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To my parents and my sisters, whose love and support represent a stable fixed point to the flow of my life.

Tackord

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Till slut vill jag nämna **Annekathrin Müller-Lohmann**, som gjorde mig uppmärksam på möjligheten att skriva mitt examensarbete i Göteborg.

Preface

This thesis is structured as follows: After a short introduction I use Chapter 2 to very briefly review some physical and technical concepts that are essential for understanding the following discussions. In Chapter 3, I introduce the two-impurity Kondo model (TIKM) and present some previous results that build the starting point of my own research which I then present in Chapters 4 and 5. The thesis concludes with a summary of my results. Some lengthy calculations can be found in the Appendix.

I have attached the preprint of a paper which I submitted for publication together with my supervisor Henrik Johannesson at the very end of my thesis.

Contents

David F. Mross and Henrik Johannesson, “The Two-Impurity Anderson Model at Quantum Criticality”, arXiv:0712.2868 (submitted for publication).

Introduction

Recent advances in semiconductor physics have opened up new possibilities to experimentally realize physical systems and observe effects that were previously restricted to purely theoretical treatment [? ?]. A prominent example are quantum impurity models, which can be realized by trapping a small, well defined number of electrons in an almost point like (0-dimensional) region [? ?]. Such quantum dots can be thought of as artificial analogues to atoms, with the energy levels of the dots corresponding to various atomic orbitals. The advantage of such nanoscopic structures is, that many properties, like various coupling constants, energy levels etc. can be very well controlled in a laboratory which in many cases allows for the suppression of perturbations in order to single out the effect of interest. The Kondo effect is arguably the most well known and well understood effect that arises from the interplay of a localized, quantum degree of freedom with a continuous many-body state. The ordinary Kondo effect can be observed in naturally occurring metals, while its related cousins, the multi-channel and multi-impurity Kondo effect, have so far not been observed in any known material. Nonetheless, they are believed to be a crucial ingredient for understanding other problems, like Heavy Fermion physics [?]. Both the two-channel Kondo model (TCKM) and the two-impurity Kondo model (TIKM) are believed to undergo a quantum phase transition, where the electrons form a very exotic non-Fermi liquid state. Experimental setups to realize both of these models in terms of quantum dots have been proposed [? ?] and in case of the TCKM already implemented to some success [?].

The present thesis focuses on the TIKM and generalizations thereof. Apart from its aforementioned connection to fundamental properties of certain material, it is also relevant to Quantum Information Processing (QIP). Here, spin-1/2 quantum dots have been proposed as a realization of qubits [?]. The TIKM is one of the simplest interacting models of two such qubits. From the point of view of QIP, the entanglement between the two qubits is of central importance. In this thesis I investigate the entanglement in

CHAPTER 1: INTRODUCTION

the presence of spin-orbit interactions which must always be expected to occur in these kinds of two-dimensional nanostructures. For an eventual realization it is important to know whether these effects can be neglected, whether they are harmful or whether they might even be put to good use.

Of a more fundamental interest is the generalization of the TIKM to the two-impurity Anderson model by allowing charge to fluctuate between the conduction bands and the impurity. A theoretic description is important for verifying future experiments on an artificial realization of such a model, as well as for explaining behavior or certain metallic compounds where the interplay between two or more Anderson-type impurities may play an important role. In my thesis I present a conformal field theory description of the TIAM and use it to calculate various properties.

Physical concepts

To give a truly satisfactory introduction into any of the ideas and techniques which I employ in the following chapters is certainly beyond the scope of this thesis, and is also not its purpose. Nonetheless, I deem it useful to mention some of the aspects and results that are central to my own work, to either remind the reader or give him a “working understanding”.

2.1 Entanglement

Entanglement, referred to by Schrödinger as “*the* characteristic trait of quantum mechanics” [?], lies at the very heart of interpreting the often highly counterintuitive implications of quantum behavior. In their famous analysis - commonly referred to as the “EPR-Paradox” [?] - Einstein, Rosen and Podolsky showed that a quantum theory which allows for entanglement, is not compatible with the concept of local reality. In this thesis I will not concern myself with these sometimes rather philosophical debates but instead focus on describing the phenomenon and how it can be quantified.

Physically, entanglement can be defined by calling a set of states entangled, if there are correlations between them, that could not be, even in principle, obtained by any classical setup [?]. More formally, a state Ψ living in a Hilbert space $\mathcal{H}_\psi = \bigotimes_i \mathcal{H}_i$ is entangled if it cannot be written as a tensor product of states ψ_i from the individual Hilbert spaces \mathcal{H}_i . To make things more concrete, consider a system of two spins 1/2, which is the only system that will be of importance in this thesis. As long as this system is isolated, the most general pure state of this system can be written as:

$$|\Psi\rangle = \sum_{\sigma, \sigma' = \uparrow, \downarrow} m_{\sigma, \sigma'} |\sigma \otimes \sigma'\rangle, \quad (2.1.1)$$

where $m_{\sigma, \sigma'}$ are the components of a two-by-two matrix m . If $\det m = 0$ then the matrix m can be written as the outer product of two vectors, i.e. $m_{\sigma, \sigma'} = a_\sigma b_{\sigma'}$. In this case Ψ

can be written as

$$|\Psi\rangle = \left(\sum_{\sigma} a_{\sigma} |\sigma\rangle \right) \otimes \left(\sum_{\sigma'} b_{\sigma'} |\sigma'\rangle \right), \quad (2.1.2)$$

and is thus not entangled. This condition is in fact both necessary and sufficient [?]. $|\det m|$ quantifies entanglement in a very natural way, ranging from 0 for no entanglement to $1/2$ for maximum entanglement. $2 \times |\det m|$ is called the von Neumann concurrence. It is a special case of the concurrence of formation which I use as a measure of entanglement in this thesis.

If the two-spin system is entangled with another system, then by the very definition of entanglement given above, the decomposition $\Phi_{\text{total}} = \Psi_{2\text{Spin}} \otimes \Psi_{\text{other}}$ is not possible and therefore the state in the two-spin sub-system cannot be expressed in the form of eq. (??). In other words, the two-spin sub-system is in a mixed state, which is typically written in the form of a density matrix. The density matrix is defined as

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|, \quad (2.1.3)$$

where p_i are the probabilities for the system to be in the states $|\psi_i\rangle$. In contrast to a superposition of (pure) states, which is again a pure state, there is no well defined phase relation between the different $|\psi_i\rangle$ of a mixed state. In this case the state is described by the (reduced) density matrix. To emphasize the difference between the two, compare the density matrix for a single spin mixed state where both spin directions occur with equal probability

$$\rho_{\text{mix}} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (2.1.4)$$

with the density matrix for the pure state $|\Psi\rangle = \frac{1}{\sqrt{2}} |\uparrow\rangle + \frac{e^{i\phi}}{\sqrt{2}} |\downarrow\rangle$, expressed in the same basis:

$$\rho_{\text{pure}} = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix}. \quad (2.1.5)$$

The phase information is given by the off-diagonal entries in the density matrix, which are called coherences.

Expectation values of physical quantities are calculated by $\langle \Omega \rangle = \text{Tr}(\rho \Omega)$. If the operator Ω acts only on some subspace \mathcal{H}_1 of the total Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, then its expectation value can be expressed as $\langle \Omega \rangle = \text{Tr}(\rho^{(1)} \Omega)$, where $\rho^{(1)} = \text{Tr}_2 \rho$. The subscript-two means that the trace is only taken with respect to the states of the second Hilbert space. $\rho^{(1)}$ is called the reduced density matrix. It contains all the information about correlations within \mathcal{H}_1 . Note that even if ρ describes a pure state, $\rho^{(1)}$ in general does not.

Most measures for entanglement are expressed in terms of the (reduced) density matrix.

A number of such measures have been proposed and in general there is no agreement on a single measure of entanglement that should always be used. However, for a two-spin system the concurrence of formation, which I shall from now on refer to simply as concurrence, is commonly considered to be a good measure [? ?]. For a density matrix ρ given in the “magic basis”:

$$\begin{aligned} |e_1\rangle &= |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle \\ |e_2\rangle &= i|\uparrow\uparrow\rangle - i|\downarrow\downarrow\rangle \\ |e_3\rangle &= i|\uparrow\downarrow\rangle + i|\downarrow\uparrow\rangle \\ |e_4\rangle &= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle, \end{aligned} \tag{2.1.6}$$

the concurrence is given by [?]:

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{2.1.7}$$

where λ_i are the square roots of the eigenvalues of $\rho\rho^*$ in decreasing order. As indicated above, for a pure state of the form shown in eqn.(??) the concurrence is equivalent to the very natural measure $|\det m|$ (up to a factor 2).

Since the amount of entanglement in a certain subsystem is completely determined by the reduced density matrix, it is possible to calculate it in the presence of interactions with a larger system, even if all the details of the full system are not known. There are, in general, many possible ways to prepare a system, leading to the same density matrix. A particularly interesting situation occurs, when a finite number of discrete degrees of freedom interact with a larger, continuous “bath”. One of the simplest examples for such a system is given by magnetic impurities embedded within a sea of conduction electrons. If the magnetic impurities interact with the electrons only via a local spin-exchange interaction, this is known as the Kondo model.

2.2 Kondo effect

Already in the early 1930s it was observed, that in certain metallic compounds, the resistivity as a function of temperature has a minimum at low temperatures and increases as $T \rightarrow 0$. This was inexplicable for quite a long time, because all known mechanisms predicted a decreasing resistivity for low temperatures. The interactions between electrons contribute as $\rho(T)_{el.} \sim T^2$, the one between electrons and phonons as $\rho(T)_{ph.} \sim T^5$ and the scattering of the electrons on (non-magnetic) lattice defects gives a constant contribution $\rho(T) \rightarrow \rho_0$. In the case of a superconductor, the resistivity even drops all the way to zero at very low temperatures.

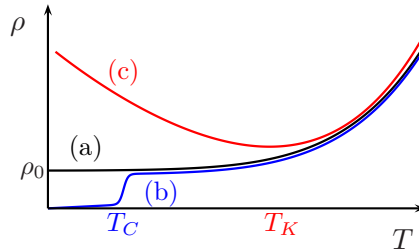


Figure 2.1: Qualitative behavior of the resistivity at low temperatures. Curve (a) describes an ordinary metal, curve (b) describes a material becoming superconductive below T_C and curve (c) shows the Kondo effect. Typical values for the Kondo temperature are in the order of $10K$.

The origin of this increase in the resistivity was uncovered in 1964 by Jun Kondo [?], using a very simple model Hamiltonian:

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger \sigma} \psi_{\mathbf{k}, \sigma} + \frac{J}{2} \mathbf{S} \cdot \sum_{\mathbf{k}, \mathbf{k}'} \psi_{\mathbf{k}}^{\dagger \sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{\mathbf{k}', \sigma'}, \quad (2.2.1)$$

where \mathbf{S} is the impurity spin, τ_i are the Pauli matrices, $J > 0$ is called the Kondo coupling and summation over spin-indices is implied. From this model he derived that in second order of perturbation theory there is a contribution $\rho^{(2)}(T) \sim \log \frac{1}{T}$, which diverges as $T \rightarrow 0$. This explains the minimum in the resistivity, but fails to capture the full low-temperature behavior, as the actual resistivity does not diverge but remains finite. The behavior at very low temperatures can not be explained by ordinary perturbation theory because all higher order terms also diverge. To access this region, new techniques were necessary and this led to the development of the very powerful concept of scaling and the renormalization group. By now the single-channel Kondo model, i.e. the Hamiltonian of eq. (??) which was introduced by Clarence Zener in Ref. [?], has been studied extensively and is very well understood. In a physical picture the conduction electrons screen the impurity spin by forming a many-body singlet with it. For infinite Kondo coupling, one electron is locked in this singlet with the impurity, screening it entirely. To the rest of the conduction electrons this acts like a localized, non-magnetic impurity. For finite coupling the screening is not achieved by a single electron but rather by all electrons close to the impurity. Thus, there is a screening cloud of finite size, outside of which the magnetic moment is completely screened. This so-called “dressed” impurity again acts as a pure non-magnetic scattering potential. This is the reason why the conduction electrons can, in this case, be described by a (local) Fermi liquid: The electrons keep their quantum numbers, they just undergo scattering phase shifts.

A particular feature of the Kondo interaction, i.e. the second term in (eq. ??), is that it is point like. Upon Fourier transformation to real space one obtains $H_{\text{Kondo}} \sim \mathbf{S} \cdot \psi^{\dagger}(0) \boldsymbol{\tau} \psi(0)$, which allows the model to be mapped exactly to an equivalent one-

dimensional model (see Appendix ?? for details). This simplifies most calculation by drastically reducing the available Hilbert space and even allows for entirely new approaches that are not possible in higher dimensions.

2.3 Peculiarities in 1D: Bosonization

One-dimensional systems are substantially different in many ways than their higher dimensional counterparts. In particular, the Fermi surface (for a typical quadratic dispersion) consists only of two discrete points (see Fig. ??). This suggests a decomposi-

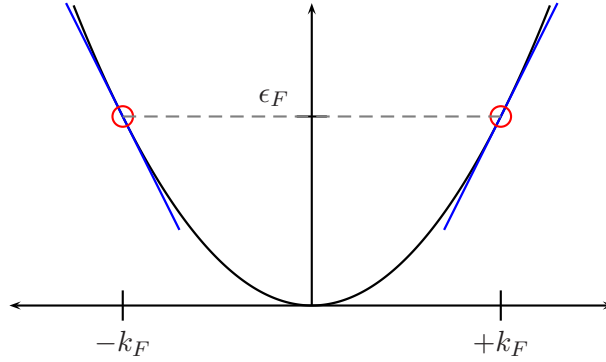


Figure 2.2: The Fermi “surface” of a one-dimensional system consists only of two, disconnected points. ϵ_F is the Fermi energy and k_F the corresponding momentum.

tion of the electron fields close to the Fermi energy into “left-movers”, corresponding to $k \approx -k_F$ and “right-movers”, corresponding to $k \approx +k_F$, both living on the infinite line $-\infty < x < \infty$:

$$\psi_{L,R}(x) = e^{\pm k_F x} \int_{\pm k_F - \Lambda}^{\pm k_F + \Lambda} \frac{dk}{2\pi} e^{ikx} \psi_k. \quad (2.3.1)$$

Here ψ_k is the annihilation operator for an electron with momentum k and Λ is an energy cut-off, such that the left- and right-movers are made up by electron-fields close to the Fermi points only, where the dispersion can be linearized to a good approximation $\epsilon_k \approx \frac{k_F}{m}(k - k_F)$. Writing down the time dependence of these electron fields explicitly, i.e.

$$\psi_{L,R}(x, t) \sim e^{\mp i(k - k_F)x} e^{-i \frac{k_F}{m}(k - k_F)t} \quad (2.3.2)$$

one notices that

$$\partial_- \psi_L(x, t) \equiv \left(\frac{k_F}{m} \frac{\partial}{\partial x} - \frac{\partial}{\partial t} \right) \psi_L(x, t) = 0 \quad (2.3.3)$$

and likewise $\partial_+ \psi_R(x, t) = 0$, as it should be for a purely right- or left-moving field. In the absence of interaction terms, left- and right-movers are decoupled on the infinite line. This changes in the presence of a boundary, e.g. if the system is defined on the

semi-infinite line $0 \leq x < \infty$ only. In order for charge to be conserved, a left-moving fermion that reaches the boundary must be reflected, i.e. turned into a right-moving fermion at the boundary. The simplest boundary condition that achieves this is the requirement $\psi_R(0) = \psi_L(0)$. This condition allows the right-moving electron to be considered as the analytic continuation of the left moving one to negative values of x , i.e. $\psi_L(x, t) = \psi_R(-x, t)$ for $x < 0$ (note that the replacement $x \rightarrow -x$ while t is kept the same, turns a right-mover into a left-mover and vice-versa). Thus, a theory of both left- and right-movers on the half-line can be written as a theory of only left-movers (or right-movers) on the full line. The kinetic energy of the electrons can then be written as:

$$H_{\text{kin.}} = \int dk \epsilon(k) \psi_k^\dagger \psi_k \approx \frac{k_F}{2\pi m} \int_{-\infty}^{\infty} dx \psi_L^\dagger(x) i \frac{d}{dx} \psi_L(x). \quad (2.3.4)$$

The expression on the right-hand side defines a (1+1) dimensional *relativistic* theory for *chiral* fermions. This theory is trivially scale invariant since it is both free and massless (Gaussian fixed point). The importance of scale invariance will be discussed in the following chapter.

Bosonization, i.e. expressing the fermionic theory equivalently in terms of bosonic fields, is most conveniently done in terms of currents. Define the charge current as:

$$J_L^c(x) =: \psi_L^\dagger(x) \psi_L(x) :. \quad (2.3.5)$$

The double dots stand for a regularization that needs to be employed because the expression on the right hand side is singular otherwise. This can for instance be achieved via ‘‘point-splitting’’

$$J_L^c(x) = \lim_{\epsilon \rightarrow 0} \left\{ \psi_L(x) \psi_L^\dagger(x + \epsilon) - \langle 0 | \psi_L(x) \psi_L^\dagger(x + \epsilon) | 0 \rangle \right\}, \quad (2.3.6)$$

but the exact nature of this is of no significance for what follows. If one also considers spin, one can define a spin current

$$\mathbf{J}_L^s(x) =: \psi_L^{\dagger\sigma}(x) \frac{\boldsymbol{\tau}_\sigma^{\sigma'}}{2} \psi_{L\sigma'}(x) :, \quad (2.3.7)$$

where τ^i are the Pauli matrices and summation over spin-indices is implied. Using these definitions it is straightforward to see that the free relativistic Hamiltonian (eq. ??) can be expressed as:

$$H_{\text{kin.}} = \frac{1}{4\pi} \int dx (J_L^c(x))^2 \quad (2.3.8)$$

or

$$H_{\text{kin.}} = \frac{1}{8\pi} \int dx (J_L^c(x))^2 + \frac{1}{6\pi} \int dx (\mathbf{J}_L^s(x))^2 \quad (2.3.9)$$

in the spinful case. The units have been chosen such that $k_F/m = 1$. The spinless Hamiltonian of eq. (??) is identical to the Hamiltonian of a free left moving boson ϕ_L

upon the identification $\sqrt{\pi}\partial_+\phi_L(x) = J_L^c(x)$:

$$H_{\text{Boson}} = \frac{1}{4} \int dx \left(\frac{\partial}{\partial x} \phi_L \right)^2 + \left(\frac{\partial}{\partial x} \theta_L \right)^2 = \frac{1}{4} \int dx (\partial_+ \phi_L)^2 = \frac{1}{4\pi} \int dx (J_L^c(x))^2. \quad (2.3.10)$$

Here θ_L is the dual boson with $\partial_x \theta_L(x, t) = \partial_t \phi_L(x, t)$ and the second equality holds because $\phi_L(x, t) = \phi_L(x + t)$ is a left-mover. To show that this Hamiltonian is fully equivalent to the one of eq. (??) it is necessary to verify that the $J_L^c(x)$, as defined in terms of the bosons and in terms of the fermions, obey the same commutation relations, which they in fact do [?]. For the spinless case the commutator of the charge current is

$$[J_L^c(x), J_L^c(y)] = 2\pi i \frac{d}{dx} \delta(x - y), \quad (2.3.11)$$

If spin is included then there is an additional factor 2 on the right hand side and the components of the spin current behave as:

$$[(J_L^s(x))^i, (J_L^s(y))^j] = 2\pi i \epsilon^{ijk} (J_L^s(x))^k \delta(x - y) + \pi i \frac{d}{dx} \delta(x - y) \delta^{ij}. \quad (2.3.12)$$

These are known as *Kac-Moody-Algebras* of $U(1)$ and $SU(2)$ respectively [?]. The coefficient multiplying the Schwinger term $\sim \frac{d}{dx} \delta(x - y)$ is called the level. Up to that term, the currents obey the usual $U(1)$ and $SU(2)$ commutation rules.

To conclude this section, consider as an instructive example the Kondo Hamiltonian of eq. (??). In bosonized form, the free electron part is given by eq. (??), while the interaction is given simply by $\mathbf{J}\mathbf{S} \cdot \mathbf{J}_L^s(0)$, using the definition of the spin-current. For $J = -\frac{1}{3\pi}$ the spin current can be redefined as $\mathbf{J}_L^s(x) \rightarrow \mathbf{J}_L^s(x) + \delta(x)\mathbf{S}$ to cancel the interaction term. Since $[S^i, S^j] = \epsilon^{ijk}$ and $[S^i, J^j] = 0$, the redefined current fulfills the same commutation relations as the original one, thus the Hamiltonian (up to an additive constant) is again the free one (eq. ??), in particular it is explicitly scale-invariant. In fact, it corresponds to the strong coupling fixed point of the Kondo model ¹.

2.4 Renormalization group (RG)

In both previous chapters we have already stumbled upon the concepts of renormalization and scale invariance. A brief digression into the renormalization group, where these are formalized is therefore appropriate, in particular because the subsequent chapter on CFT and the entire thesis relies heavily on these concepts.

Loosely speaking, the idea behind the RG is to integrate out all high energy (=short range) degrees of freedom of a microscopic theory to obtain an effective theory that describes the low energy physics. To make this explicit, consider a fairly general microscopic

¹As pointed out in Ref. [?], J is not the actual physical coupling. The infinite physical coupling constant at the unstable fixed point can become finite under a redefinition that is valid for this approach.

Hamiltonian:

$$H_0(\Lambda) = \sum_{i \in \mathcal{I}_0} \int^{\Lambda} d^d k_1 \dots \int^{\Lambda} d^d k_N \lambda_i^0 \mathcal{O}_i(\{\mathbf{k}_1, \dots, \mathbf{k}_N\}). \quad (2.4.1)$$

Here Λ is a high energy cut-off, \mathcal{O}_i are all (second quantized) operators that appear in the Hamiltonian with the coupling constants λ_i^0 , and \mathcal{I}_0 is an appropriate set of indices. Now the RG transformation can be performed in two steps:

For the first step all integrals are separated according to $\int^{\Lambda} = \int^{\Lambda/b} + \int_{\Lambda/b}^{\Lambda}$. The original Hamiltonian can be rewritten as:

$$H_0(\Lambda) = H_0(\Lambda/b) + H_{\text{high-energy}}(\Lambda, b), \quad (2.4.2)$$

where $H_{\text{high-energy}}$ contains all terms, where at least one integration goes from Λ/b to Λ . If we now perform all the integrations over $[\Lambda/b, \Lambda]$, we are left with a Hamiltonian that we can again write in the general form as

$$H_1(\Lambda/b) = \sum_{i \in \mathcal{I}_1} \int^{\Lambda/b} d^d k_1 \dots \int^{\Lambda/b} d^d k_N \lambda_i^1 \mathcal{O}_i(\{\mathbf{k}_1, \dots, \mathbf{k}_N\}). \quad (2.4.3)$$

Note that not only the values of the coupling constants may be different now, but also new operators that were not present in H_0 may appear as suggested by labeling the set of indices by \mathcal{I}_1 . In general, *all operators that are allowed by the symmetries of the original Hamiltonian must be expected to occur at some point.*

In the second step the momenta are rescaled as $\mathbf{k} \rightarrow b\mathbf{k}$, so that the new Hamiltonian can be compared to the original one. This procedure is iterated to go to ever lower energies:

$$H_0(\Lambda) \rightarrow H_1(\Lambda) \rightarrow H_2(\Lambda) \rightarrow H_3(\Lambda) \dots \quad (2.4.4)$$

The RG transformation can be understood as a function $\mathcal{F}(H_i) = H_{i+1}$, living on the space of Hamiltonian, which is spanned by all allowed operators. It is in general non-linear and all but impossible to treat analytically on its entire domain. A special case arises when $\mathcal{F}(H) = H$. In this case, which is called a fixed point, all successive applications of the RG transformation will not change the Hamiltonian. In the study of phase transitions, one is usually interested in the flow of the RG close to such a fixed point. The nature of the flow determines the critical exponents which describe the temperature dependence of physical observables, such as the specific heat, susceptibility etc. Around the fixed point, \mathcal{F} can be linearized by a multi-variable Taylor expansion in the couplings of all operators that appear in the critical Hamiltonian. It can then be diagonalized, that is to say, a basis of operators can be found, each of which generates only itself under renormalization in the linear approximation. If a system is very close to, but not precisely on the fixed point, the only things that change under renormalization are the

coupling constants. This leads to the very important concept of *relevance*: An operator, whose coupling constant decreases under renormalization is called *irrelevant*. A system that deviates from the fixed point in the direction of this operator will flow back to the fixed point. An operator, whose coupling increases is consequently called *relevant*; it will drive the system away from the fixed point. If a coupling constant does not change (in this approximation) it is called *marginal*. In case such an operator occurs, higher order terms may need to be taken into account. As an example, consider an operator \mathcal{O} with $\mathcal{O}(b\mathbf{k}) = b^\Delta \mathcal{O}(\mathbf{k})$. Its contribution to the Hamiltonian renormalizes as:

$$H_{\mathcal{O}} = \int^\Lambda d^d k \mathcal{O}(\mathbf{k}) \rightarrow b^d \int^{\Lambda/b} d^d(k/b) b^{-\Delta} \mathcal{O}(b\mathbf{k}) = b^{d-\Delta} H_{\mathcal{O}}. \quad (2.4.5)$$

Here the high momentum contributions have been neglected, which is in the spirit of the linear approximation. Clearly, \mathcal{O} is relevant for $\Delta < d$ and irrelevant for $\Delta > d$. It is a general result that it depends upon the (effective) dimensionality of the system whether an operator with a given scaling dimension is relevant or not.

2.5 Conformal field theory (CFT)

Conformal field theory is a very powerful and well developed approach that allows to describe various different systems around RG-fixed points. At a critical point, by its very definition, a system is invariant under scale transformations, in addition to its original symmetries, e.g. translation and rotation invariance. In a large class of systems those three symmetries are sufficient for the system to have full conformal invariance - that is invariance under all transformations that conserve angles. More formally, the conformal group consists of all transformations that leave the metric invariant up to a scale factor, i.e.

$$g'_{\mu\nu}(\mathbf{x}') = \Lambda(\mathbf{x}) g_{\mu\nu}(\mathbf{x}). \quad (2.5.1)$$

In addition to the aforementioned rotations, translations and scale transformations (dilations) this group also includes the *special conformal transformations* (SCT) which can be expressed as:

$$\frac{x'^\mu}{x'^2} = \frac{x^\mu}{x^2} - b^\mu. \quad (2.5.2)$$

By Noether's theorem, with every symmetry of a system comes a conserved quantity which imposes restriction upon the dynamics and can in many cases be used to simplify a problem considerably. In the particular case of a two-dimensional system, the conformal group has an infinite number of generators which in many cases allows for complete solutions to a conformal field theory, in the sense that all correlation functions can, in principle, be computed exactly, without having to resort to perturbation theory.

2.5.1 Boundary conformal field theory (BCFT)

In conformal field theories it is most convenient to express the two-dimensional space-time coordinates (x, t) in terms of the complex variable $z = t + ix$. In particular, consider a system defined on the upper complex half-plane (UHP) which is the natural geometry for treating quantum impurity problems, as we saw in Section ?? where the left- and right-moving fermion fields were defined on the same geometry. In terms of the complex variable z these fields appear in the conformal field theory as holomorphic and antiholomorphic fields, depending only on z and z^* , respectively. While they are decoupled on the full complex plane, they are related on the UHP by the boundary. This was already the case for the free fermions in Section ?? which were related by the trivial boundary condition $\psi_L(0, t) = \psi_R(0, t)$. It is obvious, that this system cannot be invariant under the full conformal group, in particular it lacks translational variance in the x direction. The conformal group in this geometry consists of all analytic functions that map the UHP upon itself. They can be written in a Taylor expansion as

$$w(z) = \sum_{n=0}^{\infty} a_n z^n \quad a_n \in \mathbb{R}. \quad (2.5.3)$$

In particular, although the presence of the boundary has reduced the number of conformal generators by half compared to the unbounded case, there is still an infinite number of them. The generators of these transformations fulfill the *Virasoro Algebra*

$$[L_n, L_m] = (n - m)L_{n+m} + \frac{c}{12}n(n^2 - 1)\delta_{n+m,0}, \quad (2.5.4)$$

where the *conformal anomaly* c depends on the particular system that is being considered. The Hilbert space of the conformal field theory can be organized in representations of this algebra. A highest weight state of this algebra, i.e. one state for which

$$\begin{aligned} L_n|h\rangle &= 0, \quad n > 0 \\ L_0|h\rangle &= h|h\rangle \end{aligned} \quad (2.5.5)$$

is called primary state of conformal dimension h . From the Virasoro Algebra one sees that $[L_0, L_{-m}] = mL_{-m}$, i.e. the ladder operator L_{-m} creates a state with conformal dimension $m + h$. It is called a descendant at level m . A primary field together with all of its descendants is called a *conformal tower*. States within such a conformal tower transform, by construction, only among themselves under conformal transformations. The field operator corresponding to a primary state, i.e.

$$\phi_h(0)|0\rangle = |h\rangle \quad (2.5.6)$$

is called a primary field of dimension h and analogously, the field $L_{-m}\phi_h$ is called a descendant field and has dimension $h + m$. A primary field transforms under conformal

transformations as

$$\phi_h(w) = \left(\frac{dw}{dz} \right)^{-h} \phi_h(z). \quad (2.5.7)$$

This behavior restricts the form of correlation functions, e.g. on the boundary $z_1 = t_1$, $z_2 = t_2$ the conformal transformation $t \rightarrow \frac{t-t_1}{t_2-t_1}$ fixes the form of the two-point function:

$$\begin{aligned} \langle \phi_{(h)}(t_1) \psi_{(h')}(t_2) \rangle &= \left(\frac{d}{dt} \left(\frac{t-t_1}{t_2-t_1} \right) \right)_{t=t_1}^h \left(\frac{d}{dt} \left(\frac{t-t_1}{t_2-t_1} \right) \right)_{t=t_2}^{h'} \langle \phi_{(h)}(0) \psi_{(h)}(1) \rangle \\ &= \frac{\langle \phi_{(h)}(1) \psi_{(h')}(0) \rangle}{(t_1-t_2)^h (t_1-t_2)^{h'}} \equiv \frac{C_{\phi,\psi} \delta_{h,h'}}{(t_1-t_2)^{2h}}. \end{aligned} \quad (2.5.8)$$

The Kronecker delta appears in the last line due to translation invariance (in the time-direction) and $C_{\phi,\psi}$ is some constant.

Since any analytic function can be written as a Laurent series around an arbitrary point, e.g.

$$\psi(z) = \sum_n \psi_n(z-w)^n, \quad (2.5.9)$$

it is likewise possible to express any product of fields as a linear combination of fields acting on one point

$$\phi_1(z_1) \phi_2(z_2) = \sum_i \sum_{\{k\}} C_{1,2}^{i\{k\}} (z_2 - z_1)^{h_p - h_1 - h_2 + n_k} \phi_p^{\{k\}}(z_2). \quad (2.5.10)$$

Here $n_k = \sum_{k \in \{k\}} k$ is the level of $\phi_p^{\{k\}}$, in particular $n_k = 0$ when the field is primary. The part on the right hand side that diverges for $z_1 \rightarrow z_2$ is called the operator product expansion (OPE). Once the OPE is known, any product of fields within a correlator can be replaced by their OPE in order to reduce the number of fields of any n -point function. In most situations there are strong restrictions what fields may appear on the right hand side of an OPE, which are known as ‘‘Fusion rules’’.

2.5.2 WZW-Models: Gluing conditions

In many physical systems of interest, there is another symmetry group, in addition to the conformal one. Two such examples have already been encountered in the previous section - the spinless fermion has $U(1)$ - and the spinful fermion has $U(1) \otimes SU(2)_1$ -symmetry. Such models have been studied extensively [?] and are known as WZW-models. For $SU(2)_n$ with $n \in \mathbb{N}$, the primary fields are n non-abelian bosons with spins $1/2, \dots, n/2$. The Fourier modes of the currents

$$\mathbf{J}_n \equiv \int_{-l}^l dx e^{i \frac{nx}{l} \pi} \mathbf{J}(x), \quad (2.5.11)$$

which for the $SU(2)_k$ spin current obey the commutation relations (see eq.??)

$$[J_n^i, J_m^j] = i \epsilon^{ijk} J_{n+m}^k + \frac{1}{2} k n, \delta_{m+n,0} \quad (2.5.12)$$

act as raising and lowering operators, like the Virasoro modes. Analogously, states that are annihilated by all $J_n, n > 0$ are called WZW-primary states and states obtained by acting with J_{-n} on a primary state are called WZW-descendants. The Virasoro modes are related to the WZW-modes via

$$L_n = \frac{1}{2+k} \sum_{m=-\infty}^{\infty} : J_{-n} J_{n+m} :, \quad (2.5.13)$$

where normal ordering means that the highest mode appears on the right. In particular this implies that any WZW-primary state is also Virasoro primary, while the inverse implication does not hold. By comparing the commutator one finds that just like L_{-n} , J_{-n} also raises the level of a state by n .

If the theory is composed of more than one sector, e.g. $U(1)$ and $SU(2)$ for electrons, then a boundary condition decides how the conformal towers of the two theories may be combined. For free electrons, the only fundamental excitations carry charge $Q = 1$ and spin $j = 1/2$. There are thus two composite primary fields in $U(1) \otimes SU(2)$ with free fermion boundary conditions: The trivial identity field which is given by combining the identity field of the charge sector with the identity field of the spin sector

$$(Q = 0, j = 0) \quad (2.5.14)$$

and the fermion

$$(Q = 1, j = 1/2). \quad (2.5.15)$$

The rules how the conformal towers are combined are called gluing conditions.

2.5.3 New boundary conditions: Fusion

So far no other boundary conditions than those for free fermions have been considered. In general it is a rather complicated task to specify a nontrivial boundary condition, that is conformally invariant. An elegant way to construct new, conformally invariant, boundary conditions from already known ones is ‘‘Fusion’’ [?]. Here, each conformal tower is mapped into a set of other conformal towers, which is specified by the OPE of the conformal tower with the tower that is used for fusion.

To make this explicit, consider the example of free fermions described above. There are four conformal towers, namely $(Q = 0), (Q = 1), (j = 0), (j = 1/2)$. Fusion with the $(j = 1/2)$ conformal tower does not affect the charge sector but exchanges the two spin-towers. This can be understood as adding angular momenta $(0) \otimes (1/2) = (1/2)$ and $(1/2) \otimes (1/2) = (0) \oplus (1)$. Since there is no $(j = 1)$ conformal tower in the theory, only the $(j = 0)$ tower appears in the fusion of $(1/2)$ with $(1/2)$. By this fusion the

gluing conditions of free fermions given above are changed into

$$\begin{aligned}(Q = 1, j = 0) \\ (Q = 0, j = 1/2).\end{aligned}\tag{2.5.16}$$

This fusion is the formal way to express the redefinition of the spin-current $\mathbf{J}(x) \rightarrow \mathbf{J}(x) + \delta(x)\mathbf{S}$ of Section ???. Thus these gluing conditions describe the strong coupling fixed point of the Kondo model.

The two-impurity Kondo model (TIKM)

The atoms of many rare earth and transition metals have an empty low-lying d - or f -level. When such atoms occur in a conductor, the conduction electrons may hop from the conduction band into the low-lying level and back. This can be described by the Anderson model which is defined by the Hamiltonian:

$$H_{\text{Anderson}} = \int d^3k \epsilon_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger\sigma} \psi_{\mathbf{k},\sigma} + V \int d^3k \left(\psi_{\mathbf{k}}^{\dagger\sigma} d_{\sigma} + d^{\dagger\sigma} \psi_{\mathbf{k},\sigma} \right) + \epsilon_d n + U n_{\uparrow} n_{\downarrow}. \quad (3.0.1)$$

Here $\psi_{\mathbf{k}}^{\dagger\sigma}$ is the creation operator for a conduction electron with momentum \mathbf{k} and spin σ , $d^{\dagger\sigma}$ is the creation operator for an electron with spin σ on the low-lying level, $n \equiv d^{\dagger\sigma} d_{\sigma}$ and summation over spin-indices is implied. V is the amplitude for the hopping process, ϵ_d is the chemical potential of the low-lying level (impurity), measured with respect to the Fermi energy of the conduction electron and U is the Coulomb repulsion between two electrons at the same impurity site (Fig. ??). Summation over spin-indices is implied, except for the last term. In general, the ground state of the system will contain states

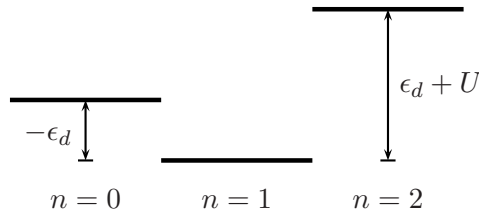


Figure 3.1: Level scheme for the doubly-, singly- and unoccupied subspaces of an Anderson impurity.

where there are zero, one and two electrons in the impurity. If $-\epsilon_d \gg V$ and $U \rightarrow \infty$ there is always one electron in the low-lying level and only virtual transitions between

CHAPTER 3: THE TWO-IMPURITY KONDO MODEL (TIKM)

that level and the conduction electrons are allowed, due to energy conservation. Here we consider the case of two such impurities, i.e. the two-impurity Anderson model (TIAM). In this limit a Schrieffer-Wolff type transformation yields the two-impurity Kondo model (TIKM) [?]:

$$H = H_{\text{kin}} + H_{\text{Kondo}} + H_{\text{RKKY}}, \quad (3.0.2)$$

where in the symmetric case, i.e. if V , ϵ_d and U are equal for both impurities:

$$\begin{aligned} H_{\text{kin}} &= \int d^3k \epsilon_{\mathbf{k}} \psi_{\mathbf{k}}^{\sigma\dagger} \psi_{\sigma, \mathbf{k}}, \\ H_{\text{Kondo}} &= J \int d^3k_1 \int d^3k_2 \psi_{\mathbf{k}_1}^{\sigma\dagger} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{\sigma', \mathbf{k}_2} \cdot \left(\mathbf{S}_1 e^{i\mathbf{R}\cdot(\mathbf{k}_1 - \mathbf{k}_2)} + \mathbf{S}_2 e^{-i\mathbf{R}\cdot(\mathbf{k}_1 - \mathbf{k}_2)} \right), \\ H_{\text{RKKY}} &= K \mathbf{S}_1 \cdot \mathbf{S}_2. \end{aligned} \quad (3.0.3)$$

Here \mathbf{S}_i are the spins of the localized electron on impurity i and \mathbf{R} is the difference vector between the two impurity sites. In addition to the Kondo effect which tends to screen the impurity spins, there is a direct interaction between the impurity spins, the RKKY interaction, which is generated in second order of the Kondo interaction [? ? ?]. If $K > 0$, it tends to lock the impurity spins in a singlet and it is in competition with the Kondo effect which tries to screen the impurities. In fact, in the limiting case of infinitely large RKKY interaction, the impurities are either locked in the $s = 0$ singlet (antiferromagnetic) or the $s = 1$ triplet (ferromagnetic), depending on the sign of K . In the former case there is no Kondo effect, because the Kondo interaction couples to the spin only and the singlet has spin 0. In the ferromagnetic limit the model describes a single spin-1 impurity coupled to two channels of electrons. The resulting model is known as the exactly screened two-channel Kondo model, where in the low energy regime the impurity is screened by the conduction electrons and the system exhibits Fermi liquid behavior [?]. It is in the intermediate regime that things become the most interesting: By numerical renormalization group (nRG) calculations, an unstable fixed point was found for a particular value of the initial coupling constants [?] and it is around this fixed point that I will focus in this thesis.

In order to treat the TIKM as a conformal field theory it is essential to map it onto a (1+1)-dimensional model. It is a rather important point that we do not start with a one-dimensional model. In one dimension we would have to take strong interactions between the electrons into account, while in two or three dimensions it is usually safe to work with free electrons, in the Fermi liquid picture. Here we can exploit the fact that only a restricted part of the Hilbert space takes part in the Kondo interaction and work in this restricted Hilbert space. The technical details for this mapping can be found in Appendix ???. The result is a one-dimensional theory with two linearly independent electron fields that can be expressed in a basis of well defined parity (Fig. ??). After

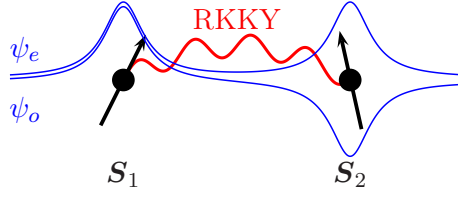


Figure 3.2: Two-impurity Kondo model. The two channels of electrons are even and odd under parity.

some trivial redefinitions the Hamiltonian thus obtained can be written as:

$$H = H_{\text{kin}} + H_{\text{Kondo}} + H_{\text{RKKY}}, \quad (3.0.4)$$

where:

$$H_{\text{kin}} = \int dE E \left(\psi_{1,E}^{\dagger\sigma} \psi_{1,E,\sigma} + \psi_{2,E}^{\dagger\sigma} \psi_{2,E,\sigma} \right),$$

$$H_{\text{Kondo}} = \int dE \int dE', \sigma' \left\{ J_+ \left[\psi_{1,E}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{1,E',\sigma'} + \psi_{2,E}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{2,E',\sigma'} \right] \cdot [\mathbf{S}_1 + \mathbf{S}_2] \right. \quad (3.0.5)$$

$$+ J_m \left[\psi_{E,1}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{1,E',\sigma'} - \psi_{2,E}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{2,E',\sigma'} \right] \cdot [\mathbf{S}_1 - \mathbf{S}_2] \quad (3.0.6)$$

$$\left. + J_- \left[\psi_{E,1}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{2,E',\sigma'} + \psi_{2,E}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{1,E',\sigma'} \right] \cdot [\mathbf{S}_1 + \mathbf{S}_2] \right\} \quad (3.0.7)$$

$$H_{\text{RKKY}} = K \mathbf{S}_1 \cdot \mathbf{S}_2.$$

Here $\psi_{1,E,\sigma}, \psi_{2,E,\sigma}$ are linear combinations of the one-dimensional fields with energy E and spin σ , the couplings J_+, J_-, J_m are related to the Kondo coupling J and the electron dispersion $\epsilon_{\mathbf{k}}$, and summation over spin-indices is implied.

3.1 Symmetry analysis

The BFCT solution relies fundamentally on exploiting the symmetries of the Hamiltonian.

Charge and spin: By inspection it is obvious that the total charge

$$Q = \int dE \left(\psi_{1,E}^{\dagger\sigma} \psi_{1,E,\sigma} + \psi_{2,E}^{\dagger\sigma} \psi_{2,E,\sigma} \right) \quad (3.1.1)$$

and total spin

$$S^z \text{ and } \mathbf{S}^2, \quad (3.1.2)$$

where

$$\mathbf{S} = \int dE \left(\psi_{1,E}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{1,E,\sigma'} + \psi_{2,E}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{2,E,\sigma'} \right) + \mathbf{S}_1 + \mathbf{S}_2 \quad (3.1.3)$$

are conserved.

Parity symmetry: For a spherically symmetric dispersion, the original three-dimensional Hamiltonian of eq. (??) is invariant under the transformation

$$\psi_{\mathbf{k}} \leftrightarrow \psi_{-\mathbf{k}}, \quad \mathbf{S}_1 \leftrightarrow \mathbf{S}_2. \quad (3.1.4)$$

In the one-dimensional form this translates to invariance under:

$$\psi_1 \leftrightarrow \psi_2, \quad \mathbf{S}_1 \leftrightarrow \mathbf{S}_2. \quad (3.1.5)$$

Particle-hole symmetry: The presence of particle-hole symmetry depends in a rather complicated way on the details of the microscopic Hamiltonian. In the simplest case, where all couplings in the Hamiltonian of eq. (??) are constants (up to irrelevant terms), it is easy to see that it is invariant under the transformations

$$\psi_{i,E,\sigma} \leftrightarrow \epsilon_{\sigma,\sigma'} \psi_{i,-E}^{\dagger,\sigma'}. \quad (3.1.6)$$

As it will turn out, particle-hole symmetry is crucial to the occurrence of the unstable fixed point.

Isospin: By explicit calculation it can be verified that the operator

$$I^- \equiv \int dE (\psi_{1,E,\uparrow} \psi_{1,-E,\downarrow} + \psi_{2,E,\uparrow} \psi_{2,-E,\downarrow}) \quad (3.1.7)$$

commutes with the Hamiltonian if particle-hole symmetry is present. This operator, its hermitian conjugate $I^+ \equiv (I^-)^\dagger$ and the total charge $I^z = \frac{1}{2}Q$ fulfill the $SU(2)$ commutation relations, thus the $U(1)$ charge symmetry is, in the presence of particle-hole symmetry, extended to an $SU(2)_2$ isospin symmetry.

Separate charge conservation: In the special case of $J_- = 0$ the charges of the two channels are separately conserved. This in turn leads to two separate $SU(2)_1$ -Isospin symmetries.

3.2 Bosonization of the TIKM

In the presence of particle-hole symmetry the TIKM can be written in terms of two $SU(2)_1$ isospin bosonic theories (corresponding to charge) and two $SU(2)_1$ spin bosonic theories. Each $SU(2)_1$ theory contains two primary fields, the spin-0 identity and a spin-1/2 WZW-field. The gluing conditions are the ones for free fermions, separately for

the two channels of electrons, i.e. $(i_{1,2} = 0, j_{1,2} = 0)$ and $(i_{1,2} = 1/2, j_{1,2} = 1/2)$. The energies of primary fields can be read off from the bosonized Hamiltonian

$$H = \frac{\pi}{3l} \sum_{a=1,2} \sum_{n=-\infty}^{\infty} (: (\mathbf{J}_a)_{-n} \cdot (\mathbf{J}_a)_n : + : (\mathbf{I}_a)_{-n} \cdot (\mathbf{I}_a)_n :), \quad (3.2.1)$$

where l is the size of the system, as

$$E = \frac{\pi}{3l} \sum_i (j_a(j_a + 1) + i_a(i_a + 1)). \quad (3.2.2)$$

Since the Kondo interaction breaks down the spin $SU(2)_1 \otimes SU(2)_1$ symmetry to the diagonal $SU(2)_2$, it is convenient to express the spin fields in such a way that keeps the remaining $SU(2)_2$ explicit. An elegant way to do this is given by the GKO-Coset construction [?] which in this case allows $SU(2)_1 \otimes SU(2)_1$ to be expressed in terms of $SU(2)_2$ and an Ising model¹, which contains three primary fields ($\mathbb{I}, \sigma, \epsilon$) with dimensions $(0, \frac{1}{16}, \frac{1}{2})$. Their OPEs are $\sigma \times \epsilon = \sigma \times \mathbb{I} = \sigma$ and $\sigma \times \sigma = \mathbb{I} + \epsilon$. In terms of the $SU(2)_2$ and Ising fields the gluing conditions are listed in Tab. ???. The energy spectrum is given by

$$E = \frac{\pi}{l} \left(\frac{i_1(i_1 + 1)}{3} + \frac{j(j + 1)}{4} + \Phi \right), \quad (3.2.3)$$

where $\Phi = 0, \frac{1}{16}, \frac{1}{2}$ for the Ising fields $\mathbb{I}, \sigma, \epsilon$, respectively.

Table 3.1: Gluing conditions for free fermions

i_1	i_2	j_1	j_2	j	Ising	El/π
0	0	0	0	0	\mathbb{I}	0
1/2	0	1/2	0	1/2	σ	1/2
0	1/2	0	1/2	1/2	σ	1/2
0	0	0	0	1	ϵ	1
1/2	1/2	1/2	1/2	1	\mathbb{I}	1
1/2	1/2	1/2	1/2	0	ϵ	1

The bosonized form of the Kondo interaction in eq. (??) can be obtained by matching symmetries and dimensions. The fermionic of the Kondo interaction parts all have both dimension and spin one. For the first term (??) it is

$$\begin{aligned} \int dE dE' \left(\psi_{1,E}^{\dagger\sigma} \tau_{\sigma}^{\sigma'} \psi_{1,E',\sigma'} + \psi_{2,E}^{\dagger\sigma} \tau_{\sigma}^{\sigma'} \psi_{2,E',\sigma'} \right) &= \int dx \delta(x) \left(\psi_1^{\dagger\sigma}(x) \tau_{\sigma}^{\sigma'} \psi_{1,\sigma'}(x) + \psi_2^{\dagger\sigma}(x) \tau_{\sigma}^{\sigma'} \psi_{2,\sigma'}(x) \right) \\ &= \left(\psi_1^{\dagger\sigma}(0) \tau_{\sigma}^{\sigma'} \psi_{1,\sigma'}(0) + \psi_2^{\dagger\sigma}(0) \tau_{\sigma}^{\sigma'} \psi_{2,\sigma'}(0) \right), \end{aligned} \quad (3.2.4)$$

¹What is meant here is the conformal field theory that has been shown to describe the continuum limit of the Ising model at the critical point.

where $\psi_{i,\sigma}(x+t) = \int dE e^{-iE(x+t)} \psi_{i,E,\sigma}$ are the (left moving) electron fields in position space. This is by definition the total spin current $\mathbf{J}(x) = \mathbf{J}_1(x) + \mathbf{J}_2(x)$ at $x = 0$ (see eq. ??). This operator does not appear explicitly in Tab. ?? since it is not primary but rather a Kac-Moody descendant of the identity. The operator $\psi_1^{\dagger\sigma}(0) \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{1,\sigma'}(0) - \psi_2^{\dagger\sigma}(0) \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{2,\sigma'}(0)$, appearing in the second term (??), contains only the identity in the charge sector since the charges in both channels remain unchanged. The only operator with these properties, other than the total spin current, is $\epsilon(0)\phi(0)$, $\phi(x)$ being the ($j = 1$) primary field. The fermionic part of the third term (??), $\psi_1^{\dagger\sigma}(0) \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{2,\sigma'}(0) + \psi_2^{\dagger\sigma}(0) \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{1,\sigma'}(0)$, changes the charges in both electron channels. It must therefore contain nontrivial contributions in both isospin sectors. Together with spin and dimension, it follows that it must be $h_1(0)h_2(0)\phi(0)$, where $h_a(x)$ are the ($i_a = 1/2$)-primary fields. The bosonized interaction is thus given by [?]

$$H_{\text{Kondo}} \sim (J_+ \mathbf{J}(0) + J_- h_1(0)h_2(0)\phi(0)) \cdot (\mathbf{S}_1 + \mathbf{S}_2) + J_m \epsilon(0)\phi(0) \cdot (\mathbf{S}_1 - \mathbf{S}_2). \quad (3.2.5)$$

This is not necessarily a simplification compared to the original Hamiltonian, since the spin and isospin fields are rather complicated objects. Instead it serves as a preparation for the BCFT solution for which it is useful to have a description where the symmetries of the system appear explicitly.

3.3 BCFT-solution

The BCFT-solution [?] is based upon the bosonization scheme described above. The very idea of this approach is, that at the critical point, the model can be described by a conformally invariant boundary condition on a free theory. Note that this is an assumption, there is no formal proof that this has to be so. Instead, excellent agreement with a separate numerical calculation was used to argue that the conformal field theory gives a good description of the physics at the critical point. Moreover, the fact that the same argument has been used successively on various similar problems, where again the results were compared to numerical or different analytical approaches, e.g. the Bethe Ansatz gives confidence about the validity of this approach.

The boundary condition that describes the unstable fixed point of the TIKM is obtained by fusion as described in Section ???. It was found that fusion with the Ising field σ , or equivalently with the total spin field ($j = 1/2$), yields the correct energy spectrum. The operator content at the critical point is obtained by fusing with σ twice². It should be noted that although the system is two-dimensional (one space- and one time-dimension)

²The scaling dimensions of operators on the half plane are related to their energies on the strip geometry [?], hence the double fusion: One for each side of the strip.

Table 3.2: Operator content at the unstable fixed point

i_1	i_2	j	Ising	$\Delta = El/\pi$
0	0	0	\mathbb{I}	0
0	0	0	ϵ	1/2
1/2	0	1/2	σ	1/2
0	1/2	1/2	σ	1/2
0	0	1	\mathbb{I}	1/2
1/2	1/2	0	\mathbb{I}	1/2
0	0	1	ϵ	1
1/2	1/2	1	\mathbb{I}	1
1/2	1/2	0	ϵ	1
1/2	1/2	1	ϵ	3/2

the marginal dimension is *one*. This is due to the fact that these operators live on the boundary $x = 0$, which is one-dimensional [?]. All operators apart from the first two in Table ?? are forbidden by the various symmetries. The relevant ϵ operator comes with a scaling field $\sim (K - K^*)$ that measures the difference of the RKKY coupling from its value at the critical point. As ϵ is relevant, the coefficient to that field grows under renormalization and drives the system away from the critical point. The operators with the quantum numbers ($i_1 = i_2 = 1/2, j = 0, \text{Ising} = \mathbb{I}, \epsilon$) are forbidden only if there is particle-hole symmetry or if $J_- = 0$, i.e. if there is no transfer of charge between the channel of conduction electrons that couples to the first spin and the ones that couple to the second spin. Since the first of these operators (the one with the identity field \mathbb{I} in the Ising sector) is relevant, it follows that one of these two conditions must be fulfilled for the fixed point to be stable, even for $K = K^*$.

3.4 TIKM in quantum dots

In a recent publication Zaránd *et al.* [?] suggested, that an experimentally controlled approach to the TIKM quantum critical state may in fact be achieved by using a special type of spinful double-quantum dot system, realized in a gated semiconductor heterostructure. With a design where the two dots are connected to two separate electron reservoirs, and RKKY coupled via a magnetic insulator, they predicted that the quantum critical becomes stable in the presence of electron-hole symmetry breaking.

In this thesis I propose a variant of their suggestion that allows for better experimental

control over the RKKY interaction, which in my proposal is generated in the usual way, by local spin-exchange interaction with a bath of conduction electrons. The setup (Fig. ??) consists of two infinite leads that are each coupled to a quantum dot via tunneling junctions. The two quantum dots are also coupled to a finite, auxiliary electron reservoir. To understand the low energy behavior of this device, consider first $V_1 = V_2 = 0$, i.e. just

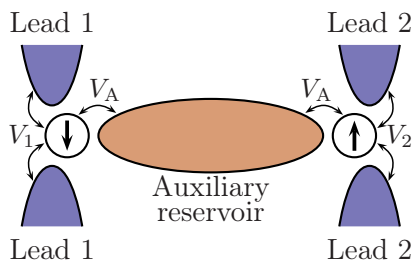


Figure 3.3: The physical setup I propose. The different V are the tunneling rates between the dots. The auxiliary reservoir is operated in the Coulomb blockade regime, where charge transfer between the reservoir and the leads (and thus also between the two leads) is strongly suppressed.

the two quantum dots with the auxiliary reservoir. If the parameters are set such that both of the dots as well as the reservoir are in the center of their respective Coulomb blockade valleys, charge fluctuation between the dots and the reservoir are strongly suppressed. Virtual transitions however, give rise to local spin exchange interactions between the electrons on the dots and the electrons in the reservoir. This is precisely the Kondo interaction, which implies that the two dots, together with the auxiliary electrons, already constitute a full TIKM. However, as long as T_A , the Kondo temperature associated with V_A is small compared to the RKKY interaction, $T_A \ll K \sim V_A^4$, the auxiliary reservoir acts as a pure RKKY interaction between the two quantum dots. By tuning up $V_{1,2}$ until $V_{1,2} \gg V_A$, the TIKM without any charge transfer between the two leads is obtained.

In the following chapter I continue by examining the critical behavior of the TIKM in the presence of spin-orbit interactions (for the conduction electrons). The advantage of the setup which I just described over the “orthodox” TIKM³, lies in the separation of the conduction electrons responsible for the RKKY interaction from those responsible for the Kondo screening. This allows me to consider the effect of spin-orbit interactions on the RKKY interaction and on the Kondo screening separately, before I put everything together in the end.

³In the TIKM as introduced in the beginning of this chapter (eq. ??), there are two impurities located within an infinite sea of conduction electrons.

Entanglement in the TIKM with spin-orbit interactions

Solid state quantum dots as qubits are believed to be one possible way of realizing qubits for quantum information processing [?]. They have the advantage of good scalability, i.e. it is relatively easy to increase the number of such qubits. So far, the problem lies with stability of such qubits. In a solid there is a huge number of interactions coupling to the qubit and destroying coherence. In order to perform algorithms on the qubits it is necessary that the qubits maintain coherence for a time that is large compared to the time it takes to perform the operations [?]. An important mechanism that leads to decoherence is spin-phonon coupling, which can arise, for instance due to spin-orbit interactions [?]. In this chapter I investigate the effect of spin-orbit interactions on the TIKM, in particular with respect to the entanglement between the qubits. I consider two different kinds of spin-orbit interactions that are important in two-dimensional systems. The first of these, the Rashba spin-orbit interaction [?] for a system in the x - y plane is given by the Hamiltonian

$$H_{\text{Rashba}} = \kappa(k^x \tau^y - k^y \tau^x), \quad (4.0.1)$$

where k^x and k^y are momentum operators in the x - and y -directions, τ^x and τ^y are Pauli matrices, as usual, and κ is a coupling constant. It appears when there are electric fields perpendicular to the x - y plane, such as gate voltages in semiconductor heterostructures. The strength of this interaction can be tuned experimentally by applying additional gate voltages [?]. The second interaction I consider, the Dresselhaus spin-orbit interactions, is given by the Hamiltonian

$$H_{\text{Dresselhaus}} = \lambda(k^y \tau^y - k^x \tau^x), \quad (4.0.2)$$

where λ is a coupling constant [?]. It arises as a consequence of broken inversion symmetry, for instance in GaAs with Zinc-blende crystal structure. As both GaAs and gated

heterostructures are commonly used to experimentally realize quantum dots [?] those interactions are bound to occur and it is important to examine their effects, not only on the phase coherence of the state of individual qubits [?], but also on the coupling between them.

In order to keep qubits stable against thermal fluctuations it may be necessary to go to very low temperatures, where new effects are known to occur. For a localized spin-1/2 state (impurity) in an electron gas, one has to take the Kondo effect into account, which tries to screen the spin. Clearly that is not desirable if one wants to use interactions between the spins to couple them. The simplest system where this effect becomes apparent is the TIKM, which was introduced in the previous chapter. In the TIKM there are two competing effects, the Kondo and the RKKY interaction, and the effect of spin-orbit interactions on both of them must be taken into account.

4.1 RKKY in the presence of spin-orbit interactions

The RKKY interaction [? ? ?] is an exchange interaction between spins in an electron gas, which arises due to coupling of the spins to the conduction electrons via the Kondo interaction, i.e.

$$H = H_{kin} + J \sum_{i=1,2} \mathbf{S}_i \cdot \psi_i^{\dagger\sigma}(0) \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{i,\sigma'}(0).^1 \quad (4.1.1)$$

In second order of the Kondo coupling a direct interaction term between the two spins arises, which can be calculated as

$$H_{\text{RKKY}} = -\frac{J^2}{\pi} \text{Im} \int_{-\infty}^{\epsilon_F} dE \text{Tr} [(\mathbf{S}_1 \cdot \boldsymbol{\tau}) G(\mathbf{R}, E + i0) (\mathbf{S}_2 \cdot \boldsymbol{\tau}) G(-\mathbf{R}, E + i0)], \quad (4.1.2)$$

where $G(\mathbf{R}, E)$ is the Green's function for the conduction electrons and the spins are located at a spacial difference of \mathbf{R} [?]. The RKKY interaction between two spins in 2D (taken as the x - y plane) in the presence of Rashba spin-orbit interactions has been calculated [?]. Here I will show, as a first new result of this thesis, that using the same procedure, the form of the RKKY interaction can be calculated in the presence of both Rashba and Dresselhaus interactions of arbitrary (relative) strength². The Hamiltonian for electrons in two dimensions with both kinds of spin-orbit interactions (eqs. ?? and ??) is:

$$H = \frac{\mathbf{k}^2}{2m} + \left[\begin{pmatrix} -\lambda & -\kappa \\ \kappa & \lambda \end{pmatrix} \begin{pmatrix} k^x \\ k^y \end{pmatrix} \right] \cdot \boldsymbol{\tau} \equiv \frac{\mathbf{k}^2}{2m} + (A\mathbf{k}) \cdot \boldsymbol{\tau}, \quad (4.1.3)$$

¹This is the same Hamiltonian as for the TIKM (eq. ??) with $J_- = 0$ and $J_+ = J_m$, up to the RKKY term.

²The perturbation theory is second order in the Kondo coupling J , but the full Green's function for electrons with spin-orbit interactions is used.

where λ and κ are the coupling strengths for Dresselhaus and Rashba spin-orbit interactions, respectively [? ?]. All occurring vectors have two components, i.e. $\mathbf{k} = (k^x, k^y)$, $\boldsymbol{\tau} = (\tau^x, \tau^y)$ and the scalar product of any vector $\mathbf{m} = (m^x, m^y)$, with the vector of Pauli matrices $\boldsymbol{\tau}$, is taken in the usual way $\mathbf{m} \cdot \boldsymbol{\tau} = m^x \tau^x + m^y \tau^y$. The Green's function to the Hamiltonian in eq. (??) is

$$G(\mathbf{k}, z) \equiv (z - H(\mathbf{k}))^{-1} = \frac{1}{z - \frac{\mathbf{k}^2}{2m} - (A\mathbf{k}) \cdot \boldsymbol{\tau}} = G_0(\mathbf{k}, A, z) + G_1(\mathbf{k}, A, z) (A\mathbf{k}) \cdot \boldsymbol{\tau}, \quad (4.1.4)$$

where

$$G_0(\mathbf{k}, A, z) = \frac{z - \frac{\mathbf{k}^2}{2m}}{\left(z - \frac{\mathbf{k}^2}{2m}\right)^2 - (A\mathbf{k})^2}, \quad (4.1.5)$$

$$G_1(\mathbf{k}, A, z) = \frac{1}{\left(z - \frac{\mathbf{k}^2}{2m}\right)^2 - (A\mathbf{k})^2}.$$

Note that both G_0 and G_1 are symmetric under parity, i.e. $\mathbf{k} \rightarrow -\mathbf{k}$. The Green's function in real space is

$$G(\mathbf{R}, A, z) = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} d^2k e^{i\mathbf{k} \cdot \mathbf{R}} [G_0(\mathbf{k}, A, z) + G_1(\mathbf{k}, A, z) (A\mathbf{k}) \cdot \boldsymbol{\tau}]. \quad (4.1.6)$$

The spin dependence can be pulled in front of the integral by writing

$$(A\mathbf{k})e^{i\mathbf{k} \cdot \mathbf{R}} = -i(A\nabla)e^{i\mathbf{k} \cdot \mathbf{R}} = (A\hat{R}) \left(-i \frac{d}{d|\mathbf{R}|} e^{i\mathbf{k} \cdot \mathbf{R}} \right), \quad (4.1.7)$$

where $\hat{R} = \mathbf{R}/|\mathbf{R}|$. The Green's function takes the form

$$G(\mathbf{R}, A, z) = G_0(\mathbf{R}, A, z) + G_1(\mathbf{R}, A, z) (A\hat{R}) \cdot \boldsymbol{\tau}, \quad (4.1.8)$$

where

$$G_1(\mathbf{R}, A, z) = -\frac{i}{4\pi^2} \int_{\mathbb{R}^2} d^2k \frac{d}{d|\mathbf{R}|} e^{i\mathbf{k} \cdot \mathbf{R}} G_1(\mathbf{k}, A, z). \quad (4.1.9)$$

Both $G_0(\mathbf{R})$ and $G_1(\mathbf{R})$ are symmetric under $\mathbf{R} \rightarrow -\mathbf{R}$. Performing the traces over the Pauli matrices in eq. (??) is a straightforward task (for details see Appendix ??). Up to this point I have not specified a coordinate system; the choice $\hat{R} = \hat{x}$, for instance, leads to the following four interaction terms between the spins

$$H_{\text{RKKY}} = H_{\text{Heis.}} + H_{\text{Rashba}} + H_{\text{Dress.}} + H_{\text{Interf.}}, \quad (4.1.10)$$

where

$$\begin{aligned} H_{\text{Heis.}} &= F_0 \mathbf{S}_1 \cdot \mathbf{S}_2 \\ H_{\text{Rashba}} &= \kappa F_1 (\mathbf{S}_1 \times \mathbf{S}_2)^y + \kappa^2 F_2 S_1^y S_2^y \\ H_{\text{Dress.}} &= \lambda F_1 (\mathbf{S}_1 \times \mathbf{S}_2)^x + \lambda^2 F_2 S_1^x S_2^x \\ H_{\text{Interf.}} &= \lambda \kappa F_2 (S_1^x S_2^y + S_1^y S_2^x). \end{aligned} \quad (4.1.11)$$

Here $F_i = F_i(\kappa, \lambda, R)$ are some functions which could in principle be calculated, at least numerically. While $F_i(0, \lambda, R) = F_i(\kappa, 0, R)$ have been obtained analytically in Ref. [?], they are in general given by rather complicated integrals.

In this form, the limiting cases of no spin-orbit effects / only Rashba / only Dresselhaus as well as the interference between the latter two become obvious. While this form is the easiest to understand physically, there is a more useful choice of a coordinate system. If the system is chosen such that $\angle(\hat{R}, \hat{y}) = -\arctan(\frac{\kappa}{\lambda})$, which implies $A\hat{R} = \kappa(0, (\kappa^2 - \lambda^2) \cos \arctan \theta)$, then only τ^y appears in the Green's function. The interaction then takes the simpler form

$$H_{\text{RKKY}} = \alpha \mathbf{S}_1 \cdot \mathbf{S}_2 + \beta S_1^y S_2^y + \gamma (\mathbf{S}_1 \times \mathbf{S}_2)^y. \quad (4.1.12)$$

Since this form explicitly conserves $U(1)$ spin symmetry, while the one above does not³, it appears possible that this symmetry can be used to simplify and possibly even calculate the F_i - but that is not part of my thesis.

The form of the interaction in eq. (??) is the same that was obtained for pure Rashba spin-orbit interactions in Ref. [?]. The parameters α, β, γ on the other hand, in general depend on R and the microscopic properties differently.

It is worth noting that in the special case $|\lambda| = |\kappa|$ the same choice of coordinate system as above gives $A\hat{R} = 0$, which means only the Heisenberg term $\sim \mathbf{S}_1 \cdot \mathbf{S}_2$ appears in the RKKY interaction, like in the absence of any spin-orbit interactions.

4.2 Kondo effect with spin-orbit interactions

The single-channel Kondo model (SCKM) in two spatial dimensions (x, y) with spin-orbit couplings is described by the Hamiltonian

$$H = \int d^2k \epsilon_k \psi_{\mathbf{k}, \sigma}^{\dagger \sigma} \psi_{\mathbf{k}, \sigma} + \int d^2k \int d^2k' \psi_{\mathbf{k}}^{\dagger \sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{\mathbf{k}', \sigma'} \cdot \mathbf{S} + \int d^2k \int d^2k' \langle \mathbf{k}, \sigma | H_{s-o} | \mathbf{k}', \sigma' \rangle \psi_{\mathbf{k}}^{\dagger \sigma} \psi_{\mathbf{k}', \sigma'}, \quad (4.2.1)$$

where (see eqs. ?? and ??)

$$H_{s-o} = (\kappa k^x + \lambda k^y) \tau^y - (\lambda k^x + \kappa k^y) \tau^x, \quad (4.2.2)$$

$|\mathbf{k}, \sigma\rangle = \psi_{\mathbf{k}}^{\dagger \sigma} |0\rangle$ are momentum eigenstates and τ^i are the Pauli matrices. κ and λ are the couplings for the Rashba and Dresselhaus spin-orbit interactions, respectively, and I assume a spherically symmetric free electron dispersion ϵ_k ⁴. The single-channel Kondo model in the presence of Rashba spin-orbit interactions has recently been investigated

³Not explicitly that is, the symmetry must of course still be present.

⁴What I mean by free electron dispersion in this context is the dispersion of the electrons in the absence of Kondo and spin-orbit interactions. Whether the dispersion is a truly free quadratic dispersion or a sinusoidal tight-binding dispersion is of no consequence.

[?]. It was found, that the qualitative low energy properties are unchanged. This can be seen by writing the Kondo model with spin-orbit interactions in the form of a multichannel Kondo model, where the different channels of electrons have different couplings to the impurity spin. The spin-orbit interactions are in this case absorbed into the kinetic and Kondo terms of the Hamiltonian and no longer appear explicitly. It is straightforward to apply the same procedure to Dresselhaus spin-orbit interactions.

As usual (see for instance Chapter ??) it is convenient to expand the electrons in partial waves around the impurity location, which I choose to be $\mathbf{R} = 0$. Only the $m = 0$ fields participate in the Kondo interaction ($m \in \mathbb{Z}$ being the orbital quantum number) and the kinetic energy is diagonal in m . The Dresselhaus- and Rashba-type spin-orbit interactions both couple each field to exactly one other field (see Appendix ??):

$$\begin{array}{ccccccccccc}
 \dots & \longleftrightarrow & \psi_{m=-2,\uparrow} & \longleftrightarrow & \psi_{m=-1,\downarrow} & \longleftrightarrow & \psi_{m=0,\uparrow} & \longleftrightarrow & \psi_{m=+1,\downarrow} & \longleftrightarrow & \psi_{m=+2,\uparrow} & \longleftrightarrow & \dots \\
 & & \text{Rashba} & & \text{Dresselhaus} & & & & \text{Rashba} & & \text{Dresselhaus} & & \\
 \dots & \longleftrightarrow & \psi_{m=-2,\uparrow} & \longleftrightarrow & \psi_{m=+1,\uparrow} & \longleftrightarrow & \psi_{m=0,\downarrow} & \longleftrightarrow & \psi_{m=-1,\uparrow} & \longleftrightarrow & \psi_{m=+2,\downarrow} & \longleftrightarrow & \dots
 \end{array} \tag{4.2.3}$$

Since there are no couplings (in the kinetic or spin-orbit terms) between fields on the upper and lower line of this diagram, it is possible to choose a basis of simultaneous eigenstates of the kinetic and spin-orbit Hamiltonian, where each state only contains states from the upper *or* from the lower line, but not from both. For non-zero spin-orbit couplings, each of those fields contains one of the $m = 0$ fields and thus couples to the impurity spin. If both kinds of spin-orbit interactions are present, there is an *infinite* number of fields coupling to the impurity. Unless there is some other mechanism that truncates the angular momentum states that may appear, it is not so easy to make a statement about the resulting physics. An infinite number of fields coupling to the impurity is a similar situation as one would obtain for a long-range Kondo interaction in the absence of spin-orbit couplings.

As long as only one of the spin-orbit interactions is present, the Hamiltonian of eq. (??) can be rewritten as

$$H = \sum_{f,\sigma} \int dE E \psi_{E,f}^{\dagger\sigma} \psi_{E,f,\sigma} + \frac{J}{2} \int dE \int dE' \sum_{f,f',\sigma,\sigma'} J_{f,f'}(E, E') \psi_{E,f}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{E',f',\sigma'}, \tag{4.2.4}$$

where $\sigma = \uparrow, \downarrow$ is an $SU(2)$ pseudospin-1/2 of the electron fields, corresponding to the upper and lower line of eq. (??), $f = \pm$ is a flavor index and the electrons are expressed in terms of the energy E (for technical details see Appendix ??). This model is known as the (anisotropic) two-channel Kondo model [?]. In general, the $J_{f,f'}(E, E')$ interaction is neither diagonal, nor has degenerate eigenvalues. A non-degenerate interaction (whether diagonal or not) is known to drive the two-channel Kondo model towards the single-channel Kondo model (plus one channel of free electrons) under renormalization [? ?]. The physical explanation for this is that if one channel of electrons couples more

strongly to the impurity than the other, screening is fully achieved by that channel in the low-temperature limit. In this case, the other channel decouples and behaves like one of free electrons [?]. Therefore, the effective low-energy model for the SCKM, in the presence of spin-orbit interaction of either the Dresselhaus or the Rashba type, is the usual SCKM (without any further interaction), plus a channel of free electrons which decouples and may thus be dropped.

The same argument can be applied to the TIKM. Physically, this is easiest to understand in terms of the nanoscopic device introduced in Section ???. Here, the TIKM is understood as two single-impurity models, coupled only via the RKKY interaction. In this picture it is clear that spin-orbit effects should not change the critical behavior. I can, for instance, start with two decoupled single-impurity models, each of which flows to the single-channel fixed point. Then I add the RKKY coupling, which does not affect how the leads couple to the impurities⁵. More formally, such a model, the two-impurity two-channel Kondo model, has been studied in Refs. [? ?]. There it was found that if two channels of electrons couple to the impurities stronger than the other two, the system renormalizes to the single-channel TIKM plus *two* decoupled channels of electrons, in agreement with physical intuition. The TIKM in the presence of either type of spin-orbit interactions, which is equivalent to a two-channel TIKM, can therefore still be described by the Hamiltonian

$$H = H_{\text{Kin.}} + K\mathbf{S}_1 \cdot \mathbf{S}_2 + J\mathbf{S}_1 \cdot \boldsymbol{\sigma}_1 + J\mathbf{S}_2 \cdot \boldsymbol{\sigma}_2, \quad (4.2.5)$$

as far as the low energy behavior is concerned.

4.3 The unstable fixed point

Now the stage is set to treat spin-orbit interactions around the critical point. Since spin-orbit effects give rise to a two-channel model, which in turn renormalizes to a single-channel model, and the RKKY interaction changes as derived in Chapter ??, the effective Hamiltonian can be written as:

$$H = H_{\text{Kin.}} + \underbrace{\alpha\mathbf{S}_1 \cdot \mathbf{S}_2 + \beta S_1^y S_2^y + \gamma(\mathbf{S}_1 \cdot \mathbf{S}_2)^y}_{H_{\text{RKKY}}} + J\mathbf{S}_1 \cdot \boldsymbol{\sigma}_1 + J\mathbf{S}_2 \cdot \boldsymbol{\sigma}_2. \quad (4.3.1)$$

For convenience I rotate all the spins (of the electrons as well as of the impurities) around the x -axis by an angle of $\pi/2$, which in the above Hamiltonian exchanges the y and z component of the spins. Defining the parameters $K^z \equiv \frac{1}{2}(\alpha + \beta)$ and $K^\perp e^{i\theta} \equiv \beta + i\gamma$, I

⁵The physics does not, of course, depend on the order in which I set up the system. I could provide a similar argument for starting with the RKKY coupling and then adding the Kondo screening channels.

write the RKKY part of the rotated Hamiltonian as

$$H_{\text{RKKY}} = K^z S_1^z S_2^z + K^\perp e^{i\theta} S_1^+ S_2^- + h.c. \quad (4.3.2)$$

As pointed out above, the Kondo screening behavior is not effected qualitatively; under renormalization the system flows to the same fixed point as without spin-orbit interactions. What may change is the value of the Kondo temperature T_K [?]. Since small deviations around the critical value of $K \equiv K^\perp = K^z \approx 2.2T_K$ are relevant, changing the Kondo temperature while keeping everything else fixed may drive the system away from the critical point⁶. To keep the system on the fixed point, it may therefore be necessary to fine tune the interactions, which is certainly possible in the proposed nanoscopic device. From here on, I assume any changes in T_K to be compensated by modifying K accordingly.

The only way how spin-orbit interactions can then influence the critical behavior is by the symmetry-breaking $SU(2) \rightarrow U(1)$, by which new operators may appear. In terms of the RKKY interaction in eq. (??), both ($K^z \neq K^\perp, \theta = 0$) and ($\theta \neq 0, K^\perp = K^z$) break $SU(2)$ to $U(1)$. For obvious reasons I will refer to the former as a longitudinal anisotropy, while I call the latter a transversal anisotropy. The effect of this symmetry breaking depends on the presence of charge transfer between the two channels of conduction electrons, as I will show⁷. There are various cases to consider. I begin with the simplest case of purely transversal perturbations:

Transversal anisotropies without charge transfer

If $K^\perp = K^z$ and charge transfer is suppressed, the Hamiltonian for $\theta \neq 0$ can be simplified substantially by a unitary transformation. The transformation consists of rotating \mathbf{S}_2 around the z -axis

$$\mathbf{S}'_2 = e^{i\theta S_2^z} \mathbf{S}_2 e^{-i\theta S_2^z}, \quad (4.3.3)$$

in which case the RKKY interaction becomes [?]

$$H_{\text{RKKY}} = K \mathbf{S}_1 \cdot \mathbf{S}'_2, \quad (4.3.4)$$

and rotating the spins of the conduction electrons coupled to that spin similarly, i.e.

$$\psi'_2 = e^{-i\theta \frac{\tau_z}{2}} \psi_2 e^{i\theta \frac{\tau_z}{2}}. \quad (4.3.5)$$

⁶Conversely, a system that is not critical at first may become critical upon introducing spin-orbit interactions.

⁷It should be kept in mind that in the presence of charge transfer, the critical point is stable only in the case of particle-hole symmetry, as discussed in Section ??.

The kinetic energy is invariant under these transformations, as are \mathbf{S}_1 and ψ_1 . Under these rotations, the Kondo Hamiltonian becomes

$$H = H_{\text{Kin.}} + K\mathbf{S}_1 \cdot \mathbf{S}'_2 + J\mathbf{S}_1 \cdot \boldsymbol{\sigma}_1 + J\mathbf{S}'_2 \cdot \boldsymbol{\sigma}'_2. \quad (4.3.6)$$

This is precisely the same Hamiltonian as for the isotropic two-impurity Kondo model (eq.??). This result does *not* mean that changing θ is an irrelevant perturbation under which the system flows back to the isotropic fixed point. Instead, the fixed points for all values of θ should be identified, since they arise from the same Hamiltonian. It should be clear that a charge transfer term $\sim \psi_1^\dagger \psi_2$ is *not* invariant under this transformation, indicating that something different may happen in that case. I will return to that later, after considering the second easiest case of purely longitudinal anisotropies:

Longitudinal anisotropies with or without charge transfer

If $K^z \neq K^\perp$ and $\theta = 0$, the Hamiltonian cannot simply be reduced to the isotropic one, even in the absence of charge transfer between the two leads. However, this perturbation is known to be irrelevant from the conformal field theory solution, even in the presence of charge transfer [?]. In fact, breaking $SU(2)$ to $U(1)$ in this way does not produce a new *leading* irrelevant operator either, which means that for longitudinal anisotropies the system flows back to the isotropic fixed point under renormalization and the scaling behavior of thermodynamic quantities is unaffected.

It should be noted that in spite of this, changing K^z while keeping K^\perp constant is a relevant perturbation. This is due to the fact that $K^\perp, K^z \rightarrow K^\perp + \delta, K^z + \delta$, where δ is some small number, drives the system away from the special case $K^\perp = K^z \approx 2.2T_K$, which is relevant, as I mentioned earlier (see Chapter ??). In the linearized RG-flow around the fixed point, this means that the irrelevant direction must be perpendicular to this. Only $K^\perp, K^z \rightarrow K^\perp + \delta, K^z - \delta$ can be irrelevant, i.e. K^\perp and K^z need to be changed simultaneously for the system to remain on the fixed point (see Figure ??).

Both longitudinal and transversal anisotropies, no charge transfer

As long as there is no charge transfer in the leads, the two previous results can be easily combined to determine what happens for both longitudinal and transversal anisotropies: By the unitary transformation, the Hamiltonian of such a system reduces to a Hamiltonian where there are only longitudinal anisotropies present. These are irrelevant as noted in the previous case.

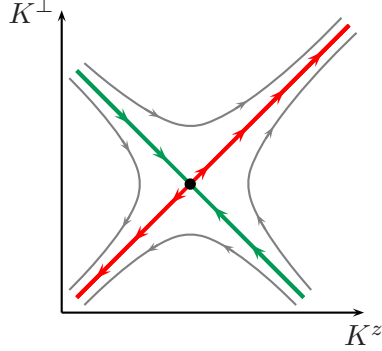


Figure 4.1: Linearized RG flow in the K^z - K^\perp plane. The red line marks the relevant direction known from the nRG solution [?] and the dot marks the fixed point. The irrelevant direction (green line) is perpendicular to the relevant one.

Both longitudinal and transversal anisotropies as well as charge transfer

As pointed out before, the presence of charge transfer disallows the unitary transformation that I used in the previous cases. From the CFT solution I find, that an exactly marginal operator ($h_1 h_2 \phi^z$ in the CFT language) is allowed when both transversal anisotropies and charge transfer are present⁸. The isospin component $h_1 h_2$ of this operator is only allowed when the charges of the two channels are *not* separately conserved. The spin component ϕ^z is allowed if spin-symmetry is broken down to $U(1)$ and symmetry under discrete rotations by an angle π around the x -axis and the y -axis is broken as well. This is only the case if $\theta \neq 0$, i.e. in the presence of transversal anisotropies. I expect this operator to stretch out the critical point into a critical line. While there is no formal proof, there are good arguments to explain the nature of the marginal operator: For the impurities, a charge transfer term $\sim \psi_1^\dagger \psi_2 + \psi_2^\dagger \psi_1$ translates into a term $|\lambda|(S_1^+ S_2^- + S_1^- S_2^+)$, where $|\lambda|$ is a real number that depends on the details of the system. Absorbing this into the RKKY interaction, changes the phase θ to an effective phase θ_{eff}

$$K^\perp e^{i\theta} S_1^+ S_2^- + |\lambda| S_1^+ S_2^- + h.c. = K' e^{i\theta_{\text{eff}}} S_1^+ S_2^- + h.c. \quad (4.3.7)$$

The effective phase θ_{eff} is made up of contributions by θ and by the coupling to the charge transfer terms, which appears as J_- in eq. (??). The models for different values of θ can therefore no longer be identified as before, instead it is plausible that there is now a line of fixed points, parameterized by θ_{eff} and connected via the marginal operator.

Further away from the critical point

It should be kept in mind, that the irrelevance of operators only carries meaning very close to the critical point. For larger differences between K^z and K^\perp the situation may

⁸In the original solution in Ref. [?] this case was not considered.

be very different. In fact, for $K^\perp = 0$, an entirely different quantum phase transition is expected to occur at a particular value of K^z [?]. On the other hand, for $K^z = 0$ the situation is very much the same for $K^\perp = K^z$:

For sufficiently large values of K^\perp , the impurities form a decoupled singlet, while for $K^\perp = K^z = 0$ the system flows to the two-channel fixed point [?]. This suggests that

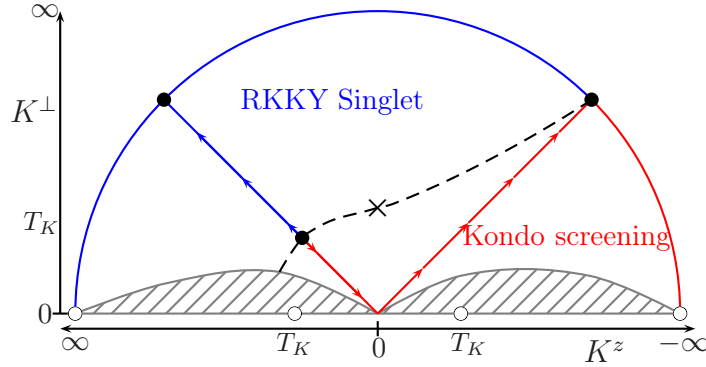


Figure 4.2: Qualitative RG flow of the anisotropic model. The solid dots and the solid line are the known results from the isotropic model. The gray area marks the system close to a different model of quantum dots coupled via the Ising interaction, where different behavior might occur. The cross represents the conjectured transversal fixed point. The dashed, line which I argue for in the text, connects this fixed point with the isotropic one and the point in the RKKY limit (given by the semicircle), which separates the singlet from the screened phase. Its curvature is not meant to suggest any deeper knowledge about some structure; a straight line is impossible, however, since close to the isotropic fixed point it follows the direction of irrelevant longitudinal anisotropies, and the point in the RKKY limit $K^\perp = -K^z$ does not lie on that line.

for some value $K^\perp \sim T_K$ there is a phase transition similar to the $K^\perp = K^z$ case. In fact, in the presence of particle-hole symmetry a phase transition *must* occur (see the discussion in Ref. [?], p. 9530). Furthermore, the same line of arguments used in [?] to solve the TIKM can be applied in this case⁹. Since there is no other energy scale in the system, I expect that there is no further phase transition away from $K^\perp = 0$. In the flow diagram, this suggests a line, separating the decoupled antiferromagnetic singlet phase from the Kondo screened ferromagnetic phase, which stretches all the way from the known $K^\perp = K^z = 2.2T_K$ critical point through the conjectured $K^z = 0, K^\perp \sim T_K$ critical point to the $K^\perp = -K^z \gg T_K$ point, which separates the singlet from the triplet state for very large RKKY interactions (Fig. ??).

⁹Note however, that this approach is justified by referring to NRG and CFT results. It is therefore, at least in principle possible, that something happens that invalidates that approach. This fixed point is conjectured by analogy, not rigorously derived.

4.4 Density matrix and concurrence

Returning to the original motivation for treating this problem, i.e. calculating the entanglement between the two impurity spins in the presence of spin-orbit interactions, I now consider the most general density matrix of the system that is compatible with conservation of the z -component of total spin. It can be written in matrix form in the standard basis of the impurity spins, i.e. $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ as

$$\rho = \begin{pmatrix} \rho_{(-1-1)}^1 c_{11} & \rho_{(-10)}^1 c_{12} & \rho_{(-10)}^2 c_{13} & \rho_{(-1+1)}^1 c_{14} \\ \rho_{(-10)}^{1\dagger} c_{21} & \rho_{(00)}^1 c_{22} & \rho_{(00)}^2 c_{23} & \rho_{(0+1)}^\alpha c_{24} \\ \rho_{(-10)}^{2\dagger} c_{31} & \rho_{(00)}^{2\dagger} c_{32} & \rho_{(00)}^3 c_{33} & \rho_{(0+1)}^\beta c_{34} \\ \rho_{(-1+1)}^{1\dagger} c_{41} & \rho_{(0+1)}^{1\dagger} c_{42} & \rho_{(0+1)}^{1\dagger} c_{43} & \rho_{(+1+1)}^1 c_{44} \end{pmatrix}, \quad (4.4.1)$$

where $c_{ij} = c_{ji}^*$ and $\rho_{\sigma,\sigma'}^i$ ($i = 1, 2, 3$, $\sigma, \sigma' = +1, 0, -1$) describe the conduction electrons and are given by $\rho_{\sigma,\sigma'}^i = \sum_a d_{ab}^i |\sigma, a\rangle \langle \sigma', b|$, d_{ab}^i being (complex) numbers and $|\sigma, a\rangle$ being conduction-electron states with spin equal to the total spin of the full system plus σ . The indices a, b contain all other quantum numbers of the conduction-electron states. From this I obtain the reduced density matrix of the two-spin subsystem by taking the trace over all conduction-electron states

$$\rho_{12} \equiv \sum_{a,\sigma} \langle \sigma, a | \rho | \sigma, a \rangle = \begin{pmatrix} |a_1| & 0 & 0 & 0 \\ 0 & |a_2| & b & 0 \\ 0 & b^* & |a_3| & 0 \\ 0 & 0 & 0 & |a_4| \end{pmatrix}, \quad (4.4.2)$$

which is fairly simple due to $U(1)$ -symmetry, i.e. $\langle \sigma', b | \sigma, a \rangle \sim \delta_{\sigma,\sigma'}$. The parameters $|a_i|$, $i \in [1, 4]$ are real numbers and b is a complex number.

I find it convenient to express the density matrix in terms of five spin-spin expectation values¹⁰

$$\begin{aligned} 3I &\equiv \langle S_z^1 S_z^2 \rangle - \langle S_x^1 S_x^2 \rangle \\ D &\equiv \langle S_x^1 S_y^2 \rangle - \langle S_y^1 S_x^2 \rangle \\ 3H &\equiv \langle \mathbf{S}^1 \cdot \mathbf{S}^2 \rangle \\ X^\pm &\equiv \langle S_z^1 \rangle \pm \langle S_z^2 \rangle. \end{aligned} \quad (4.4.3)$$

Expectation values are calculated in the usual way $\langle \mathcal{O} \rangle = \text{Tr}[\mathcal{O} \rho_{12}]$. The operators in the two-spin basis can be easily obtained from the Pauli matrices for single spins, since the basis states are product states. As an example consider $S_x^1 S_x^2$: This operator flips both spins without changing the sign, i.e. $|\uparrow\uparrow\rangle \leftrightarrow |\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle \leftrightarrow |\downarrow\uparrow\rangle$. In this basis it is

¹⁰The last one of the original six parameters is fixed since the density matrix has trace unity.

therefore given by

$$S_x^1 S_x^2 = \frac{1}{4} \tau_x^1 \tau_x^2 = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (4.4.4)$$

Note that the way the parameters (eq. ??) are defined allows for an easy reduction to various limiting cases. For example $H \neq 0, I = D = X^\pm = 0$ corresponds to the $SU(2)$ case, that is given by a pure Heisenberg interaction between the spins. Actually, in the system I consider, the parameters X^\pm are always zero by symmetry, i.e. there is no spontaneous magnetization, neither uniform nor staggered. I still keep them for now in order to derive an expression for the concurrence that is also valid for more general situations, e.g. in the presence of magnetic fields. I find it more convenient to work in the “magic basis”, given by

$$\begin{aligned} |e_1\rangle &= |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle \\ |e_2\rangle &= i|\uparrow\uparrow\rangle - i|\downarrow\downarrow\rangle \\ |e_3\rangle &= i|\uparrow\downarrow\rangle + i|\downarrow\uparrow\rangle \\ |e_4\rangle &= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle. \end{aligned} \quad (4.4.5)$$

In this basis the concurrence can be written as

$$C = \max \{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \quad (4.4.6)$$

where λ_i are the decreasingly ordered square roots of the eigenvalues of $\rho_{12}^{\text{magic}} \rho_{12}^{\text{magic}*}$ [?], where ρ_{12}^{magic} is ρ_{12} in the magic basis. In terms of the parameters defined above it is

$$\rho_{12}^{\text{magic}} = \begin{pmatrix} \frac{1}{4} + H + 2I & -iX^+ & 0 & 0 \\ iX^+ & \frac{1}{4} + H + 2I & 0 & 0 \\ 0 & 0 & \frac{1}{4} + H - 4I & D + iX^- \\ 0 & 0 & D - iX^- & \frac{1}{4} - 3H \end{pmatrix}. \quad (4.4.7)$$

Since $\rho\rho^*$ is block diagonal, it is a straightforward task to calculate the eigenvalues from quadratic equations (see Appendix ?? for details). They are

$$\begin{aligned} \lambda_{1,2}^2 &= \left(\left(\frac{1}{4} + H + 2I \right)^2 - (X^+)^2 \right) \\ \lambda_{\pm}^2 &= \left\{ D^2 - (X^-)^2 + (2I - 2H)^2 + \left(2I + H - \frac{1}{4} \right)^2 \right. \\ &\quad \left. \pm 2 \sqrt{((2I - 2H)^2 + D^2) \left(\left(2I + H - \frac{1}{4} \right)^2 - (X^-)^2 \right)} \right\}. \end{aligned} \quad (4.4.8)$$

Note that the parameters are not fully independent; all eigenvalues are positive numbers. To calculate the concurrence by the above formula, it is necessary to order them by size.

Clearly λ_- can never be the largest eigenvalue, thus there are only two cases: First, look at $\lambda_+ > \lambda_1$. In this case the concurrence is

$$C = \max\{0, \lambda_+ - \lambda_- - 2\lambda_1\}, \quad (4.4.9)$$

in particular it is zero for $\lambda_+ - \lambda_- \leq 2\lambda_1$.

The second possibility is $\lambda_1 > \lambda_+$. Clearly the concurrence is zero in this case, since $\lambda_1 - \lambda_2 = 0$ and $\lambda_{\pm} \geq 0$. However,

$$\lambda_+ - \lambda_- \leq \lambda_+ \leq \lambda_1 \leq 2\lambda_1, \quad (4.4.10)$$

thus the concurrence also vanishes by eq. (??). The second case is already contained in that formula and it is not necessary to treat any separate cases. In the case of $X^+ = X^- = 0$ the eigenvalues take the simpler form

$$\begin{aligned} \lambda_1 &= \frac{1}{4} + H + 2I \\ \lambda_{\pm} &= \sqrt{D^2 + (2I - 2H)^2} \pm \left| 2I + H - \frac{1}{4} \right| \end{aligned} \quad (4.4.11)$$

It is worth noting that in the case $X^+ = X^- = 0$ the parameter D does not affect the concurrence, since it only depends on the difference $\lambda_+ - \lambda_-$.

4.5 Entanglement properties

To calculate the concurrence of any state of the two-spin subsystem (arising from a total Hamiltonian conserving $U(1)$ spin symmetry) we can use the formula derived above. Here, some clarification might be in order: The effective Hamiltonian for the subsystem does not necessarily obey the same symmetry as the full Hamiltonian. Nonetheless, the concurrence is determined solely by the reduced density matrix that has been obtained using the $U(1)$ symmetry of the full system. The same already applies in the $SU(2)$ case: The only interaction between two spins that obeys this symmetry is $H = K\mathbf{S}_1 \cdot \mathbf{S}_2$. Such a Hamiltonian allows for only three possible values of the spin-spin correlation, corresponding to the triplet, the singlet and the decoupled case. Still, in the isotropic TIKM, where $SU(2)$ is obeyed, it continuously takes all values between the triplet and singlet values and fully determines the entanglement [? ?].

In the RKKY regime, far away from the critical point, the spins can only appear in three different states: In a singlet state

$$\rho_{\text{singlet}}(\theta) \equiv \frac{1}{2} \left(|\uparrow\downarrow\rangle - e^{i\theta} |\downarrow\uparrow\rangle \right) \left(\langle\uparrow\downarrow| - e^{-i\theta} \langle\downarrow\uparrow| \right), \quad (4.5.1)$$

in the Ising ground state

$$\rho_{\text{Ising}} = \frac{1}{2} |\uparrow\uparrow\rangle\langle\uparrow\uparrow| + \frac{1}{2} |\downarrow\downarrow\rangle\langle\downarrow\downarrow|, \quad (4.5.2)$$

or the triplet state

$$\rho_{\text{triplet}}(\theta) = \frac{1}{3}\rho_{\text{singlet}}(\theta) + \frac{1}{3}|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + \frac{1}{3}|\downarrow\downarrow\rangle\langle\downarrow\downarrow|, \quad (4.5.3)$$

corresponding to the cases $K^\perp > -K^z$, $K^\perp < -K^z$ (or $|K^z| > K^\perp = 0$) and $K^\perp = -K^z$, respectively. This can be read off immediately from the level scheme in Figure ???. Using the formulas derived above, it is easy to verify that the concurrence is unity for

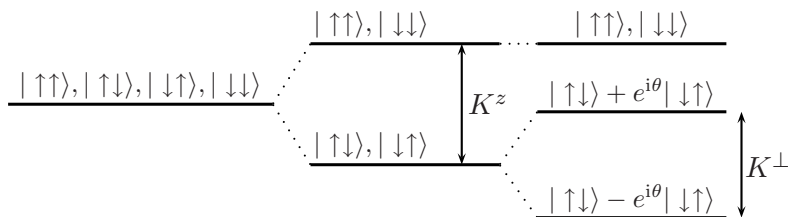


Figure 4.3: Level splitting due to the RKKY interaction, shown for $K^z > 0$.

the singlet while it always vanishes in the latter two cases (see Appendix ?? for details). In the critical regime I can revert to Ref. [?], where it was shown that in the isotropic Kondo model the spins are in the state

$$\rho_{\text{Kondo}}(\theta = 0) = \frac{1}{2}\rho_{\text{singlet}}(0) + \frac{1}{4}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)(\langle\uparrow\uparrow| + \langle\downarrow\downarrow|). \quad (4.5.4)$$

In this case, it is easy to see that $D = I = 0$ and $H = -\frac{1}{12}$. According to eq. (??), this implies $\lambda_+ = 1/2$, $\lambda_- = \lambda_1 = 1/6$. The concurrence is

$$C = \max\left\{0, \lambda_+ - \lambda_- - 2\lambda_1 = \frac{1}{2} - \frac{3}{6}\right\} = 0, \quad (4.5.5)$$

reproducing the result of Ref. [?]. In the anisotropic case, one of the spins is rotated around the z axis, while the other one is not. The state $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$ is not effected by this, but the singlet state changes to $|\uparrow\downarrow\rangle - e^{i\theta}|\downarrow\uparrow\rangle$. The state at the critical point generalizes to $\rho_{\text{Kondo}}(\theta)$ for any values of $\theta \in [0, 2\pi]$. The parameters are then given by

$$\begin{aligned} H(\theta) &= \frac{1}{8} \left(1 + \frac{1}{3} \sin^2 \frac{\theta}{2} - \cos^2 \frac{\theta}{2} \right) \\ I(\theta) &= -\frac{1}{12} \sin^2 \frac{\theta}{2} \end{aligned} \quad (4.5.6)$$

By eq. (??) this means $\lambda_+ - \lambda_- = 1/2$ and $\lambda_1 = 1/4$. Thus the concurrence is

$$C(\theta) = \max\left\{0, \frac{1}{2} - \frac{2}{4}\right\} = 0, \quad (4.5.7)$$

as in the isotropic case.

4.6 Conclusions

From the calculations I found that spin-orbit interactions do *not* affect entanglement in the TIKM around the unstable fixed point. The concurrence always vanishes identically, as in the isotropic case. The origin of the spin-orbit interactions, i.e. whether they are of the Rashba or the Dresselhaus type, is not important in this context, since they can be treated in the same way. Away from the fixed point I was able to derive the form of the RKKY interaction in the presence of *both* kinds of spin-orbit interactions. It is the same as in the presence of just one kind of spin-orbit interactions, the only difference being in the values of the coupling constants.

To use such a system for quantum information processing, this means that, just like in the isotropic case [?], the RKKY interaction needs to be large compared to the Kondo temperature in order to have a non-vanishing concurrence, as is required for quantum computing. Spin-orbit interactions may have to be taken into account for the stability of individual qubits, but they do not have to be worried about in the interaction between them.

This result is not surprising, since I demonstrated in the previous sections that spin-orbit interactions only have a minor effect on the TIKM, i.e. only appear in the RKKY interaction. In fact, in the absence of charge transfer, the same result could have been obtained immediately by using the Hamiltonian of eq. (??) and writing the density matrix in the rotated basis, where it explicitly has $SU(2)$ -symmetry, thus reducing to the result of Ref. [?]. It is only in the presence of charge transfer, that $SU(2)$ is truly broken down to $U(1)$ and the more involved procedure I presented above becomes necessary. The result, however, is the same in all cases.

Effects of charge fluctuations

As I pointed out in Chapter ??, the TIKM is a particular limit of the TIAM, where there is always an electron on each impurity and only virtual transitions between the dots and the leads are allowed. In this chapter I now investigate what happens real transitions are allowed and charge may fluctuate between the leads and the dots. Apart from being a very natural generalization of the TIKM, this also extends the parameter space where potential experiments can be compared to the theory. To be specific, I consider the setup already introduces in Section ??, with the difference that I now allow charges to hop from [into] each dot into [from] the corresponding lead, while there are still only virtual hopping processes between each of the dots and the auxiliary reservoir (Fig. ??). In this

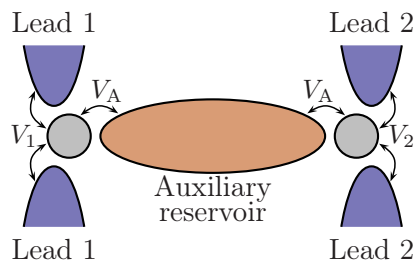


Figure 5.1: The physical system I study in this chapter. The different V are the tunneling rates between the dots. The auxiliary reservoir is operated in the Coulomb blockade regime, where charge transfer between the reservoir and dots (and thus also between the two leads) is strongly suppressed.

figure I have replaced the well defined spins that were present on the dots in the Kondo limit by a gray area, to emphasize that there is not necessarily a well defined spin. The state of the dot is in general a quantum superposition (pure state) of the states with zero, one and two electrons on the dot. To analyze this system it is easiest to start with the case where $V_A = 0$, which corresponds to two decoupled ($i = 1, 2$) single-impurity

Anderson models (SIAMs), which can be mapped to the 1-dim Hamiltonian:

$$\begin{aligned}
 H_i &= \int dE E \psi_{i,E}^{\dagger\sigma} \psi_{i,E,\sigma} + \int dE (V_i \psi_{i,E}^{\dagger\sigma} d_{i,\sigma} + h.c.) \\
 &+ U_i (d_{i,\uparrow}^{\dagger\uparrow} d_{i,\uparrow}) (d_{i,\downarrow}^{\dagger\downarrow} d_{i,\downarrow}) + \epsilon_i d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma}.
 \end{aligned} \tag{5.0.1}$$

Here $\psi_{i,E}^{\dagger\sigma}$ is a creation operator for an s -electron in lead i with energy E and spin σ , and $d_{i,\sigma}^{\dagger\sigma}$ is the creation operator for an electron with spin σ localized on dot i . U_i is the corresponding charging energy and ϵ_i the chemical potential. E and ϵ_i are measured from the common Fermi level of the leads, and repeated spin-indices are summed over. At the special point $\epsilon_i = -U_i/2$, which in the language of the quantum dot corresponds to the center of the Coulomb blockade valley, the impurity has integer ground state valence $n_i \equiv \langle d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma} \rangle = 1$. This is not only true for the Kondo limit $U_i \rightarrow \infty$ but also for small values of U_i , which can be seen by the fact that the Hamiltonian for the SIAM is invariant under the particle-hole transformation $\psi_{i,E,\sigma} \rightarrow \psi_{i,-E}^{\dagger\sigma}$, $d_{i,\sigma} \rightarrow -d_{i,\sigma}^{\dagger\sigma}$. The invariance of the first line in eq. (??) under these transformations is immediately obvious. For the terms in the second line write

$$\begin{aligned}
 U_i n_{i\uparrow} n_{i\downarrow} + \epsilon_i d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma} &\rightarrow U_i (1 - d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma} + n_{i\uparrow} n_{i\downarrow}) + \epsilon_i (2 - d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma}) \\
 &= U_i n_{i\uparrow} n_{i\downarrow} + \epsilon_i d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma} - (U_i + 2\epsilon_i) d_{i,\sigma}^{\dagger\sigma} d_{i,\sigma} + \text{const.}
 \end{aligned} \tag{5.0.2}$$

For $\epsilon_i = -U_i/2$ the last term vanishes and the Hamiltonian is unchanged, up to a constant. From this it follows that $n_i = 2 - n_i = 1$. Here the $n_i = 0$ and $n_i = 2$ states appear with equal amplitude in the impurity state. In particular in the Kondo limit, they both have zero amplitudes. As $|\epsilon_i|$ increases particle-hole symmetry is broken. The impurity state becomes asymmetric and n_i will decrease¹.

It is sufficient to treat the $n_i \leq 1$ situation exclusively because it is related to the $n_i \geq 1$ case which occurs for $\epsilon_i < -U_i/2$ via an electron-hole transformation, i.e. a reflection around the symmetric point mentioned above. The $n_i = 0$ case has to be excluded; it defines a free electron system for which the following theory does not apply. At sufficiently low temperatures, $T < T_i \sim \sqrt{\Gamma_i U_i} \exp(-2\Gamma_i/\pi|\epsilon_i|)$, the physics of the SIAM is controlled by a strong coupling fixed line, generated by electron-impurity spin exchange, together with potential scattering [?]. The critical theory is that of a local Fermi liquid, with the quasiparticle wave functions phase shifted by an amount determined by the impurity valence (“Friedel-Langreth sum rule” [?]). This picture will change as the two dots are connected by switching on V_A . I here consider the case where, by tuning a nearby gate voltage, charge transfer between the auxiliary reservoir and the dots is suppressed by Coulomb blockade, leaving only spin exchange as a viable interaction

¹If the system started in the Kondo limit, n_i will start decreasing only as ϵ_i approaches Γ_i (the width of the impurity level).

(where, in the mixed valence regimes of the dots, only the singly occupied subspaces participate). Double spin-exchange processes will then generate an RKKY interaction $\sim K \sim V_A^4$ between the dots. By tuning the tunneling rate V_A such, that the associated Kondo temperature T_A is small compared to K , the auxiliary reservoir will, in effect, act as an RKKY messenger between the two dots. I thus obtain the Hamiltonian for the TIAM with separated electron reservoirs:

$$H = \sum_{i=1,2} H_i + K \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, \quad (5.0.3)$$

where $\boldsymbol{\sigma}_i = d_{i\alpha}^\dagger \boldsymbol{\tau}_{\alpha\beta} d_{i\beta}$ with $\boldsymbol{\tau}$ being the vector of Pauli matrices. The width of the auxiliary reservoir is here to be chosen so that $K > 0$. Apart from the kinetic term for the itinerant electrons in the auxiliary reservoir (which decouple from the conduction electrons in the leads), these are the only terms that appear in the Hamiltonian. Additional terms may be generated under renormalization, and I will discuss the most relevant of those below. Note that the two $SU(2)_1$ spin symmetries of the free conduction electrons are broken down to their diagonal subgroup $SU(2)_2$ as in the TIKM (Section ??), and that only their average charge is conserved. The important point is, that there is no mixing between charges of the two reservoirs 1 and 2. Away from the symmetric SIAM point $\epsilon_i = -U_i/2$ electron-hole symmetry is broken, as pointed out above.

To probe for the quantum critical properties of the model, I exploit the BCFT approach where a quantum impurity (or, in the present case, a *pair* of impurities) is absorbed into a conformally invariant boundary condition for a 1D effective theory that involves the conduction electrons only. The boundary condition is encoded in a set of selection rules for combining quantum numbers of the effective (conformal field) theory. The gluing conditions, in turn, constrain the finite-size energy spectrum from which the dimensions of the scaling operators – and thus the critical scaling of observables – are extracted (see Chapter ??).

5.1 CFT description of the critical TIAM

To obtain the finite-size spectrum for the TIAM, I start with the known spectrum of the TIKM, see Section ?. Its spectral levels are labeled by the quantum numbers $Q_{1,2} \in \mathbb{Z}^2$, $j \in \{0, 1/2, 1\}$ (total $SU(2)_2$ spin), and $\Phi \in \{0, 1/16, 1/2\}$ as in Section ?. The selection rules that constrain the allowed combinations of quantum numbers are obtained from the ones for free fermions via *fusion* with σ [?]. To take into account the fact that,

²The net charge in the respective reservoir replaces the isospins in the absence of particle-hole symmetry.

unlike a Kondo impurity, an Anderson impurity (still in the $n_i=1$ limit) carries charge, I redefine the charges as $Q_i \rightarrow Q_i - 1$. To keep the correct physics, the selection rules must be modified accordingly. Since the Q_i are defined *mod* 2, this redefinition swaps the conformal towers ($Q_i = 0$) and ($Q_i = 1$), which is equivalent to fusion with j_i , as explained in Section ???. The correct boundary conditions, if both charges are redefined in this way, can therefore be obtained by fusing with $(j_1 = 1/2) \times (j_2 = 1/2)$. In terms of the combined fields, this corresponds to fusion with either ϵ in the Ising sector or ($j = 1$) in the spin-sector. Choosing fusion with ϵ is a bit more convenient because then all fusions take place in the Ising sector. The generalization to non-integer impurity valences $n_i < 1$ is determined by the Friedel-Langreth sum rule [?], which relates the charge n_i of a local perturbation to the electronic scattering phase shift ($\delta_{F_i} = \pi n_i/2$), at the Fermi level. This phase shift is imparted by an exactly marginal operator which is present due to the electron-hole symmetry breaking for $\epsilon_i \neq -U_i/2$, and it follows that the charges must be redefined as $Q_i \rightarrow Q_i - n_i$, with the same fusion as in the integer case [?]. The resulting spectrum can be written as

$$E = E_0 + \frac{\pi}{4l} \left[\sum_{i=1,2} (Q_i - n_i)^2 + j(j+1) + 4\Phi \right], \quad (5.1.1)$$

with l being the width of the system. The impurity valences n_i contribute to the energy spectrum as $E(n_i) = \frac{\pi}{4l} \sum_{i=1,2} (n_i^2 - 2n_i Q_i)$. The quadratic term is identical for all states, regardless of their quantum numbers and just offsets the ground-state energy. The linear part shifts the energy of states with different charges relative to each other. This shift is of the same order as the energy gaps between the different states and changes the spectrum qualitatively. The lowest energy excitation in the pure Kondo case for instance, becomes degenerate with the second lowest at $n_{1,2} = 3/4$ and has higher energy for even lower values of $n_{1,2}$.

In contrast to this, the scaling dimensions of the operators which determine thermodynamics and transport do *not* depend on the impurity valences. The dimensions are related to the energy levels of the finite system with the same boundary condition on either endpoint. As explained in Ref. [?], the replacement $Q_i \rightarrow Q_i - n_i$ at the lower boundary corresponds to the replacement $Q_i \rightarrow Q_i + n_i$ at the upper boundary, thus the contributions from both endpoints cancel each other and there is no n_i -dependence. After *double fusion* with $\sigma \times \epsilon = \sigma$ as in Ref. [?], there are five allowed operators with dimension $\Delta < 2$ (Tab. ??).

Table 5.1: Operator content ($\Delta < 2$) of the TIAM at criticality.

Operator	Δ
ϵ	1/2
$J_i^c \sim \psi_i^\dagger \psi_i$	1
$\mathbf{J}_{-1}^s \cdot \phi$	3/2
$J_i^c \epsilon \sim \psi_i^\dagger \psi_i \epsilon$	3/2
$L_{-1} \epsilon$	3/2

Here ϕ is the $j = 1$ WZW-field. The first operator in the table is the only relevant one, and comes with a scaling field $\sim (K - K_c)$ that measures the distance to the critical surface, just as in the TIKM. The exactly marginal charge currents J_i^c extend the TIKM unstable fixed point to a surface of unstable fixed points parametrized by n_i [?]. Moreover, the charge currents impart a phase shift $\delta_{Fi} = \pi n_i/2$ to the electrons at the Fermi level, as required by the Friedel-Langreth sum rule. The third operator, $\mathbf{J}_{-1}^s \cdot \phi$, is only allowed if parity $\psi_1, d_1 \leftrightarrow \psi_2, d_2$ is broken. It also appears in the overscreened two-channel Kondo model as the leading irrelevant operator [?]. The fourth operator, $J_i^c \epsilon$ has (to my knowledge) not been discussed anywhere before. A similar operator might in fact occur for the related model of two Ising-coupled Kondo impurities [?]³, but so far there is no known CFT solution for that model. By this list of operators, the thermodynamics and transport properties close to the fixed point are determined.

5.2 Thermodynamics

Thermodynamic properties can be obtained from the partition function

$$Z = e^{-\beta F}, \quad (5.2.1)$$

where β is the inverse temperature and F the free energy. Close to the critical point, the Hamiltonian is given by the fixed point Hamiltonian and all allowed operators,

$$H = H_* + H_{\text{scaling}} \equiv H_* + \sum_d H_d. \quad (5.2.2)$$

³Similar to the TIKM, there is an unstable fixed point expected at an intermediate parameter value of (the Ising coupling) I . This suggests that there is a relevant operator, associated with the difference of the Ising coupling from its critical values $\sim (I_c - I)$. In the absence of particle-hole symmetry the charge current J^c is allowed and could be combined with the relevant operator, much like $J_i^c \epsilon$.

Here H_* is the fixed point Hamiltonian and the H_d contains all operators of dimension d , e.g.

$$\begin{aligned} H_{\frac{3}{2}} &= \lambda^I L_{-1}\epsilon + \lambda_i^{c,1} J_i \epsilon + \lambda^{s,1} \mathbf{J}_{-1}^s \cdot \phi \\ H_2 &= \lambda_i^{c,2} (J_i^c)^2 + \lambda^{s,2} (\mathbf{J}^s)^2 + \lambda^{I,2} T^I, \end{aligned} \quad (5.2.3)$$

where the various λ s are coupling constants. Note that $\lambda_i^{c,1}$ and $\lambda^{s,1}$ are zero in the cases of particle-hole and parity symmetry, respectively. $T^I = L_{-2}\mathbb{I}$ is the Ising energy momentum tensor. The partition function for H can be expressed in terms of the partition function of H_* as

$$Z = e^{-\beta F} = e^{-\beta F_*} \left\langle \exp \int_{-\beta/2}^{\beta/2} d\tau H_{\text{scaling}}(\tau) \right\rangle_T. \quad (5.2.4)$$

Here F^* is the free energy at the fixed point and the correlator is calculated in the finite-temperature geometry, i.e. the infinite cylinder with period β in the (imaginary) time direction, as indicated by the subscript T . The change in the free energy due to the irrelevant operators, $\delta F = F - F_*$ can be expressed via a cumulant expansion as [?]:

$$\begin{aligned} \delta F &= -\frac{1}{\beta} \int_{\beta/2}^{\beta/2} d\tau \langle H_{\text{scaling}}(\tau) \rangle_{T,c} \\ &\quad - \frac{1}{2\beta} \int_{\beta/2}^{\beta/2} \int_{\beta/2}^{\beta/2} d\tau_1 d\tau_2 \langle H_{\text{scaling}}(\tau_1) H_{\text{scaling}}(\tau_2) \rangle_{T,c} \\ &\quad + \dots \end{aligned} \quad (5.2.5)$$

Here $\langle \dots \rangle_{T,c}$ denote cumulants, i.e. the connected part of the correlators. It remains to evaluate the various correlators that may appear. Fortunately, this can be done very easily employing results from conformal field theory.

In Ref. [?] it was suggested, that the operator $L_{-1}\epsilon$ governs the low-temperature thermodynamics as well as transport properties. However, any correlator containing the operator $L_{-1}\epsilon$ vanishes:

$$\begin{aligned} \int_{-\beta/2}^{\beta/2} d\tau \langle L_{-1}\epsilon(\tau, 0) \dots \rangle_T &= \int_{-\beta/2}^{\beta/2} d\tau \partial_\tau \langle \epsilon(\tau, 0) \dots \rangle_T \\ &= \langle \epsilon(\beta/2) \dots \rangle_T - \langle \epsilon(-\beta/2) \dots \rangle_T = 0. \end{aligned} \quad (5.2.6)$$

The last equality holds, due to the periodicity of the finite temperature geometry. Clearly, this operator does not affect the low-temperature scaling behavior, to any order. This result is neither specific for this model, nor for the particular operator $L_{-1}\epsilon$, since it is a consequence of symmetries only: Virasoro first descendants do not affect low-temperature scaling properties.

Next, note that all one-point-functions of (chiral) primary fields, i.e. $J_i^c \epsilon$ and $\mathbf{J}_{-1}^s \cdot \phi$, also vanish, due to conformal symmetry. Next, all the operators appearing in H_2 are just the energy momentum tensors of four sectors – Ising, spin and the two charge sectors. Their expectation values are determined by the central charges of their respective sector

$$\langle T^\alpha \rangle_T = \frac{c^\alpha \pi^2}{6\beta^2}, \quad (5.2.7)$$

where in the present case $c^I = 1/2$, $c^s = 3/2$ and $c_i^c = 1$ [?]. Thus in first order of the couplings, only the $d = 2$ operators give a contribution to the free energy. It is of the form

$$\delta F_2 = \text{const} \times T^2. \quad (5.2.8)$$

This is the usual behavior one gets in Fermi-liquid theory, which is expected because this operator is always allowed, even at the trivial decoupled fixed point. To get the leading effects of the non-Fermi liquid operators from $H_{\frac{3}{2}}$, I must therefore go to higher orders. Two point functions containing operators of different dimensions, i.e. cross terms between $H_{\frac{3}{2}}$ and H_2 , vanish directly by conformal symmetry. Next I consider the cross term between the two primary operators in $H_{\frac{3}{2}}$:

$$\langle J_i^c \epsilon \mathbf{J}_{-1}^s \cdot \phi \rangle_T = \langle J_i^c \rangle_T \langle \epsilon \rangle_T \langle \mathbf{J}_{-1}^s \cdot \phi \rangle_T = 0. \quad (5.2.9)$$

Because the four sectors are independent, it decomposes into one-point functions which vanish as before. The non-vanishing two-point function is determined by conformal invariance up to a normalization constant. On the boundary it is

$$\left\langle H_{\frac{3}{2}}(\tau_1) H_{\frac{3}{2}}(\tau_2) \right\rangle_T = A \frac{(\lambda^{s,1})^2 + (\lambda^{c,1})^2}{\left| \frac{\beta}{\pi} \sin \left(\frac{\pi}{\beta} (\tau_1 - \tau_2) \right) \right|^3}. \quad (5.2.10)$$

Now the contribution to the free energy can be calculated:

$$\begin{aligned} \delta F_{\frac{3}{2}} &\sim \frac{1}{\beta} \int_{-\beta/2}^{\beta/2} \int_{-\beta/2}^{\beta/2} d\tau_1 d\tau_2 \frac{1}{\left| \frac{\beta}{\pi} \sin \left(\frac{\pi}{\beta} (\tau_1 - \tau_2) \right) \right|^3} \\ &= \frac{\pi^3}{\beta^3} \int_0^{\beta/2} d\tau \frac{2}{\sin^3 \left(\frac{\pi}{\beta} \tau \right)} \\ &= 2 \frac{\pi^3}{\beta^2} \int_\epsilon^\infty dx \frac{\sqrt{1+x^2}}{x^3}. \end{aligned} \quad (5.2.11)$$

Here I had to introduce the low temperature cutoff $\epsilon = \arctan \frac{\tau_o}{\beta}$ because the integral diverges in the infrared. For $\epsilon \gg 0$ the integral is finite. To investigate the behavior for small $\epsilon \approx \tau_o T$, I first perform a partial integration:

$$\delta F_{\frac{3}{2}} \sim T^2 \int_{\tau_o T}^\infty dx \frac{1}{x \sqrt{1+x^2}} + T^2 \frac{\sqrt{1+(\tau_o T)^2}}{(\tau_o T)^2}. \quad (5.2.12)$$

The second term just gives contributions of the order T^2 and higher, thus nothing new happens there. For the first term I split the integral into two pieces $[\tau_0 T, 1]$ and $[1, \infty]$, where the latter gives a constant of order unity that multiplies T^2 . For the first piece I expand the integrand in x to determine the infrared behavior:

$$\delta F_{\frac{3}{2}}^{\text{IR}} \sim T^2 \int_{\tau_0 T}^1 dx \left(\frac{1}{x} - 2 + O(x) \right) = T^2 \ln \left(\frac{1}{\tau_0 T} \right) + O(T^2). \quad (5.2.13)$$

This singularity in the free energy also appears in the specific heat:

$$c(T) \sim T \frac{\partial^2}{\partial T^2} F(T) \sim T \ln \frac{1}{\tau_0 T} + O(T). \quad (5.2.14)$$

This is the same distinct non-Fermi liquid behavior that has been found for the TCKM [?] and that for the TIKM has been predicted in Ref. [?], albeit attributed to the wrong irrelevant operator. At this point I would like to emphasize, that this non-Fermi liquid behavior only occurs if particle-hole or parity symmetry are broken. In the symmetric case [?], the lowest dimensional operators that affect the scaling properties have dimension $d = 2$ and give rise only to Fermi liquid contributions.

In order to calculate the magnetic susceptibility

$$\chi = - \frac{\partial^2}{\partial h^2} F(h, T) \Big|_{h=0}, \quad (5.2.15)$$

where h is the z -component of an external magnetic field, I need to take a magnetic field into account in the partition function:

$$Z(h) = e^{-\beta F_*} \left\langle \exp \left(\int_{-\beta/2}^{\beta/2} d\tau H_{\text{scaling}}(\tau) + h \int_{-\beta/2}^{\beta/2} d\tau \int_{-\infty}^{\infty} dx J_z^s(\tau, x) \right) \right\rangle_T. \quad (5.2.16)$$

As before, I perform a cumulant expansion to determine the leading contribution. Only correlation functions proportional to h^2 contribute to the susceptibility.

Physically, it is clear that only fields that contain a non-trivial $SU(2)_2$ component can contribute, because only they can couple to a magnetic field. Formally this comes about by the independence of the four different sectors of the conformal field theory describing the model. Expectation values of independent fields decompose, e.g.

$$\langle J_z^s(\tau_1, x_1) J_z^s(\tau_2, x_2) J\epsilon(\tau_3) \dots J\epsilon(\tau_N) \rangle = \langle J_z^s(\tau_1, x_1) J_z^s(\tau_2, x_2) \rangle \langle J\epsilon(\tau_3) \dots J\epsilon(\tau_N) \rangle. \quad (5.2.17)$$

When cumulants are expressed in terms of ordinary expectation values, terms like the one on the left hand side always appear together with the one on the right hand side, but with opposite sign. Thus all these cumulants vanish. The leading operators containing non-trivial $SU(2)_2$ content are $(\mathbf{J}^s)^2$ and $\mathbf{J}_{-1}^s \cdot \phi$. In the parity symmetric case only the former is allowed. As for the specific heat, it gives rise only to a Fermi liquid like contribution

$$\delta \chi_{\mathbf{J}^2} = \text{const.} + O(T). \quad (5.2.18)$$

If parity symmetry is broken, the operator $\mathbf{J}_{-1}^s \cdot \phi$ gives rise to a logarithmic singularity, similar to the one in the specific heat [?]

$$\delta\chi_{\mathbf{J}_{-1} \cdot \phi} \sim \ln \frac{1}{\tau_o T} + O(T). \quad (5.2.19)$$

5.3 Finite temperature Green's functions

In Ref. [?] it was found that at zero temperature the scattering matrix $S^{(1)}$, which governs the asymptotic behavior of the electron-electron Green's function via

$$G(z_1, z_2) = \langle \psi(z_1) \psi^\dagger(z_2) \rangle \sim \frac{S^{(1)}}{z_1 - z_2}, \quad (5.3.1)$$

vanishes at the critical point. The corrections for finite temperatures are again determined by the scaling dimensions of the leading irrelevant operators. The finite temperature (Matsubara) Green's function is defined as

$$\begin{aligned} G(x_1, \tau_1, x_2, \tau_2) &= - \left\langle \mathsf{T}_\tau \left\{ \psi(x_1, \tau_1) \psi^\dagger(x_2, \tau_2) \right\} \right\rangle \\ &= - \frac{\text{Tr} [e^{-\beta H} \mathsf{T}_\tau \left\{ \psi(x_1, \tau_1) \psi^\dagger(x_2, \tau_2) \right\}]}{\text{Tr} [e^{-\beta H}]} \\ &= - \frac{\text{Tr} [e^{-\beta H_*} \mathcal{S}(\beta, 0) \mathsf{T}_\tau \left\{ \psi(x_1, \tau_1) \psi^\dagger(x_2, \tau_2) \right\}]}{\text{Tr} [e^{-\beta H_*} \mathcal{S}(\beta, 0)]}. \end{aligned} \quad (5.3.2)$$

Here T_τ denotes time ordering in imaginary time τ and

$$\mathcal{S}(\tau, \tau') \equiv e^{\tau H_*} e^{H(\tau' - \tau)} e^{-\tau' H_*} = \mathsf{T}_\tau \left\{ \exp \left(- \int_\tau^{\tau'} d\tau'' H_{\text{scaling}}(\tau'') \right) \right\}. \quad (5.3.3)$$

Expanding the exponential, the first order contribution (in H_{scaling}) to the Green's function is

$$\delta G(\beta, x_1, \tau_1, x_2, \tau_2) = \int_0^\beta d\tau \left\langle H_{\text{scaling}}(\tau) \mathsf{T}_\tau \left\{ \psi(x_1, \tau_1) \psi^\dagger(x_2, \tau_2) \right\} \right\rangle_T \quad (5.3.4)$$

By the same argument as before (eq. ??) the (Virasoro first descendant) operator $L_{-1}\epsilon$ does not give any contributions. In contrast to the thermodynamics, here the primary dim-3/2 operators give contributions in first order. This can be seen by decomposing the correlation function in question into the various sectors. Each fermion field can be written as $\psi(z) = \sigma(z)g(z)h(z)$, where σ is the Ising-field with dimension 1/16, g is a spin-1/2 field of the $SU(2)_1$ WZW-model with dimension 3/16 and h is a $U(1)$ -charge boson of dimension 1/4. The decompositions are

$$\begin{aligned} \langle \mathbf{J}\epsilon(z) \psi(z_1) \psi^\dagger(z_2) \rangle_T &= \langle \epsilon(z) \sigma(z_1) \sigma(z_2) \rangle_T \langle g(z_1) g(z_2) \rangle_T \langle \mathbf{J}(z) h(z_2) h(z_2) \rangle_T \\ \langle \mathbf{J}_{-1} \cdot \phi(z) \psi(z_1) \psi^\dagger(z_2) \rangle_T &= \langle \sigma(z_1) \sigma(z_2) \rangle_T \langle \mathbf{J}_{-1} \cdot \phi(z) g(z_1) g(z_2) \rangle_T \langle h(z_2) h(z_2) \rangle_T. \end{aligned} \quad (5.3.5)$$

CHAPTER 5: EFFECTS OF CHARGE FLUCTUATIONS

All of the correlators on the right hand side are, in general, non-vanishing. Even though these correlation functions are fixed by conformal invariance, i.e.

$$\langle J\epsilon(z)\psi(z_1)\psi^\dagger(z_2)\rangle_T \sim \langle \mathbf{J}_{-1} \cdot \boldsymbol{\phi}(z)\psi(z_1)\psi^\dagger(z_2)\rangle_T \sim \frac{\sin \frac{\pi}{\beta} z_1 - z_2}{(\sin \frac{\pi}{\beta} z - z_1)^{\frac{3}{2}} (\sin \frac{\pi}{\beta} z - z_2)^{\frac{3}{2}}}, \quad (5.3.6)$$

it is still a formidable task to extract the temperature dependence from the integral over this function. However, the same integral also appears for the TCKM where the leading temperature dependence has been found to be [?]

$$\delta G(T) \sim \sqrt{T}. \quad (5.3.7)$$

In terms of physical observables, this scaling behavior will show up in the conductance which is directly proportional to this Green's function.

5.4 Boundary-changing operators

Another interesting physical property that can be calculated very elegantly from the BCFT solution is related to Fermi-edge exponents and the Anderson orthogonality catastrophe. The Fermi-edge problem [?] is concerned with the process where a core electron is suddenly excited into the conduction band, e.g. by an x -ray photon, leaving a hole which serves as a local scattering potential. The ground state of the conduction electrons in the presence of such a potential is orthogonal to the original ground state [?], which causes the system after such a process to decay into its ground state very slowly, typically with a power-law rather than exponentially. By a Fourier transformation the relaxation process is connected to the x -ray absorption/emission spectrum, where the power-law decay shows up as a singularity at the Fermi energy. The exponents that determine the singularity in the x -ray spectrum have been calculated for a variety of systems. Of particular interest are those cases where the system exhibits exotic phases, as for instance the Luttinger liquid [?], or where additional degrees of freedom are involved, e.g. spin in the Kondo/Anderson model [?]. Similar to the TCAM [?], the TIAM falls into both of these categories.

In the device which I propose for a realization of the TIAM a similar process can be realized: By tuning the gate voltages properly, one of the impurities can be effectively removed from the system. The physical system then consists of one single-impurity Anderson model for the first lead and a completely decoupled free electron theory in the second lead. Tuning the gate voltages back to the values for the critical TIAM will reinsert the impurity, and the electrons in *both* channels subsequently rearrange to form the non-Fermi liquid ground state of the TIAM (see Fig. ??). In the language of BCFT,

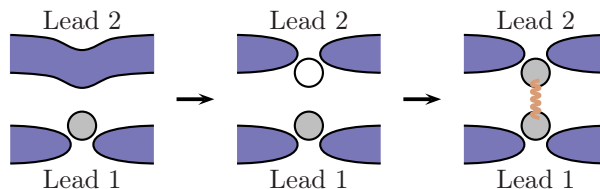


Figure 5.2: One of the physical processes I consider. In the first step there is a SIAM and a decoupled channel of free electrons. In the second step an (empty) dot has been inserted into lead 2. In the last step the system has relaxed to its ground state where the two channels of electrons are coupled via the RKKY interaction between the dots.

the impurities only appear via the boundary condition. The physical process of inserting an impurity at time $t = t_0$, thus corresponds to changing the boundary conditions which can be described by an appropriate *boundary-changing operator* acting on the system

at t_0 . To make this a bit clearer, I introduce the following notation for each of the two channels:

i	—	Free electrons	$\times \mathbb{I}$
i	—●—	Kondo Model	$\times j_i$
i	—○—	Anderson Model	$Q_i \rightarrow Q_i \mp m_i$

Figure 5.3: Notation for the single reservoirs ($i = 1, 2$) and corresponding fusions/redefinitions. Here $m_i \equiv \langle d_i^\dagger d_i \rangle$ is the net charge on the dot.

Note that fusions only effects the gluing conditions and not the expression for the energy, while the reverse is true for redefinitions. Since the system consists of two reservoirs, both must known in order to specify a given system. A remark is in order concerning m_i , the net charge on the dot i when it is decoupled from the other one. It does not have to equal to n_i , the net charge of the same dot at the critical point of the TIKM. In fact, I expect that $n_i \leq m_i$ ($n_i, m_i \in [0, 1]$); since only the singly occupied subspaces participate in the RKKY interactions, the effective RKKY coupling increases with increasing n_i . The RKKY coupling is antiferromagnetic ($K > 0$) and the spin-spin expectation value at the critical point is negative (see Section ??), thus larger values of n_i are energetically favorable. I mark a decoupled system by writing the two subsystems parallel to each other. The system can be connected only by the RKKY interaction which I denote by a red line connecting the impurities, i.e.:

1	—●—	Two-impurity	$\times \sigma$
2	—●—	Kondo Model	
1	—○—	Two-impurity	$\times \sigma, Q_{1,2} \rightarrow Q_{1,2} \mp n_{1,2}$
2	—○—	Anderson Model	

Figure 5.4: Notation for coupled reservoirs and corresponding fusions/redefinitions.

Using this notation, I write the process of adding or removing an impurity at $\tau = \tau_0 = it_0$ as:

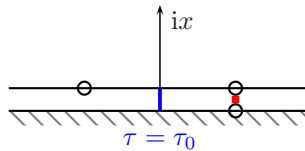


Figure 5.5: Adding an impurity at $\tau = \tau_0$ changes the boundary conditions of the system from that time on.

The quantity that measures how far the system has evolved from its initial state after a time $\Delta\tau$, is given by the Green's function of the (yet undetermined) boundary-changing

operator \mathcal{O} :

$$G(\tau) = \langle 0, I | \mathcal{O}(\tau_0 + \Delta\tau) \mathcal{O}^\dagger(\tau_0) | 0, I \rangle \sim (\Delta\tau)^{-2x}, \quad (5.4.1)$$

where x is the conformal dimension of \mathcal{O} and $|0, I\rangle$ is the initial ground state of the system. The boundary-changing operator is assumed to be a primary field⁴, thus the Green function is fixed to the given asymptotic form by conformal invariance (see eq.??). To relate x to the energy spectrum, I map the half plane onto the infinite strip via the conformal transformation $u + iv = \frac{l}{\pi} \ln(\tau + ix)$ (Fig. ??).

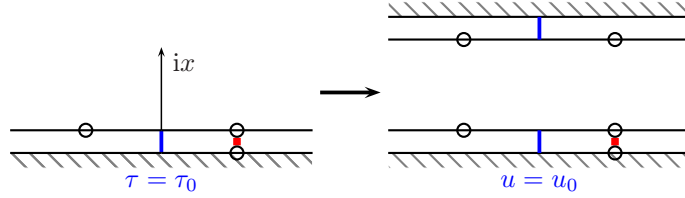


Figure 5.6: Mapping to the strip geometry.

Under this transformation the propagator becomes ($u_0 = \frac{l}{\pi} \ln(\tau_0)$):

$$\langle 0, II | \mathcal{O}(u_0 + \Delta u) \mathcal{O}^\dagger(u_0) | 0, II \rangle = \left(\frac{2l}{\pi} \sinh \frac{\pi}{2l} \Delta u \right)^{-2x}. \quad (5.4.2)$$

Here I denote the ground state of the system on the strip geometry (same boundary condition on both sides) by $|0, II\rangle$. In the limit $\Delta u \gg l$ this becomes

$$\left(\frac{2l}{\pi} \sinh \frac{\pi}{2l} \Delta u \right) \rightarrow \frac{\pi}{l} e^{\frac{\pi}{l} x \Delta u}. \quad (5.4.3)$$

Alternatively, the propagator can also be evaluated in the strip geometry by inserting a complete set of states. Note that since \mathcal{O} changes the boundary conditions, the eigenstates of the system after applying \mathcal{O} are not the same as the ones before (see Fig. ??). I label states with boundary condition I on the top and boundary F on the bottom by $|n, IF\rangle$. These are the eigenstates after applying \mathcal{O} and a complete basis of them should therefore be inserted

$$\begin{aligned} \langle 0, II | \mathcal{O}(u_0 + \Delta u) \mathcal{O}^\dagger(u_0) | 0, II \rangle &= \sum_n \langle 0, II | e^{-H\Delta u} \mathcal{O}(u_0) e^{H\Delta u} | n, IF \rangle \langle n, IF | \mathcal{O}^\dagger(u_0) | 0, II \rangle \\ &= \sum_n |\langle 0, II | \mathcal{O}(u_0) | n, IF \rangle| e^{-\Delta u (E_0^{II} - E_n^{IF})}. \end{aligned} \quad (5.4.4)$$

In the limit of large Δu only the lowest-energy state $|n_0, IF\rangle$ contribute and by comparison with eq. (??) I get:

$$x = \frac{l}{\pi} (E_{n_0}^{IF} - E_0^{II}). \quad (5.4.5)$$

⁴A descendant field has a higher dimension than the primary field from which it is derived and thus decays faster asymptotically.

So far, no particular boundary-changing operator has been specified. Since the scaling dimensions of a boundary-changing operator depend only on the energy of a corresponding state on the strip, with one type of boundary condition at the bottom and another kind of boundary condition on the top, the possible boundary operators are determined by the gluing conditions in this geometry. Using the notation I introduced in the beginning of this chapter (Figures ?? and ??), it is a straightforward task to find the correct boundary operators and their scaling dimensions:

The energy is measured with respect to the ground state of the system with boundary conditions II , the spectrum of which is given by

$$E = E_0 + \frac{\pi}{4l} \left[\sum_{i=1,2} (Q_i - n_i)^2 + j(j+1) + 4\Phi \right], \quad (5.4.6)$$

with the gluing conditions given in Tab. ??. The boundary condition II corresponds to

Table 5.2: Gluing conditions for free fermions

Q_1	Q_2	j	Ising
0	0	0	\mathbb{I}
1/2	0	1/2	σ
0	1/2	1/2	σ
0	0	1	ϵ
1/2	1/2	1	\mathbb{I}
1/2	1/2	0	ϵ

a SIAM and a decoupled channel of free electrons on each side of the strip (Fig. ??). According to Fig. ?? this does not affect the gluing conditions and the redefinitions of

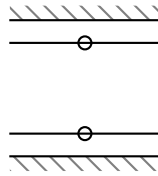


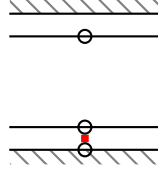
Figure 5.7: Strip with boundary condition II .

the charge cancel: $Q_i \rightarrow Q_i + m_i - m_i = Q_i$. Thus E_0^{II} is equal to the ground-state energy of the free fermion theory E_0 .

For the case IF , the boundary conditions are those of an SIAM and free electrons at the top and those of the TIAM at the bottom of the strip (Fig. ??).

By the Figures ?? and ?? this translates into fusion with σ and the redefinitions $Q_1 \rightarrow Q_1 - n_1 + m_1, Q_2 \rightarrow Q_2 - n_2$. The energy for states with these boundary conditions is

$$E = E_0 + \frac{\pi}{4l} \left[(Q_1 - n_1 + m_1)^2 + (Q_2 - n_2)^2 + j(j+1) + 4\Phi \right], \quad (5.4.7)$$


Figure 5.8: Strip with boundary condition IF .

with the gluing conditions given in Tab. ???. Among these, I exclude the last four by the physical requirement, that inserting the dot in lead 2 does not affect the charge in lead 1⁵. There remain two physically different processes: The inserted impurity may either

Table 5.3: Gluing conditions and energies for the boundary condition IF

Q_1	Q_2	j	Ising	El/π
0	0	0	σ	$\frac{1}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2)$
0	0	1	σ	$\frac{9}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2)$
0	1	1/2	\mathbb{I}	$\frac{7}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2n_2)$
0	1	1/2	ϵ	$\frac{15}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2n_2)$
1	0	1/2	\mathbb{I}	$\frac{7}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2(n_1 - m_1))$
1	1	0	σ	$\frac{9}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2(n_2 + n_1 - m_1))$
1	0	1/2	ϵ	$\frac{15}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2(n_1 - m_1))$
1	1	1	σ	$\frac{17}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2(n_2 + n_1 - m_1))$

have no charge initially, which is described by the first two operators or carry charge one, which is described by the third and fourth. Among these, the first and the third operator always have the lowest dimension for their respective process and will dominate the asymptotic behavior. Their scaling dimensions can be read off from eq. (??) as:

$$x_1(\mathcal{O}_1) = \frac{1}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2), \quad (5.4.8)$$

$$x_3(\mathcal{O}_3) = \frac{7}{16} + \frac{1}{4} ((n_1 - m_1)^2 + n_2^2 - 2n_2). \quad (5.4.9)$$

The Green's function for the boundary-changing operators is

$$G(\tau) = \langle I | \mathcal{O}_i(t_0 + \Delta t) \mathcal{O}_j^\dagger(\tau_0) | I \rangle \sim (\Delta\tau)^{-2x_i} \delta_{i,j}, \quad (5.4.10)$$

where the off-diagonal components are zero due to charge conservation. A smaller value of x_i means that it takes longer for the system to reach its ground state. Note that the time scale for reaching the non-Fermi liquid critical ground state decreases (increases)

⁵As the system relaxes to its ground state, the *net* charge m_1 on the dot will change to n_1 however, as I mentioned earlier.

with increasing n_2 when the $i = 2$ dot is initially empty (occupied). This parallels the property of the Fermi edge singularities in the SIAM, where the X-ray photoemission (X-ray absorption) spectrum gets softer as the impurity valence increases (decreases) [? ?] (For a quick derivation in the BCFT formalism, see Appendix ??). In fact, for $n_1 = m_1$ the exponents that I found for the TIAM (eqs. ?? and ??) differ from those for the SIAM, i.e.

$$\begin{aligned} x_1 &= \frac{1}{4}n^2 \\ x_2 &= \frac{1}{2} + \frac{1}{4}(n^2 - 2n), \end{aligned} \tag{5.4.11}$$

by an additive constant ($1/16$) only. The fact that the final state impurity valence guides the respective processes in similar ways is notable, considering that the SIAM critical ground state is of the Fermi liquid type, while the TIAM critical ground state is not.

Summary

6.1 Spin-orbit effects

As the first of two problems that I have addressed in my thesis, I investigated the effects of spin-orbit interactions on the RKKY interaction in two dimensions, as well as on the SIKM in the low-temperature (strong-coupling) regime and on the TIKM at the quantum critical point. I have derived the form of the RKKY interaction in the presence of both, the Rashba and the Dresselhaus spin-orbit interactions. For the SIKM I have shown that Dresselhaus spin-orbit interactions can be treated in the same way as Rashba spin-orbit interactions and as long as only one of them is present, the qualitative low-energy behavior is not affected. The critical behavior of the TIKM does not change either, except when there is charge transfer between the two channels of conduction electrons. In the presence of charge transfer, I have shown that a marginal operator appears and provided arguments for its interpretation.

I have derived a general formula for the concurrence of two spin-1/2 qubits coupled via interactions that conserve only the z -component of the total spin, and found that the concurrence vanishes at the critical point of the TIKM, as it does in the isotropic case. For the TIKM with spin-orbit interactions away from criticality, I have conjectured an RG-flow diagram using symmetry arguments, limiting cases and analogies to known models.

6.2 Charge fluctuations

As the second project, which I presented in Chapter ??, I have presented a conformal field theory description of the TIAM at quantum criticality and proposed a device to realize it experimentally. I have found a new leading irrelevant operator that is allowed

CHAPTER 6: SUMMARY

only if particle-hole symmetry is broken and shown that it is responsible for non-Fermi liquid scaling of physical observables like the specific heat and the conductance. While non-Fermi liquid behavior has already been predicted for this model in Ref. [?], I have now supplied the operator(s) from which this behavior originates and shown how the occurrence of non-Fermi liquid behavior in the TIAM depends on the presence of particle-hole and/or parity symmetry.

I have also calculated how the exponents, that set the timescale for the build-up of the non-Fermi liquid quantum critical ground state, depend on the amount of charge on the dots and found the trend to be similar to the physically very different single-impurity Anderson model.

Mapping the Kondo model to one dimension

Let us start by considering the simplest example: The single-impurity Kondo model. Its interaction $\sim \delta(x) \mathbf{S} \cdot \psi^\dagger \boldsymbol{\tau} \psi$ has spherical symmetry suggesting¹ an expression of the wave functions in terms of a radial quantum number and spherical harmonics:

$$|E, l, m\rangle = \int d^3k \delta(\epsilon_{\mathbf{k}} - E) \mathcal{Y}_{lm}(\hat{\mathbf{k}}) |\mathbf{k}\rangle = \int dk k \delta(\epsilon_k - E) ||\mathbf{k}\rangle, l, m\rangle. \quad (\text{A.0.1})$$

Here, spin-indices have been suppressed as they are mere spectators for this procedure. Since $\langle \mathbf{r} = 0 | |\mathbf{k}\rangle, l, m\rangle$ is nonzero only for $m = l = 0$ and the interaction is a point interaction at the origin, $|E\rangle \equiv |E, 0, 0\rangle$ are the only states that may contribute. Dropping all the decoupled states, we are left with a one dimensional theory.

Next consider a coordinate system where the impurity lies at some arbitrary position \mathbf{R} but with the quantum numbers still being defined with respect to the origin. Formally this means \mathbf{k}' , valid for the reference system in question, are related to the shifted ones, \mathbf{k} by:

$$\langle \mathbf{r} | \mathbf{k}\rangle = \langle \mathbf{r} - \mathbf{R} | \mathbf{k}'\rangle. \quad (\text{A.0.2})$$

In this case many, in fact infinitely many, angular momentum modes are expected to contribute, namely all those for which $\langle \mathbf{r} | |\mathbf{k}\rangle, l, m\rangle_{\mathbf{r}=\mathbf{R}} \neq 0$. This is somewhat inconvenient, but there is a solution: Noting that the operator \mathbf{k} generates translations we can write

$$\langle \mathbf{r} - \mathbf{R} | \mathbf{k}'\rangle = \langle \mathbf{r} | e^{-i\mathbf{k}\cdot\mathbf{R}} | \mathbf{k}'\rangle. \quad (\text{A.0.3})$$

¹Spherical symmetry is by no means necessary for this reduction scheme, it just serves as a motivation and for a clear physical picture. The necessary and sufficient condition is, that the impurity couples only to a finite set of *bulk* states. The generalization is obtained by replacing l and m by some other set of quantum numbers and $\hat{\mathbf{k}}$ and $|\mathbf{k}|$ by some orthogonal functions of \mathbf{k} . If more than one state couples to the impurity, then an equal number of one-dimensional states will appear in the new theory.

APPENDIX A: MAPPING THE KONDO MODEL TO ONE DIMENSION

Thus $|\mathbf{k}\rangle = e^{-i\mathbf{k}\cdot\mathbf{R}}|\mathbf{k}'\rangle$ and only the zero angular momentum modes of that term will contribute, i.e. of all the

$$|E, l, m\rangle = \int d^3k \delta(\epsilon_{\mathbf{k}} - E) \mathcal{Y}_{lm}(\hat{k}) e^{-i\mathbf{R}\cdot\mathbf{k}} |\mathbf{k}\rangle \quad (\text{A.0.4})$$

only $|E\rangle \equiv |E, 0, 0\rangle$ appears in the Kondo interaction.

Now we have set the ground to treat the general case: Consider N impurities located at the sites \mathbf{R}_i . We can construct a basis for each of the impurity sites:

$$|E, i, l, m\rangle = \int d^3k \delta(\epsilon_{\mathbf{k}} - E) \mathcal{Y}_{lm} e^{-i\mathbf{R}_i\cdot\mathbf{k}} |\mathbf{k}\rangle. \quad (\text{A.0.5})$$

Note that the $|E, i, l, m\rangle$ actually form a basis although they already do so for any fixed $i \in [1, N]$. This is of course possible since the basis is infinite.

For the Kondo effect only the s -waves couple to each single impurity (the generalization to some arbitrary, finite number of states coupling to each impurity should be obvious). The basis given by $|E, i, l, m\rangle$ is not orthogonal, but using standard techniques it is always possible to construct a basis containing all the $|E, i\rangle \equiv |E, i, 0, 0\rangle$ and an infinite set of other states being orthogonal to *each* of the $|E, i\rangle$. All those states couple to neither of the impurities and can thus be safely dropped. What remains is a finite-dimensional basis of one-dimensional fields.

APPENDIX B

Traces over Pauli matrices

To derive the form of the RKKY interaction, it is necessary to perform traces over various combinations of Pauli matrices. This is a straightforward task using the relation

$$(\boldsymbol{\tau} \cdot \mathbf{A})(\boldsymbol{\tau} \cdot \mathbf{B}) = (\mathbf{A} \cdot \mathbf{B}) + i(\mathbf{A} \times \mathbf{B}) \cdot \boldsymbol{\tau}. \quad (\text{B.0.1})$$

from which all necessary formulas can be derived easily. Firstly

$$\text{Tr}[(\boldsymbol{\tau} \cdot \mathbf{A})(\boldsymbol{\tau} \cdot \mathbf{B})] = 2\mathbf{A} \cdot \mathbf{B}, \quad (\text{B.0.2})$$

which is trivial, using the fact that Pauli matrices are traceless. Secondly:

$$\begin{aligned} \text{Tr}[(\boldsymbol{\tau} \cdot \mathbf{A})(\boldsymbol{\tau} \cdot \mathbf{B})\tau_i] &= i(\mathbf{A} \times \mathbf{B}) \cdot \text{Tr}[\boldsymbol{\tau}\tau_i] \\ &= 2i(\mathbf{A} \times \mathbf{B})_i, \end{aligned} \quad (\text{B.0.3})$$

again using the traceless property as well as the relation $\tau_i\tau_j = \delta_{ij} + i\epsilon_{ijk}\tau_k$. A Pauli matrix appearing between the spin operators can of course always be brought into that position using the cyclic property of the trace. Finally I also need the somewhat less trivial relation:

$$\begin{aligned} \text{Tr}[(\boldsymbol{\tau} \cdot \mathbf{A})\tau_j(\boldsymbol{\tau} \cdot \mathbf{B})\tau_i] &= \text{Tr}[(\boldsymbol{\tau} \cdot \mathbf{A})(\mathbf{e}_j \cdot \boldsymbol{\tau})(\boldsymbol{\tau} \cdot \mathbf{B})(\mathbf{e}_i \cdot \boldsymbol{\tau})] \\ &= \text{Tr}[(\mathbf{A} \cdot \mathbf{e}_j + i(\mathbf{A} \times \mathbf{e}_j) \cdot \boldsymbol{\tau})(\mathbf{B} \cdot \mathbf{e}_i + i(\mathbf{B} \times \mathbf{e}_i) \cdot \boldsymbol{\tau})] \\ &= 2A_jB_i - \text{Tr}[(\mathbf{A} \times \mathbf{e}_j) \cdot \boldsymbol{\tau}][(\mathbf{B} \times \mathbf{e}_i) \cdot \boldsymbol{\tau}] \\ &= 2A_jB_i - \sum_{a,b,c,d,k,l} A^a e_j^b B^c e_i^d \epsilon_{abk} \epsilon_{cdl} \text{Tr}[\tau^l \tau^k] \\ &= 2A_jB_i - 2 \sum_{a,b,c,d} A^a \delta_j^b B^c \delta_i^d (\delta_{ac} \delta_{bd} - \delta_{ad} \delta_{bc}) \\ &= 2A_jB_i - 2(\delta_{i,j} \mathbf{A} \cdot \mathbf{B} - A_i B_j) \\ &= -2\delta_{i,j} \mathbf{A} \cdot \mathbf{B} + 2A_i B_j + 2A_j B_i. \end{aligned} \quad (\text{B.0.4})$$

RKKY interaction for $\hat{R} = \hat{x}$

For the case $\hat{R} = \hat{x}$ as discussed in the text (Chapter ??) the Green function is:

$$G = G_0 + G_1\alpha\tau_z - G_1\beta\tau_x \quad (\text{B.0.5})$$

The RKKY interaction is proportional to

$$\text{Tr} [(\mathbf{S}_1 \cdot \boldsymbol{\tau})G(\mathbf{R})(\mathbf{S}_2 \cdot \boldsymbol{\tau})G(-\mathbf{R})]. \quad (\text{B.0.6})$$

Plugging in G and using the formulas derived above, I obtain:

$$\begin{aligned} \text{Tr}[\dots] &= G_0^2 \text{Tr} [(\mathbf{S}_1 \cdot \boldsymbol{\tau})(\mathbf{S}_2 \cdot \boldsymbol{\tau})] \\ &\quad + G_0 G_1 \text{Tr} [(\mathbf{S}_1 \cdot \boldsymbol{\tau})(\mathbf{S}_2 \cdot \boldsymbol{\tau}) (-\alpha\tau_z + \beta\tau_x)] \\ &\quad + G_0 G_1 \text{Tr} [(\mathbf{S}_2 \cdot \boldsymbol{\tau})(\mathbf{S}_1 \cdot \boldsymbol{\tau}) (+\alpha\tau_z - \beta\tau_x)] \\ &\quad + G_1^2 \text{Tr} [(\mathbf{S}_1 \cdot \boldsymbol{\tau}) (-\alpha\tau_z + \beta\tau_x) (\mathbf{S}_2 \cdot \boldsymbol{\tau}) (+\alpha\tau_z - \beta\tau_x)] \\ &= 2G_0^2 \mathbf{S}_1 \cdot \mathbf{S}_2 \quad (\text{B.0.7}) \\ &\quad - 4G_0 G_1 i\alpha (\mathbf{S}_1 \times \mathbf{S}_2)^z + 4i\beta (\mathbf{S}_1 \times \mathbf{S}_2)^x \\ &\quad + 2G_1^2 \alpha^2 (\mathbf{S}_1 \cdot \mathbf{S}_2 - 2S_1^z S_2^z) \\ &\quad + 2G_1^2 \beta^2 (\mathbf{S}_1 \cdot \mathbf{S}_2 - 2S_1^x S_2^x) \\ &\quad + 4G_1^2 \alpha\beta (S_1^x S_2^z + S_1^z S_2^x). \end{aligned}$$

Second quantization of Rashba and Dresselhaus interactions

The Hamiltonian for Rashba and Dresselhaus spin-orbit interactions in two dimensions, which I take as the x - y plane, is (see eqs. ?? and ??):

$$H_{s-o} = (\kappa k^x + \lambda k^y) \tau^y - (\kappa k^y + \lambda k^x) \tau^x. \quad (\text{C.0.1})$$

The second quantized Hamiltonian is given by:

$$H_{s-o}^{2\text{nd}} = \int dk \int dk' \sum_{m,m'} \langle k, m, \sigma | H_{s-o} | k', m', \sigma' \rangle \psi_{k,m}^{\dagger\sigma} \psi_{k',m',\sigma'}, \quad (\text{C.0.2})$$

where the states are labeled by total momentum $k = \sqrt{(k^z)^2 + (k^x)^2}$ and the orbital quantum number m . The matrix elements are

$$\begin{aligned} \langle k, m, \sigma | H_{s-o} | k', m', \sigma' \rangle &= (\tau^+)_{\sigma}^{\sigma'} \langle k, m | (-\kappa k^y + \lambda k^x) + i(\lambda k^y + \kappa k^x) | k', m' \rangle \\ &\quad - (\tau^-)_{\sigma}^{\sigma'} \langle k, m | ((\lambda k^x + \kappa k^y) - i(\kappa k^x + \lambda k^y)) | k', m' \rangle, \end{aligned} \quad (\text{C.0.3})$$

where $\tau^{\pm} = \frac{1}{2}(\tau^x \mp i\tau^y)$ are the spin raising operators. I insert a complete basis of states $\int_0^{\infty} dr \int_0^{2\pi} d\phi |r, \phi\rangle \langle r, \phi|$ to write the momentum operators in polar coordinates, i.e. $k_x = k \sin \phi$ and $k_y = k \cos \phi$. Noting that

$$\langle r, \phi | k_y \mp i k_x | k, m \rangle = \langle r, \phi | k e^{\mp i\phi} | k, m \rangle = \langle r, \phi | k L_{\pm} | k, m \rangle, \quad (\text{C.0.4})$$

where L_{\pm} are the ladder operators for angular momentum in 2D, I remove the complete basis again to obtain the matrix elements

$$\begin{aligned} \langle k, m, \sigma | H_{s-o} | k', m', \sigma' \rangle &= -k\delta(k - k') \left(\kappa \left((\tau^-)_{\sigma}^{\sigma'} \langle m | L_+ | m' \rangle + (\tau^+)_{\sigma}^{\sigma'} \langle m | L_- | m' \rangle \right) \right. \\ &\quad \left. + i\lambda \left((\tau^-)_{\sigma}^{\sigma'} \langle m | L_- | m' \rangle + (\tau^+)_{\sigma}^{\sigma'} \langle m | L_+ | m' \rangle \right) \right). \end{aligned} \quad (\text{C.0.5})$$

APPENDIX C: SECOND QUANTIZATION OF RASHBA AND DRESSELHAUS INTERACTIONS

The 2nd quantized Hamiltonian can thus be written as

$$H_{s-o}^{2\text{nd}} = \int dk \sum_m k \left(\kappa \psi_{k,m+1}^{\dagger\sigma} (\tau^+)_{\sigma}^{\sigma'} \psi_{k,m,\sigma'} + i\lambda \psi_{k,m-1}^{\dagger\sigma} (\tau^-)_{\sigma}^{\sigma'} \psi_{k,m,\sigma'} \right) + h.c. \quad (\text{C.0.6})$$

Kondo model in the presence of Dresselhaus or Rashba interactions

The Hamiltonian for the 2D Kondo Model in the presence of Rashba or Dresselhaus spin-orbit interactions in two dimensions can be written as:

$$H = H_{\text{kin}} + H_{s-o} + H_{\text{Kondo}}, \quad (\text{D.0.1})$$

where (see previous section)

$$\begin{aligned} H_{\text{kin}} &= \int dk \sum_m \sum_{\sigma=\uparrow,\downarrow} \epsilon_k \psi_{k,m}^{\dagger\sigma} \psi_{k,m,\sigma} \\ H_{s-o} &= \int dk \sum_m k \left(\kappa \psi_{k,m+1}^{\dagger\sigma} (\tau^+)_{\sigma}^{\sigma'} \psi_{k,m,\sigma'} + i\lambda \psi_{k,m-1}^{\dagger\sigma} (\tau^-)_{\sigma}^{\sigma'} \psi_{k,m,\sigma'} \right) + h.c. \\ H_{\text{Kondo}} &= J \int dk \int dk' \sum_{\sigma,\sigma'=\uparrow,\downarrow} \psi_{k,0}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{k',0,\sigma'} \cdot \mathbf{S}. \end{aligned} \quad (\text{D.0.2})$$

To diagonalize the spin-orbit part, I define new fields as

$$\begin{aligned} \psi_{k,m,\uparrow,\pm} &= \frac{1}{\sqrt{2}} \left(\psi_{k,\uparrow,m} \pm i^{\frac{1}{2}(n-1)} \psi_{k,\downarrow,m+n} \right) \\ \psi_{k,m,\downarrow,\pm} &= \frac{1}{\sqrt{2}} \left(\psi_{k,\downarrow,m} \pm i^{\frac{1}{2}(n-1)} \psi_{k,\uparrow,m-n} \right), \end{aligned} \quad (\text{D.0.3})$$

where $n = 1$ in the Rashba case and $n = -1$ in the Dresselhaus case. In terms of these fields, the three terms of the Hamiltonian (??) are

$$\begin{aligned} H_{\text{kin}} &= \int dk \sum_m \sum_{f=\pm} \sum_{\sigma=\uparrow,\downarrow} \epsilon_k \psi_{k,m,f}^{\dagger\sigma} \psi_{k,m,\sigma,f} \\ H_{s-o} &= \mu \int dk k \sum_m \sum_{f=\pm} \sum_{\sigma=\uparrow,\downarrow} f \psi_{k,m,f}^{\dagger\sigma} \psi_{k,m,\sigma,f} \\ H_{\text{Kondo}} &= \frac{J}{2} \int dk \int dk' \sum_{\sigma,\sigma'=\uparrow,\downarrow} \sum_{f,f'=\pm} \psi_{k,0,f}^{\dagger\sigma} \boldsymbol{\tau}_{\sigma}^{\sigma'} \psi_{k',0,\sigma',f'} \cdot \mathbf{S}, \end{aligned} \quad (\text{D.0.4})$$

APPENDIX D: KONDO MODEL IN THE PRESENCE OF DRESSELHAUS OR RASHBA INTERACTIONS

where $\mu = \kappa$ if the spin-orbit interactions are of the Rashba type and $\mu = \lambda$ if they are of the Dresselhaus type. Since all terms are diagonal in m and only the $m = 0$ fields take part in the Kondo interaction, I can drop all other fields from the description. I will also suppress the m quantum number which is always zero from here on to lighten the notation. Defining $\epsilon_k^\pm = \epsilon_k \pm k$, I combine H_{kin} and H_{s-o} to

$$\tilde{H}_{\text{kin}} = \int dk \sum_{f,\sigma} \epsilon_k^f \psi_{k,f}^{\dagger\sigma} \psi_{k,\sigma,f}. \quad (\text{D.0.5})$$

I now define a final set of fields as

$$\psi_{E,\sigma,f} = \frac{1}{\int dk \delta(E - \epsilon_k^f)} \int dk \delta(E - \epsilon_k^f) \psi_{k,\sigma,f}. \quad (\text{D.0.6})$$

Calling $N^f(E) = \int dk \delta(E - \epsilon_k^f)$, the final Hamiltonian is

$$H = \sum_{f,\sigma} \int dE E \psi_{E,f}^{\dagger\sigma} \psi_{E,f,\sigma} + \frac{J}{2} \int dE \int dE' \sum_{f,f',\sigma,\sigma'} N^f(E) N^{f'}(E') \psi_{E,f}^{\dagger\sigma} \tau_\sigma^{\sigma'} \psi_{E',f',\sigma'}. \quad (\text{D.0.7})$$

Concurrence related calculations

E.1 Eigenvalues for the concurrence formula

To calculate the concurrence it is necessary to determine the eigenvalues of $M \equiv \rho_{12}^{\text{magic}} \rho_{12}^{\text{magic}*}$, where (see eq.??)

$$\rho_{12}^{\text{magic}} = \begin{pmatrix} \frac{1}{4} + H + 2I & -iX^+ & 0 & 0 \\ iX^+ & \frac{1}{4} + H + 2I & 0 & 0 \\ 0 & 0 & \frac{1}{4} + H - 4I & D + iX^- \\ 0 & 0 & D - iX^- & \frac{1}{4} - 3H \end{pmatrix}. \quad (\text{E.1.1})$$

Since ρ_{12}^{magic} is block diagonal in $S_z = \pm 1$ and $S_z = 0$, it is only necessary to solve quadratic equations to obtain the eigenvalues. The upper block ($S_z = \pm 1$) of $\rho_{12}^{\text{magic}} \rho_{12}^{\text{magic}*}$, call it M_1 is diagonal, thus the eigenvalues can be read off immediately:

$$M_1 = \begin{pmatrix} (1/4 + H + 2I)^2 - (X^+)^2 & 0 \\ 0 & (1/4 + H + 2I)^2 - (X^+)^2 \end{pmatrix}. \quad (\text{E.1.2})$$

The lower block ($S_z = 0$), call it M_0 is:

$$M_0 = \begin{pmatrix} (\frac{1}{4} + H - 4I)^2 + (D + iX^-)^2 & (D + iX^-)(\frac{1}{4} - 3H) + (D - iX^-)(\frac{1}{4} + H - 4I) \\ (D + iX^-)(\frac{1}{4} - 3H) + (D - iX^-)(\frac{1}{4} + H - 4I) & (\frac{1}{4} - 3H)^2 + (D - iX^-)^2 \end{pmatrix}. \quad (\text{E.1.3})$$

The characteristic polynomial of M_0 is

$$P(\lambda) = \lambda^2 - p\lambda + q, \quad (\text{E.1.4})$$

where:

$$\begin{aligned} p &= \text{tr}M_0 = (1/4 + H - 4I)^2 + (D + iX^-)^2 + (1/4 - 3H)^2 + (D - iX^-)^2 \\ &= 2 \left(D^2 - (X^-)^2 + (2I - 2H)^2 + (2I + H - 1/4)^2 \right) \end{aligned} \quad (\text{E.1.5})$$

APPENDIX E: CONCURRENCE RELATED CALCULATIONS

and

$$\begin{aligned}
q = \det M_0 &= \left((1/4 + H - 4I)^2 + (D + iX^-)^2 \right) \left((1/4 - 3H)^2 + (D - iX^-)^2 \right) \\
&\quad - \left((D + iX^-)(1/4 - 3H) + (D - iX^-)(1/4 + H - 4I) \right)^2 \\
&= \left((2I - 2H)^2 - (2I + H - 1/4)^2 + D^2 + (X^-)^2 \right)^2.
\end{aligned} \tag{E.1.6}$$

The solutions to $P(\lambda) = 0$ are

$$\begin{aligned}
\lambda_{\pm} &= -\frac{p}{2} \pm \sqrt{\frac{p^2}{4} - q} \\
&= D^2 - (X^-)^2 + (2I - 2H)^2 + (2I + H - 1)^2 \pm 2\sqrt{\left((2I - 2H)^2 + D^2 \right) \left((2I + H - 1)^2 - (X^-)^2 \right)}.
\end{aligned} \tag{E.1.7}$$

E.2 Concurrences of various states

To calculate the concurrence for a given density matrix by the formula I derived, it is necessary to calculate spin-expectation values. In the magic basis the involved operators are:

$$\begin{aligned}
S_1^z S_2^z - S_1^x S_2^x &= \frac{1}{4} \text{diag}(0, 2, -2, 0) \\
\mathbf{S}_1 \cdot \mathbf{S}_2 &= \frac{1}{4} \text{diag}(1, 1, 1, -3) \\
S_1^x S_2^y - S_1^y S_2^x &= \frac{1}{4} \text{diag} \left(\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -2 \\ -2 & 0 \end{pmatrix} \right).
\end{aligned} \tag{E.2.1}$$

The singlet state (eq. ??) in the magic basis is

$$\rho_{\text{singlet}}(\theta) = \text{diag} \left(\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} \sin^2 \frac{\theta}{2} & \frac{1}{2} \sin \theta \\ \frac{1}{2} \sin \theta & \cos^2 \frac{\theta}{2} \end{pmatrix} \right). \tag{E.2.2}$$

It is now a simple task to multiply $\rho_{\text{singlet}}(\theta)$ with the matrices in eq. (??) and take the trace to obtain the parameters H, I and D as defined in eq. (??):

$$\begin{aligned}
H_{\text{singlet}}(\theta) &= \frac{1}{3} \text{Tr} [\mathbf{S}_1 \cdot \mathbf{S}_2 \rho_{\text{singlet}}(\theta)] = \frac{1}{12} \text{Tr} \left[\begin{pmatrix} \sin^2 \frac{\theta}{2} & \frac{1}{2} \sin \theta \\ \frac{3}{2} \sin \theta & -3 \cos^2 \frac{\theta}{2} \end{pmatrix} \right] = \frac{1}{12} \sin^2 \frac{\theta}{2} - \frac{1}{4} \cos^2 \frac{\theta}{2} \\
I_{\text{singlet}}(\theta) &= \frac{1}{3} \text{Tr} [(S_1^z S_2^z - S_1^x S_2^x) \rho_{\text{singlet}}(\theta)] = \frac{1}{12} \text{Tr} \left[\begin{pmatrix} -2 \sin^2 \frac{\theta}{2} & -\sin \theta \\ 0 & 0 \end{pmatrix} \right] = -\frac{1}{6} \sin^2 \frac{\theta}{2} \\
D_{\text{singlet}}(\theta) &= \text{Tr} [(S_1^x S_2^y - S_1^y S_2^x) \rho_{\text{singlet}}(\theta)] = \frac{1}{4} \text{Tr} \left[\begin{pmatrix} -\sin \theta & -2 \cos^2 \frac{\theta}{2} \\ -2 \sin^2 \frac{\theta}{2} & -\sin \theta \end{pmatrix} \right] = -\frac{1}{2} \sin \theta.
\end{aligned} \tag{E.2.3}$$

As I mentioned before (see Section ??), it is not necessary to calculate the parameter D to determine the concurrence, I chose to still give it for completion. calculate the concurrence, the values of λ_1 and $\lambda_+ - \lambda_-$ (eq. ??) are needed. They are:

$$\begin{aligned}
\lambda_1 &= \frac{1}{4} + H + 2I = \frac{1}{4} - \frac{1}{4} \cos^2 \frac{\theta}{2} - \frac{1}{4} \sin^2 \frac{\theta}{2} = 0 \\
\lambda_+ - \lambda_- &= 2 \left| -\frac{1}{4} + H + 2I \right| = \frac{1}{4} + \frac{1}{4} \cos^2 \frac{\theta}{2} + \frac{1}{4} \sin^2 \frac{\theta}{2} = 1.
\end{aligned} \tag{E.2.4}$$

APPENDIX E: CONCURRENCE RELATED CALCULATIONS

By eq. (??) this means that the concurrence for the singlet state is one, independent of θ , i.e. the singlet state is always maximally entangled. The Ising doublet (eq. ??) has the density matrix

$$\rho_{\text{doublet}} = \text{diag}(1/2, 1/2, 0, 0). \quad (\text{E.2.5})$$

By inspection the parameters are $H_{\text{doublet}} = I_{\text{doublet}} = 1/12$, $D_{\text{doublet}} = 0$, which implies $\lambda_1 = 1/2$ and $\lambda_+ - \lambda_- = 0$, thus the concurrence is zero.

The parameters for $\rho_{\text{triplet}}(\theta)$ can easily be obtained from the ones of $\rho_{\text{singlet}}(\theta)$ and ρ_{doublet} since all those density matrices as well as the spin-operators are block diagonal. They are

$$\begin{aligned} H_{\text{triplet}}(\theta) &= \frac{1}{3}H_{\text{singlet}}(\theta + \frac{\pi}{2}) + \frac{2}{3}H_{\text{doublet}} = \frac{1}{18} + \frac{1}{36}\cos^2\frac{\theta}{2} - \frac{1}{12}\sin^2\frac{\theta}{2} \\ I_{\text{triplet}}(\theta + \frac{\pi}{2}) &= \frac{1}{3}I_{\text{singlet}}(\theta) + \frac{2}{3}I_{\text{doublet}} = \frac{1}{18}\left(1 - \cos^2\frac{\theta}{2}\right) \\ D_{\text{triplet}}(\theta + \frac{\pi}{2}) &= \frac{1}{3}D_{\text{singlet}}(\theta) + \frac{2}{3}D_{\text{doublet}} = -\frac{1}{6}\cos\theta. \end{aligned} \quad (\text{E.2.6})$$

From this $\lambda_1 = \lambda_+ - \lambda_- = 1/3$ and the concurrence is zero. The state at the TIKM critical point is (see eq. ??)

$$\rho_{\text{Kondo}}(\theta) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \sin^2\frac{\theta}{2} & \frac{1}{2}\sin\theta \\ 0 & 0 & \frac{1}{2}\sin\theta & \cos^2\frac{\theta}{2} \end{pmatrix} \quad (\text{E.2.7})$$

The parameters are

$$\begin{aligned} H_{\text{triplet}}(\theta) &= \frac{1}{2}H_{\text{singlet}}(\theta) + \frac{1}{8} = \frac{1}{8}\left(1 + \frac{1}{3}\sin^2\frac{\theta}{2} - \cos^2\frac{\theta}{2}\right) \\ I_{\text{triplet}}(\theta) &= \frac{1}{2}I_{\text{singlet}}(\theta) = -\frac{1}{12}\sin^2\frac{\theta}{2} \\ D_{\text{triplet}}(\theta) &= \frac{1}{2}D_{\text{singlet}}(\theta) = -\frac{1}{4}\sin\theta. \end{aligned} \quad (\text{E.2.8})$$

This implies $\lambda_1 = \frac{1}{4}$ and $\lambda_+ - \lambda_- = \frac{1}{2}$. The concurrence $C = \max\{0, \lambda_+ - \lambda_- - 2\lambda_1\}$ vanishes for these values. It should be noted that in the previous cases, i.e. the doublet and the triplet, the difference $\lambda_+ - \lambda_- - 2\lambda_1$ was always a finite, negative, number and the concurrence vanished by virtue of taking the maximum with zero. In this case the difference of the λ s is zero itself, which means that a small deviation from this state could lead to a non-zero value for the concurrence. In other words, the point where the concurrence first vanishes marks the fixed-point.

Fermi-edge exponents of the SIAM

In the notation of Section ?? the process of removing the impurity is described by Figure ?. According to Figure ?? there is no fusion of conformal towers, thus the boundary-changing operators have free-electron quantum numbers, i.e.

$$\begin{aligned} (Q = 0, j = 0) \\ (Q = 1, j = 1/2). \end{aligned} \tag{F.0.1}$$

On the strip with the SIAM boundary condition at the bottom and the free-electron

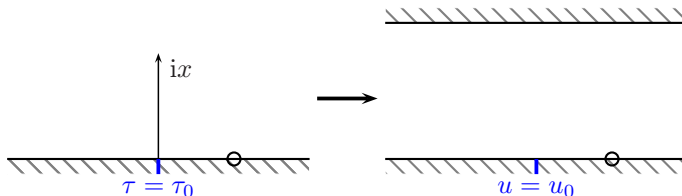


Figure F.1: Boundary changing process in the SIAM.

boundary condition at the top (right hand side of Figure ?? for $u > u_0$), the energy spectrum is

$$E = E_0 + \frac{\pi}{l} \left(\frac{j(j+1)}{3} + \frac{(Q-n)^2}{4} \right), \tag{F.0.2}$$

where n is the average amount of charge on the impurity and E_0 is the ground-state energy of free electrons. The scaling dimensions of the two boundary changing operators are determined by the energy via eq. (??):

$$\begin{aligned} x_1(Q = 0, j = 0) &= \frac{1}{4}n^2 \\ x_2\left(Q = 1, j = \frac{1}{2}\right) &= \frac{1}{2} + \frac{1}{4}(n^2 - 2n). \end{aligned} \tag{F.0.3}$$

Paper

David F. Mross and Henrik Johannesson, “The Two-Impurity Anderson Model at Quantum Criticality”, arXiv:0712.2868 (submitted for publication).