\downarrow}(\tau_2) \eta(\tau) \eta^{\dagger}(0) \right] \right\rangle_0 \\ &= \frac{J^2}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_{0c}(\tau_1 - \tau_2) G_{0c}(\tau_2 - \tau) \\ &\times \left\langle T_{\tau} \left[ f^{\dagger}(\tau_1) \eta(\tau_1) \eta^{\dagger}(\tau_2) f(\tau_2) \eta(\tau) \eta^{\dagger}(0) \right] \right\rangle_0 \\ &= \frac{J^2}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_{0c}(\tau_1 - \tau_2) G_{0c}(\tau_2 - \tau_1) G_f(\tau_2 - \tau_1) \\ &\times \left\langle T_{\tau} \left[ \eta(\tau_1) \eta^{\dagger}(\tau_2) \eta(\tau) \eta^{\dagger}(0) \right] \right\rangle_0. \end{aligned}$$
(5.12)

Since the fermionic Majorana fields are real  $\eta = \eta^{\dagger}$  the remaining average over those 4 fields leads to two different contributions given by

$$\left\langle T_{\tau} \left[ \eta(\tau_1) \eta(\tau_2) \eta(\tau) \eta(0) \right] \right\rangle_0 = - \left\langle T_{\tau} \left[ \eta(\tau) \eta^{\dagger}(\tau_2) \right] \right\rangle_0 \left\langle T_{\tau} \left[ \eta(\tau_1) \eta^{\dagger}(0) \right] \right\rangle_0$$
(5.13)

and

$$\left\langle T_{\tau} \left[ \eta(\tau_1) \eta(\tau_2) \eta(\tau) \eta(0) \right] \right\rangle_0 = \left\langle T_{\tau} \left[ \eta(\tau) \eta^{\dagger}(\tau_1) \right] \right\rangle_0 \left\langle T_{\tau} \left[ \eta(\tau_2) \eta^{\dagger}(0) \right] \right\rangle_0.$$
(5.14)

These two contributions can be used for equation (5.12). Changing the imaginary times  $\tau_1 \leftrightarrow \tau_2$  leads to

$$G_{\eta}^{(2.1)}(\tau) = -\frac{J^2}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_{0c}(\tau_1 - \tau_2) G_{0c}(\tau_2 - \tau_1) \\ \times G_{0\eta}(\tau - \tau_2) \left[ G_{0f}(\tau_2 - \tau_1) - \underbrace{G_{0f}(\tau_1 - \tau_2)}_{= -G_{0f^*}(\tau_2 - \tau_1)} \right] G_{0\eta}(\tau_1)$$
(5.15)  
$$= -\frac{J^2}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_{0\eta}(\tau - \tau_2) \Sigma_{\eta}^{2.1}(\tau_2 - \tau_1) G_{0\eta}(\tau_1),$$

70

where the self-energy is given by

$$\Sigma_{\eta}^{2.1}(\tau_2 - \tau_1) = G_{0c}(\tau_1 - \tau_2) \left[ \Pi_{0f}(\tau_2 - \tau_1) + \Pi_{0f^*}(\tau_2 - \tau_1) \right].$$
(5.16)

As before there is a second possibility  $G_{\eta}^{(2,2)}(\tau)$  which corresponds to a correction where  $\tau_1$  and  $\tau_2$  are exchanged and thus gives a factor 2 for the diagram. We conclude that the final result is given by

$$\Sigma_{\eta}(\tau) = -\frac{J^2}{2} G_{0c}(-\tau) \left[ \Pi_{0f}(\tau) + \Pi_{0f^*}(\tau) \right].$$
(5.17)

#### 5.1.3. Dyson's equation

The two self-energies are computed in appendix C.2 and the results can be used to correct the two propagators  $G_f(\tau)$  and  $G_\eta(\tau)$ . We remember in Fourier space Dyson's equation separates into a product which is given by



where the double dashed lines are the full propagators  $G_f(\tau)$  or  $G_\eta(\tau)$ , respectively, and the single dashed lines the free propagators  $G_{0f}(\tau)$  or  $G_{0\eta}(\tau)$ . Dyson's equation can be written as

$$G_{f,\eta}(i\omega_n) = \frac{1}{[G_{0f,\eta}]^{-1}(i\omega_n) - \Sigma_{f,\eta}(i\omega_n)}$$
(5.19)

or after the analytical continuation  $i\omega_n \rightarrow \omega + i0^+$  with retarded propagators as

$$G_{f,\eta}^{R}(\omega) = \frac{1}{[G_{0f,\eta}^{R}]^{-1}(\omega) - \Sigma_{f,\eta}^{R}(\omega)}.$$
(5.20)

The imaginary parts of the retarded Green's functions are given by

$$G_{f}^{''R}(\omega) = \frac{\Sigma_{f}^{''R}(\omega)}{[\omega - B - \Sigma_{f}^{''R}(\omega) - \Sigma_{cf}]^{2} + [\Sigma_{f}^{R''}(\omega)]^{2}}$$

$$G_{\eta}^{''R}(\omega) = \frac{\Sigma_{\eta}^{''R}(\omega)}{[\omega - \Sigma_{\eta}^{''R}(\omega)]^{2} + [\Sigma_{\eta}^{R''}(\omega)]^{2}}.$$
(5.21)

The self-energies are plotted in Figure 5.1 where  $\Sigma_{\eta}^{''R}(\omega) = 0$  for  $|\omega| \leq B$  which leads to a cut in the magnetic susceptibility too.



Figure 5.1.: In these two Figures the self-energies in presence of a magnetic field are shown. The self-energy  $\Sigma_{\eta}$  is cut at  $|\omega| \leq B$  due to the magnetic field. In this plot we have chosen B = 0.005 and  $B/T_K = 5 \cdot 10^4$ . This will consequently cut the magnetic susceptibility too. The self-energy  $\Sigma_f$  is anti-symmetric. From this it can be seen that for the real part the self-energy  $\Sigma_{cf}$  is important to obtain correctly  $\Sigma_f'(0)$  which shows the importance of that diagram.

# 5.2. Discussion of the magnetic susceptibility

In this section the modified propagators are used to discuss the magnetic susceptibilities  $\chi_3(\tau) = -\langle T_\tau [S^z(\tau)S^z(0)] \rangle$  and  $\chi_{+-}(\tau) = -\langle T_\tau [S^+(\tau)S^-(0)] \rangle$ . The spin operators are replaced by  $S^z = \Phi \eta$ ,  $S^+ = \sqrt{2} \Phi f^{\dagger}$  and  $S^- = \sqrt{2} \Phi f$  (see chapter 4) leading to

$$\chi_3(\tau) = G_{\Phi}(\tau)G_{\eta}(\tau)$$
  

$$\chi_{+-}(\tau) = 2G_{\Phi}(\tau)G_f(\tau).$$
(5.22)

The imaginary parts of these susceptibilities  $\chi_3^{''R}$  and  $\chi_{+-}^{''R}$  are given by

$$\chi_{3}^{''R}(\omega) = -\frac{1}{2} \tanh\left(\frac{\beta\omega}{2}\right) G_{\eta}^{''R}(\omega)$$

$$\chi_{+-}^{''R}(\omega) = -\tanh\left(\frac{\beta\omega}{2}\right) G_{f}^{''R}(\omega).$$
(5.23)

The two needed self-energies for the propagators  $G_f$  and  $G_\eta$  are computed in appendix C.2 and are given by

$$\Sigma_{\eta}^{''R}(\omega) = -\frac{J^2}{4}\rho_0 \int_{-D}^{D} \left[ \Pi_{0f}^{''R}(\omega_1 + \omega) + \Pi_{0f^*}^{''R}(\omega_1 + \omega) \right] \left( \text{sign}(\omega_1 + \omega) - \text{sign}(\omega_1) \right) d\omega_1$$
  
$$\Sigma_f^{''R}(\omega) = -\frac{J^2}{4}\rho_0 \int_{-D}^{D} \left[ \Pi_{0f}^{''R}(\omega_1 + \omega) + \Pi_{0\eta}^{''R}(\omega_1 + \omega) \right] \left( \text{sign}(\omega_1 + \omega) - \text{sign}(\omega_1) \right) d\omega_1,$$
  
(5.24)

from which the real part of the self-energies can be obtained by applying the Kramers-Kronig relation. The three polarization diagrams are given by

$$\Pi_{0\eta}^{''R}(\omega) = \pi \frac{\rho_0}{2} \operatorname{sign}(\omega) \Theta(D^2 - \omega^2)$$
(5.25)

$$\Pi_{0f}^{''R}(\omega) = \pi \rho_0 \Theta(\omega - B) \Theta(D^2 - (\omega - B)^2)$$
(5.26)

$$\Pi_{0f^*}^{''R}(\omega) = -\pi\rho_0\Theta(-\omega - B)\Theta(D^2 - (\omega + B)^2)$$
(5.27)

The self-energy  $\Sigma_{cf}$  is given by

$$\Sigma_{cf} = -\frac{J^2}{4} \int_0^\beta d\tau G_{0c}(\tau) G_{0c}(-\tau)$$
  
=  $-\frac{J^2}{4} \rho_0^2 \int_{-D}^D d\omega_1 \int_{-D}^D d\omega_2 \frac{n_F(\omega_1) - n_F(\omega_2)}{\omega_1 - \omega_2}$   
=  $-\frac{J^2}{4} \rho_0^2 2 \int_{-D}^D \int_{-D}^0 \frac{1}{\omega_1 - \omega_2}$   
=  $\frac{J^2}{4} \rho_0 \log(4).$  (5.28)

The susceptibilities are shown in Figure 5.2. The plots of the susceptibilities will help



Figure 5.2.: These two graphs show the magnetic susceptibilities calculated with by the DM-NRG and using Majorana fermions. For the DM-NRG we used the same parameters as before and in the graphs only the result for the broadening parameter b = 0.55 is given. The magnetic susceptibility in the upper plot is cut for energies below B. The magnetic susceptibility in the lower plot has a sharp peak at B which is not very well resolved by the NRG and the optimal *b*-broadening (*b*-trick) was applied [55]

us to understand the role of the spin relaxation time for the  $\mathcal{T}$ -matrix. We assert, that the analytical result for  $\langle S^z S^z \rangle$  does not describe energies below B. The analytical result shows a sharp resonance for  $\langle S^-S^+ \rangle$  in the analytical calculation. This peak can not be well resolved by the NRG. We applied the *b*-trick which fits the optimal broadening parameter for each part of the whole spectrum which leads to a better resolved peak [55]. From this point it can be seen that the DM-NRG overestimates the width of the resonance in the  $\mathcal{T}$ -matrix. To verify this the DM-NRG calculation should be extended using *z*-averaging [54] and *b*-trick.

# 5.3. Spin relaxation time for the T-matrix

The spin relaxation time is included to the  $\mathcal{T}$ -matrix thus the free propagators  $G_{0f}$  and  $G_{0\eta}$  are replaced by the dressed propagators  $G_f$  and  $G_\eta$  and the polarization diagrams are given by

$$\Pi_{f,\eta}^{''R}(\omega) = \rho_0 \int_{-\infty}^{\infty} \Theta(D^2 - (\omega_1 - \omega)^2) \left[ n_F(\omega_1) - n_F(\omega - \omega_1) \right] G_{f,\eta}^{''R}(\omega_1)$$
(5.29)

from which the real part can be obtained from the Kramers-Kronig relation. Figure 5.3 shows the inclusion of the spin relaxation time in lowest order to the  $\mathcal{T}$ -matrix and it can be seen that the divergence is cut but the peaks stays narrow. This can be understood from the susceptibility  $\langle S^-S^+ \rangle$  where it can be seen that the self-energy the resonance stays narrow compared to the result of the DM-NRG. We conclude that the self-energy helps us to cut the divergence but there are higher order diagram which are important. The discrepancy is however hard to estimate because we have shown that the NRG lacks resolution at the Zeeman split Kondo resonance.



Figure 5.3.: This plot of the  $\mathcal{T}$ -matrix shows that the divergence is cut or reduced but we have to include more self-energy diagrams to describe the resonance for the anti-ferromagnetic Kondo model where the DM-NRG result is likewise questionable. For the ferromagnetic Kondo model the singularity vanishes after the inclusion of the spin relaxation time.

## 5.4. Summary

The discussion of the self-energy shows that the resonance of the  $\mathcal{T}$ -matrix is obtained too narrow by the RPA and too broad by the DM-NRG. Further, the inclusion of the second-order self-energy to the  $\mathcal{T}$ -matrix is in question because the RPA for the  $\mathcal{T}$ -matrix renormalized the Kondo coupling J and the self-energy is calculated with free vertices. Nevertheless, it can be seen that the spin relaxation time is important to understand the transport-properties of a quantum dot. It helps us to cut the divergence which is clearly a problem of using lowest order perturbation theory for the self-energy [66, 67]. The analytical result can be improved by summing up more self-energy diagrams.

# 6. Conclusion

## 6.1. Summary

In this work we have shown how the Kondo effect can emerge in quantum dots leading to an anomalous logarithmic increase of the conductance at low temperatures. In particular, the magneto-conductance which was in the focus of this work has been shown to correspond to the situation where a magnetic field is applied to the impurity. For the discussion the relation between the conductance and the  $\mathcal{T}$ -matrix was used. The  $\mathcal{T}$ -matrix of the Kondo model describes the spin dynamics of the impurity and the spin dynamics has been expressed by Majorana fermion propagators with following advantages

- Wick's theorem which can not be applied directly to spin operators can be applied to Majorana fermions.
- $\mathcal{T}$ -matrix can be expressed as a usual response function which makes the perturbation theory clearer.
- No restrictions of the Hilbert space are needed as it is the case for Abrikosov pseudo-fermions.
- Dyson's equation allows to discuss the spin relaxation time.

It was further shown that the NRG was the first method to correctly describe the cross-over regime in the Kondo model while all perturbative methods fail due to divergence of the Kondo coupling J for low energies. In absence of a magnetic field the NRG produces results agreeing qualitatively with experiments. The discussion of the  $\mathcal{T}$ -matrix at finite magnetic field raises the question of the reliability of the NRG. The applied magnetic field defines through the Zeeman energy a second energy scale. It was seen that the problem is that the NRG does not describe the transitions from the ground state to higher excited states in the first few iterations where only high energies are described [26]. Thus, a more generalized technique namely the DM-NRG was applied to calculate the  $\mathcal{T}$ -matrix at finite magnetic field where we used the DM-NRG code written by O. Legeza et al. [25] and which can by found on http://www.phy.bme.hu/~dmnrg/. Those results have been compared to the RPA result of the  $\mathcal{T}$ -matrix which was obtained by using the Majorana fermion diagrammatic with free propagators. The evaluation of the RPA result was done in two steps. First, the RPA was carried out in absence of a magnetic field, where the result matched the poor man's scaling result. We have shown a systematic way of the evaluation of the RPA and then, in the second step we applied this procedure to the  $\mathcal{T}$ -matrix at finite magnetic field. This result

was discussed for anti-ferromagnetic and then for ferromagnetic coupling J. For the anti-ferromagnetic Kondo model we asserted:

- For  $\max(B, \omega) \gg T_K$  the RPA agrees well with DM-NRG result except for  $\omega \approx B$  where the resonances of the two methods do not agree. The resonance obtained by the DM-NRG computation is a large resonance while the resonance obtained by the RPA is very narrow one which additionally diverges. Furthermore, there are not enough points in the DM-NRG run for  $\omega \approx B$  which leads to an overestimated width of the resonance after the broadening of the obtained delta peaks in the Lehman representation of the  $\mathcal{T}$ -matrix. On the other hand, for the RPA free propagators were used neglecting the spin relaxation time from which is expected that it cuts the divergence and enlarges the peak.
- The RPA result does not match the critical magnetic field for the Zeeman splitting which is a property of the anti-ferromagnetic Kondo effect.
- The RPA procedure neglects the particle-hole channel diagram which becomes important for low energies. The problem is that the RPA yields an artefact for low energies where the  $\mathcal{T}$ -matrix is increasing again. It could be shown, however, that this artefact in the RPA vanishes using an approximation for the particle-hole channel.

Then, we compared the ferromagnetic Kondo model at finite magnetic field with the underscreened S = 1 anti-ferromagnetic Kondo model. The following interpretation exists for the underscreened Kondo model. In contrast to the screened  $S = \frac{1}{2}$  Kondo effect where the spin of the impurity is fully screened by the spin of the conduction electrons, the spin S = 1 can not be fully screened. It remains a  $S = \frac{1}{2}$  which is ferromagnetically coupled to the spin of the conduction electrons. The discussion of the underscreened Kondo model is motivated by its recent observation in molecular transistors. It should be mentioned again that the ferromagnetic Kondo model can be fully described by the perturbation theory because the Kondo coupling J does not diverge during the renormalization. We concluded for the RPA and the DM-NRG for the ferromagnetic Kondo model:

- The RPA and the DM-NRG show a Zeeman splitting which remains for  $B \rightarrow 0$ . The RPA result at finite magnetic field converges to the RPA result at zero magnetic field. The splitting for any magnetic field is present because there is no Kondo singlet which has first to be destroyed before it can be split. The ferromagnetically coupled spin can be polarized for arbitrary small B.
- The  $\mathcal{T}$ -matrix shows again a behaviour that is fast varying at  $\omega \approx B$ . The result of RPA and the DM-NRG differ at  $\omega \approx B$  which was quite remarkable. The problem is here as before that there are not enough points for energies in the neighbourhood of B. Thus the peak is too broad in the DM-NRG. The neglected spin relaxation time leads here to the obtained singularity in the RPA for  $\omega = B$ .

These results were compared with the results obtained from a experimental study of the molecular transistor [32]. In this experiment it has been found that the splitting of the spectral function begins for small B leading to a differential conductance which is also split for  $B \to 0$ . This is the same physics as the ferromagnetic Kondo model with  $S = \frac{1}{2}$ .

In the end of the work the role of the spin relaxation time was discussed. It was shown which diagrams have to be summed up in Dyson's equation. In particular the first nonvanishing diagram was summed up which was found in second order perturbation theory. We concluded that the spin relaxation time cuts the divergences. But unfortunately it is only weakly enlarged so that it does not match the DM-NRG result. During the discussion of the magnetic susceptibilities it was shown, that the DM-NRG results at finite magnetic field are too large and the RPA results too narrow. This underlines that the behaviour is between the DM-NRG and the RPA result.

# 6.2. Outlook

We can mention several points here. The ferromagnetic Kondo model at finite magnetic field can help to understand new physics where the spin is underscreened. The underscreened Kondo effect has also been found in spin S = 1 molecules by J.J. Parks et al. [70] and might be important for the conductance of atomic nano-contacts [71].

The problem of the resolution of the DM-NRG should be further discussed. Therefore, improved techniques of broadening can be used such as *b*-trick where an optimal broadening parameter is found leading to better resolved resonances [55]. The results can be further improved by using *z*-averaging where much more points are generated [54].

In the Majorana diagrammatics the role of the neglected particle-hole channel has to be discussed in more detail. This diagram has to be summed up to make the calculation equivalent to a one-loop renormalization group. Furthermore, the self-energy of the Majorana fermion is questionable since the inclusion seems to be uncontrolled. Thus, the technique has to be studied more thoroughly where the focus should be on whether there is a way to perform a RPA for the self-energy. This could avoid some inconsistencies due to the inclusion of the self-energy in second order to the RPA. Recently, S. Kehrein has been calculated the susceptibilities and the  $\mathcal{T}$ -matrix in a magnetic field for the non-equilibrium Kondo model [72]. The susceptibilities obtained by equilibrium Majorana Green's function can also be extended to a non-equilibrium calculation using the Keldysh formalism.

# A. Zero temperature Green's functions and Fermi liquid theory

In this appendix Green's functions will be introduced and they will be related to the Fermi liquid picture where quasi-particles have the same properties as the noninteracting Fermi gas [35, 37]. The idea is that the interaction is switched on adiabatically and that there is a one-to-one correspondence between the eigenstates of the free and the interacting system. We are going to show how interactions modify the free electrons and in which regime the Fermi liquid picture is valid.

# A.1. Schrödinger, Heisenberg and Interaction picture

Here three different but well known representations of quantum mechanics are introduced [41]. Since perturbation theory is carried out in the interaction picture, it is important to give a short summary of them. In general, the idea is to solve the timedependent Schrödinger equation and to find the time-evolution of the eigenstates.

#### A.1.1. Schrödinger picture

The Schrödinger picture is useful for time-independent Hamiltonians. This point is very important for the solution. The solution of the Schrödinger equation  $i\partial_t |\psi(t)\rangle = H|\psi(t)\rangle$  is given by

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle,\tag{A.1}$$

where  $|\psi(0)\rangle$  indicates the initial state begins. In this picture the states are timedependent and the operators, which are measured, may be time-dependent.

#### A.1.2. Heisenberg picture

In the Heisenberg picture all the time-dependence is transferred to the operators. This transformation is done by

$$\langle \psi_1(t)|A|\psi_2(t)\rangle = \langle \psi_1(0)|\underbrace{e^{iHt}Ae^{-iHt}}_{A(t)}|\psi_2(0)\rangle, \tag{A.2}$$

where A can be any operator which is measured. Again, the Hamiltonian does not depend on time and also the states do not depend on time any more. In this picture one has to solve the Heisenberg equation which is given by

$$\dot{A}(t) = i \left[ H, A(t) \right] + (\partial_t A)(t). \tag{A.3}$$

The last part is only non-zero when the operator A has an explicit time-dependence.

#### A.1.3. Interaction picture

This picture will be useful for the Green's function method. If the Hamiltonian H can be separated into  $H = H_0 + V(t)$  and the eigenstates of  $H_0$  are known, this picture is very powerful. Further, the Hamiltonian  $H_0$  does not depend on time. The states and operators are transformed by

$$\begin{aligned} |\Psi(t)\rangle &= e^{iH_0t}|\psi(t)\rangle \\ A_I(t) &= e^{iH_0t}Ae^{-iH_0t} \end{aligned} \tag{A.4}$$

Using this transformation for the Schrödinger equation the time evolution is given by

$$i\partial_t |\Psi(t)\rangle = V_I(t)|\Psi(t)\rangle.$$
 (A.5)

After this transformation, only the interaction Hamiltonian V(t) affects the time evolution of the transformed states. The solution of equation (A.5) is given by

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle$$

with

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{i}\right)^n \int_{t_0}^t dt_1 \cdots \int_{t_0}^t dt_n T_t(V_I(t_1) \cdots V_I(t_n)) = T_t\left(e^{-i\int_{t_0}^t V_I(t_1)dt_1}\right),$$
(A.6)

where  $T_t$  is the time-ordering operator, which occurs because time dependent Hamiltonians do not commutate at different times. Later, equation (A.6) will be used to develop the Green's function in a perturbation series. For this perturbation series,  $U(t, t_0)$  has some important properties:

$$U^{\dagger}(t, t_0) = U^{-1}(t, t_0) = U(t_0, t)$$
  

$$U(t, t_1)U(t_1, t_0) = U(t, t_0).$$
(A.7)

## A.2. Green's functions

The classical Green's function occurs the first time in classical mechanics and classical electrodynamic where the driven harmonic oscillator with friction or Poisson's equation is solved [37]. For the Schrödinger equation the Green's function  $G(\mathbf{r_1}, t_1, \mathbf{r_2}, t_2)$  is defined by the property

$$[i\partial_t - H(\mathbf{r}_1)]G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2),$$
(A.8)

where  $H(\mathbf{r}_1)$  is given by

$$H(\mathbf{r}_1) = H_0(\mathbf{r}_1) + V(\mathbf{r}_1).$$
 (A.9)

The full Hamiltonian is separated into a part  $H_0$ , which is exactly solvable and the interaction part V which is treated as perturbation. If the Green's function in A.8 is known, the solution for the Schrödinger equation

$$[i\partial_t - H_0(\mathbf{r}_1) - V(\mathbf{r}_1)]\Psi(\mathbf{r}_1, t_1) = 0$$
(A.10)

is given by the following convolution

$$\Psi(\mathbf{r}_1, t_1) = \Psi^0(\mathbf{r}_1, t_1) + \int dt_2 \int d\mathbf{r}_2 G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) V(\mathbf{r}_2) \Psi^0(\mathbf{r}_2, t_2), \qquad (A.11)$$

where  $\Psi^0(\mathbf{r}_1, t_1)$  is the solution for the exact solvable part of the Hamiltonian. Unfortunately,  $G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2)$  can not be found exactly in general. The retarded Green's function  $G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2)$  is defined by

$$G^{R} = -i\Theta(t_{1} - t_{2})\langle 0| \left\{ \Psi(\boldsymbol{r}_{1}, t_{1}), \Psi^{\dagger}(\boldsymbol{r}_{2}, t_{2}) \right\} |0\rangle,$$
(A.12)

where  $\Psi^{\dagger}(\Psi)$  are fermion field creation (destruction) operators, respectively. They create (destroy) an electron at time t at position r. Using equation of motion theory and the anti-commutation rule of fermions

$$\left\{ \Psi_{\sigma_1}(\boldsymbol{r}_1, t_1), \Psi_{\sigma_2}^{\dagger}(\boldsymbol{r}_2, t_2) \right\} = \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \delta(t_1 - t_2) \delta_{\sigma_1, \sigma_2}$$

$$\left\{ \Psi_{\sigma_1}^{(\dagger)}(\boldsymbol{r}_1, t_1), \Psi_{\sigma_2}^{(\dagger)}(\boldsymbol{r}_2, t_2) \right\} = 0,$$
(A.13)

one can see that equation (A.12) solves equation (A.8). In the case of free fermions, where the Hamiltonian H is bilinear  $H_0 = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$ , the retarded Green's function in Fourier-space  $G(\boldsymbol{k}\sigma,\omega)$  is given by

$$G_0^R(\boldsymbol{k}\sigma,\omega) = \frac{1}{\omega - \epsilon_{\boldsymbol{k}} + i0^+}.$$
(A.14)

The fermion field operators are related to the given fermion operators via a Fourier transformation. The important corresponding spectral function  $A_0(\mathbf{k}\sigma,\omega)$  and the normalized spectral function  $\rho_0(\mathbf{k}\sigma,\omega)$  are given by

$$A_0(\boldsymbol{k}\sigma,\omega) = -2G_0^{''R}(\boldsymbol{k}\sigma,\omega) = 2\pi\delta(\omega-\epsilon_{\boldsymbol{k}})$$
  

$$\rho_0(\boldsymbol{k}\sigma,\omega) = -\frac{1}{\pi}G_0^{''R}(\boldsymbol{k}\sigma,\omega) = \delta(\omega-\epsilon_{\boldsymbol{k}}),$$
(A.15)

where  $G''^R = \text{Im}(G^R)$ . The spectral functions is a very sharp resonance for energy  $\epsilon_{\mathbf{k}}$  of the particle. If scattering processes are switched on, represented by the interaction  $V(\mathbf{r})$  above, the fermion particles will not stay in the state  $\mathbf{k}$ . They will be scattered out of this state so that again a relaxation time  $\tau$  is introduced which broadens the sharp peak. The retarded Green's function  $G^R(\mathbf{k}\sigma,\omega)$  with interaction is then given by

$$G^{R}(\boldsymbol{k}\sigma,t) \approx -i\Theta(t)e^{-i\epsilon_{\boldsymbol{k}}t}e^{-\frac{t}{\tau}}.$$
(A.16)

The corresponding spectral function is given by the following broadened form

$$A(\boldsymbol{k}\sigma,\omega) = \frac{\frac{2}{\tau}}{(\omega - \epsilon_{\boldsymbol{k}})^2 + (\frac{1}{\tau})^2}.$$
(A.17)

# A.3. Perturbation theory for the Green's function

In this section it is shown how the Green's functions can be expanded into a perturbation series and that the Green's functions of the interacting system can be expressed by free Green's functions with the help of the adiabatic principle. Further it will be shown, how the relaxation time of the quasi-particles can be evaluated systematically by using Dyson's equation.

#### A.3.1. Adiabatic principle

For the beginning the potential V(t) is assumed to be spin-independent, i.e. spin-flip processes are not possible. On this way, the introduction of Feynman diagrams is easier. In many-particle quantum mechanics, the full Green's function G is defined by

$$G(1,2) = -i\langle \Phi_0 | T_t \left( \psi(1)\psi^{\dagger}(2) \right) | \Phi_0 \rangle, \qquad (A.18)$$

where the abbreviation  $1 = \{\mathbf{r}_1, t_1, \sigma_1\}$  is introduced.  $\psi(1)$  destroys a particle at position  $\mathbf{r}_1$  at time  $t_1$  and spin  $\sigma_1$ . Likewise  $2 = \{\mathbf{r}_2, t_2, \sigma_2\}$ , so that  $\psi^{\dagger}(2)$  creates a particle at position  $\mathbf{r}_2$  at time  $t_2$  and with spin  $\sigma_2$ . The operators in equation (A.18) are given in the Heisenberg picture and have the same properties as in equation (A.13). The Green's function can be interpreted as a propagator, giving the probability for a transition of the particle from 2 to 1. The perturbation series of the Green's function is given by [35, 36, 38]

$$G(1,2) = \frac{\langle \Phi_0 | T_t \left( U(\infty, -\infty) \Psi(1) \Psi^{\dagger}(2) \right) | \Phi_0 \rangle_0}{\langle \phi_0 | U(\infty, -\infty) | \phi_0 \rangle_0} \\ = \frac{\langle \Phi_0 | \sum_{n=0}^{\infty} \left( \frac{-i}{n!} \right)^n \int_{-\infty}^{\infty} dt_1 \cdots dt_n T_t \left( V_I(t_1) \cdots V_I(t_n) \Psi(1) \Psi^{\dagger}(2) \right) | \Phi_0 \rangle_0}{\langle \phi_0 | \sum_{n=0}^{\infty} \left( \frac{-i}{n!} \right)^n \int_{-\infty}^{\infty} dt_1 \cdots dt_n T_t \left( V_I(t_1) \cdots V_I(t_n) \right) ) | \Phi_0 \rangle_0}$$
(A.19)

where the expansion for the time-evolution operator in equation (A.6) was used, and it is important to mention that the operators are all taken in the interaction representation. The remarkable point is that the averages are taken in the system without interactions. This comes from the adiabatic principle which states that the ground-state of a nondegenerated system can not make transitions so that the ground-state of the interacting and the free system only differ by a phase factor. In principle, this expansion for the Green's function can be done for any correlation of two operators, so that the fermion creation and destruction operator in the definition are replaced. For example, one can calculate a spin-spin correlator  $\langle \Phi_0 | S(t) S(0) | \Phi_0 \rangle$ .

#### A.3.2. Feynman diagrams

We want to introduce Feynman diagrams using a spin-independent interaction potential which is given by

$$V_{I}(t) = \frac{1}{2} \int d\mathbf{r}_{1} d\mathbf{r}_{2} \Psi^{\dagger}(\mathbf{r}_{1}, t_{1}) \Psi^{\dagger}(\mathbf{r}_{2}, t_{2}) V(\mathbf{r}_{1} - \mathbf{r}_{2}) \Psi(\mathbf{r}_{2}, t_{2}) \Psi(\mathbf{r}_{1}, t_{1}), \qquad (A.20)$$

where  $V(\mathbf{r}_1 - \mathbf{r}_2)$  is the interaction potential which enters the Schrödinger equation. Further, the spin-indices were neglected due to the spin-independent  $V_I(t)$ . Before Feynman diagrams are discussed, Wick's theorem is introduced, which states that the average over 2n operators can be expressed by n averages over two operators [36, 38]. The following example should give the idea. The average of six operators, which occurs with the given interaction potential in first order of the expansion in equation (A.19)

$$\langle T_t(\Psi^{\dagger}(a)\Psi^{\dagger}(b)\Psi(b)\Psi(a)\Psi(1)\Psi^{\dagger}(2))\rangle = \langle T_t(\Psi^{\dagger}(a)\Psi^{\dagger}(b)\Psi(b)\Psi(a)\Psi(1)\Psi^{\dagger}(2))\rangle$$

$$= G_0(a,b)G_0(b,a)G_0(1,2),$$
(A.21)

where the 0 indicated the free propagators. Further, this example shows the idea of the linked cluster theorem. If the operators  $\Psi(1)$  and  $\Psi^{\dagger}(2)$  are contracted, one can only contract operators of the time-evolution series  $U(\infty, -\infty)$ . But this contractions also occur in the denominator of the expansion equation (A.19), so that the integrals are cancelled out and only the free propagator  $G_0(1,2)$  contributes. Finally, these two rules enable one two draw Feynman diagrams and to find the concerning Feynman rules and one can verify, that for the given interaction equation (A.20) the factor  $\frac{1}{n!}$  is cancelled out. Another important rule is, that each closed fermion loop contributes a factor (-1), which can be seen in the following example

$$\langle \Psi^{\dagger}(1)\Psi(1)\Psi^{\dagger}(2)\Psi(2)\Psi^{\dagger}(3)\cdots\Psi(n-1)\Psi^{\dagger}(n)\Psi(n)\rangle$$

$$= \langle \Psi^{\dagger}(1)\Psi(1)\Psi^{\dagger}(2)\Psi(2)\Psi^{\dagger}(3)\cdots\Psi(n-1)\Psi^{\dagger}(n)\Psi(n)\rangle,$$
(A.22)

because the first and the last operator have to be anti-commuted in order to get the propagator  $G_0(n, 1)$ . The interaction potential  $U(\mathbf{r}_1 - \mathbf{r}_2)$  is defined as  $U_{1,2} = U(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2)$ . Doing so leads to different contributions to the perturbation series. Each order can be represented graphically wih Feynman diagrams [35, 37, 38] using the following rules:



In Figure A.1 the popular Hartree and Fock contributions in first order perturbation theory are given. They are obtained using the given rules above. Also it is integrated over internal vertices. Further, if the system is invariant under translations, the Green's function can be defined in Fourier-space. This leads to conservation of momentum and energy at each vertex, which is more intuitive and to very similar diagrams.



Figure A.1.: This Figure shows the contributions in first order perturbation theory, the Hartree term on the left hand side and Fock term on the right hand side.

#### A.3.3. Dyson's equation and Fermi liquid theory

Dyson's equation sums irreducible diagrams of different orders up to infinity. For example in Figure A.2 the Hartree diagram of first order perturbation theory is summed up. In the series, the factor of a free Green's function and the Hartree diagram occurs. The result is a geometric series. To do this more generally, the concept of irreducible diagrams is introduced. A reducible diagram is the third contribution to the series in Figure A.2, because one can cut it into two Hartree diagrams. An exampled of an irreducible diagram is a diagram, which can not be cut into less complex diagrams. For instance the given Hartree and the given Fock diagram are irreducible (see Figure A.1). Figure A.3 shows the most important second order irreducible diagrams. All irreducible diagrams can be summed up to infinity. An irreducible diagram is called  $\Sigma$  and equation (A.24) shows, how this summation can be done systematically. In principle, the full Green's function can be obtained on this way, because a lot of diagrams are summed



Figure A.2.: The Hartree diagram of first order perturbation theory is summed up to infinity.



Figure A.3.: This Figure shows two irreducible diagrams in second order. The first one is a Hartreetype diagram, also called sunrise-diagram and the second is a Fock-type diagram.

up. The full Green's function is given by



This graphical equation leads in frequence space to the important algebraic Dyson equation [37], which is given by

$$G = G_0 + G\Sigma G_0 = \frac{1}{G_0^{-1} - \Sigma}.$$
 (A.25)

 $\Sigma$  is called self-energy. The free retarded Green's function  $G_0^R$  is given in equation (A.14). The full retarded Green's function is given by

$$G^{R}(\boldsymbol{k}\sigma,\omega) = \frac{1}{w - \epsilon_{\boldsymbol{k}} - \Sigma^{R}(\boldsymbol{k},\omega)}$$
  
= 
$$\frac{1}{w - \epsilon_{\boldsymbol{k}} - \Sigma'^{R}(\boldsymbol{k},\omega) - i\Sigma''^{R}(\boldsymbol{k},\omega)},$$
 (A.26)

where  $\Sigma'^R$  denotes the real part and  $\Sigma''^R$  the imaginary part of the retarded self-energy. The imaginary part of the retarded Green's function is related to the spectral function. The real part shifts the position of the pole. This can be understood as a mass-renormalization of the particles due to the interaction. The imaginary part determines the life-time of the quasi-particles and the irreducible diagrams in second order give the first contribution to this life-time. It can be shown that these diagrams lead to [35, 37]

$$\Sigma^{''R} \propto E_{\boldsymbol{k}}^2,$$
 (A.27)

where the renormalized mass enters the energy-dispersion  $E_k$ . The energy-dispersion helps us to find the range where the Fermi liquid picture is valid. The picture works, when the quasi-particle peaks is not broadened too much so that the quasi-particle have a exact energy-dispersion which can be used to calculate the properties of the Fermi gas.



Figure A.4.: This Figure shows the quasi-particle peak centered at  $E_k$  with weight  $0 < Z_k < 1$ . The incoherent background ensures that the spectral function remains normalized.

In other words if the weight  $Z_k$  is in the vicinity of 1 the Fermi liquid picture works well. It turns out for the Kondo model where a spin-dependent interaction term appears that the ground-state is a local Fermi liquid liquid which can be seen from typical properties. For instance a constant susceptibility or the  $T^2$  term in the conductance which indicates the relaxation time of the quasi-particles.

# B. Equations of motion technique and the $\mathcal{T}$ -matrix

In this section the  $\mathcal{T}$ -matrix is derived by using the equations of motion technique for the zero-temperature Green's function of the conduction electrons. The aim is to bring the Green's function of the conduction electrons to the equation which determines the  $\mathcal{T}$ -matrix given by

$$G^{R}_{c\boldsymbol{k}\boldsymbol{k}'\sigma}(\omega) = G^{R}_{0\boldsymbol{k}c\sigma}(\omega)\delta_{\boldsymbol{k},\boldsymbol{k}'} + G^{R}_{0\boldsymbol{k}c\sigma}(\omega)\mathcal{T}^{R}_{\boldsymbol{k}\boldsymbol{k}'\sigma}(\omega)G^{R}_{0\boldsymbol{k}'c\sigma}(\omega)$$
(B.1)

From that result, the  $\mathcal{T}$ -matrix can be transformed to imaginary-times. The full Green's function  $G_{c\boldsymbol{k},\boldsymbol{k}'\sigma}(t-t')$  of the conduction electrons is determined by the Kondointeraction and  $G_{0c\boldsymbol{k}\sigma}$  describes free conduction electrons. The full Green's function is given by

$$G_{c\boldsymbol{k}\boldsymbol{k}'\sigma}(t-t') = -i\left\langle T_t \left[ c_{\boldsymbol{k}\sigma}(t)c_{\boldsymbol{k}'\sigma}^{\dagger}(t') \right] \right\rangle$$
  
$$= -i\theta(t-t')\left\langle c_{\boldsymbol{k}\sigma}(t)c_{\boldsymbol{k}'\sigma}^{\dagger}(t') \right\rangle + i\theta(t'-t)\left\langle c_{\boldsymbol{k}'\sigma}^{\dagger}(t')c_{\boldsymbol{k}\sigma}(t) \right\rangle,$$
(B.2)

where  $T_t$  is the time ordering operator and the creation and annihilation operators are given in the Heisenberg representation. The equation of motion for the Green's function of the conduction electrons is given by

$$i\partial_t G_{c\boldsymbol{k}\boldsymbol{k}'\sigma}(t-t') = \delta(t-t') \left\langle \underbrace{\left\{ c_{\boldsymbol{k}\sigma}(t), c_{\boldsymbol{k}'\sigma}^{\dagger}(t) \right\}}_{\delta_{\boldsymbol{k}\boldsymbol{k}'}} \right\rangle + i \left\langle T\left[ \left[ H, c_{\boldsymbol{k}\sigma} \right](t) c_{\boldsymbol{k}'\sigma}^{\dagger}(t') \right] \right\rangle, \quad (B.3)$$

where anti-commutation rules for fermions are used. The two following commutationrules for any operators A, B, C and D will be useful:

$$[AB, C] = A\{B, C\} - \{A, C\}B$$

and

$$[ABC, D] = A\{BC, D\} - \{A, D\}BC.$$
(B.4)

The Kondo-Hamiltonian  $H_{\rm K} = H_0 + H_{\rm I}$  is given by the sum of a bilinear and an interaction term

$$H_{\mathrm{K}} = \underbrace{\sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma}}_{H_{0}} + \underbrace{\frac{J}{2} \sum_{\boldsymbol{k}_{1}\boldsymbol{k}_{2}\sigma_{1}\sigma_{2}} c_{\boldsymbol{k}_{1}\sigma_{1}}^{\dagger} \boldsymbol{\tau}_{\sigma_{1}\sigma_{2}} c_{\boldsymbol{k}_{2}\sigma_{2}} \cdot \boldsymbol{S}}_{H_{\mathrm{I}}}.$$

87

The first commutation-rule can be used to derive the commutator of  $c_{k\sigma}$  and the bilinear part  $H_0$  of the Kondo-Hamiltonian

$$\left[H_0, c_{\boldsymbol{k}\sigma}\right] = -\epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma},\tag{B.5}$$

while the commutator of the interaction part with  $c_{{\bm k}\sigma}$  can be derived using the second rule

$$\begin{bmatrix} H_{1}, c_{k\sigma} \end{bmatrix} = \frac{J}{2} \sum_{\boldsymbol{k}_{2}\boldsymbol{k}_{1}\sigma_{1}\sigma_{2}} \boldsymbol{\tau}_{\sigma_{2}\sigma_{1}} \left[ c_{\boldsymbol{k}_{2}\sigma_{2}}^{\dagger} c_{\boldsymbol{k}_{1}\sigma_{1}} \cdot \boldsymbol{S}, c_{\boldsymbol{k}\sigma} \right]$$

$$= \frac{J}{2} \sum_{\boldsymbol{k}_{2}\boldsymbol{k}_{1}\sigma_{1}\sigma_{2}} \boldsymbol{\tau}_{\sigma_{2}\sigma_{1}} c_{\boldsymbol{k}_{2}\sigma^{2}}^{\dagger} \underbrace{\left\{ c_{\boldsymbol{k}_{1}\sigma_{1}} \cdot \boldsymbol{S}, c_{\boldsymbol{k}\sigma} \right\}}_{=0} \right]$$

$$- \frac{J}{2} \sum_{\boldsymbol{k}_{2}\boldsymbol{k}_{1}\sigma_{1}\sigma_{2}} \boldsymbol{\tau}_{\sigma_{2}\sigma_{1}} \underbrace{\left\{ c_{\boldsymbol{k}_{2}\sigma_{2}}^{\dagger}, c_{\boldsymbol{k}\sigma} \right\}}_{=\delta_{\boldsymbol{k}_{2}\boldsymbol{k}}\delta_{\sigma_{2}\sigma}} c_{\boldsymbol{k}_{1}\sigma_{1}} \cdot \boldsymbol{S}$$

$$= -\frac{J}{2} \sum_{\boldsymbol{k}_{1}\sigma_{1}} \boldsymbol{\tau}_{\sigma\sigma_{1}} c_{\boldsymbol{k}_{1}\sigma_{1}} \cdot \boldsymbol{S} \text{ with } \sum_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma} = c_{0\sigma}.$$
(B.6)

The anti-commutator in the first step disappears due to  $[c_{k\sigma}, S] = 0$ . These two different commutators can be used to write down an intermediate equations of motion for the full Green's function which is given by

$$\left(i\partial_{t} - \epsilon_{\boldsymbol{k}}\right) G_{c\boldsymbol{k}\boldsymbol{k}'\sigma}(t-t') = \delta(t-t')\delta_{\boldsymbol{k}\boldsymbol{k}'} - i\frac{J}{2}\sum_{\sigma_{1}}\boldsymbol{\tau}_{\sigma\sigma_{1}} \cdot \left\langle T_{t}\left[c_{0\sigma_{1}}(t)\boldsymbol{S}(t)c_{\boldsymbol{k}'\sigma}^{\dagger}(t')\right]\right\rangle.$$

$$(B.7)$$

The aim of every equation of motion-derivation is to find a closed set of equation. It turns out that this can be achieved by using the derivation with respect to t' in equation equation (B.7) which is given by

$$i\partial_{t'}i\left\langle T_t\left[c_{0\sigma_1}(t)\boldsymbol{S}(t)c_{\boldsymbol{k}'\sigma}^{\dagger}(t')\right]\right\rangle = \left\langle \left\{c_{0\sigma_1}(t)\boldsymbol{S}(t),c_{\boldsymbol{k}'\sigma}^{\dagger}(t')\right\}\right\rangle \delta(t-t') - i\left\langle T_t\left[c_{0\sigma_1}(t)\boldsymbol{S}(t)\left[H,c_{\boldsymbol{k}'\sigma}^{\dagger}\right](t')\right]\right\rangle.$$
(B.8)

Again two different commutators contribute to the equation of motions where the commutator with the bilinear part of the Kondo-Hamiltonian with  $c^{\dagger}_{k\sigma}$  is given by

$$\left[H_0, c^{\dagger}_{\boldsymbol{k}'\sigma}\right] = \epsilon_{\boldsymbol{k}'} c^{\dagger}_{\boldsymbol{k}'\sigma},\tag{B.9}$$

while the commutator of  $c^{\dagger}_{{\bm k}\sigma}$  with the interaction term of the Kondo-Hamiltonian reads

$$\begin{bmatrix} H_{1}, c_{\boldsymbol{k}'\sigma}^{\dagger} \end{bmatrix} = \frac{J}{2} \sum_{\boldsymbol{k}_{2}\boldsymbol{k}\sigma_{2}\sigma_{1}} \left[ \boldsymbol{\tau}_{\sigma_{2}\sigma_{1}} c_{\boldsymbol{k}_{2}\sigma_{2}}^{\dagger} \underbrace{\left\{ c_{\boldsymbol{k}\sigma_{1}} \cdot \boldsymbol{S}, c_{\boldsymbol{k}'\sigma}^{\dagger} \right\}}_{\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\sigma\sigma_{1}}\cdot\boldsymbol{S}} - \boldsymbol{\tau}_{\sigma_{2}\sigma_{1}} \underbrace{\left\{ c_{\boldsymbol{k}_{2}\sigma_{2}}^{\dagger}, c_{\boldsymbol{k}'\sigma}^{\dagger} \right\}}_{=0} c_{\boldsymbol{k}\sigma_{1}} \cdot \boldsymbol{S} \right]$$
$$= \frac{J}{2} \sum_{\boldsymbol{k}_{2}\sigma_{2}} \boldsymbol{\tau}_{\sigma_{2}\sigma} c_{\boldsymbol{k}_{2}\sigma_{2}}^{\dagger} \cdot \boldsymbol{S}$$
$$= \frac{J}{2} \sum_{\sigma_{2}} \boldsymbol{\tau}_{\sigma_{2}\sigma} c_{0\sigma_{2}}^{\dagger} \cdot \boldsymbol{S}. \tag{B.10}$$

The equation of motion for the second Green's function is given by

$$\left( i\partial_{t'} + \epsilon_{\mathbf{k}'} \right) i \left\langle T_t \left[ c_{0\sigma_1}(t) \mathbf{S}(t) c_{\mathbf{k}'\sigma}^{\dagger}(t') \right] \right\rangle =$$

$$= \delta(t - t') \left\langle \mathbf{S} \right\rangle \delta_{\sigma\sigma_1} - i \frac{J}{2} \sum_{\sigma_2} \left\langle T_t \left[ c_{0\sigma_1}(t) \mathbf{S}(t) \boldsymbol{\tau}_{\sigma_2\sigma} c_{0\sigma_2}^{\dagger}(t') \cdot \mathbf{S}(t') \right] \right\rangle$$
(B.11)

The imaginary part of the retarded  $\mathcal{T}$ -matrix is related to the conductance of the quantum dot and therefore only the part where t > t' is taken. Furthermore, the  $\mathcal{T}$ -matrix in dependence of energies is obtained with the Fourier transformation:

$$F^{R}(\omega) = -i \int_{-\infty}^{\infty} d(t - t')\theta(t - t')F(t)e^{i\omega(t - t')}e^{\eta(t - t')},$$
 (B.12)

where  $e^{\eta t}$  is an infinitesimal small factor which regularizes the integral and represents the causality of the correlation function. The derivation with respect to t gives  $\omega + i\eta$ and that with respect to t' gives  $-\omega - i\eta$  which leads to a closed set of equations in dependence of energy  $\omega$ :

$$\left(\omega+i\eta-\epsilon_{\boldsymbol{k}}\right)G^{R}_{c\boldsymbol{k}\boldsymbol{k}'\sigma}(\omega)=\delta_{\boldsymbol{k}\boldsymbol{k}'}+\frac{J}{2}\left\langle\left\langle\boldsymbol{\tau}_{\sigma\sigma_{1}}\cdot\boldsymbol{S}(t)c_{0\sigma_{1}}(t);c^{\dagger}_{\boldsymbol{k}'\sigma}(t')\right\rangle\right\rangle$$

and

$$\left( \boldsymbol{\omega} + i\boldsymbol{\eta} - \boldsymbol{\epsilon}_{\boldsymbol{k}'} \right) \left\langle \left\langle c_{0\sigma_1}(t)\boldsymbol{S}(t); c_{\boldsymbol{k}'\sigma}^{\dagger}(t') \right\rangle \right\rangle = \\ \left\langle \boldsymbol{S} \right\rangle \delta_{\sigma\sigma_1} + \frac{J}{2} \left\langle \left\langle c_{0\sigma_1}(t)\boldsymbol{S}(t); \boldsymbol{\tau}_{\sigma_2\sigma}c_{0\sigma_2}^{\dagger}(t') \cdot \boldsymbol{S}(t') \right\rangle \right\rangle,$$

$$(B.13)$$

where  $\langle \langle \dots \rangle \rangle$  indicates the Fourier transformation of the retarded part of the  $\mathcal{T}$ -matrix. Solving this leads to the  $\mathcal{T}$ -matrix which is given by

$$G^{R}_{c\boldsymbol{k}\boldsymbol{k}'\sigma}(\omega) = G^{R}_{0c\boldsymbol{k}}(\omega)\delta_{\boldsymbol{k}\boldsymbol{k}'} + \frac{J}{2}G^{R}_{0c\boldsymbol{k}}(\omega)\underbrace{\left(\langle S^{z}\rangle + \frac{J}{2}\left\langle\left\langle c_{0\sigma_{1}}(t)\boldsymbol{\tau}_{\sigma\sigma_{1}}\cdot\boldsymbol{S}(t);c^{\dagger}_{0\sigma_{2}}(t')\boldsymbol{\tau}_{\sigma_{2}\sigma}\cdot\boldsymbol{S}(t')\right\rangle\right\rangle\right)}_{=T_{\sigma}(\omega)\frac{2}{J}}G^{R}_{0c\boldsymbol{k}'}(\omega),$$
(B.14)

where the free Green's function of the conduction electrons is given by

$$G^R_{0ck}(\omega) = \frac{1}{\omega - \epsilon_k + i0^+} \tag{B.15}$$

The time-ordered  $\mathcal{T}$ -matrix can be read-off from these equations and is given by

$$\mathcal{T}_{\sigma}(t) = -\frac{J}{2} \left\langle S^{z} \right\rangle - i \frac{J^{2}}{4} \left\langle T_{t} \left[ c_{0\sigma_{1}}(t) \boldsymbol{\tau}_{\sigma\sigma_{1}} \cdot \boldsymbol{S}(t); c_{0\sigma_{2}}^{\dagger}(0) \boldsymbol{\tau}_{\sigma_{2}\sigma} \cdot \boldsymbol{S}(0) \right] \right\rangle$$
(B.16)

and for imaginary-times it is given by

$$\mathcal{T}_{\sigma}(\tau) = -\frac{J}{2} \left\langle S^{z} \right\rangle - \frac{J^{2}}{4} \left\langle T_{\tau} \left[ c_{0\sigma_{1}}(\tau) \boldsymbol{\tau}_{\sigma\sigma_{1}} \cdot \boldsymbol{S}(\tau); c_{0\sigma_{2}}^{\dagger}(0) \boldsymbol{\tau}_{\sigma_{2}\sigma} \cdot \boldsymbol{S}(0) \right] \right\rangle, \qquad (B.17)$$

where  $T_{\tau}$  is the imaginary-time ordering symbol.

# C. Polarization diagrams and self-energies

In this appendix the polarization diagrams and the self-energies are calculated for both the cases in absence and presence of a magnetic field B.

# C.1. Polarization diagrams

In this chapter the polarization diagrams are calculated which provide the main contribution to random phase approximation for the  $\mathcal{T}$ -matrix. We will distinguish between the absence and the presence of a magnetic field B. For the computations of the diagrams we will use the introduced Matsubara Green's function technique from chapter 3. The definitions for the Fourier transformation are given by

$$G_{AB}(\tau) = \frac{1}{\beta} \sum_{\nu_1} e^{-i\nu_1 \tau} G_{AB}(i\nu_1)$$
$$G_{AB}(i\nu) = \int_0^\beta d\tau G_{AB}(\tau).$$

We will also use the analytical continuation in the following form

$$G_{AB}(i\omega_n) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega_1 G_{AB}^{\prime\prime R}(\omega_1) \frac{1}{i\nu_1 - \omega_n},$$

which has the advantage that we only have to evaluate the Matsubara sum over simple poles using equation (3.13).

#### C.1.1. Polarization diagram for B = 0

The polarization diagram in the absence of a magnetic field is given by

$$\tau$$
 $\eta$ 
 $= \Pi_{0\eta}(\tau) = G_{0\eta}(\tau)G_{0c}(\tau).$ 
(C.1)

In this equation the local conduction electron propagator  $G_{0c}(i\omega_n)$  occurs which is given by

$$G_{0c}(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{i\omega_n - \epsilon},$$

91

where  $\rho(\epsilon)$  is the density of states of the electrons which is given by a flat band

$$\rho(\epsilon) = \frac{1}{2D}\Theta(D^2 - \epsilon^2) = \rho_0\Theta(D^2 - \epsilon^2)$$

The integral  $\int d\epsilon$  occurs due to the local Kondo-interaction term. The free Majorana fermion propagator  $G_{0\eta}(i\omega_n)$  is given by

$$G_{0\eta}(i\omega_n) = \frac{1}{i\omega_n}$$

The corresponding retarded propagators can be obtained by applying the analytical continuation rule where the Matsubara frequency is replaced by  $i\omega_n \rightarrow \omega + 0^+$ . Using the introduced Matsubara formalism for Majorana fermions from chapter 3 the polarization diagram reads

$$\begin{aligned} \Pi_{0\eta}(i\omega_{b}) &= \int_{0}^{\beta} d\tau e^{i\omega_{b}\tau} G_{0\eta}(\tau) G_{0c}(\tau) \\ &= \int_{0}^{\beta} d\tau e^{i\omega_{b}\tau} \frac{1}{\beta^{2}} \sum_{\nu_{1},\nu_{2}} G_{0\eta}(i\nu_{1}) G_{0c}(i\nu_{2}) e^{-i\nu_{1}\tau} e^{-i\nu_{2}\tau} \\ &= \frac{1}{\beta} \sum_{\nu_{1}} G_{0\eta}(i\nu_{1}) G_{0c}(i\omega_{b} - i\nu_{1}) \\ &= -\frac{1}{\pi^{2}} \int_{-\infty}^{\infty} d\omega_{1} \int_{-\infty}^{\infty} d\omega_{2} \underbrace{G_{0\eta}^{''R}(\omega_{1}) G_{0c}^{''R}(\omega_{2})}_{=\pi^{2}\delta(\omega_{1})\rho_{0}\Theta(D^{2}-\omega_{2}^{2})} \underbrace{\frac{1}{\beta} \sum_{i\nu_{1}} \frac{1}{i\nu_{1}-\omega_{1}} \frac{1}{i\nu_{1}-i\omega_{b}+\omega_{2}}}_{\frac{n_{F}(\omega_{1})-n_{F}(-\omega_{2})}{\omega_{1}-i\omega_{b}+\omega_{2}}} \\ &= -\frac{\rho_{0}}{2} \int_{-\infty}^{\infty} d\omega_{2} \underbrace{(1-2n_{F}(-\omega_{2}))}_{\tanh\left(-\frac{\beta\omega_{2}}{2}\right)} \frac{1}{-i\omega_{b}+\omega_{2}} \Theta(D^{2}-\omega_{2}^{2}). \end{aligned}$$
(C.2)

Performing the analytical continuation  $i\omega_b \to \omega + i0^+$  in the limit temperature  $T \to 0$ and using  $\frac{1}{x \pm i0^+} = \mathbf{P} \mp i\pi \delta(x)$  leads to the retarded polarization diagram  $\Pi^R_{0\eta}$ 

$$\Pi_{0\eta}^{R}(\omega) = \frac{\rho_{0}}{2} \operatorname{P} \int_{-D}^{D} d\omega_{2} \frac{\operatorname{sign}(\omega_{2})}{\omega + \omega_{2}} + i\pi \frac{\rho_{0}}{2} \operatorname{sign}(\omega) \Theta(\omega^{2} - D^{2})$$

$$= \frac{\rho_{0}}{2} \log \left( \left| \frac{\omega^{2} - D^{2}}{\omega^{2}} \right| \right) + i\pi \frac{\rho_{0}}{2} \operatorname{sign}(\omega) \Theta(\omega^{2} - D^{2}), \quad (C.3)$$

where  $tanh(\beta x) = sign(x)$  for  $T \to 0$  and  $\delta(\omega - \omega_2)$  were used.

#### C.1.2. Polarization diagram for $B \neq 0$

The polarization diagram for a finite magnetic field can be obtained directly from equation C.2 when the Majorana fermion propagator  $G_{0\eta}(\tau)$  is replaced by  $G_{0f}(\tau)$ 

which is given by

$$G_{0f}(i\omega_n) = \frac{1}{i\omega_n - B}.$$
(C.4)

Doing so yields

$$\Pi_{0f}(i\omega_{b}) = -\frac{1}{\pi^{2}} \int_{-\infty}^{\infty} d\omega_{1} \int_{-\infty}^{\infty} d\omega_{2} \underbrace{\underbrace{G_{0f}^{''R}(\omega_{1})G_{0c}^{''R}(\omega_{2})}_{=\pi^{2}\delta(\omega_{1}-B)\rho_{0}\Theta(D^{2}-\omega_{2}^{2})} \underbrace{\frac{1}{\beta} \sum_{i\nu_{1}} \frac{1}{i\nu_{1}-\omega_{1}} \frac{1}{i\nu_{1}-\omega_{1}} \frac{1}{i\nu_{1}-i\omega_{b}+\omega_{2}}}_{\frac{n_{F}(\omega_{1})-n_{F}(-\omega_{2})}{\omega_{1}-i\omega_{b}+\omega_{2}}}$$
$$= -\rho_{0} \int_{-\infty}^{\infty} d\omega_{2} \underbrace{(n_{F}(B)-n_{F}(-\omega_{2}))}_{-n_{F}(-\omega_{2})} \frac{1}{B-i\omega_{b}+\omega_{2}} \Theta(D^{2}-\omega_{2}^{2}).$$
(C.5)

In the limit temperature  $T \to 0$  the Fermi-distribution function is given by  $n_F(-\omega_2) = \Theta(\omega_2)$  and the analytical continuation  $i\omega_b \to \omega + i0^+$  giving  $\delta(B - \omega + \omega_2)$  leads to

$$\Pi_{0f}^{R}(\omega) = \rho_0 P \int_0^D \frac{d\omega_2}{B - \omega + \omega_2} + i\pi\rho_0 \Theta(\omega - B)\Theta(D^2 - (\omega - B)^2)$$
  
=  $\rho_0 \log\left(\left|\frac{B - \omega + D}{B - \omega}\right|\right) + i\pi\rho_0\Theta(\omega - B)\Theta(D^2 - (\omega - B)^2).$  (C.6)

In the next chapter the polarization diagram  $\Pi_{0f*}$  becomes important to calculate the self-energy  $\Sigma_{\eta}$  in the presence of a magnetic field. In this case we have to replace the propagator  $G_{0f}$  by  $G_{0f*}$  which is given by

$$G_{0f^*}(i\omega_n) = \frac{1}{i\omega_n + B}.$$
(C.7)

This leads to the polarization diagram

$$\Pi_{0f^*}(i\omega_b) = -\rho_0 \int_{-\infty}^{\infty} d\omega_2 \underbrace{\left(n_F(-B) - n_F(-\omega_2)\right)}_{1 - n_F(-\omega_2)} \frac{1}{-B - i\omega_b + \omega_2} \Theta(D^2 - \omega_2^2), \quad (C.8)$$

and the retarded polarization diagram is given in this case by

$$\Pi_{0f^*}^R(\omega) = -\rho_0 \operatorname{P} \int_{-D}^0 \frac{d\omega_2}{-B - \omega + \omega_2} - i\pi\rho_0 \Theta(-\omega - B)\Theta(D^2 - (\omega + B)^2)$$
  
$$= \rho_0 \log\left(\left|\frac{B + \omega + D}{B + \omega}\right|\right) - i\pi\rho_0 \Theta(-\omega - B)\Theta(D^2 - (\omega + B)^2).$$
 (C.9)

# C.2. The self-energies

In this chapter the self-energies are calculated in the absence and presence of a magnetic field. The self-energies are used to discuss the spin relaxation time in the magnetic susceptibility and in the  $\mathcal{T}$ -matrix.

<sup>&</sup>lt;sup>1</sup>We mention that the Fermi level  $\epsilon_F$  is put to zero (particle-hole-symmetry).

# C.2.1. Self-energy for B = 0

In chapter 3 it is shown that the self-energy  $\Sigma_{\eta}(\tau)$  in the absence of a magnetic field is given by

$$\Sigma_{\eta}(\tau) = -J^2 G_{0c}(-\tau) \Pi_{0\eta}(\tau).$$
 (C.10)

Performing the Fourier transformation gives

$$\begin{split} \Sigma_{\eta}(i\omega_{n}) &= -J^{2} \int_{0}^{\beta} d\tau e^{i\omega_{n}\tau} \frac{1}{\beta^{2}} \sum_{\nu_{1},\omega_{b}} G_{0c}(i\nu_{1}) \Pi_{0\eta}(i\omega_{b}) e^{i\nu_{1}\tau} e^{-i\omega_{b}\tau} \\ &= -J^{2} \frac{1}{\beta} \sum_{\nu_{1}} G_{0c}(i\nu_{1}) \Pi_{0\eta}(i\nu_{1} + i\omega_{n}) \\ &= -J^{2} \frac{1}{\pi^{2}} \int_{-\infty}^{\infty} d\omega_{1} \int_{-\infty}^{\infty} d\omega_{2} G_{0c}(\omega_{1}) \Pi_{0\eta}(\omega_{2}) \\ &\times \underbrace{\frac{1}{\beta} \sum_{\nu_{1}} \frac{1}{i\nu_{1} - \omega_{1}} \frac{1}{i\nu_{1} + i\omega_{n} - \omega_{2}}}_{= \frac{n_{F}(\omega_{1}) + n_{B}(\omega)}{\omega_{1} + i\omega_{n} - \omega_{2}}} \\ &= -J^{2} \frac{1}{2\pi^{2}} \int_{-\infty}^{\infty} d\omega_{1} \int_{-\infty}^{\infty} d\omega_{2} G_{0c}(\omega_{1}) \Pi_{0\eta}(\omega_{2}) \frac{2n_{F}(\omega_{1}) - 1 + 1 + 2n_{B}(\omega_{2})}{\omega_{1} - \omega_{2} + i\omega_{n}}. \end{split}$$
(C.11)

We perform again the analytical continuation  $i\omega_n \to \omega + i0^+$  giving a  $\delta$ -function to obtain the retarded self-energy. Further, rewriting the fermionic and bosonic distribution function using  $1 - 2n_F(x) = \tanh(x/2)$  and  $1 + 2n_B(x) = \coth(x/2)$  and using the polarization diagram  $\Pi_{0\eta}^{''R}(\omega) = \pi \frac{\rho_0}{2} \operatorname{sign}(\omega) \Theta(\omega^2 - D^2)$  leads to the imaginary part of the retarded self-energy  $\Sigma_{\eta}^{''R}$  given by

$$\begin{split} \Sigma_{\eta}^{''R}(\omega) &= -\frac{J^2}{2}\rho_0 \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \delta(\omega_1 - \omega_2 + \omega) \\ &\times \Theta(D^2 - \omega_1^2) \Pi_{0\eta}^{''R}(\omega_2) \left[ \coth\left(\frac{\beta\omega_2}{2}\right) - \tanh\left(\frac{\beta\omega_1}{2}\right) \right] \\ &= -\frac{J^2}{2}\rho_0 \int_{-D}^{D} d\omega_2 \Pi_{0\eta}^{''R}(\omega_2) \left[ \coth\left(\frac{\beta\omega_2}{2}\right) - \tanh\left(\frac{\beta(\omega_2 - \omega)}{2}\right) \right] \\ &= -\frac{J^2}{4}\rho_0^2 \pi \int_{-D}^{D} d\omega_2 \left[ \coth\left(\frac{\beta\omega_2}{2}\right) - \tanh\left(\frac{\beta(\omega_2 - \omega)}{2}\right) \right] \Theta(D^2 - \omega_2^2) \operatorname{sign}(\omega_2) \\ &= \operatorname{sign}(\omega_1 + \omega) - \operatorname{sign}(\omega_1) \text{ for } T \to 0 \\ &= -\frac{J^2}{4}\rho_0^2 \pi \int_{-D}^{D} d\omega_2 \left[ \operatorname{sign}(\omega_2) - \operatorname{sign}(\omega_2 - \omega) \right] \operatorname{sign}(\omega_2) \\ &\propto -\frac{J^2}{4}\rho_0^2 \pi |\omega| \Theta(D^2 - \omega^2), \end{split}$$
(C.12)

which is called Korringa-term. The real part can be obtained by using the Kramers-Kronig relation

$$\Sigma_{\eta}^{'R}(\omega) = \frac{1}{\pi} \operatorname{P} \int_{-\infty}^{\infty} \frac{\Sigma_{\eta}^{''R}(\omega_1)}{\omega_1 - \omega} d\omega_1.$$
 (C.13)

The imaginary part of the self-energy is proportional to  $\omega$ . Using this and

$$\Sigma_{\eta}^{\prime R}(\omega) \propto \mathbf{P} \int_{a}^{b} \frac{\omega_{1}}{\omega_{1} - \omega} d\omega_{1} = \left[ \omega \log(\omega_{1} - \omega) + \omega_{1} \right]_{b}^{a}.$$
 (C.14)

the real-part can be calculated. The self-energy  $\Sigma^R_\eta$  is shown in Figure 3.4.

# C.2.2. Self-energies for $B \neq 0$

The self-energies  $\Sigma_{\eta}$  and  $\Sigma_{f}$  can be calculated with the help of equation (C.12) and are given by

$$\Sigma_{f}(\tau) = -\frac{J^{2}}{2}G_{0c}(-\tau)\left[\Pi_{0f}(\tau) + \Pi_{0\eta}(\tau)\right]$$
  

$$\Sigma_{\eta}(\tau) = -\frac{J^{2}}{2}G_{0c}(-\tau)\left[\Pi_{0f}(\tau) + \Pi_{0f^{*}}(\tau)\right].$$
(C.15)

Combining those two equations leads to

$$\Sigma_{\eta}^{''R}(\omega) = -\frac{J^2}{4}\rho_0 \int_{-\infty}^{\infty} \left[ \Pi_{0f}^{''R}(\omega_2) + \Pi_{0f^*}^{''R}(\omega_2) \right],$$

$$\times \left( \operatorname{sign}(\omega_2) - \operatorname{sign}(\omega_2 - \omega) \right) \Theta(D^2 - (\omega_2 - \omega)^2) d\omega_1$$

$$\Sigma_f^{''R}(\omega) = -\frac{J^2}{4}\rho_0 \int_{-\infty}^{\infty} \left[ \Pi_{0f}^{''R}(\omega_2) + \Pi_{0\eta}^{''R}(\omega_2) \right]$$

$$\times \left( \operatorname{sign}(\omega_2) - \operatorname{sign}(\omega_2 - \omega) \right) \Theta(D^2 - (\omega_2 - \omega)^2) d\omega_1.$$
(C.16)

The real part can be obtained by using equation (C.13).

# D. List of Symbols

Symbol	Meaning
Р	Principle value from $\frac{1}{x\pm i0^+} = P\frac{1}{x} \mp i\pi\delta(x)$
$\mathcal{T}_{\sigma}$	Transmission matrix which describes the tunneling of elec- trons through the quantum dot
G	Conductance of the quantum dot
$G_{AB}( au, au_0)$	Matsubara Green's function of the two operators $A$ and $B$ (see chapter 3)
$\operatorname{sign}(x)$	Signum-function: returns 1 for $x \ge 0$ and -1 for $x < 0$
$\Theta(x)$	Theta-functions: returns 1 for $x \ge 0$ and 0 for $x < 0$
$n_F(\omega)$	Fermi-distribution: $n_F(\omega) = 1/(\exp(\beta(\omega - \mu) + 1))$
$n_B(\omega)$	Bose-distribution: $n_B(\omega) = 1/(\exp(\beta(\omega - \mu) - 1))$
β	$\frac{1}{T}$ with temperature $T$
$i\omega_b$	bosonic Matsubara frequencies
$i\omega_n, i\nu_j \text{ for } j \in \mathbb{N}$	fermionic Matsubara frequencies
$oldsymbol{\eta},\Phi$	Majorana fermions $oldsymbol{\eta}$ and independent fermionic field $\Phi$
S,  au	Spin operators $S^x$ , $S^y$ , $S^z$ and Pauli matrices $\tau^x$ , $\tau^y$ , $\tau^z$ written as vector
$S^{\pm} = S^x \pm iS^y$	Spin ladder operators which increase or decrease the spin quantum number by one
$G_{0\eta}, G\eta$	Free and full Majorana fermion propagator (doubled and single dashed lines in diagrammatics)
Dirac fermions composed of Majorana fermions	
---	
propagator of the Dirac fermions $f, f^{\dagger}$	
free local conduction electron propagator (represented by a solid line in diagrammatics)	
polarization diagrams given by $G_{0c}(\tau)G_{0\eta,f}(\tau)$	
Density Matrix Numerical Renormalization Group	
Numerical Renormalization Group	
Random Phase Approximation	
two dimensional electron gas	
Gate voltage which allows to control the number of electrons on the dot and bias voltage which defines a potential differ- ence between the left and right lead	
Real part $F'$ and imaginary part $F''$ of a retarded correlation function $F$ related by the Kramers-Kronig relation given by	
$F'^{R}(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} dx_1 \frac{F''^{R}(x_1)}{x_1 - x}$	
full and free retarded Green's functions	
flat band approach of the spectral function	
$\rho(\omega) = \rho_0 \Theta(D^2 - \omega^2)$	
The imaginary time $\tau$ ordering and real time $t$ ordering operator	
imaginary time and real time evolution operator	
Self-energies	
Zeeman term in Kondo Hamiltonian	

$H_K$	Kondo Hamiltonian
$H_0$	The non-interacting term of the Kondo Hamiltonian
$H_{\mathrm{I}}$	Interaction term of the Kondo Hamiltonian (vertices are represented by dots in the diagrammatics)
$H_D$	Describes the energy levels and interactions of the quantum dot
$H_{L;R}$	Describes the non-interaction electrons in the reservoirs coupled to the quantum dot
$H_T$	Describes coupling between the reservoirs and the quantum dot with tunneling amplitude $t$ leading to the hybridization $\Gamma$

## Danksagung

Ich möchte mich zunächst bei Serge Florens für die Betreuung der Diplomarbeit bedanken. Durch ihn habe ich sehr viel Einsicht in die Physik bekommen. Dabei möchte ich mich besonders dafür bedanken, dass ich jederzeit Probleme, die beim Verständnis von physikalischen Sachverhalten auftauchten, ausführlich diskutieren konnte. Desweiteren möchte ich mich bei Axel Freyn für Diskussionen über die NRG und die Beantwortung von computertechnischen Fragen bedanken. Außerdem möchte ich mich bei der gesamten Arbeitsgruppe für die tolle Atmosphäre bedanken, die sich unter anderem beim Kaffeetrinken zeigte. Alexander Shnirman möchte ich für die Betreuung von Karlsruher Seite und für Diskussionen über Majorana Fermionen bedanken. Ohne die Betreuung wäre es nicht möglich gewesen wäre, die Diplomarbeit im Rahmen des Doppeldiploms in Grenoble zu schreiben. Dabei gilt auch mein der deutsch-französischen Hochschule (DFH), die den Aufenthalt finanziell unterstützte. Auch meinen Freunden danke ich, dass sie mir geholfen haben, meine Arbeit auf Rechtschreib- und Grammatikfehler zu untersuchen. Letztlich möchte ich mich noch bei meiner Familie bedanken, die mir immer mit Rat zur Seite steht und mich finanziell unterstützt.

## Bibliography

- Neil W. Ashcroft and N. David Mermin. Solid State Physics. Cengage Learning Services, January 1976.
- [2] Charles Kittel. Introduction to Solid State Physics. Wiley John + Sons, 8th ed. edition, November 2004.
- [3] Charles Kittel and Kittel. Quantum Theory of Solids. John Wiley & Sons, revised. edition, June 1987.
- [4] J. Robert Schrieffer. Theory of Superconductivity. Westview Press, revised edition, January 1971.
- [5] P. W. Anderson. Localized Magnetic States in Metals. *Physical Review*, 124(1):41, October 1961.
- [6] Philip W. Anderson. Ground State of a Magnetic Impurity in a Metal. *Physical Review*, 164(2):352, December 1967.
- [7] Alexander Cyril Hewson. The Kondo Problem to Heavy Fermions. Cambridge University Press, April 1997.
- [8] Jun Kondo. Resistance Minimum in Dilute Magnetic Alloys. Progress of Theoretical Physics, 32(1):371–49, 1964.
- [9] Kenneth G. Wilson. The renormalization group: Critical phenomena and the Kondo problem. *Reviews of Modern Physics*, 47(4):773, October 1975.
- [10] Leo Kouwenhoven and Leonid Glazman. Revival of the Kondo effect. condmat/0104100, April 2001. Physics World, v. 14, No 1, pp. 33-38.
- [11] Siegfried Mantl and Helge L. Bay. New method for epitaxial heterostructure layer growth. Applied Physics Letters, 61(3):267, 1992.
- [12] Brian R. Pamplin. Molecular Beam Epitaxy. Crystal Research and Technology, 17(6):692–692, 1982.
- [13] M. A. Kastner. The single-electron transistor. Reviews of Modern Physics, 64(3):849, July 1992.
- [14] L. L. Sohn, L. P. Kouwenhoven, and G. Schön. Mesoscopic Electron Transport. Springer, 1997. Chapter: Electron Transport in Quantum Dots.

- [15] M.A. Kastner. The single electron transistor and artificial atoms. Annalen der Physik, 9(11-12):885–894, 2000.
- [16] M. Pustilnik. Kondo effect in nanostructures. cond-mat/0512671, December 2005. phys. stat. sol. (a) 203, 1137 (2006).
- [17] We took for this figure the original one and created an equivalent axis with P<sub>Y</sub>X.
- [18] N. Roch, C. B. Winkelmann, S. Florens, V. Bouchiat, W. Wernsdorfer, and F. Balestro. Kondo effects in a C60 single-molecule transistor. *physica status solidi* (b), 245(10):1994–1997, 2008.
- [19] D. Goldhaber-Gordon, Hadas Shtrikman, D. Mahalu, David Abusch-Magder, U. Meirav, and M. A. Kastner. Kondo effect in a single-electron transistor. *Nature*, 391(6663):156–159, January 1998.
- [20] M. Pustilnik, L. I Glazman, D. H Cobden, and L. P Kouwenhoven. Magnetic fieldinduced Kondo effects in Coulomb blockade systems. *cond-mat/0010336*, October 2000. Lecture Notes in Physics, 579, 3 (2001).
- [21] M. Pustilnik and L. I. Glazman. Kondo effect induced by a magnetic field. Phys. Rev. B, 64(4):045328, Jul 2001.
- [22] M. Pustilnik and L. I Glazman. Kondo effect in quantum dots. cond-mat/0401517, January 2004. J. Phys. Condens. Matter 16, R513 (2004).
- [23] Lam H. Yu and Douglas Natelson. The Kondo Effect in C60 Single-Molecule Transistors. Nano Letters, 4(1):79–83, January 2004.
- [24] P. W. Anderson. Basic Notions of Condensed Matter Physics. Perseus, 0002 edition, November 1997.
- [25] A. I. Tóth, C. P. Moca, Ö. Legeza, and G. Zaránd. Density matrix numerical renormalization group for non-Abelian symmetries. *Physical Review B*, 78(24):245109, December 2008.
- [26] Walter Hofstetter. Generalized Numerical Renormalization Group for Dynamical Quantities. *Physical Review Letters*, 85(7):1508, 2000.
- [27] A. Rosch, T. A. Costi, J. Paaske, and P. Wölfle. Spectral function of the Kondo model in high magnetic fields. *Physical Review B*, 68(1):014430, July 2003.
- [28] T. A. Costi. Kondo Effect in a Magnetic Field and the Magnetoresistivity of Kondo Alloys. *Physical Review Letters*, 85(7):1504, 2000.
- [29] Winfried Koller, Alex C. Hewson, and Dietrich Meyer. Singular dynamics of underscreened magnetic impurity models. *Physical Review B*, 72(4):045117, July 2005.

- [30] Ph. Nozières and A. Blandin. Kondo effect in real metals. Journal de Physique, 41(3):19, 1980.
- [31] D. M. Cragg and P. Lloyd. Kondo Hamiltonians with a non-zero ground-state spin. Journal of Physics C: Solid State Physics, 12(6):215 – 218, 1978.
- [32] Nicolas Roch, Serge Florens, Theo A. Costi, Wolfgang Wernsdorfer, and Franck Balestro. Observation of the Underscreened Kondo Effect in a Molecular Transistor. *Physical Review Letters*, 103(19):197202, November 2009.
- [33] C. H. L. Quay, John Cumings, S. J. Gamble, R. de Picciotto, H. Kataura, and D. Goldhaber-Gordon. Magnetic field dependence of the spin- 1/2 and spin-1 Kondo effects in a quantum dot. *Physical Review B*, 76(24):245311, December 2007.
- [34] A. Kogan, S. Amasha, D. Goldhaber-Gordon, G. Granger, M. A. Kastner, and Hadas Shtrikman. Measurements of Kondo and Spin Splitting in Single-Electron Transistors. *Physical Review Letters*, 93(16):166602, October 2004.
- [35] Lew D Landau and Ewgeni M Lifschitz. Lehrbuch der theoretischen Physik, 10 Bde., Bd.9, Statistische Physik: Theorie des kondensierten Zustandes. Deutsch (Harri), 4., berichtigte a. edition, January 1992.
- [36] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski. Methods of quantum field theory in statistical physics. Courier Dover Publications, 1975.
- [37] Henrik Bruus and Karsten Flensberg. Many-body quantum theory in condensed matter physics: an introduction. Oxford University Press, 2004.
- [38] Alexander L. Fetter and John Dirk Walecka. *Quantum theory of many-particle systems*. Courier Dover Publications, June 2003.
- [39] Gerald D. Mahan. Many-Particle Physics. Springer Verlag Gmbh, 0002 edition, June 1990.
- [40] Alexander Altland and Ben Simons. Condensed matter field theory. Cambridge University Press, 2006.
- [41] Gordon Baym. Lectures on Quantum Mechanics. Westview Press, January 1974.
- [42] Albert Messiah. Quantenmechanik, Bd.1: Band 1. Gruyter, 2. a. edition, January 1991.
- [43] Albert Messiah. Quantenmechanik, Bd.2: Band 2. Gruyter, 3., verb. a. edition, October 1990.
- [44] P. Coleman. Local moment physics in heavy electron systems. arXiv:condmat/0206003v3, May 2002.

- [45] László Borda, Lars Fritz, Natan Andrei, and Gergely Zaránd. Theory of inelastic scattering from quantum impurities. *Physical Review B*, 75(23):235112, June 2007.
- [46] J. R. Schrieffer and P. A. Wolff. Relation between the Anderson and Kondo Hamiltonians. *Phys. Rev.*, 149(2):491–492, Sep 1966.
- [47] Gergely Zaránd, László Borda, Jan von Delft, and Natan Andrei. Theory of Inelastic Scattering from Magnetic Impurities. *Physical Review Letters*, 93(10):107204, 2004.
- [48] Yigal Meir and Ned S. Wingreen. Landauer formula for the current through an interacting electron region. *Physical Review Letters*, 68(16):2512, April 1992.
- [49] Jørgen Rammer. Quantum Field Theory of Non-equilibrium States. Cambridge University Press, illustrated edition, July 2007.
- [50] Leo Kadanoff, Gordon Baym, and David Pines. Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems. Westview Press, new ed of 2 revised ed edition, December 1994.
- [51] Ralf Bulla, Theo A. Costi, and Thomas Pruschke. Numerical renormalization group method for quantum impurity systems. *Reviews of Modern Physics*, 80(2):395, April 2008.
- [52] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson. Renormalization-group approach to the Anderson model of dilute magnetic alloys. I. Static properties for the symmetric case. *Physical Review B*, 21(3):1003, February 1980.
- [53] Lev D. Landau and Eewgeni M. Lifschitz. Lehrbuch der theoretischen Physik: in 10 Bänden. Statistische Physik, Teil 1. Harri Deutsch Verlag, 1987.
- [54] Wanda C. Oliveira and Luiz N. Oliveira. Generalized numerical renormalizationgroup method to calculate the thermodynamical properties of impurities in metals. *Physical Review B*, 49(17):11986, May 1994.
- [55] Axel Freyn and Serge Florens. Optimal broadening of finite energy spectra in the numerical renormalization group: Application to dissipative dynamics in two-level systems. *Physical Review B*, 79(12):121102, March 2009.
- [56] R. Bulla, T. A. Costi, and D. Vollhardt. Finite-temperature numerical renormalization group study of the Mott transition. *Physical Review B*, 64(4):045103, June 2001.
- [57] Ralf Bulla, Hyun-Jung Lee, Ning-Hua Tong, and Matthias Vojta. Numerical renormalization group for quantum impurities in a bosonic bath. *Physical Review B*, 71(4):045122, January 2005.

- [58] Ingo Peschel. Density-matrix renormalization: a new numerical method in physics : lectures of a seminar and workshop held at the Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany, August 24th to September 18th, 1998. Springer, 1999.
- [59] David Joshua Goldhaber-Gordon. The Kondo effect in a single-electron transistor. Master's thesis, Harvard University, 1999.
- [60] Jiwoong Park, Abhay N. Pasupathy, Jonas I. Goldsmith, Connie Chang, Yuval Yaish, Jason R. Petta, Marie Rinkoski, James P. Sethna, Hector D. Abruna, Paul L. McEuen, and Daniel C. Ralph. Coulomb blockade and the Kondo effect in singleatom transistors. *Nature*, 417(6890):722–725, June 2002.
- [61] Nicolas Roch, Serge Florens, Vincent Bouchiat, Wolfgang Wernsdorfer, and Franck Balestro. Quantum phase transition in a single-molecule quantum dot. *Nature*, 453(7195):633–637, May 2008.
- [62] Richard D. Mattuck. A Guide to Feynman Diagrams in the Many-Body Problem. Dover Pubn Inc, 0002 edition, June 1992.
- [63] Frank Wilczek. Majorana returns. Nat Phys, 5(9):614–618, 2009.
- [64] W. Mao, P. Coleman, C. Hooley, and D. Langreth. Spin Dynamics from Majorana Fermions. *Physical Review Letters*, 91(20):207203, November 2003.
- [65] P. Coleman, L. B. Ioffe, and A. M. Tsvelik. Simple formulation of the two-channel Kondo model. *Physical Review B*, 52(9):6611, 1995.
- [66] Alexander Shnirman and Yuriy Makhlin. Spin-Spin Correlators in the Majorana Representation. *Physical Review Letters*, 91(20):207204, November 2003.
- [67] L. N. Bulaevskii, M. Hruscaronka, and G. Ortiz. Tunneling measurement of quantum spin oscillations. *Physical Review B*, 68(12):125415, 2003.
- [68] O. Parcollet and C. Hooley. Perturbative expansion of the magnetization in the out-of-equilibrium Kondo model. *Physical Review B*, 66(8):085315, 2002.
- [69] A. Rosch, J. Paaske, J. Kroha, and P. Wölfle. The Kondo Effect in Non-Equilibrium Quantum Dots: Perturbative Renormalization Group. *Journal of* the Physical Society of Japan, 74:118–126, 2005.
- [70] J. J. Parks, A. R. Champagne, T. A. Costi, W. W. Shum, A. N. Pasupathy, E. Neuscamman, S. Flores-Torres, P. S. Cornaglia, A. A. Aligia, C. A. Balseiro, G. K.-L. Chan, H. D. Abruña, and D. C. Ralph. Mechanical Control of Spin States in Spin-1 Molecules and the Underscreened Kondo Effect. *Science*, 328(5984):1370 –1373, June 2010.

- [71] Procolo Lucignano, Riccardo Mazzarello, Alexander Smogunov, Michele Fabrizio, and Erio Tosatti. Kondo conductance in an atomic nanocontact from first principles. *Nat Mater*, 8(7):563–567, July 2009.
- [72] P. Fritsch and S. Kehrein. Nonequilibrium Kondo model with voltage bias in a magnetic field. *Physical Review B*, 81(3):035113, January 2010.

## Erklärung

Hiermit versichere ich, die vorliegende Arbeit selbstständig und ohne fremde Hilfe angefertigt zu haben. Verwendete Literatur und andere Unterlagen sind jeweils im Text vermerkt und im Anhang aufgelistet.

Karlsruhe, den 28.02.2011