Flow equation solution of the Kondo model with nontrivial density of states

Diplomarbeit

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Contents

Introduction

One of the fundamental problems in condensed matter theory is the analysis of many-particle systems. Though the basic features of most systems can be modeled in one- and two-body interactions, there also exist collective excitations which can only be described in a many-particle framework. Another difficulty appears in the case of strongly correlated systems: While for weak correlations mean-field or perturbative approaches lead to quite accurate results, these usually fail for strong-coupled systems. There is great interest in analytic tools that allow studying both many-particle phenomena and strong correlations. Unfortunately most analytic methods (e.g. the Bethe ansatz) are restricted to integrable models. By using the flow equation approach we are able to study the properties of strong-correlated systems in a controlled systematic expansion, even for nonintegrable perturbations. Though the ground state properties of these systems can often be derived by assuming a constant density of states, the properties at higher energies can usually only be accessed by taking the full density of states into account.

In this thesis the Kondo model with nontrivial density of states will be investigated. The latter describes the coupling of a conduction band to a single magnetic impurity. Another interesting application is the dynamical mean-field theory (DMFT): Within DMFT correlated lattice problems are reduced to an Anderson impurity or a Kondo model with nontrivial density of states.

Though there has been large theoretical activity on this topic during the last decades, a complete analytic description is still missing. In 1964 Kondo could show using perturbation theory that for a constant density of states the resistivity of such systems diverges proportional to $\ln(k_B T)$ at low temperatures. Though this result implicates the existence of resistance minima at low temperatures as observed in earlier experiments, including higher order terms did not lead to a convergence. It turned out that the calculation is only valid for temperatures larger than the Kondo temperature, which is given by the typical low energy scale of the system. (In earlier publications the Kondo temperature was also defined as the temperature at which Kondo's solution diverges.)

In a series of subsequent publications Anderson et al. (1969-1970) could show using perturbative scaling that for antiferromagnetic coupling of the impurity spin to the conduction band the coupling constant (constant density of states) grows continuously and eventually diverges. Though this calculation is also valid for temperatures lower than the Kondo temperature, the solution cannot be considered as a consistent description due to its divergence.

Also nonperturbative methods have been developed or extended to study the Kondo model like Wilson's numerical renormalization group (NRG) in 1975 or Bethe ansatz techniques (1983). Though these methods were able to describe the properties of the Kondo model with constant density of states in a satisfying way, the extension to nonintegrable perturbations was either impossible due to the construction of the method (Bethe ansatz) or could only be done in a purely numerical way (NRG).

To fill this gap we will use Wegner's flow equation method to study the Kondo model. The Kondo model with constant density of states has already been solved by Hofstetter and Kehrein (2001): In the strong-coupling regime the Hamiltonian of the anisotropic Kondo model (constant density of states) can be mapped to an effective low energy Hamiltonian of the noninteracting resonant level model (RLM), which can be solved exactly. In this thesis we will extend the latter solution to nontrivial densities of states by separating the coupling function in a momentum independent part (corresponding to a constant density of states) and a second part containing the momentum dependency as a small (nonintegrable) perturbation. We will show that by using the flow equation method we are able to map the Hamiltonian of the Kondo model with nontrivial density of states to an effective low energy Hamiltonian with constant density of states. In the strong-coupling regime the latter Hamiltonian can again be mapped to an effective RLM-Hamiltonian and thereby solved exactly.

Remarkably this calculation provides the first systematic analytic description of the Kondo model with nontrivial density of states. In contrast to earlier approaches the correct low temperature properties can be derived.

Outline

In Chapter 1 we introduce the Kondo Hamiltonian, which will be the subject of this thesis. We will also give a brief introduction into the bosonization of 1-D fermion systems (essentially based on a recent review) and present the main concepts of the flow equation approach. We will also briefly review the connection between the density of states and the hybridization function in the Kondo model.

The flow equation solution of the anisotropic Kondo model with momentum independent couplings will be reviewed in Chapter 2. We will show in detail the bosonization of the model Hamiltonian and its diagonalization using the flow equation method. The interaction will be rewritten in terms of vertex operators with a scaling dimension that depends on the longitudinal coupling. We will show that (for not too large initial couplings) the scaling dimension always flows towards the Toulouse point and that in the strong-coupling regime the latter is a fixed point of this approach. Furthermore the used operator product expansions become exact at the Toulouse point, thereby avoiding the usual strong-coupling divergence.

In Chapter 3 we will extend the earlier flow equation solution of the anisotropic Kondo model for constant densities of states to nontrivial ones. This chapter provides the original part of this thesis. We will separate the Hamiltonian into a part with constant couplings and another one containing the momentum dependency as a small perturbation. Thereby only the additional flow induced by the latter corrections has to be derived.

The derived flow equations will be analyzed in Chapter 4. We will discuss the effect of a small change in the density of states for systems with nonzero densities of states at the Fermi level. Furthermore we will shortly discuss large corrections and also solve the Kondo model with constant density of states using its fermionic representation.

1 Model and method

1.1 The Kondo model

In the 1930s resistivity minima were found in certain "pure" nonmagnetic metals at low temperatures. Though it turned out soon that this effect was caused by a small amount of magnetic impurities, the theoretical description took its time. Using the Kondo model (originally introduced by Zener in 1951 [1])

$$H = \sum_{p,\alpha} \epsilon_p c^\dagger_{p\alpha} c_{p\alpha} + \sum_{p,q,\alpha,\beta} \frac{J(p,q)}{L} \mathbf{S} \cdot c^\dagger_{p\alpha} \sigma_{\alpha\beta} c_{q\beta}, \tag{1.1}$$

Kondo showed in 1964 [2] that for small antiferromagnetic couplings and a constant density of states (implying $J(p,q) \equiv J$) the resistivity calculated in perturbation theory diverges proportional to $J^3 \ln(k_B T/D)$ at low temperatures. Here $c^{(\dagger)}_{k\alpha}$ are the creation and annihilation operators for the Bloch states of wave-vector k and spin α. $\mathbf{S}$ denotes the impurity spin-$\frac{1}{2}$ operator, $\sigma_{\alpha\beta}$ is the Pauli operator for conduction band electrons, k_B is Boltzmann's constant, L is the system size and D is the system band width [3]. Please note that the Kondo model can be derived from the Anderson impurity model by the Schrieffer-Wolff transformation [4] (see also Section 1.3). The exchange is assumed to be SU(2)-invariant.

The Kondo model (1.1) describes the coupling of a magnetic impurity to a conduction band (see Fig. 1.1). While the latter is represented by the kinetic energy term the impurity only enters the Hamiltonian via the interaction part. In the Kondo regime the impurity level is singly occupied and its ground state is degenerate due to the spin degree of freedom. The Hamiltonian is constructed in such a way that it does not lead out of this subspace. There exist two possible interactions: the spin of the scattered conduction band electron can flip (spin-flip scattering) or it stays unchanged (longitudinal scattering). It turns out that the so-called Kondo effect (the existence of a resistance minimum) is induced by the spin-flip scattering of the conduction band electrons at the impurity site, leading to the creation of a *spin compensation cloud* surrounding the impurity site and screening its induced magnetic moment.

In a subsequent series of publications ([5],[6] and [7]) Anderson et al. were able to obtain the correct low temperature physics of the Kondo model using a perturbative scaling approach. But in the antiferromagnetic case the coupling

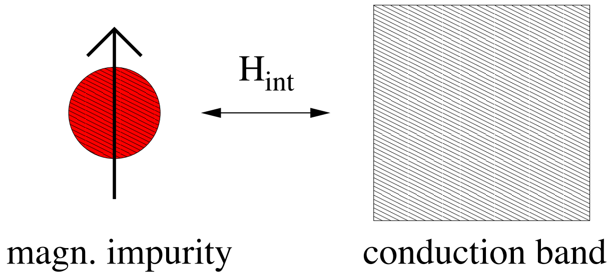


Figure 1.1: Coupling of a magnetic impurity to a conduction band.

constant grows continuously and eventually diverges. Thereby the transition between weak- and strong-coupling cannot be studied in a consistent way by using this method. Nonperturbative methods like Wilson's numerical renormalization group (NRG) [8] and Bethe ansatz [9] led to a quantitative understanding of the strong-coupling regime. For a complete introduction into the physics of the Kondo model see e.g. [10].
Most analytic methods require the integrability of the Kondo model. Using the flow equation approach we are also able to study nonintegrable perturbations, which provides the main motivation for this work.

In the following we will use the *anisotropic* Kondo Hamiltonian

$$\begin{aligned} H &= \sum_{p,\alpha} \epsilon_p c^\dagger_{p\alpha} c_{p\alpha} + \sum_{p,q,\alpha,\beta} \frac{J_\parallel(p,q)}{L} c^\dagger_{p\alpha} \sigma^z_{\alpha\beta} c_{q\beta} S^z + \\ &\quad + \sum_{p,q,\alpha,\beta} \frac{J_\perp(p,q)}{2L} \left(c^\dagger_{p\alpha} \sigma^+_{\alpha\beta} c_{q\beta} S^- + \text{h.c.} \right), \end{aligned} \tag{1.2}$$

which is a generalized form of Eq. (1.1). As pointed out by Toulouse in 1969 [11], for $J_\parallel = 2\pi\left(2-\sqrt{2}\right)$, $J_\parallel \gg |J_\perp|$, (the so called *Toulouse point*, $J_{\parallel/\perp}(p,q) \equiv J_{\parallel/\perp}$) the Kondo model is equivalent to the noninteracting resonant level model (Anderson impurity model without spin), which can be solved exactly. Its low energy scale is given by the Anderson width of the resonant level. The latter provides a suitable definition of the *Kondo temperature* as the typical low energy scale of the system.

Sometimes the Kondo temperature is also defined as the temperature of the resistivity minimum. But this definition takes the influence of phonons (and possible other excitations) on the resistivity into account, which are not included in the Kondo Hamiltonian.

To avoid the typical strong coupling divergence (see e.g. [5]), we will use a partial bosonized form of Eq. (1.2) to analyze the properties of the Kondo Model.

We will also show below that the Toulouse point is a fixed point of our approach.

To solve the Hamiltonian (1.2) we will use the flow equation solution of the anisotropic Kondo Hamiltonian with momentum independent couplings $J_{\parallel/\perp}(p,q) \equiv J_{\parallel/\perp}$ by Hofstetter and Kehrein ([12],[13]) and calculate the corrections for a nontrivial density of states in terms of a small "perturbation" proportional to $J_{\parallel/\perp}(p,q) - J_{\parallel/\perp}(0,0)$, which vanishes at the Fermi level.

1.2 Flow equations

It is an attractive goal to solve physical problems by the explicit diagonalization of the system Hamiltonian H. We will transform the Hamiltonian by a series of unitary transformations:

$$H(B) = U(B)HU^\dagger(B), \tag{1.3}$$

where $H(B=\infty)$ is the diagonalized Hamiltonian, $H(B=0)=H$ the initial Hamiltonian and $U(B)$ an unitary operator ($U^\dagger(B) = U^{-1}(B)$). The *flow parameter* B determines the sequence of the transformations. Here we will use the *flow equation* approach introduced by Wegner (1994) [14] (independently introduced in 1993 by Głazek and Wilson, *similarity renormalization scheme* [15]).
The unitary transformation is constructed by using the differential formulation of Eq. (1.3):

$$\boxed{\frac{dH(B)}{dB} = [\eta(B), H(B)],} \tag{1.4}$$

where $\eta(B) = -\eta^\dagger(B)$ is an anti-Hermitian generator. Using the ansatz [16]

$$\eta(B) = \frac{dU(B)}{dB}U^\dagger(B) \tag{1.5}$$

one finds

$$\begin{aligned}
\frac{dH(B)}{dB} &= \eta(B)H(B) + H(B)\eta^\dagger(B) \\
&\overset{(1.3),(1.5)}{=} \frac{dU(B)}{dB}U^\dagger(B)U(B)HU^\dagger(B) + \\
&\quad +U(B)HU^\dagger(B)U(B)\frac{dU^\dagger(B)}{dB} \\
&= \frac{d}{dB}\left(U(B)HU^\dagger(B)\right).
\end{aligned} \tag{1.6}$$

The integration of Eq. (1.5) leads to

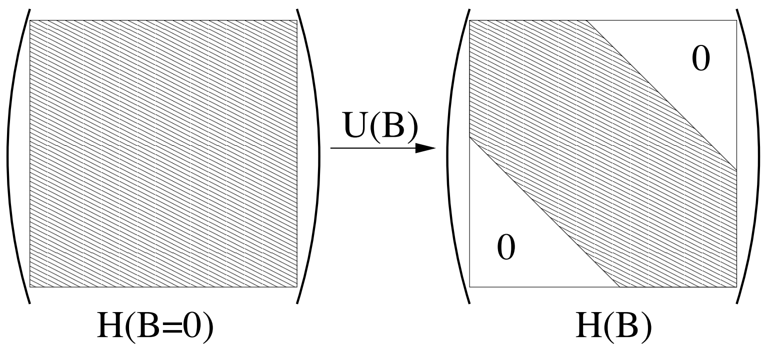


Figure 1.2: Schematic flow of the Hamiltonian

$$U(B) = T_B \exp\left(\int_0^B \eta(\tilde{B}) d\tilde{B}\right), \tag{1.7}$$

where we introduced a B-ordering operator T_B that commutes all generators $\eta(\{B_i\})$ to the left of all other generators $\eta(B_j)$ with $B_j < B_i$ and vice versa for $T_B^\dagger$. Please note that since

$$U^\dagger(B) = T_B^\dagger \exp\left(\int_0^B \eta^\dagger(\tilde{B}) d\tilde{B}\right) = T_B^\dagger \exp\left(-\int_0^B \eta(\tilde{B}) d\tilde{B}\right) = U^{-1}(B), \tag{1.8}$$

$U(B)$ really is an unitary transformation.

The main idea is now to construct $\eta(B)$ in such a way that $U(B)$ eliminates all couplings between states with energy differences larger than $|\Delta\epsilon| \propto B^{-1/2}$. Fig. 1.2 shows schematically the flow generated by $U(B)$. The off-diagonal matrix elements connecting states with large energy differences are eliminated before dealing with small energies, thereby making the Hamiltonian increasingly band-diagonal.

Starting with the Hamiltonian

$$H(B) = H_0(B) + H_{int}(B), \tag{1.9}$$

where $H_0(B)$ is the diagonal part of $H(B)$ and $H_{int}(B)$ the "interaction", Wegner chooses the anti-Hermitian generator

$$\boxed{\eta(B) = [H_0(B), H_{int}(B)].} \tag{1.10}$$

E.g. for potential scattering one can rewrite the operators in a simple matrix representation:

$$\eta = (\eta)_{pq} \text{ and } H = (h)_{pq}. \tag{1.11}$$

The reader easily shows by calculating the matrix-products that

$$\eta_{pq} = (\epsilon_p - \epsilon_q) h_{pq} \tag{1.12}$$

is fulfilled. Here $\epsilon_p \equiv h_{pp}$ was defined. The flow equations for the matrix elements of the Hamiltonian are given by:

$$\partial_B h_{pq} = -(\epsilon_p - \epsilon_q)^2 h_{pq} + \sum_{k \neq p,q} (\epsilon_p + \epsilon_q - 2\epsilon_k) h_{pk} h_{kq}. \tag{1.13}$$

In the case $\epsilon_p \neq \epsilon_q$ the first term (induced by the commutator $[\eta(B), H_0(B)]$) corresponds to an exponential decay of the matrix element.
One can also show [14] that with the above choice Eq. (1.4) is a generalization of the Jacobi method for diagonalizing matrices and that

$$\frac{d}{dB} Tr\, H_{int}^2(B) \leq 0 \tag{1.14}$$

is fulfilled. This implies that $H_{int}(B)$ usually becomes smaller during the flow and hence $H(B)$ becomes more and more diagonal. Though the latter statement cannot be proved rigorously in general, it turns out that it is true for many problems.
Please note that by choosing $\eta(B)$ in the above way the flow parameter B has the dimension of $(energy)^{-2}$.

The infinitesimal nature of this unitary transformation leads to an energy scale separation: large energy differences are eliminated before smaller ones. This also suggests to use the flow equation method to derive effective low energy Hamiltonians.

1.3 Density of states

One of the remaining essential questions is how the density of states can be included in the Kondo problem in an efficient way. Fortunately this can be easily done using earlier preliminary NRG calculations and the Schrieffer-Wolff transformation. The following review is essentially based on Refs. [17] and [4].

The Hamiltonian of the Anderson model for a single magnetic impurity is given by

$$H_A = \sum_{\mathbf{p},\alpha} \epsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} + \sum_\alpha \epsilon_d d^\dagger_\alpha d_\alpha + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \sum_{\mathbf{p},\alpha} \left(V_{\mathbf{p}} c^\dagger_{\mathbf{p}\alpha} d_\alpha + \text{ h.c. } \right). \tag{1.15}$$

Here $c^{(\dagger)}_{\mathbf{p}\alpha}$ denote the standard annihilation and creation operators of the conduction band electrons and $d^{(\dagger)}_\alpha$ the operators corresponding to the impurity orbital.

The impurity and the conduction band are mixed by the hybridization function $V_{\mathbf{p}}$ and U is the interatomic Coulomb interaction at the impurity site. The system is assumed to be SU(2)-invariant.

It is convenient to label the states by their energy rather than by their momentum. First the discrete $\mathbf{p}$'s have to be transformed into continuum $\mathbf{p}$'s:

$$
\begin{aligned}
\sum_{\mathbf{p},\alpha} \epsilon_{\mathbf{p}} c^{\dagger}_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} &\rightarrow \int d^3p \; \epsilon_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha}, \\
\sum_{\mathbf{p},\alpha} V_{\mathbf{p}} c^{\dagger}_{\mathbf{p}\alpha} &\rightarrow \left[\frac{\Omega}{(2\pi)^3}\right]^{1/2} \int d^3p \; V_{\mathbf{p}} a_{\mathbf{p}\alpha},
\end{aligned}
\tag{1.16}
$$

where $a^{(\dagger)}_{\mathbf{p}\alpha}$ denote the continuum operators, Ω is the volume of the system and we defined $p \equiv |\mathbf{p}|$.

In the next step a spherical harmonic expansion is introduced for $a_{\mathbf{p}\alpha}$:

$$
\begin{aligned}
a_{\mathbf{p}\alpha} &= \frac{1}{p} \sum_{l,m} a_{plm} Y_{lm}(\hat{\mathbf{p}}), \\
a_{plm\alpha} &= p \int d\Omega_{\hat{\mathbf{p}}} Y^{*}_{lm}(\hat{\mathbf{p}}) a_{\mathbf{p}\alpha}.
\end{aligned}
\tag{1.17}
$$

Here we defined $\hat{\mathbf{p}} \equiv \mathbf{p}/|\mathbf{p}|$.

In the following we will use the notation $\epsilon_p \equiv \epsilon_{\mathbf{p}}$ and $V_p \equiv V_{\mathbf{p}}$. The continuum representation is then given by

$$
\begin{aligned}
\int d^3p \; \epsilon_{\mathbf{p}} a^{\dagger}_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha} &= \sum_{l,m,r,s} \int d\Omega_{\hat{\mathbf{p}}} \; dp \; \epsilon_p Y^{*}_{lm}(\hat{\mathbf{p}}) Y_{rs}(\hat{\mathbf{p}}) a^{\dagger}_{plm\alpha} a_{prs\alpha} \\
&= \sum_{l,m} \int dp \; \epsilon_p a^{\dagger}_{plm\alpha} a_{plm\alpha}
\end{aligned}
\tag{1.18}
$$

and

$$
\begin{aligned}
\left[\frac{\Omega}{(2\pi)^3}\right]^{1/2} \int d^3p \; V_{\mathbf{p}} a_{\mathbf{p}\alpha} &= \left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int d^3p \; \frac{1}{\sqrt{4\pi}} V_{\mathbf{p}} a_{\mathbf{p}\alpha} \\
&= \left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int p^2 \; d\Omega_{\hat{\mathbf{p}}} \; dp \; Y^{*}_{00}(\hat{\mathbf{p}}) V_p a_{\mathbf{p}\alpha} \\
&= \left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int p \; dp \; V_p a_{p00\alpha}.
\end{aligned}
\tag{1.19}
$$

Therefore one only has to keep the $l = m = 0$ operators. For convenience the subscript "00" will be dropped in the following.

The next step is to introduce the energy representation:

$$a_{\epsilon\alpha} = \left(\frac{d\epsilon_p}{dp}\right)^{-1/2} a_{p\alpha}, \tag{1.20}$$

when $\epsilon = \epsilon_p$. Also an energy cutoff from $-D/2$ to $D/2$ about the Fermi level will be needed. One finds:

$$\begin{aligned} \int dp\ \epsilon_p a^\dagger_{p\alpha} a_{p\alpha} &= \int dp\ \epsilon_p \frac{d\epsilon_p}{dp} a^\dagger_{\epsilon\alpha} a_{\epsilon\alpha} \\ &= \int\limits_{-D/2}^{D/2} d\epsilon\ \epsilon\ a^\dagger_{\epsilon\alpha} a_{\epsilon\alpha} \end{aligned} \tag{1.21}$$

and

$$\begin{aligned} \left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int p\ dp\ a_{p00\alpha} &= \left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int p\ dp\ V_p \left(\frac{d\epsilon_p}{dp}\right)^{1/2} a_{\epsilon\alpha} \\ &= \left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int\limits_{-D/2}^{D/2} p(\epsilon)\ d\epsilon\ \left(\frac{d\epsilon_p}{dp}\right)^{1/2} V(\epsilon) a_{\epsilon\alpha}. \end{aligned} \tag{1.22}$$

In a 3-D system the density of states fulfills:

$$\rho(\mathbf{p})d\mathbf{p} = \frac{p^2\Omega}{2\pi^2} d\mathbf{p}\ \rightarrow\ \rho(\epsilon) = \frac{p^2\Omega}{2\pi^2}\frac{dp}{d\epsilon}. \tag{1.23}$$

Please note that (unlike most textbooks) we did not perform the spinsum.

Using the latter relation one can rewrite Eq. (1.22) to:

$$\left[\frac{\Omega}{2\pi^2}\right]^{1/2} \int p\ dp\ a_{p00\alpha} = \int\limits_{-D/2}^{D/2} d\epsilon\ \left[\rho(\epsilon)\right]^{1/2} V(\epsilon) a_{\epsilon\alpha}. \tag{1.24}$$

Summing up, in the continuum limit the Hamiltonian of the Anderson model for a single magnetic impurity (see Eq. (1.15)) can be transformed to:

$$\begin{aligned} H_A &= \sum_\alpha \int\limits_{-D/2}^{D/2} d\epsilon\ \epsilon\ a^\dagger_{\epsilon\alpha} a_{\epsilon\alpha} + \sum_\alpha \epsilon_d d^\dagger_\alpha d_\alpha + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \\ &+ \sum_\alpha \int\limits_{-D/2}^{D/2} d\epsilon\ \sqrt{\rho(\epsilon)}\left[V(\epsilon) a_{\epsilon\alpha} d_\alpha + \text{ h.c. }\right]. \end{aligned} \tag{1.25}$$

Remarkably both the hybridization function $V(\epsilon)$ and the density of states $\rho(\epsilon)$ only enter the Hamiltonian via the product $\sqrt{\rho(\epsilon)}V(\epsilon)$. Thereby one can model all combinations of densities of states and hybridization functions by a constant density of states ρ_0 and an energy (or a momentum) dependent hybridization function or vice versa.

In this thesis we assume a system with a constant hybridization function and a nonconstant (nontrivial) density of states. As shown in the calculation above, this system is equivalent to a system with a constant density of states and an energy (or a momentum) dependent hybridization function. To simplify the calculation we will therefore model the original system by a system with a constant density of states and a momentum dependent hybridization function.

The connection between the Kondo and the Anderson Hamiltonian (Eqs. (1.1) and (1.15)) is given by the Schrieffer-Wolff transformation [4]:

$$H_K = e^S H_A e^{-S}, \tag{1.26}$$

where

$$\begin{aligned} S \;=\; & \sum_{p,\alpha} V_p \Bigg\{ \Bigg[\frac{U}{(\epsilon_d - \epsilon_p)(\epsilon_d - \epsilon_p + U)} d^\dagger_{-\alpha} d_{-\alpha} c^\dagger_{p\alpha} d_\alpha + \\ & + \frac{1}{(\epsilon_p - \epsilon_d)} c^\dagger_{p\alpha} d_\alpha \Bigg] - \text{ h.c. } \Bigg\} \end{aligned} \tag{1.27}$$

For simplicity we already used the effective one dimensional notation. Here terms of $\mathcal{O}(V^3)$ have been neglected, since V is assumed to be a small parameter.

The coupling function of the Kondo Hamiltonian is then given by

$$J(p,q) = \frac{1}{2} V_p V_q U \left[\frac{1}{(\epsilon_d - \epsilon_p)(\epsilon_d - \epsilon_p + U)} + \frac{1}{(\epsilon_d - \epsilon_q)(\epsilon_d - \epsilon_q + U)} \right]. \tag{1.28}$$

The impurity spin operators are defined by $S^+ = d^\dagger_\uparrow d_\downarrow$, $S^- = d^\dagger_\downarrow d_\uparrow$ and $S^z = (d^\dagger_\uparrow d_\uparrow + d^\dagger_\downarrow d_\downarrow)/2$.

Usually the additional momentum dependency introduced by $\epsilon_{p/q}$ is neglected. The coupling function in the Kondo model is then formally given by

$$\boxed{J(p,q) = \frac{J_0}{\rho_0} \sqrt{\rho(\epsilon_p)} \sqrt{\rho(\epsilon_q)},} \tag{1.29}$$

where J_0 is a constant.

1.4 Bosonization

In this section we want to give a brief introduction into the bosonization of 1-dimensional (1-D) fermionic system, which is essentially a compressed version of a review by von Delft and Schoeller [18] made suitable for our needs.

Though it is clear that the action of e.g. a fermionic annihilation operator on an arbitrary state can be represented by removing the fermion on the highest occupied level of the state and creating a particle-hole excitation afterwards (or vice versa), only for 1-D systems it is possible to find a representation of the fermion field operator as a function of bosonic particle-hole excitation creation and annihilation operators and an additional operator that removes one fermion from the system (or adds on to it). The latter operator is needed since particle-hole excitations cannot change the number of particles of a state but fermion field operators do.

1.4.1 Basic definitions

We start with a set of 1-D fermion creation and annihilation operators that obey the generic anticommutation relations

$$\left\{c^{\dagger}_{p\alpha}, c_{q\beta}\right\} = \delta_{p,q}\delta_{\alpha,\beta}, \tag{1.30}$$

where p, q are the usual wave-vector indices of the form

$$p = \frac{2\pi}{L} n_p,\ n_p \in \mathbb{Z}. \tag{1.31}$$

Here L is the system size and α, β specify the type of the fermions (e.g. electron spin state)[1].
The fermion field is defined by

$$\Psi_\alpha(x) = \sqrt{\frac{2\pi}{L}} \sum_p e^{-ipx} c_{p\alpha}, \tag{1.32}$$

with the inverse

$$c_{q\alpha} = \frac{1}{\sqrt{2\pi L}} \int\limits_{-L/2}^{L/2} dx\ e^{iqx} \Psi_\alpha(x). \tag{1.33}$$

In the following we will use the operation of *fermion-normal-ordering* ": :", which is defined by

$$: AB : =\ AB - \langle 0|\, AB\, |0\rangle, \ \ \text{for } A, B \in \left\{c^{\dagger}_{p\alpha}, c_{p\alpha}\right\}. \tag{1.34}$$

[1]Different boundary conditions lead to an additional phase factor in the bosonization identity which is usually neglected.

Here $|0\rangle$ is the vacuum state:

$$c_{p\alpha}|0\rangle \equiv 0, \quad \text{for}\, p > 0, \tag{1.35}$$

$$c^\dagger_{p\alpha}|0\rangle \equiv 0, \quad \text{for}\, p \leq 0. \tag{1.36}$$

Please note that for an operator product with a vacuum state expectation value fermion-normal-ordering is equivalent to moving the operators $c_p^\dagger$ with $p \leq 0$ and c_p with $p > 0$ to the right.

The operator

$$\hat{N}_\alpha = \sum_p : c^\dagger_{p\alpha} c_{p\alpha} : \tag{1.37}$$

counts the number of α-fermions relative to $|0\rangle$. The $\vec{N}$-particle Hilbert space is defined as the set of all states with the same $\{\hat{N}_\alpha\}$-eigenvalues, where $\vec{N} = (N_\alpha, N_\beta, ...)$. Its ground state will be denoted by $|\vec{N}\rangle_0$.

We define the bosonic particle-hole creation and annihilation operators by

$$b^\dagger_{p\alpha} = \frac{i}{\sqrt{n_p}} \sum_q c^\dagger_{q+p\alpha} c_{q\alpha}, \tag{1.38}$$

$$b_{p\alpha} = \frac{-i}{\sqrt{n_p}} \sum_q c^\dagger_{q-p\alpha} c_{q\alpha}, \tag{1.39}$$

with

$$p = \frac{2\pi}{L} n_p, \quad n_p \in \mathbb{N} \setminus \{0\}. \tag{1.40}$$

The reader easily verifies the following commutation relations:

$$[b_{p\alpha}, b_{q\beta}] = [b^\dagger_{p\alpha}, b^\dagger_{q\beta}] = [\hat{N}_\alpha, b^{(\dagger)}_{p\beta}] = 0. \tag{1.41}$$

Only the commutator $[b_{p\alpha}, b^\dagger_{q\beta}]$ needs some special treatment as has been first pointed out by Mattis and Lieb in 1965 [19]:

$$\begin{aligned}
[b_{p\alpha}, b^\dagger_{q\beta}] &= \frac{1}{\sqrt{n_p n_q}} \sum_{m,n} [c^\dagger_{m-p\alpha} c_{m\alpha}, c^\dagger_{n+q\beta} c_{n\beta}] \\
&= \frac{\delta_{\alpha,\beta}}{\sqrt{n_p n_q}} \sum_{m,n} \left(c^\dagger_{m-p\alpha} c_{n\beta} \delta_{m,n+q} - c^\dagger_{n+q\beta} c_{m\alpha} \delta_{n,m-p} \right) \\
&= \frac{\delta_{\alpha,\beta}}{\sqrt{n_p n_q}} \sum_{m} \left(c^\dagger_{m-p\alpha} c_{m-q\alpha} - c^\dagger_{m-p+q\alpha} c_{m\alpha} \right).
\end{aligned} \tag{1.42}$$

In the case of $p = q$ the terms in the previous line are the occupation number operators for the α-fermions. Due to the definition of m in Eq. (1.31) the sums are divergent. To get (absolute) convergent sums one has to apply fermion normal ordering:

$$\begin{aligned}
[b_{p\alpha}, b^\dagger_{q\beta}] &= \frac{\delta_{\alpha,\beta}}{\sqrt{n_p n_q}} \sum_m \Big(\Big(: c^\dagger_{m-p\alpha} c_{m-q\alpha} : - : c^\dagger_{m-p+q\alpha} c_{m\alpha} : \Big) + \\
&\quad + \Big(\langle 0 | c^\dagger_{m-p\alpha} c_{m-q\alpha} | 0 \rangle - \langle 0 | c^\dagger_{m-p+q\alpha} c_{m\alpha} | 0 \rangle \Big) \Big) \\
&= \frac{\delta_{\alpha,\beta}}{\sqrt{n_p n_q}} \sum_m \Big(\Big(: c^\dagger_{m-p+q\alpha} c_{m\alpha} : - : c^\dagger_{m-p+q\alpha} c_{m\alpha} : \Big) + \\
&\quad + \delta_{p,q} \left[\Theta(p-m) - \Theta(-m) \right] \Big) \\
&= \frac{\delta_{\alpha,\beta}\delta_{p,q}}{n_p} \left(\sum_{n_m=-\infty}^{n_p} - \sum_{n_m=-\infty}^{0} \right) \\
&= \delta_{\alpha,\beta}\delta_{p,q}
\end{aligned} \tag{1.43}$$

Please note that

$$b_{p\alpha} | \vec{N} \rangle_0 \equiv 0, \tag{1.44}$$

since the ground state cannot contain any particle-holes excitations per definition.

Analog to the definition of fermion-normal-ordering we define *boson-normal-ordering* ": :" by

$$: AB := AB -_0 \langle \vec{N} | \, AB \, | \vec{N} \rangle_0, \quad \text{for } A, B \in \left\{ b^\dagger_{p\alpha}, b_{p\alpha} \right\}, \tag{1.45}$$

which is equivalent to moving all operators b_p to the right of all operators $b^\dagger_p$. Since boson-normal-ordered terms are per definition also fermion-normal-ordered, we will use the same notation for both types of ordering.

Unfortunately one cannot change the total number of fermions with the bosonic operators defined above. So one needs additional operators, the so called *Klein factors* $F^{(\dagger)}_\alpha$, which are defined to commute with all bosonic operators. As will be shown below, one can rewrite any state $|\Phi\rangle$ as a function $f(\{b^\dagger_{p\alpha}\})$ acting on $|\vec{N}\rangle_0$. Since one can always commute the Klein factors to the right of $f(\{b^\dagger_{p\alpha}\})$, only their action on the ground state has to be defined:
$F^\dagger_\alpha$ adds an α-fermion to the lowest empty α-level of $|\vec{N}\rangle_0$, F_α removes the α-fermion on the highest occupied α-level of $|\vec{N}\rangle_0$.

For a better understanding of the operators defined above we illustrated several exemplary actions of the latter in Fig. 1.3.

We define the *boson field* by

$$\Phi_\alpha(x) = -\sum_{p>0} \frac{1}{\sqrt{n_p}} \left(e^{-ipx} b_{p\alpha} + e^{ipx} b^\dagger_{p\alpha} \right) e^{-ap/2} \tag{1.46}$$

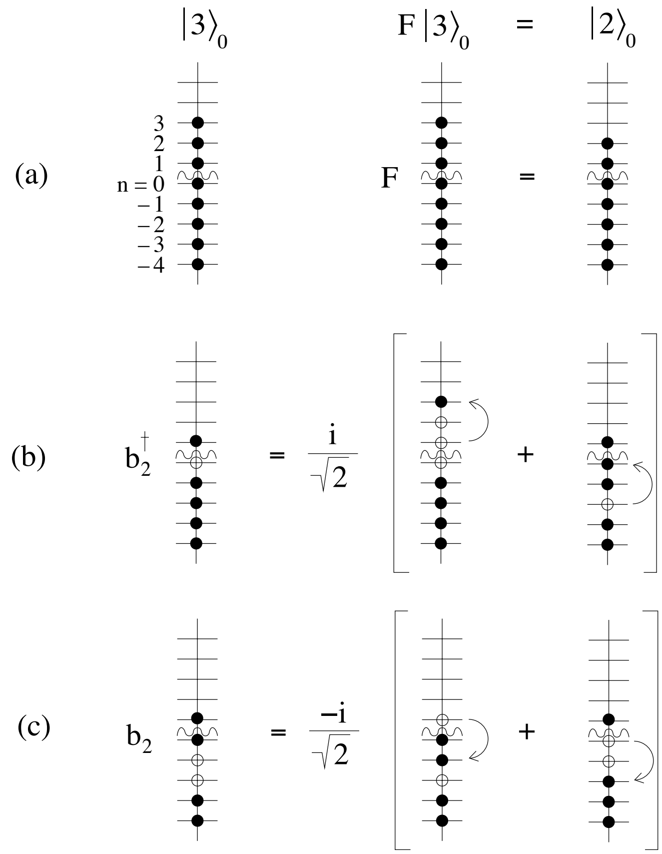


Figure 1.3: Exemplary actions of the bosonic particle-hole operators and the Klein Factors. For convenience we assume only one species of fermions. Furthermore here n_p is used as index. The wiggled line represents the Fermi "surface". Fig. (a) shows an exemplary ground state and the action of the Klein factor F on it. In Figs. (b) and (c) we illustrated the action of a particle-hole excitation creation and an annihilation operator.

$$\equiv \quad \varphi_\alpha(x) + \varphi_\alpha^\dagger(x), \tag{1.47}$$

where a is an infinitesimal positive parameter needed to regularize ultraviolet divergent momentum sums. Obviously a^{-1} is proportional to the maximum momentum transfer induced by $\Phi_\alpha(x)$.

In the following we will need the commutators

$$[\varphi_\alpha(x), \varphi_\beta(y)] = [\varphi_\alpha^\dagger(x), \varphi_\beta^\dagger(y)] = 0 \tag{1.48}$$

and

$$
\begin{aligned}
[\varphi_\alpha(x), \varphi^\dagger_\beta(y)] &= \delta_{\alpha,\beta} \sum_{q>0} \frac{1}{n_q} e^{-q[i(x-y)+a]} \\
&= -\delta_{\alpha,\beta} \ln\left(1 - e^{-\frac{2\pi}{L}[i(x-y)+a]}\right) \\
&\overset{L\to\infty}{\approx} -\delta_{\alpha,\beta} \ln\left(\frac{2\pi}{L}[i(x-y)+a]\right). \qquad (1.49)
\end{aligned}
$$

1.4.2 Coherent-state representation

To retrieve the bosonization identity we will use the coherent-state representation of eigenstates of bosonic annihilation operators (see e.g. [20]).
We assume that we found an eigenstate $|\Phi\rangle$ of the annihilation operator b_p with eigenvalue α_p:

$$
b_p|\Phi\rangle = \alpha_p|\Phi\rangle. \qquad (1.50)
$$

The eigenstate can be expanded in occupation number representation:

$$
|\Phi\rangle = \sum_{n_{p_1},n_{p_2}...n_{p_i}} \phi_{n_{p_1},n_{p_2}...n_{p_i}} |n_{p_1}, n_{p_2}...n_{p_i}\rangle. \qquad (1.51)
$$

Here $|n_{p_1}, n_{p_2}...n_{p_i}\rangle$ is a normalized symmetric state with n_{p_j} particles in state $|p_j\rangle$ and $\{|p_j\rangle\}$ is an orthonormal basis.
For an annihilation operator b_{p_j} acting on $|\Phi\rangle$ follows with Eq. (1.50):

$$
\alpha_{p_j}\phi_{n_{p_1},n_{p_2}...(n_{p_j}-1)..} = \sqrt{n_{p_j}}\phi_{n_{p_1},n_{p_2}...n_{p_j}...} \qquad (1.52)
$$

Applying this relation for all states leads to:

$$
\phi_{n_{p_1},n_{p_2}...n_{p_i}} = \frac{\alpha_{p_1}^{n_{p_1}}}{\sqrt{n_{p_1}!}} \frac{\alpha_{p_2}^{n_{p_2}}}{\sqrt{n_{p_2}!}} \cdots \frac{\alpha_{p_i}^{n_{p_i}}}{\sqrt{n_{p_i}!}} \hat{\lambda}, \quad \text{with a phase operator } \hat{\lambda}. \qquad (1.53)
$$

Using Eq. (1.51) with

$$
|n_{p_1}, n_{p_2}...n_{p_i}\rangle = \frac{(b^\dagger_{p_1})^{n_{p_1}}}{\sqrt{n_{p_1}!}} \frac{(b^\dagger_{p_2})^{n_{p_2}}}{\sqrt{n_{p_2}!}} \cdots \frac{(b^\dagger_{p_i})^{n_{p_i}}}{\sqrt{n_{p_i}!}} |\Phi\rangle_0, \qquad (1.54)
$$

where $|\Phi\rangle_0$ denotes the ground state, one finally obtains

$$
\begin{aligned}
|\Phi\rangle &= \sum_{n_{p_1},n_{p_2}...n_{p_i}} \frac{(\alpha_{p_1} b^\dagger_{p_1})^{n_{p_1}}}{n_{p_1}!} \frac{(\alpha_{p_2} b^\dagger_{p_2})^{n_{p_2}}}{n_{p_2}!} \cdots \frac{(\alpha_{p_i} b^\dagger_{p_i})^{n_{p_i}}}{n_{p_i}!} \hat{\lambda}|\Phi\rangle_0 \\
&= \exp\left(\sum_p \alpha_p b^\dagger_p\right) \hat{\lambda}|\Phi\rangle_0. \qquad (1.55)
\end{aligned}
$$

1.4.3 Bosonization identities

Using a mathematical trick one can show that $\Psi_\alpha(x)|0\rangle$ is an eigenstate of $b_{p\alpha}$:

$$\begin{aligned}
b_{p\alpha}\Psi_\alpha(x)|\vec{N}\rangle_0 &\overset{(1.44)}{=} [b_{p\alpha}, \Psi_\alpha(x)]|\vec{N}\rangle_0 \\
&= \frac{-i}{\sqrt{n_p}}\sqrt{\frac{2\pi}{L}}\sum_{q,k} e^{-ikx}[c^\dagger_{q-p\alpha}c_{q\alpha}, c_{k\alpha}]|\vec{N}\rangle_0 \\
&= \frac{-i}{\sqrt{n_p}}\sqrt{\frac{2\pi}{L}}\sum_{q,k} e^{-ikx}\left(-\delta_{k,q-p}c_{q\alpha}\right)|\vec{N}\rangle_0 \\
&= \frac{i}{\sqrt{n_p}}e^{ipx}\Psi_\alpha(x)|\vec{N}\rangle_0. \qquad (1.56)
\end{aligned}$$

Hence there exists a coherent-state representation of $\Psi_\alpha(x)|\vec{N}\rangle_0$:

$$\begin{aligned}
\Psi_\alpha(x)|\vec{N}\rangle_0 &= \exp\left(\sum_{p>0}\frac{i}{\sqrt{n_p}}e^{ipx}b_p^\dagger\right)F_\alpha\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0 \\
&\overset{(1.47)}{=} e^{-i\varphi^\dagger_\alpha(x)}F_\alpha\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0. \qquad (1.57)
\end{aligned}$$

Here the Klein factor F_α is needed since $\Psi_\alpha(x)$ removes one α-fermion. The phase operator $\hat{\lambda}_\alpha(x)$ can be evaluated using

$$\begin{aligned}
{}_0\langle\vec{N}|F^\dagger_\alpha\Psi_\alpha(x)|\vec{N}\rangle_0 &= {}_0\langle\vec{N}|F^\dagger_\alpha e^{-i\varphi^\dagger_\alpha(x)}F_\alpha\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0 \\
&= {}_0\langle\vec{N}|e^{-i\varphi^\dagger_\alpha(x)}F^\dagger_\alpha F_\alpha\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0 \\
&= \left(e^{i\varphi_\alpha(x)}|\vec{N}\rangle_0\right)^\dagger\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0 \\
&\overset{(1.44)}{=} \left(1|\vec{N}\rangle_0\right)^\dagger\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0 \\
&= \lambda_\alpha(x). \qquad (1.58)
\end{aligned}$$

On the other hand also

$$\begin{aligned}
{}_0\langle\vec{N}|F^\dagger_\alpha\Psi_\alpha(x)|\vec{N}\rangle_0 &= {}_0\langle\vec{N}|F^\dagger_\alpha\sqrt{\frac{2\pi}{L}}\sum_p e^{-ipx}c_{p\alpha}|\vec{N}\rangle_0 \\
&= \left(F_\alpha|\vec{N}\rangle_0\right)^\dagger\sqrt{\frac{2\pi}{L}}\sum_p e^{-ipx}c_{p\alpha}|\vec{N}\rangle_0 \\
&= \left(c_{(N_\alpha 2\pi/L),\alpha}|\vec{N}\rangle_0\right)^\dagger\sqrt{\frac{2\pi}{L}}\sum_p e^{-ipx}c_{p\alpha}|\vec{N}\rangle_0
\end{aligned}$$

$$
\begin{aligned}
&= {}_0\langle \vec{N}|c^\dagger_{(N_\alpha 2\pi/L),\alpha}\sqrt{\frac{2\pi}{L}}\sum_p e^{-ipx}c_{p\alpha}|\vec{N}\rangle_0 \\
&= \sqrt{\frac{2\pi}{L}}e^{-i\frac{2\pi}{L}N_\alpha x} \qquad (1.59)
\end{aligned}
$$

has to be fulfilled. Thus one finds

$$\hat{\lambda}_\alpha(x) = \sqrt{\frac{2\pi}{L}}e^{-i\frac{2\pi}{L}\hat{N}_\alpha x}. \qquad (1.60)$$

Unfortunately we did not derive the bosonization identity until now, because we could still be missing additional factors that have no action on the ground state; e.g. a factor of $\exp(-i\varphi_\alpha(x))$ (as the reader maybe already noticed), since

$$e^{-i\varphi_\alpha(x)}|\vec{N}\rangle_0 \overset{(1.44)}{=} |\vec{N}\rangle_0. \qquad (1.61)$$

Therefore one has to analyze the action of $\Psi_\alpha(x)$ on an arbitrary state $|\Phi\rangle$ in the $\vec{N}$-particle Hilbert space.
Please note that since it is possible to express $\Psi^{(\dagger)}_\alpha$ in terms of the bosonic operators $b^{(\dagger)}$ (and thus $c^\dagger_{p\alpha}c_{q\alpha}$ by using Eq. (1.33)), one can rewrite every state $|\Phi\rangle$ as a function $f(b^\dagger, b)$ acting on the ground state $|\vec{N}\rangle_0$. Because one can always commute the b-operators to the right, one finds with Eq. (1.44)

$$|\Phi\rangle = f(\{b^\dagger_{p\alpha}\})|\vec{N}\rangle_0 \qquad (1.62)$$

for all states $|\Phi\rangle$.
By commuting $\Psi_\alpha(x)$ to the right of $f(\{b^\dagger_{p\alpha}\})$ one finds

$$
\begin{aligned}
\Psi_\alpha(x)|\Phi\rangle &= \Psi_\alpha(x)f(\{b^\dagger_{p\beta}\})|\vec{N}\rangle_0 \\
&\overset{(A.8)}{=} f(\{b^\dagger_{p\beta} + \delta_{\alpha,\beta}\frac{i}{\sqrt{n_p}}e^{-ipx}\})\Psi_\alpha(x)|\vec{N}\rangle_0 \\
&\overset{(1.57)}{=} f(\{b^\dagger_{p\beta} + \delta_{\alpha,\beta}\frac{i}{\sqrt{n_p}}e^{-ipx}\})e^{-i\varphi^\dagger_\alpha(x)}F_\alpha\hat{\lambda}_\alpha(x)|\vec{N}\rangle_0 \\
&\overset{(1.41)}{=} F_\alpha\hat{\lambda}_\alpha(x)e^{-i\varphi^\dagger_\alpha(x)}f(\{b^\dagger_{p\beta} + \delta_{\alpha,\beta}\frac{i}{\sqrt{n_p}}e^{-ipx}\})|\vec{N}\rangle_0 \\
&\overset{(A.5)}{=} F_\alpha\hat{\lambda}_\alpha(x)e^{-i\varphi^\dagger_\alpha(x)}\left(e^{-i\varphi_\alpha(x)}f(\{b^\dagger_{p\beta}\})e^{i\varphi_\alpha(x)}\right)|\vec{N}\rangle_0 \\
&\overset{(1.44)}{=} F_\alpha\hat{\lambda}_\alpha(x)e^{-i\varphi^\dagger_\alpha(x)}e^{-i\varphi_\alpha(x)}f(\{b^\dagger_{p\beta}\})|\vec{N}\rangle_0 \\
&= F_\alpha\hat{\lambda}_\alpha(x)e^{-i\varphi^\dagger_\alpha(x)}e^{-i\varphi_\alpha(x)}|\Phi\rangle. \qquad (1.63)
\end{aligned}
$$

Since $|\Phi\rangle$ is an arbitrary state, the following bosonization identities are true for all states:

$$\boxed{\begin{aligned} \Psi_\alpha(x) &= F_\alpha \sqrt{\tfrac{2\pi}{L}} e^{-i\frac{2\pi}{L}\hat{N}_\alpha x} e^{-i\varphi^\dagger_\alpha(x)} e^{-i\varphi_\alpha(x)} \\ &\overset{(A.4),(1.49)}{=} F_\alpha a^{-1/2} e^{-i\frac{2\pi}{L}\hat{N}_\alpha x} e^{-i\Phi_\alpha(x)}. \end{aligned}} \tag{1.64}$$

In the following we will neglect the phase operator $\exp(-i2\pi\hat{N}_\alpha x/L)$, which is correct in the limit $L \to \infty$.

1.4.4 Hamiltonian with linear dispersion

Though by Eq. (1.33) we can express any combination of fermion creation and annihilation operators in terms of the boson field operators, the reader easily verifies that this usually is a bad idea. As an example we want to show the bosonization of a normal-ordered Hamiltonian with linear dispersion $\epsilon_p = v_F p$, setting $v_F \equiv 1$:

$$H = \sum_\alpha H_\alpha, \text{ with } \quad H_\alpha = \sum_p p : c^\dagger_{p\alpha} c_{p\alpha} : . \tag{1.65}$$

The $\vec{N}$-particle ground state is an eigenstate of H_α with eigenvalue

$$_0\langle \vec{N} | H_\alpha | \vec{N} \rangle_0 = \frac{2\pi}{L} \frac{1}{2} N_\alpha (N_\alpha + 1). \tag{1.66}$$

Also

$$\begin{aligned} [H_\alpha, b^\dagger_{q\beta}] &= \sum_{p,k} \frac{ip}{\sqrt{n_q}} [c^\dagger_{p\alpha} c_{p\alpha}, c^\dagger_{k+q\beta} c_{k\beta}] \\ &= \sum_{p,k} \frac{ip\delta_{\alpha,\beta}}{\sqrt{n_q}} \left(c^\dagger_{p\alpha} c_{k\beta} \delta_{p,k+q} - c^\dagger_{k+q\beta} c_{p\alpha} \delta_{p,k} \right) \\ &= \delta_{\alpha,\beta} \sum_p \frac{i}{\sqrt{n_q}} \left((p+q) c^\dagger_{p+q\beta} c_{p\beta} - p c^\dagger_{p+q\beta} c_{p\beta} \right) \\ &= \delta_{\alpha,\beta} q b^\dagger_{q\beta} \end{aligned} \tag{1.67}$$

is fulfilled.

Since the bosonization identities are analytic, any combination of fermion creation and annihilation operators can be expressed in terms of the boson field operators (i.e. Taylor expansion) using Eq. (1.33) and hence in terms of $b^{(\dagger)}$. The only form that reproduces Eqs. (1.66) and (1.67) is

$$\boxed{H_\alpha = \sum_{p>0} p b^\dagger_{p\alpha} b_{p\alpha} + \frac{2\pi}{L} \frac{1}{2} \hat{N}_\alpha (\hat{N}_\alpha + 1).} \tag{1.68}$$

In the limit $L \to \infty$ the second term can be neglected.

1.4.5 Vertex operators

Exponentials of boson fields are called vertex operators:

$$V_\alpha(\lambda, x) \equiv e^{i\lambda\Phi_\alpha(x)}. \tag{1.69}$$

The normal-ordering of these exponentials is defined by:

$$: e^{i\lambda\Phi_\alpha(x)} := e^{i\lambda\varphi_\alpha^\dagger(x)} e^{i\lambda\varphi_\alpha(x)} \overset{(A.4),(1.49)}{=} \left(\frac{L}{2\pi a}\right)^{\lambda^2/2} e^{i\lambda\Phi_\alpha(x)}. \tag{1.70}$$

For the product of two normal-ordered exponentials one finds:

$$\begin{aligned} : e^{i\lambda\Phi_\alpha(x)} :: e^{i\mu\Phi_\alpha(y)} : &= e^{i\lambda\varphi_\alpha^\dagger(x)} e^{i\lambda\varphi_\alpha(x)} e^{i\mu\varphi_\alpha^\dagger(y)} e^{i\mu\varphi_\alpha(y)} \\ &\overset{(A.6)}{=} e^{i\lambda\varphi_\alpha^\dagger(x)} e^{i\mu\varphi_\alpha^\dagger(y)} e^{i\lambda\varphi_\alpha(x)} \times \\ &\quad \times e^{-\lambda\mu[\varphi_\alpha(x), \varphi_\alpha^\dagger(y)]} e^{i\mu\varphi_\alpha(y)} \\ &\overset{(1.49)}{=} e^{i(\lambda\varphi_\alpha^\dagger(x) + \mu\varphi_\alpha^\dagger(y))} e^{i(\lambda\varphi_\alpha(x) + \mu\varphi_\alpha(y))} \times \\ &\quad \times \left(\frac{2\pi}{L}[i(x-y)+a]\right)^{\lambda\mu} \\ &= \; : e^{i(\lambda\Phi_\alpha(x) + \mu\Phi_\alpha(y))} : \left(\frac{2\pi}{L}[i(x-y)+a]\right)^{\lambda\mu}. \end{aligned} \tag{1.71}$$

In the following we will have to expand products of the type $V_\alpha(\lambda, x)V_\alpha(\mu, y)$:

$$\begin{aligned} V_\alpha(\lambda, x)V_\alpha(\mu, y) &\overset{(1.71)}{=} \left(\frac{L}{2\pi a}\right)^{-(\lambda+\mu)^2/2} [i(x-y)/a + 1]^{\lambda\mu} \times \\ &\quad \times : e^{i(\lambda\Phi_\alpha(x) + \mu\Phi_\alpha(y))} : . \end{aligned} \tag{1.72}$$

Using $\Phi_\alpha(x) \approx \Phi_\alpha(y) + (x-y)\partial_y\Phi_\alpha(y) + \ldots$ one finds the following operator product expansion (OPE) for the short-distance behavior ($x \to y$):

$$\begin{aligned} V_\alpha(\lambda, x)V_\alpha(\mu, y) &\approx \left(\frac{L}{2\pi a}\right)^{-(\lambda+\mu)^2/2} [i(x-y)/a + 1]^{\lambda\mu} \times \\ &\quad \times : \exp\left[i(\lambda+\mu)\Phi_\alpha(y) + i\lambda(x-y)\partial_y\Phi_\alpha(y) + \ldots\right] : \\ &= \left(\frac{L}{2\pi a}\right)^{-(\lambda+\mu)^2/2} [i(x-y)/a + 1]^{\lambda\mu} \times \\ &\quad \times \exp\left[i\lambda(x-y)\partial_y\varphi_\alpha^\dagger(y) + \ldots\right] \times \\ &\quad \times : \exp\left[i(\lambda+\mu)\Phi_\alpha(y)\right] : \exp\left[i\lambda(x-y)\partial_y\varphi_\alpha(y) + \ldots\right] \end{aligned}$$

$$
\begin{aligned}
&= \left(\frac{L}{2\pi a}\right)^{-(\lambda+\mu)^2/2} [i(x-y)/a+1]^{\lambda\mu} \times \\
&\quad \times \left[1 + i\lambda(x-y)\partial_y \varphi_\alpha^\dagger(y) + \ldots\right] \times \\
&\quad \times \left[1 + i(\lambda+\mu) : \Phi_\alpha(y) : + \ldots\right] \left[1 + i\lambda(x-y)\partial_y \varphi_\alpha(y) + \ldots\right] \\
&\approx \left(\frac{L}{2\pi a}\right)^{-(\lambda+\mu)^2/2} [1 + i(x-y)/a]^{\lambda\mu} \times \\
&\quad \times \left[1 + i\lambda(x-y)\partial_y \Phi_\alpha(y) + \ldots\right].
\end{aligned} \tag{1.73}
$$

For the anticommutation relation of two vertex operators follows:

$$
\begin{aligned}
\{V_\alpha(\lambda, x), V_\alpha(\mu, y)\} &= \left([1 + i(x-y)/a]^{\lambda\mu} + [1 - i(x-y)/a]^{\lambda\mu}\right) \times \\
&\quad \times \left(\frac{L}{2\pi a}\right)^{-(\lambda+\mu)^2/2} \left[1 + i\lambda(x-y)\partial_y \Phi_\alpha(y) + \ldots\right].
\end{aligned} \tag{1.74}
$$

Please note that in the case $\lambda = 1$, $\mu = -1$ the right hand side is proportional to a delta function.

2 The anisotropic Kondo model

In this section we want to review the flow equation analysis of the anisotropic Kondo model by Hofstetter and Kehrein ([12],[13]).

2.1 Bosonization of the Hamiltonian

For momentum independent couplings the Hamiltonian of the anisotropic Kondo model (1.2) can be rewritten to

$$\begin{aligned} H &= \sum_{p,\alpha} \epsilon_p c^\dagger_{p\alpha} c_{p\alpha} + \frac{J_\parallel}{2\pi} \sum_{\alpha,\beta} \Psi^\dagger_\alpha(0) \sigma^z_{\alpha\beta} \Psi_\beta(0) S^z + \\ & + \frac{J_\perp}{4\pi} \sum_{\alpha,\beta} \left(\Psi^\dagger_\alpha(0) \sigma^+_{\alpha\beta} \Psi_\beta(0) S^- + \text{ h.c. } \right), \end{aligned} \tag{2.1}$$

where $\Psi^{(\dagger)}_\alpha(0) = \sqrt{2\pi/L} \sum_p c^{(\dagger)}_{k\alpha}$. Assuming a linear dispersion for the noninteracting conduction band and using the bosonization identities from Eqs. (1.64) and (1.68) one finds

$$\begin{aligned} H &= \sum_\alpha \sum_{p>0} p b^\dagger_{p\alpha} b_{p\alpha} + \frac{J_\parallel}{2\pi a} \sum_{\alpha,\beta} F^\dagger_\alpha e^{i\Phi_\alpha(0)} \sigma^z_{\alpha\beta} F_\beta e^{-i\Phi_\beta(0)} S^z + \\ & + \frac{J_\perp}{4\pi a} \sum_{\alpha,\beta} \left(F^\dagger_\alpha e^{i\Phi_\alpha(0)} \sigma^+_{\alpha\beta} F_\beta e^{-i\Phi_\beta(0)} S^- + \text{ h.c. } \right). \end{aligned} \tag{2.2}$$

Here the constant $\sum_{p,\alpha} p\langle 0|c^\dagger_{p\alpha} c_{p\alpha}|0\rangle$ has been dropped and v_F has been set to 1.

Due to the special structure of the Kondo model it is convenient to introduce bosonic charge and spin density modes (see e.g. [21] or [22]):
We define the charge density modes by

$$\begin{aligned} \rho(p) &= \sqrt{\frac{1}{2|p|}} \sum_q \left(c^\dagger_{q+p\uparrow} c_{q\uparrow} + c^\dagger_{q+p\downarrow} c_{q\downarrow} \right) \\ &= \sqrt{\frac{L}{4\pi}} \begin{cases} -i(b^\dagger_{p\uparrow} + b^\dagger_{p\downarrow}), \ p > 0 \\ i(b_{-p\uparrow} + b_{-p\downarrow}), \ p < 0 \end{cases}, \end{aligned} \tag{2.3}$$

and the spin density modes by

$$\begin{aligned}\sigma(p) &= \sqrt{\frac{1}{2|p|}}\sum_q\left(c^\dagger_{q+p\uparrow}c_{q\uparrow}-c^\dagger_{q+p\downarrow}c_{q\downarrow}\right)\\ &= \sqrt{\frac{L}{4\pi}}\begin{cases}-i(b^\dagger_{p\uparrow}-b^\dagger_{p\downarrow}),\ p>0\\ i(b_{-p\uparrow}-b_{-p\downarrow}),\ p<0\end{cases}.\end{aligned}\tag{2.4}$$

Please note that $\rho^\dagger(p)=\rho(-p)$ and $\sigma^\dagger(p)=\sigma(-p)$ are fulfilled. Using Eqs. (1.41) and (1.43) one easily verifies

$$[\rho(p),\rho(q)]=[\sigma(p),\sigma(q)]=0,\ \text{for } p,q>0,\tag{2.5}$$

$$[\rho(-p),\rho(q)]=[\sigma(-p),\sigma(q)]=\delta_{p,q}\frac{L}{2\pi},\ \text{for } p,q>0,\tag{2.6}$$

$$[\rho(p),\sigma(q)]=0.\tag{2.7}$$

By inserting the definitions of $\rho(p)$ and $\sigma(p)$ (Eqs. (2.3) and (2.4)) one easily shows:

$$\frac{2\pi}{L}\sum_{p>0}p\left[\rho(p)\rho(-p)+\sigma(p)\sigma(-p)\right]=\sum_\alpha\sum_{p>0}pb^\dagger_{p\alpha}b_{p\alpha}.\tag{2.8}$$

Introducing the bosonic field corresponding to the spin density modes

$$\Phi(x)=-\frac{2\pi i}{L}\sum_{q\neq 0}\frac{\sqrt{|q|}}{q}e^{-iqx-a|q|/2}\sigma(q)=\frac{1}{\sqrt{2}}\left[\Phi_\uparrow(x)-\Phi_\downarrow(x)\right]\tag{2.9}$$

one can rewrite Eq. (2.2) to

$$\begin{aligned}H &= \frac{2\pi}{L}\sum_{p>0}p\left[\rho(p)\rho(-p)+\sigma(p)\sigma(-p)\right]-\frac{J_\parallel}{2\sqrt{2}\pi}\partial_x\Phi(0)S^z+\\ &\quad+\frac{J_\perp}{4\pi a}\left(e^{i\sqrt{2}\Phi(0)}F^\dagger_\uparrow F_\downarrow S^-+\text{ h.c. }\right).\end{aligned}\tag{2.10}$$

For convenience the Klein factors will be absorbed by redefining the spin operators:

$$F^\dagger_\uparrow F_\downarrow S^-\to S^-,\ F^\dagger_\downarrow F_\uparrow S^+\to S^+ \text{ and } S^z\to S^z.\tag{2.11}$$

Since the charge density modes in Eq. (2.10) decouple completely they can be omitted:

$$\begin{aligned}H &= \frac{2\pi}{L}\sum_{p>0}p\sigma(p)\sigma(-p)-\frac{J_\parallel}{2\sqrt{2}\pi}\partial_x\Phi(0)S^z+\\ &\quad+\frac{J_\perp}{4\pi a}\left(e^{i\sqrt{2}\Phi(0)}S^-+\text{ h.c. }\right)\\ &\equiv H_0+H_\parallel+H_\perp\end{aligned}\tag{2.12}$$

The longitudinal coupling $H_\parallel$ can be eliminated by an (unitary) Emery-Kivelson transformation [23]:

$$U = e^{i\mu\Phi(0)S^z}. \tag{2.13}$$

Here μ is a free parameter.
Using

$$[\sigma(p), \Phi(0)] = -\frac{i}{\sqrt{|p|}} e^{-a|p|/2} \tag{2.14}$$

one finds with Eq. (A.5):

$$\begin{aligned} UH_0U^\dagger &= \frac{2\pi}{L}\sum_{p>0} p\left(\sigma(p) - \mu S^z\sqrt{\frac{1}{|p|}}e^{-a|p|/2}\right)\left(\sigma(-p) - \mu S^z\sqrt{\frac{1}{|p|}}e^{-a|p|/2}\right) \\ &= H_0 - \frac{2\pi}{L}\mu S^z \sum_{p>0}\sqrt{|p|}\,[\sigma(p)+\sigma(-p)]\,e^{-a|p|/2} + \text{ const.} \\ &= H_0 + \mu\partial_x\Phi(0)S^z + \text{ const. .} \end{aligned} \tag{2.15}$$

Since both $\Phi(0)$ and $\partial_x\Phi(0)$ are linear in $\sigma(p)$,

$$[\partial_x\Phi(0), \Phi(0)] = \text{ const.} \tag{2.16}$$

is fulfilled. With Eq. (A.3) follows

$$UH_\parallel U^\dagger = H_\parallel + \text{ const. .} \tag{2.17}$$

Unfortunately one cannot directly use the operator identities in Appendix A to evaluate $UH_\perp U^\dagger$, since $[S^\pm, S^z]$ does not commute with S^z.
Denoting the impurity spin state up by $\binom{1}{0}$ and the spin down state $\binom{0}{1}$ one can represent the impurity spin operators by

$$S^+ = F_\downarrow^\dagger F_\uparrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ S^- = F_\uparrow^\dagger F_\downarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \text{ and } S^z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}. \tag{2.18}$$

By explicit calculation of the matrix products one finds:

$$\begin{aligned} Ue^{i\sqrt{2}\Phi(0)}S^-U^\dagger &= \exp\begin{pmatrix} i\mu\Phi(0)/2 & 0 \\ 0 & -i\mu\Phi(0)/2 \end{pmatrix} e^{i\sqrt{2}\Phi(0)} F_\uparrow^\dagger F_\downarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \times \\ &\quad \times \exp\begin{pmatrix} -i\mu\Phi(0)/2 & 0 \\ 0 & i\mu\Phi(0)/2 \end{pmatrix} \\ &= \begin{pmatrix} \exp[i\mu\Phi(0)/2] & 0 \\ 0 & \exp[-i\mu\Phi(0)/2] \end{pmatrix}\begin{pmatrix} 0 & 0 \\ \exp[i\sqrt{2}\Phi(0)] & 0 \end{pmatrix} \times \\ &\quad \times \begin{pmatrix} \exp[-i\mu\Phi(0)/2] & 0 \\ 0 & \exp[i\mu\Phi(0)/2] \end{pmatrix} F_\uparrow^\dagger F_\downarrow \\ &= \exp[i(\sqrt{2}-\mu)\Phi(0)]F_\uparrow^\dagger F_\downarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ &= e^{i(\sqrt{2}-\mu)\Phi(0)}S^-. \end{aligned} \tag{2.19}$$

After the analog transformation of the second spin-flip term one arrives at:

$$UH_\perp U^\dagger = \frac{J_\perp}{4\pi a}\left(e^{i(\sqrt{2}-\mu)\Phi(0)}S^- + \text{ h.c. }\right). \tag{2.20}$$

Choosing

$$\mu = \frac{J_\parallel}{2\sqrt{2}\pi} \tag{2.21}$$

obviously eliminates the longitudinal scattering term. Dropping the constants and defining

$$g_0 = \frac{J_\perp}{4\pi a},\quad \lambda_0 = \sqrt{2} - \mu \text{ and } V(\lambda, x) = \exp[i\lambda\Phi(x)], \tag{2.22}$$

one finds for the transformed Hamiltonian:

$$UHU^\dagger = H_0 + g_0\left[V(\lambda_0, 0)S^- + \text{ h.c. }\right]. \tag{2.23}$$

The parameter λ defined above is also called *scaling dimension*. Please note that the value of $\lambda = 1$ is equivalent to the Toulouse point, where the model can be mapped onto a noninteracting Anderson model. The latter can be solved exactly. Also $V(\lambda, x) \equiv V_\uparrow\left(\lambda/\sqrt{2}, x\right) V_\downarrow\left(-\lambda/\sqrt{2}, x\right)$ is fulfilled.

In the following we will need the normalized Fourier-transformed vertex operators

$$C_p = \frac{1}{\alpha_p\sqrt{L}}\int dx\; e^{-ipx}V(-\lambda, x) \;\text{ and }\; C_p^\dagger = \frac{1}{\alpha_p\sqrt{L}}\int dx\; e^{ipx}V(\lambda, x), \tag{2.24}$$

with $\alpha_p^2 = 2\pi a|pa|^{\lambda^2-1}/\Gamma(\lambda^2)$. Please not that by this definition $C_p^{(\dagger)}$ changes the systems energy by $|p|$.
During the flow the interaction will become increasingly nonlocal, which is taken into account by rewriting the Hamiltonian in the form

$$H(B) = H_0 + \int dx\; g(B, x)\left[V(\lambda, x)S^- + \text{ h.c. }\right], \tag{2.25}$$

with $g(B, x) = \sum_p g_p(B)e^{ipx}/\sqrt{L}$, $g_p(B = 0) = g_0/\sqrt{L}$ and $g_p(B) = g_{-p}(B)$. It is convenient to use the equivalent form

$$\boxed{H = H_0 + \sum_p g_p\alpha_p\left(C_p^\dagger S^- + C_p S^+\right)} \tag{2.26}$$

as starting point for the flow equation approach. In the following we will use the convention $H = H_0 + H_\perp$.

2.2 Flow equations

To calculate the generator $\eta(B)$ and its induced flow, some preliminary relations have to be evaluated:

$$\begin{aligned}
[H_0, C_q^\dagger] &= \frac{2\pi}{L}\sum_{p>0} p[\sigma(p)\sigma(-p), C_q^\dagger] \\
&= \frac{2\pi}{L\sqrt{L}\alpha_q}\sum_{p>0} p \int dx\; e^{iqx}[\sigma(p)\sigma(-p), V(\lambda, x)] \\
&\overset{(A.3)}{=} \frac{1}{\sqrt{L}\alpha_q}\int dx\; e^{iqx}\sum_{p>0}\frac{2\pi\lambda}{L}\sqrt{p}\left[\sigma(p)e^{-ipx-a|p|/2}V(\lambda, x)+\right. \\
&\quad \left. + e^{ipx-a|p|/2}V(\lambda, x)\sigma(-p)\right] \\
&= \frac{i}{\sqrt{L}\alpha_q}\int dx\; e^{iqx}\partial_x V(\lambda, x) \\
&= \frac{q}{\sqrt{L}\alpha_q}\int dx\; e^{iqx} V(\lambda, x) \\
&= q\, C_q^\dagger.
\end{aligned} \tag{2.27}$$

And analog:

$$[H_0, C_q] = -q\, C_q. \tag{2.28}$$

Keeping only the leading non-vanishing term of the OPE (1.74) one finds the anticommutation relations:

$$\boxed{\begin{aligned}
\{C_p^\dagger, C_q\} &= \delta_{p,q}, \\
\{C_p, C_q\} &= 0, \\
\{C_p^\dagger, C_q^\dagger\} &= 0.
\end{aligned}} \tag{2.29}$$

Please note that the anticommutation relations (2.29) become exact at the Toulouse point $\lambda = 1$.

The main part of the generator $\eta(B)$ is chosen as Wegner proposed (Eq. (1.10)):

$$\boxed{\eta^{(1)} = [H_0, H_\perp] \overset{(2.27),(2.28)}{=} \sum_p p g_p \alpha_p \left(C_p^\dagger S^- - C_p S^+\right).} \tag{2.30}$$

A second generator part $\eta^{(2)}$ will be introduced later to simplify the structure of the Hamiltonian.

The conduction band is transformed using Eqs. (2.27) and (2.28):

$$[\eta^{(1)}, H_0] = -\sum_p p^2 g_p \alpha_p \left(C_p^\dagger S^- + C_p S^+\right), \tag{2.31}$$

leading to an exponential decay in the couplings g_p. Using the anticommutation relations (2.29), one finds for the interaction term:

$$\begin{aligned}
[\eta^{(1)}, H_\perp] &= \sum_{p,q} p g_p g_q \alpha_p \alpha_q [C_p^\dagger S^- - C_p S^+, C_q^\dagger S^- + C_q S^+] \\
&= \sum_{p,q} (p+q) g_p g_q \alpha_p \alpha_q \left(C_p^\dagger C_q S^- S^+ - C_q C_p^\dagger S^+ S^- \right) \\
&= \sum_{p,q} (p+q) g_p g_q \alpha_p \alpha_q \left(\frac{1}{2}[C_p^\dagger, C_q] - \{C_p^\dagger, C_q\} S^z \right) \\
&\equiv \partial_B H_{ps} + \partial_B H_\parallel^{(2)}. \qquad (2.32)
\end{aligned}$$

While the first term corresponds to potential scattering, the second leads to a coupling of the impurity to the conduction band similar to the previous eliminated longitudinal scattering. Please note that due to the special prefactor the anticommutation relations (2.29) will not be used to evaluate the second term. Here the second non-vanishing term in the OPE (1.74) plays an important role and has to be taken into account:

$$\begin{aligned}
\partial_B H_\parallel^{(2)} &= -\int\int dx\, dy\, \frac{1}{L} \sum_{p,q} (p+q) g_p g_q e^{ipx} e^{-iqy} \{V(\lambda, x), V(-\lambda, y)\} S^z \\
&= i \int\int dx\, dy\, (\partial_x - \partial_y) g(x) g(y) \{V(\lambda, x), V(-\lambda, y)\} S^z \\
&\approx -\lambda \int\int dx\, dy\, (\partial_x - \partial_y) g(x) g(y) \left([1 + i(x-y)/a]^{-\lambda^2} + \right. \\
&\quad \left. + [1 - i(x-y)/a]^{-\lambda^2} \right) (x-y) \partial_y \Phi(y) S^z, \qquad (2.33)
\end{aligned}$$

where the leading term in the OPE (1.74) dropped out due to the antisymmetric integration measure. For convenience we define

$$H_\parallel^{(2)} \equiv \int dx\, f(x) \partial_x \Phi(x) S^z, \qquad (2.34)$$

where

$$\begin{aligned}
\partial_B f(x) &= -\lambda \int dy\, (\partial_x - \partial_y) g(x) g(y) (x-y) \times \\
&\quad \times \left([1 + i(x-y)/a]^{-\lambda^2} + [1 - i(x-y)/a]^{-\lambda^2} \right). \qquad (2.35)
\end{aligned}$$

Since $H_\parallel^{(2)}$ has the same structure as the already eliminated longitudinal scattering term $H_\parallel$ (except the position dependence), it can also be eliminated by an Emery-Kivelson transformation. Due to the integral structure of $H_{\|}^{(2)}$ the applied transformation has to be infinitesimal:

$$U = \exp\left(i\int dx\ r(x)\Phi(x)S^z\right). \tag{2.36}$$

Transforming the conduction band using Eq. (A.5) leads to

$$UH_0U^\dagger = H_0 + \int dx\ r(x)\partial_x\Phi(x)S^z + const.\ . \tag{2.37}$$

$H_{\|}^{(2)}$ is again invariant under the transformation U (up to a constant) and with the choice

$$\partial_B r(x) = -\partial_B f(x) \tag{2.38}$$

it is compensated by the new term in Eq. (2.37). The constants will be dropped as usual.
The transformation of $H_\perp$ again leads to a change in the scaling dimension. Since the coupling $g(x)$ is assumed to be localized (and consequently $f(x)$), one can use the short-distance expansion $\Phi(x) = \Phi(y) + (x-y)\partial_y\Phi(y) + \ldots$ to evaluate the change:

$$\begin{aligned} UV(\lambda,y)S^-U^\dagger &\overset{(A.2)}{=} V(\lambda,y)S^- + \int dx\ [V(\lambda,y)S^-, if(x)\Phi(x)S^z] + \mathcal{O}(r^2) \\ &\approx V(\lambda,y)S^- + i\int dx\ f(x)\Big(V(\lambda,y)\Phi(x)S^- - \\ &\quad -\frac{1}{2}[V(\lambda,y),\Phi(x)]\Big) \\ &= V(\lambda,y)S^- + i\int dx\ f(x)\Phi(y)V(\lambda,y)S^- + \mathcal{O}(x-y) \\ &\approx V(\lambda+d\lambda,y)S^-, \end{aligned} \tag{2.39}$$

where

$$d\lambda = \int dx\ f(x) = dB\int dx\ \partial_B f(x) \tag{2.40}$$

has been defined. The assumption of localization is only valid on the length scale

$$d_{eff} \sim \sqrt{B}, \tag{2.41}$$

because some modes have already been integrated out. Therefore one separates the bosonic field into a "fast" and a "slow" part (modes with large energy-differences are integrated out faster than ones with smaller):

$$V(\lambda,x) = e^{i\lambda\Phi_{slow}(x)}e^{i\lambda\Phi_{fast}(x)}, \tag{2.42}$$

where

$$\begin{aligned}\Phi_{slow}(x) &= -\frac{2\pi i}{L}\sum_{\substack{|p|<1/\sqrt{B},\\ p\neq 0}}\frac{\sqrt{|p|}}{p}e^{-ipx-a|p|/2}\sigma(p)\\ &\approx -\frac{2\pi i}{L}\sum_{p\neq 0}\frac{\sqrt{|p|}}{p}e^{-ipx-\sqrt{B}|p|/2}\sigma(p)\end{aligned} \tag{2.43}$$

contains the modes with small energy differences and $\Phi_{fast}(x)$ the rest. Since the assumption of localization is only valid for the slow modes, the shift of the scaling dimension in Eq. (2.39) can only be applied to Φ_{slow}:

$$UV(\lambda,y)S^{-}U^{\dagger} = e^{i(\lambda+d\lambda)\Phi_{slow}(x)}e^{i\lambda\Phi_{fast}(x)}. \tag{2.44}$$

To avoid a momentum-dependence of the scaling dimension the expression above is approximated by a single renormalized vertex operator with one scaling dimension for all modes. The renormalization factor ξ is chosen to ensure equal vacuum state expectation values:

$$\langle 0|e^{i(\lambda+d\lambda)\Phi_{slow}(x)}e^{i\lambda\Phi_{fast}(x)}|0\rangle = \langle 0|\xi e^{i(\lambda+d\lambda)\Phi(x)}|0\rangle. \tag{2.45}$$

Using Eq. (1.70) and $\langle 0| : e^{i\lambda\Phi(x)} : |0\rangle = 1$ one finds

$$\langle 0|e^{i(\lambda+d\lambda)\Phi_{slow}(x)}e^{i\lambda\Phi_{fast}(x)}|0\rangle = \left(\frac{L}{2\pi\sqrt{B}}\right)^{-(\lambda+d\lambda)^2/2}\left(\frac{\sqrt{B}}{a}\right)^{-\lambda^2/2} \tag{2.46}$$

and

$$\langle 0|\xi e^{i(\lambda+d\lambda)\Phi(x)}|0\rangle = \xi\left(\frac{L}{2\pi a}\right)^{-(\lambda+d\lambda)^2/2}, \tag{2.47}$$

implying

$$\xi = \left(\frac{\sqrt{B}}{a}\right)^{\lambda d\lambda}. \tag{2.48}$$

Here terms to the power of $(d\lambda)^2$ have been neglected. The renormalization will be taken into account by a *running coupling*

$$g(x) \to g(x)\left(\frac{\sqrt{B}}{a}\right)^{\lambda d\lambda}, \tag{2.49}$$

which will lead to the additional term

$$\frac{1}{2}g_p \ln\left(\frac{B}{a^2}\right)\lambda\partial_B\lambda \tag{2.50}$$

in the g_p flow equations.

Having assured the correctness of the localization approximation, one can proceed to evaluate the flow of λ. Using the definitions (2.40) and (2.35) one obtains

$$\partial_B \lambda^2 = \frac{8\pi a \lambda^2(1-\lambda^2)}{\Gamma(\lambda^2)} \sum_p g_p g_{-p} |pa|^{\lambda^2-1}. \tag{2.51}$$

Obviously the Toulouse point $\lambda = 1$ is a fixed point of this differential equation.

The potential scattering induced in Eq. (2.32) leads to an additional interaction in the Hamiltonian:

$$H_{ps} = \sum_{p,q} \omega_{pq} \left(C_p^\dagger C_q - C_p C_q^\dagger \right). \tag{2.52}$$

To simplify the numerical evaluation, the generation of non-diagonal terms can be suppressed by introducing a second generator part

$$\boxed{\eta^{(2)} = \sum_{p,q} \eta_{pq}^{(2)} \left(C_p^\dagger C_q - C_q C_p^\dagger \right),} \tag{2.53}$$

where the coefficients have to fulfill

$$\eta_{pq}^{(2)} = -\eta_{qp}^{(2)}, \tag{2.54}$$

so that $\eta^{(2)}$ is anti-Hermitian. One obtains using Eqs. (2.27) and (2.28):

$$\begin{aligned}
[\eta^{(2)}, H_0] &= \sum_{p,q} [\eta_{pq}^{(2)} \left(C_p^\dagger C_q - C_q C_p^\dagger \right), H_0] \\
&= -\sum_{p,q} (p-q) \eta_{pq}^{(2)} \left(C_p^\dagger C_q - C_p C_q^\dagger \right) \\
&= -\sum_{p,q} (p-q) \eta_{pq}^{(2)} \left(C_p^\dagger C_q + C_q^\dagger C_p \right).
\end{aligned} \tag{2.55}$$

Using the anticommutation relations (2.29) the reader easily verifies:

$$\begin{aligned}
[\eta^{(2)}, H_\perp] &= \sum_{k,p,q} \eta_{pq}^{(2)} \alpha_k g_k [C_p^\dagger C_q - C_q C_p^\dagger, C_k^\dagger S^- + C_k S^+] \\
&= 2\sum_{p,q} \eta_{pq}^{(2)} \alpha_q g_q \left(C_p^\dagger S^- + C_p S^+ \right),
\end{aligned} \tag{2.56}$$

$$\begin{aligned}
[\eta^{(1)}, H_{ps}] &= \sum_{k,p,q} k g_k \alpha_k \omega_{pq} [C_k^\dagger S^- + C_k S^+, C_p^\dagger C_q - C_p C_q^\dagger] \\
&= -2\sum_{p,q} q g_q \alpha_q \omega_{pq} \left(C_p^\dagger S^- + C_p S^+ \right)
\end{aligned} \tag{2.57}$$

and

$$\begin{aligned}
[\eta^{(2)}, H_{ps}] &= \sum_{k,l,p,q} \eta^{(2)}_{pq} \omega_{kl} [C^\dagger_p C_q - C_q C^\dagger_p, C^\dagger_k C_l - C_k C^\dagger_l] \\
&= 2 \sum_{k,p,q} \eta^{(2)}_{pq} \left((C^\dagger_p C_k + C^\dagger_k C_p) \omega_{qk} - (C^\dagger_q C_k + C^\dagger_k C_q) \omega_{pk} \right) \\
&= 2 \sum_{p,q} \eta^{(2)}_{pq} (C^\dagger_p C_q + C^\dagger_q C_p)(\omega_{qq} - \omega_{pp}). \qquad (2.58)
\end{aligned}$$

By Eqs. (2.32), (2.55) and (2.58) no off-diagonal potential scattering terms are induced, if for $p \neq q$

$$\frac{1}{2}(p+q) g_p g_q \alpha_p \alpha_q - (p-q)\eta^{(2)}_{pq} + 2\eta^{(2)}_{pq}(\omega_q - \omega_p) = 0 \qquad (2.59)$$

or equivalently

$$\eta^{(2)}_{pq} = \frac{1}{2} \frac{(p+q) g_p g_p \alpha_p \alpha_q}{p - q + 2(\omega_p - \omega_q)} \qquad (2.60)$$

is fulfilled. Here for convenience

$$\omega_p \equiv \omega_{pp} \qquad (2.61)$$

has been defined. From the antisymmetric definition (2.54) follows

$$\eta^{(2)}_{pp} = 0. \qquad (2.62)$$

After eliminating the off-diagonal potential scattering terms one arrived at the Hamiltonian

$$\boxed{H(B) = H_0 + \sum_p g_p \alpha_p \left(C^\dagger_p S^- + C_p S^+ \right) + \sum_p \omega_p \left(C^\dagger_p C_p - C_p C^\dagger_p \right)} \qquad (2.63)$$

with the closed set of flow equations

$$\boxed{\begin{aligned}
\partial_B \lambda^2 &= \frac{8\pi a \lambda^2 (1-\lambda^2)}{\Gamma(\lambda^2)} \sum_p g_p g_{-p} |pa|^{\lambda^2 - 1}, \\
\partial_B g_p &= -p^2 g_p + 2 \sum_{q \neq p} \frac{\alpha_q}{\alpha_p} \eta^{(2)}_{pq} g_q + \frac{1}{2} g_p \ln\left(\frac{B}{a^2}\right) \lambda \partial_B \lambda - 2p g_p \omega_p, \\
\partial_B \omega_p &= p \alpha_p^2 g_p^2,
\end{aligned}} \qquad (2.64)$$

as already found in [12],[13]. The latter were derived using the generator

$$\boxed{\eta = \sum_p p g_p \alpha_p \left(C^\dagger_p S^- - C_p S^+ \right) + \sum_{p,q} \eta^{(2)}_{pq} \left(C^\dagger_p C_q - C_q C^\dagger_p \right).} \qquad (2.65)$$

Due to the complicated structure of the differential equations a complete analytic solution is almost impossible. Apart from the strong-coupling fixed point $\lambda^2 = 1$ the potential scattering can be neglected and an approximate evaluation is possible.

2.3 Phase diagram

Neglecting terms of $\mathcal{O}(g_p^3)$ (terms induced by the potential scattering and $\eta^{(2)}$) the flow equation of the coupling g_p can be approximated by

$$\partial_B g_p = -p^2 g_p + \frac{1}{4} g_p \ln(B) \partial_B \lambda^2. \tag{2.66}$$

For convenience the regularization parameter a is set to 1 throughout this section. Using the ansatz

$$g_p(B) = \tilde{g}(B) e^{-Bp^2}, \tag{2.67}$$

one finds

$$\begin{aligned} \sum_p g_p g_{-p} |p|^{\lambda^2-1} &= 2\tilde{g}^2 \sum_{p>0} p^{\lambda^2-1} e^{-2Bp^2} \\ &= \tilde{g}^2 \frac{L}{\pi} \int_0^\infty dp\, (p^2)^{(\lambda^2-1)/2} e^{-2Bp^2} \\ &= \tilde{g}^2 \frac{L}{2\pi} 2^{-\lambda^2/2} B^{-\lambda^2/2} \Gamma\left(\frac{\lambda^2}{2}\right), \end{aligned} \tag{2.68}$$

leading to the two coupled flow equations

$$\partial_B \tilde{g} = \frac{1}{4} \tilde{g} \ln(B) \partial_B \lambda^2 \tag{2.69}$$

and

$$\partial_B \lambda^2 = L H(\lambda^2) B^{-\lambda^2/2} \tilde{g}^2. \tag{2.70}$$

Here

$$H(\lambda^2) = \frac{2^{2-\lambda^2/2} \lambda^2 (1-\lambda^2) \Gamma(\lambda^2/2)}{\Gamma(\lambda^2)} \tag{2.71}$$

has been introduced. Please note that the Toulouse point $\lambda^2 = 1 \;\rightarrow\; \partial_B \lambda^2 = 0$ is a fixed point of both differential equations. Using a logarithmic measure of the flow parameter

$$x = \ln(B) \tag{2.72}$$

Eq. (2.69) can be integrated:

$$\tilde{g}(x) = \tilde{g}_0 \exp\left[\frac{1}{4}\left(\lambda^2(x) x - \int_{x_0}^{x} dy \lambda^2(y)\right)\right]. \tag{2.73}$$

Defining new couplings

$$u(x) = \frac{1}{2}\left(1 - \frac{\lambda^2(x)}{2}\right), \; u(0) = \frac{J_\parallel}{4\pi} + \mathcal{O}(J_\parallel^2) \tag{2.74}$$

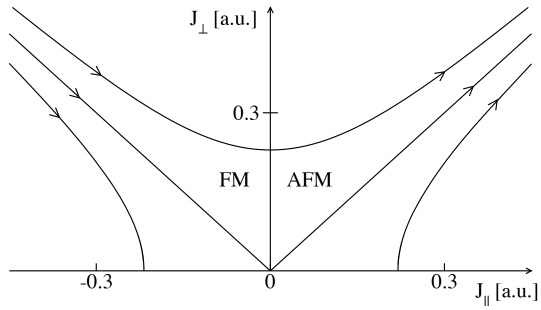


Figure 2.1: Phase diagram of the Kondo model

and

$$v(x) = \sqrt{L}\tilde{g}(x)\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right),\ v(0) = \frac{J_\perp}{4\pi}, \tag{2.75}$$

one finds

$$\begin{aligned} \partial_x u(x) &= -\frac{1}{4}LH(\lambda^2)\exp\left[x\left(1-\frac{\lambda^2}{2}\right)\right]\tilde{g}^2 \\ &= -\frac{1}{4}H(\lambda^2)v^2(x) \end{aligned} \tag{2.76}$$

and

$$\begin{aligned} \partial_x v(x) &= \sqrt{L}\tilde{g}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2\right)\left(\frac{1}{2} - \frac{1}{4}x\lambda^2\right) + \\ &\quad +\sqrt{L}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2\right)\left(-\frac{1}{4}\tilde{g}x\partial_x\lambda^2\right) + \\ &\quad +\sqrt{L}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2\right)\partial_x\tilde{g} \\ &= u(x)v(x). \end{aligned} \tag{2.77}$$

In the limit of small couplings $J_\parallel$ and using

$$\lim_{\lambda^2\to 2} H(\lambda^2) = -4, \tag{2.78}$$

one obtains the scaling equations derived by Anderson [7]:

$$\boxed{\begin{aligned} \partial_x u(x) &= v^2(x) \\ \partial_x v(x) &= u(x)v(x) \end{aligned}} \tag{2.79}$$

and also the Kosterlitz-Thouless phase diagram (Fig. 2.1).

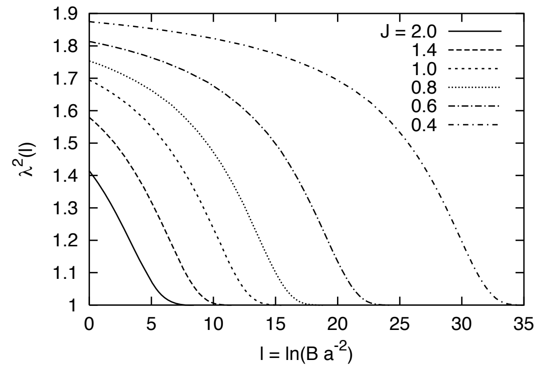


Figure 2.2: Flow of the scaling dimension towards the Toulouse point [13], $J_\| = J_\perp = J$

2.4 Flow of the scaling dimension

Though a complete analytic solution of the flow equations (2.64) is only hard to achieve, the numerical solution is straightforward. Fig. (2.2) shows the flow of the scaling dimension found by Hofstetter and Kehrein [13] for various symmetric antiferromagnetic initial values $J_\| = J_\perp = J$.

The Kondo temperature is the characteristic low energy scale of the system. In the limit $B \to \infty$ the scaling dimension always flows to the Toulouse point and the Hamiltonian is equivalent to the noninteracting resonant level model, whose low energy scale is given by the *Anderson width* of the resonant level. Therefore one can conclude

$$T_K \sim \frac{1}{a}\tilde{g}^2(B = \infty). \qquad (2.80)$$

This relation will be of key importance for the following chapters.

From the flow equations (2.64) follows that the "speed" of the flow of the scaling dimension from one point λ_1 to another point $\lambda_2 < \lambda_1$ only depends on the size of the g_p's. Or using the results from Section 2.3 it depends mainly on the prefactor $\tilde{g}(B)$. Obviously a large $\tilde{g}(B)$ corresponds to a fast flow and a small $\tilde{g}(B)$ to a slow flow. Choosing e.g. $\lambda_2 = 1$ one can determine the size of $\tilde{g}(B = \infty)$ by analyzing the speed of the flow and therefore by using Eq. (2.80) one can give an estimation on the dependency of the Kondo temperature on the initial couplings.

Interpreting Fig. (2.2) leads to the expected conclusion that larger couplings lead to higher Kondo temperatures than smaller ones do. For a derivation of the functional dependence of the Kondo temperature from the initial couplings see [12] and [13].

2.5 Summary

In this chapter we reviewed the flow equation solution of the anisotropic Kondo model with constant density of states. By using Wegner's flow equation approach (and within the OPE) the bosonized Hamiltonian of the anisotropic Kondo model can be mapped (in the strong-coupling regime) to an effective low energy Hamiltonian of the noninteracting resonant level model (RLM), which can be solved exactly. Unlike earlier scaling approaches in fermionic language no divergence of the renormalized coupling constants occurs.

3 The Kondo model with nontrivial density of states

In this chapter we will extend the previously derived solution of the anisotropic Kondo model with a constant density of states ([12],[13]) to systems with a nontrivial one. This extension provides the original part of this thesis.

3.1 Motivation

The flow equation solution of the anisotropic Kondo model (2.1) with momentum independent couplings $J_{\parallel/\perp}(p,q) \equiv J_{\parallel/\perp}(0,0)$ was reviewed in the previous chapter. But for strong-correlating systems the latter assumption is definitive wrong, e.g. cuprate superconductors and certain semi-conductors show a pseudogap density of states

$$\rho(\epsilon) \sim |\epsilon|^r,\ r \neq 0, \tag{3.1}$$

leading to a strong momentum-dependency of the couplings. As has been shown in earlier NRG calculations (see e.g. [24] and [25]) for these systems it is of key importance to take the momentum-dependency into account. Another interesting application are systems that can be studied in a DMFT-framework.

In the following we will use Wegner's flow equation approach to map the Hamiltonian of the anisotropic Kondo model with momentum-dependent couplings to an effective RLM-Hamiltonian, similar to the calculations in the previous chapter.

Though it is possible to completely bosonize the Hamiltonian

$$\begin{aligned} H &= \sum_{p,\alpha} p c^\dagger_{p\alpha} c_{p\alpha} + \sum_{p,q,\alpha,\beta} \frac{J_\parallel(p,q)}{L} c^\dagger_{p\alpha} \sigma^z_{\alpha\beta} c_{q\beta} S^z + \\ &\quad + \sum_{p,q,\alpha,\beta} \frac{J_\perp(p,q)}{2L} \left(c^\dagger_{p\alpha} \sigma^+_{\alpha\beta} c_{q\beta} S^- + \text{ h.c. } \right), \end{aligned} \tag{3.2}$$

it turns out that a partial bosonization is the more appropriate tool. We will rewrite the Hamiltonian above to

$$H = \sum_{p,\alpha} p c^\dagger_{p\alpha} c_{p\alpha} + \sum_{p,q,\alpha,\beta} \frac{J_\parallel(0,0)}{L} c^\dagger_{p\alpha} \sigma^z_{\alpha\beta} c_{q\beta} S^z +$$

$$
\begin{aligned}
& + \sum_{p,q,\alpha,\beta} \frac{J_\perp(0,0)}{2L} \left(c^\dagger_{p\alpha} \sigma^+_{\alpha\beta} c_{q\beta} S^- + \text{ h.c. } \right) + \\
& + \sum_{p,q,\alpha,\beta} \frac{J_\parallel(p,q) - J_\parallel(0,0)}{L} c^\dagger_{p\alpha} \sigma^z_{\alpha\beta} c_{q\beta} S^z + \\
& + \sum_{p,q,\alpha,\beta} \frac{J_\perp(p,q) - J_\perp(0,0)}{2L} \left(c^\dagger_{p\alpha} \sigma^+_{\alpha\beta} c_{q\beta} S^- + \text{ h.c. } \right) \\
\equiv \; & H_0 + H^{(0,0)}_\parallel + H^{(0,0)}_\perp + \tilde{H}_\parallel + \tilde{H}_\perp \qquad (3.3)
\end{aligned}
$$

and use this form as the starting point of our approach. While the terms $H^{(0,0)}_\parallel$ and $H^{(0,0)}_\perp$ can again be easily bosonized, we will keep the fermionic representation of $\tilde{H}_\parallel$ and $\tilde{H}_\perp$. H_0 will be treated in both fermionic and bosonic representation. Please note that the charge density modes only affect the fermionic part of the Hamiltonian.
In the semi-bosonized form we can reuse the results of the previous chapter and we only have to calculate the flow induced by the corrections $\tilde{H}_\parallel$ and $\tilde{H}_\perp$. Since the terms induced by the additional potential scattering only become important at energies of the order of the Kondo scale, corrections proportional to them can be neglected.

3.2 Additional longitudinal scattering

In this section we want to calculate the main parts of the flow induced by the corrections to the longitudinal scattering $\tilde{H}_\parallel$. For convenience we define

$$
\begin{aligned}
\tilde{H}_\parallel &= \sum_{p,q,\alpha,\beta} \frac{J_\parallel(p,q) - J_\parallel(0,0)}{L} c^\dagger_{p\alpha} \sigma^z_{\alpha\beta} c_{q\beta} S^z \\
&\equiv \sum_{p,q} f_\parallel(p,q) \left(c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow} \right) S^z \qquad (3.4) \\
&\equiv \tilde{\sigma}_\parallel S^z. \qquad (3.5)
\end{aligned}
$$

To calculate the flow induced by the generator $\eta^{(1)}$ (Eq. (2.30)) we will need the commutators $[\tilde{\sigma}_\parallel, \sigma(k)]$ and $[\tilde{\sigma}_\parallel, \Phi(x)]$. Neglecting normal-ordered terms we find

$$
\begin{aligned}
[\tilde{\sigma}_\parallel, \sigma(k)] &= \sum_{p,q,l} \frac{f_\parallel(p,q)}{\sqrt{2|k|}} [c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}, c^\dagger_{l+k\uparrow} c_{l\uparrow} - c^\dagger_{l+k\downarrow} c_{l\downarrow}] \\
&= \sum_{p,q,\alpha} \frac{f_\parallel(p,q)}{\sqrt{2|k|}} \left(c^\dagger_{p\alpha} c_{q-k\alpha} - c^\dagger_{p+k\alpha} c_{q\alpha} \right)
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{p,q,\alpha} \frac{f_\parallel(p,q)}{\sqrt{2|k|}} \Big(:c^\dagger_{p\alpha} c_{q-k\alpha}: - :c^\dagger_{p+k\alpha} c_{q\alpha}: + \\
&\quad + \langle 0| c^\dagger_{p\alpha} c_{q-k\alpha} |0\rangle - \langle 0| c^\dagger_{p+k\alpha} c_{q\alpha} |0\rangle \Big) \\
&\approx 2 \sum_p \frac{f_\parallel(p,p+k)}{\sqrt{2|k|}} \left[\Theta(-p) - \Theta(-p-k)\right] \\
&\equiv A_k \qquad (3.6)
\end{aligned}
$$

and

$$
\begin{aligned}
[\tilde{\sigma}_\parallel, \Phi(x)] &= -\frac{2\pi i}{L} \sum_{k\neq 0} \frac{\sqrt{|k|}}{k} \exp\left(-ikx - a|k|\frac{1}{2}\right) [\tilde{\sigma}_\parallel, \sigma(k)] \\
&= -\frac{2\pi i}{L} \sum_{k\neq 0} \frac{\sqrt{|k|}}{k} \exp\left(-ikx - a|k|\frac{1}{2}\right) A_k. \qquad (3.7)
\end{aligned}
$$

Within this approximation $\tilde{H}_\parallel$ is (up to a constant) invariant under Emery-Kivelson transformations of the form

$$
U = \exp\left(i \int dx\ f(x)\Phi(x) S^z\right), \qquad (3.8)
$$

because

$$
\begin{aligned}
U \tilde{H}_\parallel U^\dagger &\overset{(A.3)}{=} \tilde{H}_\parallel - i \int dx\ f(x) [\tilde{\sigma}_\parallel, \Phi(x)] (S^z)^2 \\
&= \tilde{H}_\parallel + \text{const.}\ . \qquad (3.9)
\end{aligned}
$$

The generator part according to $\tilde{H}_\parallel$ can be easily calculated using the fermionic representation of H_0:

$$
\begin{aligned}
[H_0, \tilde{H}_\parallel] &= \sum_{k,p,q} k f_\parallel(p,q) S^z [c^\dagger_{k\uparrow} c_{k\uparrow} + c^\dagger_{k\downarrow} c_{k\downarrow}, c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}] \\
&= \sum_{p,q} (p-q) f_\parallel(p,q) (c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}) S^z, \qquad (3.10)
\end{aligned}
$$

leading to:

$$
\boxed{\eta^{(3)} = \sum_{p,q} (p-q) f_\parallel(p,q) (c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}) S^z.} \qquad (3.11)
$$

For the main part of the flow of $f_\parallel(p,q)$ we find

$$
\begin{aligned}
[\eta^{(3)}, H_0] &= \sum_{k,p,q} k(p-q) f_\parallel(p,q) [c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}, c^\dagger_{k\uparrow} c_{k\uparrow} + c^\dagger_{k\downarrow} c_{k\downarrow}] S^z \\
&= -\sum_{p,q} (p-q)^2 f_\parallel(p,q) (c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}) S^z, \qquad (3.12)
\end{aligned}
$$

which corresponds to an exponential decay as expected. Unfortunately the calculation of the remaining commutators is slightly more complicated but straightforward:

$$
\begin{aligned}
[\eta^{(1)}, \tilde{H}_{\|}] &= \sum_p \eta_p^{(1)} [C_p^\dagger S^- - C_p S^+, \tilde{\sigma}_{\|} S^z] \\
&= \sum_p \eta_p^{(1)} \left(C_p^\dagger \tilde{\sigma}_{\|} [S^-, S^z] + [C_p^\dagger, \tilde{\sigma}_{\|}] S^z S^- - \right. \\
&\quad \left. - C_p \tilde{\sigma}_{\|} [S^+, S^z] - [C_p, \tilde{\sigma}_{\|}] S^z S^+ \right) \\
&= \frac{1}{2} \sum_p \eta_p^{(1)} \left(\{\tilde{\sigma}_{\|}, C_p^\dagger\} S^- + \{\tilde{\sigma}_{\|}, C_p\} S^+ \right). \qquad (3.13)
\end{aligned}
$$

To calculate the OPE of $\{\tilde{\sigma}_{\|}, C_p^{(\dagger)}\}$ we will rewrite $\tilde{\sigma}_{\|}$ in terms of particle-hole-excitation creation and annihilation operators $\alpha^+(p)$ and $\alpha^-(p)$. Using Eq. (A.3) we will commute the $\alpha^-(p)$ terms to the right of $C_p^{(\dagger)}$ and the $\alpha^+(p)$ terms to the left of these. By doing this we can achieve the normal-ordering of these terms (see boson-normal-ordering, Eq. (1.45)). Keeping only the not normal-ordered terms we already found a suitable OPE as will turn out in the following.
The new particle-hole-excitation creation and annihilation operators are defined by

$$
\begin{aligned}
\tilde{\sigma}_{\|} &= \sum_{p,q} f_{\|}(p,q) \left(c_{p\uparrow}^\dagger c_{q\uparrow} - c_{p\downarrow}^\dagger c_{q\downarrow} \right) \\
&= \sum_p \Big(f_{\|}(p,p)(c_{p\uparrow}^\dagger c_{p\uparrow} - c_{p\downarrow}^\dagger c_{p\downarrow}) + \\
&\quad + \sum_{q>0} f_{\|}(p+q,p)(c_{p+q\uparrow}^\dagger c_{p\uparrow} - c_{p+q\downarrow}^\dagger c_{p\downarrow}) + \\
&\quad + \sum_{q>0} f_{\|}(p-q,p)(c_{p-q\uparrow}^\dagger c_{p\uparrow} - c_{p-q\downarrow}^\dagger c_{p\downarrow}) \Big) \\
&\equiv \sum_p \left(\alpha^0(p) + \alpha^+(p) + \alpha^-(p) \right). \qquad (3.14)
\end{aligned}
$$

In the following we will need the commutation relations

$$
\begin{aligned}
\sum_p [\alpha^-(p), \Phi(x)] &= \sum_p \sum_{q>0} \frac{-\sqrt{2}\pi i}{L} \sum_{k\neq 0} f_{\|}(p-q,p) \frac{1}{k} e^{-ikx - a|k|/2} \times \\
&\quad \times \sum_l [c_{p-q\uparrow}^\dagger c_{p\uparrow} - c_{p-q\downarrow}^\dagger c_{p\downarrow}, c_{l+k\uparrow}^\dagger c_{l\uparrow} - c_{l+k\downarrow}^\dagger c_{l\downarrow}] \\
&\equiv \sum_{p,l,\alpha} \sum_{q>0} \sum_{k\neq 0} g(p,q,k,x) [c_{p-q\alpha}^\dagger c_{p\alpha}, c_{l+k\alpha}^\dagger c_{l\alpha}]
\end{aligned}
$$

$$\begin{aligned}
&= \sum_{p,l,\alpha} \sum_{q>0} \sum_{k\neq 0} g(p,q,k,x) \left(c^\dagger_{p-q\alpha} c_{l\alpha} \delta_{p,l+k} - c^\dagger_{l+k\alpha} c_{p\alpha} \delta_{p-q,l} \right) \\
&= \sum_{p,\alpha} \sum_{q>0} \sum_{k\neq 0} g(p,q,k,x) \Big(: c^\dagger_{p-q\alpha} c_{p-k\alpha} : - : c^\dagger_{p-q+k\alpha} c_{p\alpha} : + \\
&\quad + \langle 0 | c^\dagger_{p-q\alpha} c_{p-k\alpha} | 0 \rangle - \langle 0 | c^\dagger_{p-q+k\alpha} c_{p\alpha} | 0 \rangle \Big) \\
&= \sum_{p,\alpha} \sum_{q>0} \sum_{k\neq 0} \left[g(p+k,q,k,x) - g(p,q,k,x) \right] : c^\dagger_{p-q+k\alpha} c_{p\alpha} : + \\
&\quad + 2 \sum_{p} \sum_{q>0} \sum_{k\neq 0} g(p,q,k,x) \delta_{q,k} \left[\Theta(-p+q) - \Theta(-p) \right] \\
&\approx 2 \sum_{p} \sum_{q>0} g(p,q,q,x) \left[\Theta(-p+q) - \Theta(-p) \right] \\
&= -\frac{2\sqrt{2}\pi i}{L} \sum_{p} \sum_{q>0} \frac{f_\parallel(p-q,p)}{q} e^{-iqx - a|q|/2} \times \\
&\quad \times \left[\Theta(-p+q) - \Theta(-p) \right]
\end{aligned} \tag{3.15}$$

and

$$\begin{aligned}
\sum_p [\alpha^+(p), \Phi(x)] &= \frac{2\sqrt{2}\pi i}{L} \sum_p \sum_{q>0} \frac{f_\parallel(p+q,p)}{q} e^{iqx - a|q|/2} \times \\
&\quad \times \left[\Theta(-p-q) - \Theta(-p) \right],
\end{aligned} \tag{3.16}$$

which can be derived analog. We calculate the OPE of $V(\lambda,x)\tilde{\sigma}_\parallel$ by

$$\begin{aligned}
V(\lambda,x)\tilde{\sigma}_\parallel &= V(\lambda,x) \sum_p \left(\alpha^0(p) + \alpha^+(p) + \alpha^-(p) \right) \\
&= V(\lambda,x) \sum_p \left(\alpha^0(p) + \alpha^-(p) \right) + \sum_p \alpha^+(p) V(\lambda,x) + \\
&\quad + \sum_p [V(\lambda,x), \alpha^+(p)] \\
&= :: V(\lambda,x) : \left(\frac{L}{2\pi a} \right)^{-\lambda^2/2} \sum_p \alpha^0(p) : + \\
&\quad + : V(\lambda,x) \sum_p \alpha^-(p) : + : \sum_p \alpha^+(p) V(\lambda,x) : - \\
&\quad - \sum_p [\alpha^+(p), e^{i\lambda\Phi(x)}] \\
&\overset{(A.3)}{\approx} -i\lambda \sum_p [\alpha^+(p), \Phi(x)] V(\lambda,x)
\end{aligned}$$

$$\begin{aligned}
&= \frac{2\sqrt{2}\pi\lambda}{L}\sum_p\sum_{q>0}\frac{f_\parallel(p+q,p)}{q}e^{iqx-a|q|/2}\times \\
&\quad\times\left[\Theta(-p-q)-\Theta(-p)\right]V(\lambda,x) \\
&\equiv \lambda\sum_{q>0}\frac{B_q}{|q|}e^{iqx}V(\lambda,x). \qquad (3.17)
\end{aligned}$$

For the OPE of $\tilde{\sigma}_\parallel V(\lambda,x)$ we find

$$\tilde{\sigma}_\parallel V(\lambda,x) = \lambda\sum_{q<0}\frac{B_q}{|q|}e^{iqx}V(\lambda,x), \qquad (3.18)$$

leading to

$$\{\tilde{\sigma}_\parallel, V(\lambda,x)\} = \lambda\sum_{q\neq 0}\frac{B_q}{|q|}e^{iqx}V(\lambda,x). \qquad (3.19)$$

Using the definition of $C_p^{(\dagger)}$ from Eq. (2.24) one finds

$$\begin{aligned}
\{\tilde{\sigma}_\parallel, C_p^\dagger\} &= \frac{1}{\alpha_p\sqrt{L}}\int dx e^{ipx}\{\tilde{\sigma}_\parallel, V(\lambda,x)\} \\
&= \frac{1}{\alpha_p\sqrt{L}}\lambda\sum_{q\neq 0}\frac{B_q}{|q|}\int dx e^{i(p+q)x}V(\lambda,x) \\
&= \lambda\sum_{q\neq 0}\frac{B_q}{|q|}\frac{\alpha_{p+q}}{\alpha_p}C_{p+q}^\dagger \qquad (3.20)
\end{aligned}$$

and

$$\{\tilde{\sigma}_\parallel, C_p\} = -\lambda\sum_{q\neq 0}\frac{B_q}{|q|}\frac{\alpha_{p-q}}{\alpha_p}C_{p-q}. \qquad (3.21)$$

Using the OPEs above we can easily continue the previous calculation:

$$\begin{aligned}
[\eta^{(1)}, \tilde{H}_\parallel] &= \frac{1}{2}\sum_p \eta_p^{(1)}\left(\{\tilde{\sigma}_\parallel, C_p^\dagger\}S^- + \{\tilde{\sigma}_\parallel, C_p\}S^+\right) \\
&= \frac{1}{2}\sum_p \eta_p^{(1)}\lambda\sum_{q\neq 0}\frac{B_q}{|q|\alpha_p}\left(\alpha_{p+q}C_{p+q}^\dagger S^- - \alpha_{p-q}C_{p-q}S^+\right) \\
&= -\sum_p\left(\sum_{q\neq 0}\frac{\lambda}{2}\frac{B_q}{|q|}\alpha_p\frac{\eta_{p+q}^{(1)}}{\alpha_{p+q}}\right)\left(C_p^\dagger S^- + C_p S^+\right) \\
&= -\sum_p\sum_{q\neq 0}\sum_k\frac{\sqrt{2}\pi\lambda}{L}\frac{f_\parallel(k+q,k)}{|q|}e^{-a|q|/2}\left[\Theta(-k-q)-\right. \\
&\quad \left.-\Theta(-k)\right](p+q)g_{p+q}\alpha_p\left(C_p^\dagger S^- + C_p S^+\right). \qquad (3.22)
\end{aligned}$$

Since the main longitudinal scattering part of the Hamiltonian $H_{\parallel}^{(0,0)}$ has already been eliminated by the Emery-Kivelson transformation, we are left with the commutator:

$$\begin{aligned}
[\eta^{(3)}, H_{\perp}^{(0,0)}] &= \sum_p \alpha_p g_p [\tau^z S^z, C_p^\dagger S^- + C_p S^+] \\
&= \sum_p \alpha_p g_p \left(\tau^z C_p^\dagger [S^z, S^-] + \tau^z C_p [S^z, S^+]\right. \\
&\quad \left. + [\tau^z, C_p^\dagger] S^- S^z + [\tau^z, C_p] S^+ S^z\right) \\
&= \frac{1}{2} \sum_p \alpha_p g_p \left(-\{\tau^z, C_p^\dagger\} S^- + \{\tau^z, C_p\} S^+\right),
\end{aligned} \tag{3.23}$$

where for convenience

$$\tau^z \equiv \sum_{p,q} (p-q) f_{\parallel}(p,q)(c_{p\uparrow}^\dagger c_{q\uparrow} - c_{p\downarrow}^\dagger c_{q\downarrow}) \tag{3.24}$$

has been defined. Analog to the OPE of $\{\tilde{\sigma}_{\parallel}, C_p^{(\dagger)}\}$ (Eqs. (3.20) and (3.21)) we find the relations

$$\{\tau^z, C_p^\dagger\} = \lambda \sum_{q\neq 0} \mathrm{sgn}(q) B_q \frac{\alpha_{p+q}}{\alpha_p} C_{p+q}^\dagger \tag{3.25}$$

and

$$\{\tau^z, C_p\} = -\lambda \sum_{q\neq 0} \mathrm{sgn}(q) B_q \frac{\alpha_{p-q}}{\alpha_p} C_{p-q}. \tag{3.26}$$

Within these OPEs we find:

$$\begin{aligned}
[\eta^{(3)}, H_{\perp}^{(0,0)}] &= \frac{1}{2} \sum_p \alpha_p g_p \left(-\{\tau^z, C_p^\dagger\} S^- + \{\tau^z, C_p\} S^+\right) \\
&= -\frac{1}{2} \sum_p \alpha_p g_p \left(\lambda \sum_{q\neq 0} \mathrm{sgn}(q) B_q \frac{\alpha_{p+q}}{\alpha_p} C_{p+q}^\dagger S^- + \right. \\
&\quad \left. + \lambda \sum_{q\neq 0} \mathrm{sgn}(q) B_q \frac{\alpha_{p-q}}{\alpha_p} C_{p-q} S^+\right) \\
&= -\frac{\lambda}{2} \sum_{q\neq 0} \sum_p g_{p+q} \mathrm{sgn}(q) B_q \alpha_p \left(C_p^\dagger S^- + C_p S^+\right) \\
&= -\sum_p \sum_{q\neq 0} \sum_k \frac{\sqrt{2}\pi\lambda}{L} \frac{f_{\parallel}(k+q,k)}{|q|} e^{-a|q|/2} g_{p+q} \alpha_p q \times \\
&\quad \times [\Theta(-k-q) - \Theta(-k)] \left(C_p^\dagger S^- + C_p S^+\right).
\end{aligned} \tag{3.27}$$

The addition of the previous commutators leads to:

$$
\begin{aligned}
[\eta^{(1)}, \tilde{H}_{\|}] + [\eta^{(3)}, H_{\perp}^{(0,0)}] &= -\sum_{p}\sum_{q\neq 0}\sum_{k} \frac{\sqrt{2}\pi\lambda}{L} \frac{(p+2q) f_{\|}(k+q,k)}{|q|} e^{-a|q|/2} \times \\
&\quad \times g_{p+q}\alpha_p \left[\Theta(-k-q) - \Theta(-k)\right] \times \\
&\quad \times \left(C_p^{\dagger} S^{-} + C_p S^{+}\right). \qquad (3.28)
\end{aligned}
$$

3.3 Additional spin-flip scattering

The calculation of the flow induced by $\tilde{H}_{\perp}$ is slightly more difficult because we cannot use the OPE derived in the previous section as we will see below. We will therefore rewrite the vertex operators in their series representation keeping only terms of $\mathcal{O}(J_{\|}^{(0,0)})$ and use an expansion similar to Wick's theorem to reduce complicated fermionic multi-particle objects to single-particle excitations.
Again we rewrite the interaction to

$$
\begin{aligned}
\tilde{H}_{\perp} &= \sum_{p,q} \frac{J_{\perp}(p,q) - J_{\perp}(0,0)}{2L} (c_{p\uparrow}^{\dagger} c_{q\downarrow} S^{-} + c_{p\downarrow}^{\dagger} c_{q\uparrow} S^{+}) \\
&\equiv \sum_{p,q} f_{\perp}(p,q) (c_{p\uparrow}^{\dagger} c_{q\downarrow} S^{-} + c_{p\downarrow}^{\dagger} c_{q\uparrow} S^{+}) \qquad (3.29) \\
&\equiv \tilde{\sigma}_{\perp}^{+} S^{-} + \tilde{\sigma}_{\perp}^{-} S^{+}. \qquad (3.30)
\end{aligned}
$$

Calculating the commutator relations with the spin density modes we find e.g.

$$
\begin{aligned}
[\tilde{\sigma}_{\perp}^{+}, \sigma(k)] &= \sum_{l,p,q} \frac{f_{\perp}(p,q)}{\sqrt{2|k|}} [c_{p\uparrow}^{\dagger} c_{q\downarrow}, c_{l+k\uparrow}^{\dagger} c_{l\uparrow} - c_{l+k\downarrow}^{\dagger} c_{l\downarrow}] \\
&= -\sum_{p,q} \frac{f_{\perp}(p,q)}{\sqrt{2|k|}} (c_{p+k\uparrow}^{\dagger} c_{q\downarrow} + c_{p\uparrow}^{\dagger} c_{q-k\downarrow}) \\
&= -\sum_{p,q} \frac{f_{\perp}(p-k,q) + f_{\perp}(p,q+k)}{\sqrt{2|k|}} c_{p\uparrow}^{\dagger} c_{q\downarrow}. \qquad (3.31)
\end{aligned}
$$

Dropping the normal-ordered terms as in the previous section leads to

$$
[\tilde{\sigma}_{\perp}^{+}, \Phi(x)] = [\tilde{\sigma}_{\perp}^{-}, \Phi(x)] = 0. \qquad (3.32)
$$

Within this approximation the unitary transformations of the form

$$
U = \exp\left(i \int dx\; f(x)\Phi(x) S^{z}\right) \qquad (3.33)
$$

lead to

$$\begin{aligned} U\tilde{H}_\perp U^\dagger &= \tilde{\sigma}_\perp^+ U S^- U^\dagger + \tilde{\sigma}_\perp^- U S^+ U^\dagger \\ &= \tilde{\sigma}_\perp^+ S^-[1+\mathcal{O}(f)] + \tilde{\sigma}_\perp^- S^+[1+\mathcal{O}(f)] \\ &\approx \tilde{H}_\perp. \end{aligned} \tag{3.34}$$

Therefore we will assume that both Emery-Kivelson transformation leave $\tilde{H}_\perp$ unchanged, which is correct for small couplings $f(x)$.

To derive the generator corresponding to $\tilde{H}_\perp$ one has to calculate the commutator:

$$\begin{aligned} [H_0, \tilde{H}_\perp] &= \sum_{k,p,q} k f_\perp(p,q)[c^\dagger_{k\uparrow}c_{k\uparrow} + c^\dagger_{k\downarrow}c_{k\downarrow}, c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\downarrow}c_{q\uparrow}S^+] \\ &= \sum_{p,q}(p-q)f_\perp(p,q)\left(c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\downarrow}c_{q\uparrow}S^+\right) \\ &\equiv \tau^+S^- + \tau^-S^+. \end{aligned} \tag{3.35}$$

By

$$\boxed{\eta^{(4)} = \sum_{p,q}(p-q)f_\perp(p,q)\left(c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\downarrow}c_{q\uparrow}S^+\right)} \tag{3.36}$$

we have derived the final part of the generator η. Again the commutator

$$\begin{aligned} [\eta^{(4)}, H_0] &= \sum_{k,p,q} k(p-q) f_\perp(p,q)[c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\downarrow}c_{q\uparrow}S^+, c^\dagger_{k\uparrow}c_{k\uparrow} + c^\dagger_{k\downarrow}c_{k\downarrow}] \\ &= -\sum_{p,q}(p-q)^2 f_\perp(p,q)\left(c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\downarrow}c_{q\uparrow}S^+\right), \end{aligned} \tag{3.37}$$

leads to an exponential decay of the coupling. As in the previous section the remaining commutators lead to more complicated structures, e.g.:

$$\begin{aligned} [\eta^{(1)}, \tilde{H}_\perp] &= \sum_k k\alpha_k g_k[C^\dagger_k S^- - C_k S^+, \tilde{\sigma}_\perp^+ S^- + \tilde{\sigma}_\perp^- S^+] \\ &= \sum_k k\alpha_k g_k \Big(C^\dagger_k \tilde{\sigma}_\perp^-[S^-,S^+] + [C^\dagger_k, \tilde{\sigma}_\perp^-]S^+S^- - \\ &\quad - C_k\tilde{\sigma}_\perp^+[S^+,S^-] - [C_k, \tilde{\sigma}_\perp^+]S^-S^+\Big) \\ &\approx -\sum_k 2k\alpha_k g_k\left(C^\dagger_k\tilde{\sigma}_\perp^- + C_k\tilde{\sigma}_\perp^+\right)S^z. \end{aligned} \tag{3.38}$$

Unfortunately we could not find a way to expand the operator products $C_k^{(\dagger)}\tilde{\sigma}_\perp^\pm$ in the bosonic representation. We will therefore expand these expressions in fermionic language by using the relation

$$
\begin{aligned}
e^{i\lambda\Phi(x)} &= e^{i\sqrt{2}\Phi(x)}e^{-i\mu\Phi(x)} \\
&= \frac{2\pi a}{L}\sum_{p,q} e^{i(p-q)x}c^{\dagger}_{p\uparrow}c_{q\downarrow}e^{-i\mu\Phi(x)} \\
&= \frac{2\pi a}{L}\sum_{p,q} e^{i(p-q)x}c^{\dagger}_{p\uparrow}c_{q\downarrow}(1-i\mu\Phi(x)+\mathcal{O}(\mu^2)),
\end{aligned}
\tag{3.39}
$$

where for convenience we defined

$$
\mu = \frac{J_{\|}(0,0)}{2\sqrt{2}\pi}
\tag{3.40}
$$

as in the previous chapter. The occurring many-particle objects will be expanded to single-particle excitations by using

$$
\begin{aligned}
c^{\dagger}_{k\alpha}c_{l\beta}c^{\dagger}_{p\gamma}c_{q\delta} - \langle 0|c^{\dagger}_{k\alpha}c_{l\beta}c^{\dagger}_{p\gamma}c_{q\delta}|0\rangle \; &= :c^{\dagger}_{k\alpha}c_{l\beta}c^{\dagger}_{p\gamma}c_{q\delta}: + \\
+\langle 0|c^{\dagger}_{k\alpha}c_{l\beta}|0\rangle : c^{\dagger}_{p\gamma}c_{q\delta}: &+ \langle 0|c^{\dagger}_{k\alpha}c_{q\delta}|0\rangle : c_{l\beta}c^{\dagger}_{p\gamma}: + \\
+\langle 0|c_{l\beta}c^{\dagger}_{p\gamma}|0\rangle : c^{\dagger}_{k\alpha}c_{q\delta}: &+ \langle 0|c^{\dagger}_{p\gamma}c_{q\delta}|0\rangle : c^{\dagger}_{k\alpha}c_{l\beta}: \; .
\end{aligned}
\tag{3.41}
$$

In the following we will neglect normal-ordered many-particle objects and constants. Please note that this expansion can be successively extended to higher orders by taking contractions of many-particle objects into account. In Appendix B we collected all expansions of this type used in this thesis.
Within these approximations we find

$$
\begin{aligned}
e^{i\lambda\Phi(x)}\tilde{\sigma}^{-}_{\perp} &= e^{i\sqrt{2}\Phi(x)}e^{-i\mu\Phi(x)}\tilde{\sigma}^{-}_{\perp} \\
&= \frac{2\pi a}{L}\sum_{k,k'} e^{i(k-k')x}c^{\dagger}_{k\uparrow}c_{k'\downarrow}e^{-i\mu\Phi(x)}\sum_{p,q} f_{\perp}(p,q)c^{\dagger}_{p\downarrow}c_{q\uparrow} \\
&\approx \frac{2\pi a}{L}\sum_{k,k'} e^{i(k-k')x}c^{\dagger}_{k\uparrow}c_{k'\downarrow}(1-i\mu\Phi(x))\sum_{p,q} f_{\perp}(p,q)c^{\dagger}_{p\downarrow}c_{q\uparrow} \\
&= \frac{2\pi a}{L}\sum_{k,k'} e^{i(k-k')x}c^{\dagger}_{k\uparrow}c_{k'\downarrow}(1-\frac{2\pi\mu}{\sqrt{2}L}\sum_{m\neq 0}\sum_{l}\frac{1}{m}e^{-imx-a|m|/2}\times \\
&\quad \times(c^{\dagger}_{l+m\uparrow}c_{l\uparrow}-c^{\dagger}_{l+m\downarrow}c_{l\downarrow}))\sum_{p,q} f_{\perp}(p,q)c^{\dagger}_{p\downarrow}c_{q\uparrow} \\
&= \frac{2\pi a}{L}\sum_{k,k',p,q} e^{i(k-k')x}f_{\perp}(p,q)c^{\dagger}_{k\uparrow}c_{k'\downarrow}c^{\dagger}_{p\downarrow}c_{q\uparrow} - \\
&\quad -\frac{4\pi^2 a\mu}{\sqrt{2}L^2}\sum_{k,k',p,q,l}\sum_{m\neq 0} e^{i(k-k')x}f_{\perp}(p,q)\frac{1}{m}e^{-imx-a|m|/2}\times
\end{aligned}
$$

$$
\begin{aligned}
&\times c^\dagger_{k\uparrow} c_{k'\downarrow} c^\dagger_{l+m\uparrow} c_{l\uparrow} c^\dagger_{p\downarrow} c_{q\uparrow} + \\
&+\frac{4\pi^2 a\mu}{\sqrt{2}L^2} \sum_{k,k',p,q,l} \sum_{m\neq 0} e^{i(k-k')x} f_\perp(p,q) \frac{1}{m} e^{-imx-a|m|/2} \times \\
&\times c^\dagger_{k\uparrow} c_{k'\downarrow} c^\dagger_{l+m\downarrow} c_{l\downarrow} c^\dagger_{p\downarrow} c_{q\uparrow} \\
\approx\ & \frac{2\pi a}{L} \sum_{p,q} \Bigg(\sum_k f_\perp(k,q) e^{i(p-k)x} \Theta(k) c^\dagger_{p\uparrow} c_{q\uparrow} - \\
&- \sum_k f_\perp(p,k) e^{i(k-q)x} \Theta(-k) c^\dagger_{p\downarrow} c_{q\downarrow} \Bigg) + \\
&+\frac{4\pi^2 a\mu}{\sqrt{2}L^2} \sum_{k,p,q} \sum_{m\neq 0} \frac{1}{m} e^{-imx-a|m|/2} \times \\
&\times \Big[\Big(- e^{i(p-m-k)x} f_\perp(k,q) \Theta(-p+m) \Theta(k) - \\
&e^{i(k-p)x} f_\perp(p,k+m) \Theta(-k) \Theta(-(k+m)) + \\
&+ e^{i(p-(k+m))x} f_\perp(k,q) \Theta(k+m) \Theta(k) \Big) c^\dagger_{p\uparrow} c_{q\uparrow} + \\
&+ \Big(e^{i(k-p)x} f_\perp(p,k+m) \Theta(-k) \Theta(-(k+m)) - \\
&- e^{i(k-(q+m))x} f_\perp(p,k) \Theta(-k) \Theta(q+m) - \\
&- e^{i(k-q)x} f_\perp(q-m,p) \Theta(-p) \Theta(q-m) \Big) c^\dagger_{p\downarrow} c_{q\downarrow} \Big] + \\
&+\frac{4\pi^2 a\mu}{\sqrt{2}L^2} \sum_{k,l} e^{i(l-k)x} f_\perp(k,l) \Theta(-l) \Theta(k) \times \\
&\times \sum_{p\neq q} \frac{1}{p-q} e^{i(p-q)x-a|p-q|/2} c^\dagger_{p\downarrow} c_{q\downarrow}
\end{aligned}
\tag{3.42}
$$

and analog

$$
\begin{aligned}
e^{-i\lambda\Phi(x)} \tilde{\sigma}^+_\perp \ = \ & \frac{2\pi a}{L} \sum_{p,q} \Bigg(\sum_k e^{i(p-k)x} f_\perp(k,q) \Theta(k) c^\dagger_{p\downarrow} c_{q\downarrow} - \\
&- \sum_k e^{i(k-q)x} f_\perp(p,k) \Theta(-k) c^\dagger_{p\uparrow} c_{q\uparrow} \Bigg) - \\
&+\frac{4\pi^2 a\mu}{\sqrt{2}L^2} \sum_{k,p,q} \sum_{m\neq 0} \frac{1}{m} e^{-imx-a|m|/2} \times \\
&\times \Big[\Big(- e^{i(p-m-k)x} f_\perp(k,q) \Theta(-p+m) \Theta(k) - \\
&- e^{i(k-p)x} f_\perp(p,k+m) \Theta(-k) \Theta(-(k+m)) +
\end{aligned}
$$

$$
\begin{aligned}
&+e^{i(p-(k+m))x} f_\perp(k,q)\Theta(k+m)\Theta(k)\Big) c^\dagger_{p\downarrow} c_{q\downarrow} + \\
&+\Big(e^{i(k-p)x} f_\perp(p,k+m)\Theta(-k)\Theta(-(k+m)) - \\
&-e^{i(k-(q+m))x} f_\perp(p,k)\Theta(-k)\Theta(q+m) - \\
&-e^{i(k-q)x} f_\perp(q-m,p)\Theta(-p)\Theta(q-m)\Big) c^\dagger_{p\uparrow} c_{q\uparrow}\Big] + \\
&+\frac{4\pi^2 a\mu}{\sqrt{2}L^2}\sum_{k,l} e^{i(l-k)x} f_\perp(k,l)\Theta(-l)\Theta(k) \times \\
&\times \sum_{p\neq q} \frac{1}{p-q} e^{i(p-q)x - a|p-q|/2} c^\dagger_{p\uparrow} c_{q\uparrow}. \qquad (3.43)
\end{aligned}
$$

The integration of these terms leads to δ-functions of the momentum. Summing up we find

$$
\begin{aligned}
[\eta^{(1)}, \tilde{H}_\perp] &= -\sum_k 2k\alpha_k g_k \left(C^\dagger_k \tilde{\sigma}^-_\perp + C_k \tilde{\sigma}^+_\perp\right) S^z \\
&= \sum_{p,q}\sum_k \frac{-8\pi^2 a}{L\sqrt{L}}\Big[(k-p) f_\perp(k,q)\Theta(k) g_{k-p} - \\
&\quad -(k-q) f_\perp(p,k)\Theta(-k) g_{k-q}\Big](c^\dagger_{p\uparrow}c_{q\uparrow} - c^\dagger_{p\downarrow}c_{q\downarrow}) S^z + \\
&\quad +\frac{16\pi^3 a\mu}{\sqrt{2}\sqrt{L}L^2}\sum_{k,p,q}\sum_{m\neq 0}\frac{1}{m} e^{-a|m|/2} \times \\
&\quad \times\Big[(p-k-2m) g_{p-2m-k} f_\perp(k,q)\Theta(-p+m)\Theta(k) + \\
&\quad +(k-p-m) g_{k-p-m} f_\perp(p,k+m)\Theta(-k)\Theta(-(k+m)) + \\
&\quad +(k+2m-p) g_{p-k-2m} f_\perp(p,k+m)\Theta(k+m)\Theta(k) + \\
&\quad +(p+m-k) g_{k-p-m} f_\perp(p,k+m)\Theta(-k)\Theta(-(k+m)) + \\
&\quad +(k-q-2m) g_{k-q-2m} f_\perp(p,k)\Theta(-k)\Theta(q+m) + \\
&\quad +(k-q-m) g_{k-q-2m} f_\perp(q-m,p)\Theta(-p)\Theta(q-m)\Big] \times \\
&\quad \times\left(c^\dagger_{p\uparrow}c_{q\uparrow} - c^\dagger_{p\downarrow}c_{q\downarrow}\right) S^z + \\
&\quad +\frac{16\pi^3 a\mu}{\sqrt{2}\sqrt{L}L^2}\sum_{k,l} f_\perp(k,l)\Theta(-l)\Theta(k) \times \\
&\quad \times\sum_{p\neq q}\frac{k+q-p-l}{p-q} g_{-(p-q+l-k)} e^{-a|p-q|/2} \times \\
&\quad \times\left(c^\dagger_{p\uparrow}c_{q\uparrow} - c^\dagger_{p\downarrow}c_{q\downarrow}\right) S^z. \qquad (3.44)
\end{aligned}
$$

By an analog derivation we find for the remaining commutator:

$$
\begin{aligned}
[\eta^{(4)}, H_{\perp}^{(0,0)}] &= \sum_k \alpha_k g_k [\tau^+ S^- + \tau^- S^+, C_k^\dagger S^- + C_k S^+] \\
&= \sum_k \alpha_k g_k \Big(\tau^+ C_k [S^-, S^+] + [\tau^+, C_k] S^+ S^- + \\
&\quad + \tau^- C_k^\dagger [S^+, S^-] + [\tau^-, C_k^\dagger] S^- S^+ \Big) \\
&\approx \sum_k 2\alpha_k g_k \left(-\tau^+ C_k + \tau^- C_k^\dagger \right) S^z \\
&= \sum_{p,q} \sum_k \frac{-8\pi^2 a}{L\sqrt{L}} \Big[-(k-p) f_\perp(p,k) \Theta(k) g_{k-q} + \\
&\quad + (k-q) f_\perp(k,q) \Theta(-k) g_{k-p} \Big] (c_{p\uparrow}^\dagger c_{q\uparrow} - c_{p\downarrow}^\dagger c_{q\downarrow}) S^z + \\
&\quad - \sum_{p,q} \sum_k \sum_{m \neq 0} \frac{16\pi^3 a\mu}{\sqrt{2}\sqrt{L} L^2} \times \\
&\quad \times \Big[\frac{p-k}{m} f_\perp(p,k) g_{k-q-2m} e^{-a|m|/2} \Theta(k) \Theta(q+m) - \\
&\quad - \frac{p-m-k}{m} f_\perp(p-m,k) g_{k-q-m} e^{-a|m|/2} \Theta(-p+m) \Theta(k) + \\
&\quad + \frac{p-k-m}{m} f_\perp(p,k+m) g_{k-q-m} e^{-a|m|/2} \Theta(k+m) \Theta(-k) + \\
&\quad + \frac{k-q}{m} f_\perp(k,q) g_{p-k-2m} e^{-a|m|/2} \Theta(-k) \Theta(k+m) - \\
&\quad - \frac{k-q}{m} f_\perp(k,q) g_{p-2m-k} e^{-a|m|/2} \Theta(-k) \Theta(-k+m) + \\
&\quad + \frac{k-q-m}{m} f_\perp(k,q+m) g_{p-k-m} e^{-a|m|/2} \Theta(-k) \Theta(q+m) \Big] \times \\
&\quad \times (c_{p\uparrow}^\dagger c_{q\uparrow} - c_{p\downarrow}^\dagger c_{q\downarrow}) S^z - \\
&\quad - \frac{16\pi^3 a\mu}{\sqrt{2}\sqrt{L} L^2} \sum_{p \neq q} \sum_{k,m} \frac{k-m}{p-q} f_\perp(k,m) g_{m-k-p+q} \times \\
&\quad \times e^{-a|p-q|/2} \Theta(-k) \Theta(m) \left(c_{p\uparrow}^\dagger c_{q\uparrow} - c_{p\downarrow}^\dagger c_{q\downarrow} \right) S^z. \qquad (3.45)
\end{aligned}
$$

3.4 Large corrections

If $J_{\|/\perp}(p,q)$ is large compared to the couplings $J_{\|/\perp}(0,0)$ as e.g. in pseudogap-systems, one also has to take terms quadratic in the corrections into account. The occurring fermionic multi-particle excitations will be expanded as in the previous section and are also collected in Appendix B.
Due to their similar structure we will combine the commutators

$$\begin{aligned}[]
[\eta^{(3)},\tilde{H}_\perp] &= \sum_{p,q,k,l}(p-q)f_\|(p,q)f_\perp(k,l)\times \\
&\quad\times[c^\dagger_{p\uparrow}c_{q\uparrow}S^z - c^\dagger_{p\downarrow}c_{q\downarrow}S^z, c^\dagger_{k\uparrow}c_{l\downarrow}S^- + c^\dagger_{k\uparrow}c_{l\downarrow}S^+]
\end{aligned}\tag{3.46}$$

and

$$\begin{aligned}[]
[\eta^{(4)},\tilde{H}_\|] &= \sum_{p,q,k,l}(p-q)f_\perp(p,q)f_\|(k,l)\times \\
&\quad\times[c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\uparrow}c_{q\downarrow}S^+, c_{k\uparrow}c_{l\uparrow}S^z - c_{k\downarrow}c_{l\downarrow}S^z] \\
&= -\sum_{p,q,k,l}(k-l)f_\perp(k,l)f_\|(p,q)\times \\
&\quad\times[c_{p\uparrow}c_{q\uparrow}S^z - c_{p\downarrow}c_{q\downarrow}S^z, c^\dagger_{k\uparrow}c_{l\downarrow}S^- + c^\dagger_{k\uparrow}c_{l\downarrow}S^+]
\end{aligned}\tag{3.47}$$

to

$$\begin{aligned}[]
[\eta^{(3)},\tilde{H}_\perp]+[\eta^{(4)},\tilde{H}_\|] &= \frac{1}{2}\sum_{p,q,k,l}(p-q+l-k)\, f_\|(p,q)f_\perp(k,l)\times \\
&\times\Big[\Big(2c^\dagger_{p\downarrow}c_{q\downarrow}c^\dagger_{k\uparrow}c_{l\downarrow} - 2c^\dagger_{p\uparrow}c_{q\uparrow}c^\dagger_{k\uparrow}c_{l\downarrow} + \delta_{l,p}c^\dagger_{k\uparrow}c_{q\downarrow} + \delta_{k,q}c^\dagger_{p\uparrow}c_{l\downarrow}\Big)S^- + \\
&+\Big(2c^\dagger_{p\uparrow}c_{q\uparrow}c^\dagger_{k\downarrow}c_{l\uparrow} - 2c^\dagger_{p\downarrow}c_{q\downarrow}c^\dagger_{k\downarrow}c_{l\uparrow} + \delta_{l,p}c^\dagger_{k\downarrow}c_{q\uparrow} + \delta_{k,q}c^\dagger_{p\downarrow}c_{l\uparrow}\Big)S^+\Big] \\
&\approx \frac{1}{2}\sum_{p,q,k,l}(p-q+l-k)\, f_\|(p,q)f_\perp(k,l)\times \\
&\times\Big[\Big(\delta_{p,l}(1-2\Theta(-p))c^\dagger_{k\uparrow}c_{q\downarrow} + \delta_{k,q}(1-2\Theta(q))c^\dagger_{p\uparrow}c_{l\downarrow}\Big)S^- + \\
&+\Big(\delta_{p,l}(1-2\Theta(-p))c^\dagger_{k\downarrow}c_{q\uparrow} + \delta_{k,q}(1-2\Theta(q))c^\dagger_{p\downarrow}c_{l\uparrow}\Big)S^+\Big] \\
&= \sum_{p,q}\sum_k\frac{1}{2}(2k-p-q)\mathrm{sgn}(k)\left(f_\|(k,q)f_\perp(p,k)+f_\|(p,k)f_\perp(k,q)\right)\times \\
&\times\left(c^\dagger_{p\uparrow}c_{q\downarrow}S^- + c^\dagger_{p\downarrow}c_{q\uparrow}S^+\right).
\end{aligned}\tag{3.48}$$

This term will play an important role for pseudogap-systems as we will see in the following. The potential scattering induced by

$$[\eta^{(3)},\tilde{H}_\|] = \sum_{p,q,k,l}(p-q)f_\|(p,q)f_\|(k,l)[c^\dagger_{p\uparrow}c_{q\uparrow} - c^\dagger_{p\downarrow}c_{q\downarrow}, c^\dagger_{k\uparrow}c_{l\uparrow} - c^\dagger_{k\downarrow}c_{l\downarrow}]\,(S^z)^2$$

$$= \sum_{p,q} \frac{1}{4} \sum_{k} (p+q-2k) f_{\|}(p,k) f_{\|}(k,q) \left(c^{\dagger}_{p\uparrow} c_{q\uparrow} + c^{\dagger}_{p\downarrow} c_{q\downarrow} \right) \tag{3.49}$$

will be neglected, because these effects are only important at energies of the Kondo scale. We will also only keep the first term of the commutator

$$\begin{aligned}
[\eta^{(4)}, \tilde{H}_{\perp}] &= \sum_{p,q,k,l} (p-q) f_{\perp}(p,q) f_{\perp}(k,l) \times \\
&\quad \times [c^{\dagger}_{p\uparrow} c_{q\downarrow} S^{-} + c^{\dagger}_{p\downarrow} c_{q\uparrow} S^{+}, c^{\dagger}_{k\uparrow} c_{l\downarrow} S^{-} + c^{\dagger}_{k\downarrow} c_{l\uparrow} S^{+}] \\
&\approx \sum_{p,q,k,l} (p-q) f_{\perp}(p,q) f_{\perp}(k,l) \times \\
&\quad \times \Big\{ \Big[\delta_{k,q} \left(\Theta(k) c^{\dagger}_{p\uparrow} c_{l\uparrow} + \Theta(-k) c^{\dagger}_{p\downarrow} c_{l\downarrow} \right) - \\
&\quad - \delta_{p,l} \left(\Theta(l) c^{\dagger}_{k\uparrow} c_{q\uparrow} + \Theta(-l) c^{\dagger}_{k\downarrow} c_{q\downarrow} \right) \Big] S^{-} S^{+} + \\
&\quad + \Big[\delta_{k,q} \left(\Theta(k) c^{\dagger}_{p\downarrow} c_{l\downarrow} + \Theta(-k) c^{\dagger}_{p\uparrow} c_{l\uparrow} \right) - \\
&\quad - \delta_{p,l} \left(\Theta(l) c^{\dagger}_{k\downarrow} c_{q\downarrow} + \Theta(-l) c^{\dagger}_{k\uparrow} c_{q\uparrow} \right) \Big] S^{+} S^{-} \Big\} \\
&= \sum_{p,q} \sum_{k>0} 2(2k-p-q) f_{\perp}(k,q) f_{\perp}(p,k) \times \\
&\quad \times \left(c^{\dagger}_{p\uparrow} c_{q\uparrow} - c^{\dagger}_{p\downarrow} c_{q\downarrow} \right) S^{z} + \\
&\quad + \sum_{p,q,k} (p+q-2k) f_{\perp}(k,q) f_{\perp}(p,k) \times \\
&\quad \times \left(c^{\dagger}_{p\uparrow} c_{q\uparrow} S^{+} S^{-} + c^{\dagger}_{p\downarrow} c_{q\downarrow} S^{-} S^{+} \right).
\end{aligned} \tag{3.50}$$

3.5 Flow equations

Summarizing the previous sections, we obtained within our approximations the Hamiltonian

$$\boxed{\begin{aligned}
H &= H_0 + \sum_{p} g_p \alpha_p \left(C^{\dagger}_{p} S^{-} + C_p S^{+} \right) + \sum_{p} \omega_p \left(C^{\dagger}_{p} C_p - C_p C^{\dagger}_{p} \right) + \\
&\quad + \sum_{p,q} f_{\|}(p,q) \left(c^{\dagger}_{p\uparrow} c_{q\uparrow} - c^{\dagger}_{p\downarrow} c_{q\downarrow} \right) S^{z} + \\
&\quad + \sum_{p,q} f_{\perp}(p,q) \left(c^{\dagger}_{p\uparrow} c_{q\downarrow} S^{-} + c^{\dagger}_{p\downarrow} c_{q\uparrow} S^{+} \right)
\end{aligned}} \tag{3.51}$$

with the following closed set of flow equations:

$$
\boxed{\begin{aligned}
\partial_B \lambda^2 &= \frac{8\pi a \lambda^2(1-\lambda^2)}{\Gamma(\lambda^2)} \sum_p g_p g_{-p} |pa|^{\lambda^2-1}, \\
\partial_B g_p &= -p^2 g_p + 2\sum_{q\neq p} \frac{\alpha_q}{\alpha_p} \eta^{(2)}_{pq} g_q + \frac{1}{2} g_p \ln\left(\frac{B}{a^2}\right) \lambda \partial_B \lambda - \\
&\quad - \frac{\sqrt{2}\pi\lambda}{L} \sum_{q\neq 0} \sum_k g_{p+q} f_{\|}(k+q,k) \frac{p+2q}{|q|} e^{-a|q|/2} \times \\
&\quad \times \left[\Theta(-k-q) - \Theta(-k)\right] - 2p g_p \omega_p, \\
\partial_B f_{\|}(p,q) &= -(p-q)^2 f_{\|}(p,q) + \sum_k A(k,p,q) + \\
&\quad + \sum_k \sum_{m\neq 0} B(k,m,p,q) + (1-\delta_{p,q}) \sum_{k,m} C(k,m,p,q) + \\
&\quad + \sum_{k>0} 2(2k-p-q) f_{\perp}(k,q) f_{\perp}(p,k), \\
\partial_B f_{\perp}(p,q) &= -(p-q)^2 f_{\perp}(p,q) + \\
&\quad + \sum_k \frac{1}{2}(2k-p-q)\,\mathrm{sgn}(k) \times \\
&\quad \times \left[f_{\|}(k,q) f_{\perp}(p,k) + f_{\|}(k,p) f_{\perp}(q,k)\right], \\
\partial_B \omega_p &= p\alpha_p^2 g_p^2.
\end{aligned}} \tag{3.52}
$$

The flow equations were derived using the generator

$$
\boxed{\begin{aligned}
\eta &= \sum_p p\alpha_p g_p \left(C_p^\dagger S^- - C_p S^+\right) + \sum_{p,q} \eta^{(2)}_{pq} \left(C_p^\dagger C_q - C_q C_p^\dagger\right) + \\
&\quad + \sum_{p,q} (p-q) f_{\|}(p,q) \left(c^\dagger_{p\uparrow} c_{q\uparrow} - c^\dagger_{p\downarrow} c_{q\downarrow}\right) S^z + \\
&\quad + \sum_{p,q} (p-q) f_{\perp}(p,q) \left(c^\dagger_{p\uparrow} c_{q\downarrow} S^- + c^\dagger_{p\downarrow} c_{q\uparrow} S^+\right).
\end{aligned}} \tag{3.53}
$$

For convenience we defined:

$$
\begin{aligned}
A(k,p,q) &= \frac{-8\pi^2 a}{L\sqrt{L}} \Big(k\left[f_{\perp}(k,q) g_{k-p} - f_{\perp}(p,k) g_{k-q}\right] + \\
&\quad + \left[p\Theta(k) + q\Theta(-k)\right]\left[g_{k-q} f_{\perp}(p,k) - g_{k-p} f_{\perp}(k,q)\right] \Big),
\end{aligned} \tag{3.54}
$$

$$
\begin{aligned}
B(k,m,p,q) &= \frac{16\pi^3 a\mu}{\sqrt{2}\sqrt{L}L^2} \frac{1}{m} e^{-a|m|/2} \times \\
&\quad \times \Big[(p-k-2m) g_{p-2m-k} f_{\perp}(k,q) \Theta(-p+m) \Theta(k) + \\
&\quad + (k-p-m) g_{k-p-m} f_{\perp}(p,k+m) \Theta(-k) \Theta(-(k+m)) + \\
&\quad + (k+2m-p) g_{p-k-2m} f_{\perp}(p,k+m) \Theta(k+m) \Theta(k) + \\
&\quad + (p+m-k) g_{k-p-m} f_{\perp}(p,k+m) \Theta(-k) \Theta(-(k+m)) +
\end{aligned}
$$

$$
\begin{aligned}
&+(k-q-2m)g_{k-q-2m}f_\perp(p,k)\Theta(-k)\Theta(q+m)+\\
&+(k-q-m)g_{k-q-2m}f_\perp(q-m,p)\Theta(-p)\Theta(q-m)-\\
&-(p-k)f_\perp(p,k)g_{k-q-2m}\Theta(k)\Theta(q+m)+\\
&+(p-m-k)f_\perp(p-m,k)g_{k-q-m}\Theta(-p+m)\Theta(k)-\\
&-(p-k-m)f_\perp(p,k+m)g_{k-q-m}\Theta(k+m)\Theta(-k)-\\
&-(k-q)f_\perp(k,q)g_{p-k-2m}\Theta(-k)\Theta(k+m)+\\
&+(k-q)f_\perp(k,q)g_{p-2m-k}\Theta(-k)\Theta(-k+m)-\\
&-(k-q-m)f_\perp(k,q+m)g_{p-k-m}\Theta(-k)\Theta(q+m)\Big], \quad (3.55)
\end{aligned}
$$

$$
\begin{aligned}
C(k,m,p,q) \;=\; & \frac{16\pi^3 a\mu}{\sqrt{2}\sqrt{L}L^2}f_\perp(k,m)e^{-a|p-q|/2}\times\\
&\times\left(\frac{k+q-p-m}{p-q}g_{-p+q-m+k}\Theta(-m)\Theta(k)-\right.\\
&\left.-\frac{k-m}{p-q}g_{m-k-p+q}\Theta(m)\Theta(-k)\right). \quad (3.56)
\end{aligned}
$$

Remarkably, due to the construction of our Hamiltonian the corrections enter the flow of the unperturbed system via g_p. While the longitudinal correction enters directly, the spin-flip correction generates an additional flow of the longitudinal correction.

4 Results

In this chapter we will first study the effect of a small change in the density of states for systems with nonzero densities of states at the Fermi level. Staying in the picture of perturbation theory we will only investigate the influence of the first order corrections - which are linear in $f_{\|/\perp}(p,q)$ - on the flow.

We will also shortly discuss the additional flow created by terms quadratic in the corrections, which become important for large perturbations.

4.1 Flow of the scaling dimension

From their definitions in Eqs. (3.4) and (3.29) the corrections have to obey the relations

$$f_{\|/\perp}(0,0) \equiv 0 \tag{4.1}$$

and

$$f_{\|/\perp}(p,q) \equiv f_{\|/\perp}(q,p). \tag{4.2}$$

As an example we will choose the circle

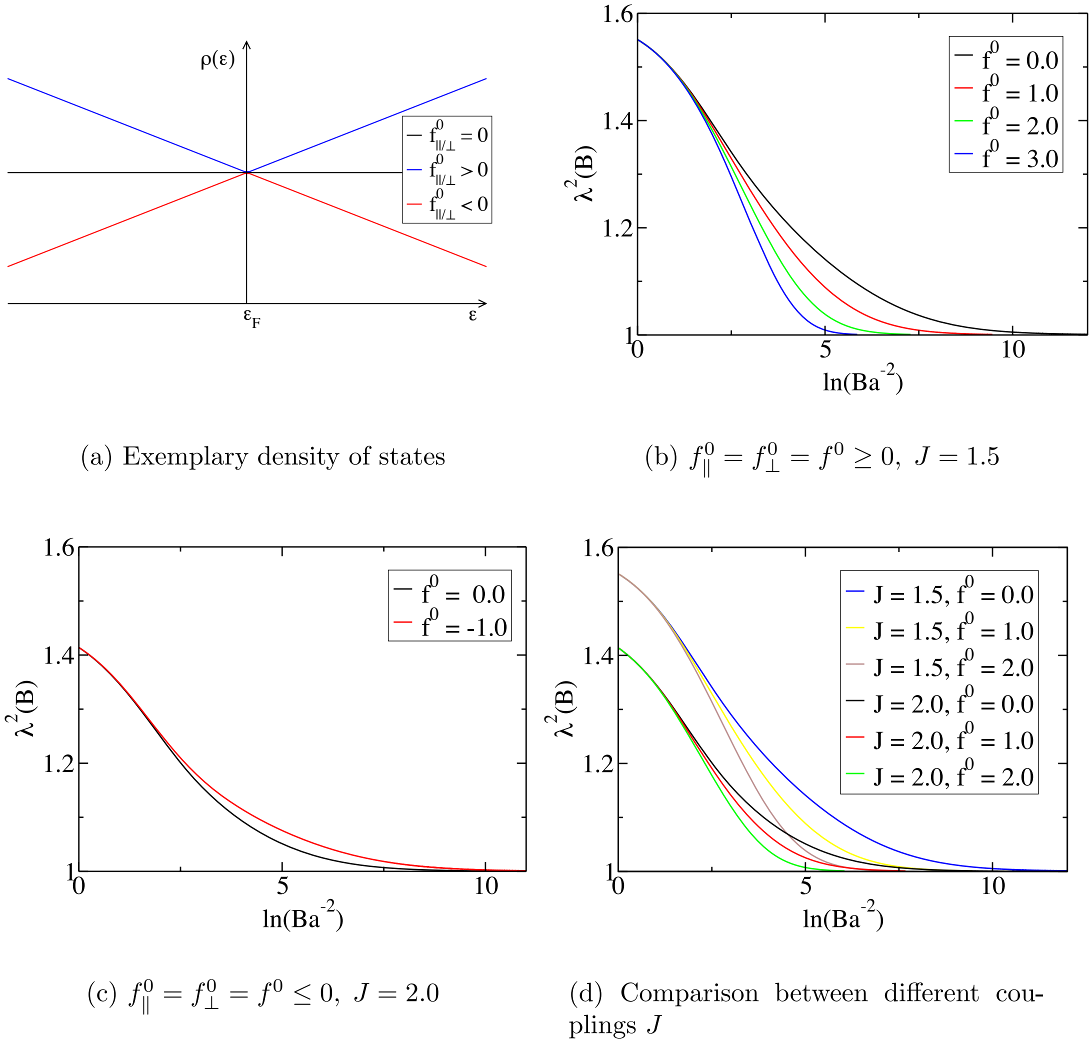
$$f_{\|/\perp}(p,q) = f^0_{\|/\perp}\sqrt{p^2+q^2}(2L)^{-1} \tag{4.3}$$

as the initial values of the additional couplings, which is equivalent to total couplings of the form

$$J_{\|/\perp}(p,q) = J_{\|/\perp}(0,0) + f^0_{\|/\perp}\sqrt{p^2+q^2}. \tag{4.4}$$

Please note that with the above choice a positive (negative) $f^0_{\|/\perp}$ an approximate linear increasing (decreasing) density of states measured from the Fermi level is modeled (see Fig. 4.1(a)).

In Figs. 4.1(b) and 4.1(c) we plotted the flow of the scaling dimension for several positive and negative corrections. We again considered only symmetric antiferromagnetic couplings $J_\|(0,0) = J_\perp(0,0) = J > 0$. As expected positive (negative) corrections lead to a faster (slower) flow of the scaling dimension, corresponding to a higher (lower) Kondo temperature. For a comparison of the flow of the scaling dimension between different couplings J see Fig. 4.1(d). Similar results can be obtained for other initial values than (4.3).



(a) Exemplary density of states

(b) $f^0_{\|} = f^0_{\perp} = f^0 \geq 0,\ J = 1.5$

(c) $f^0_{\|} = f^0_{\perp} = f^0 \leq 0,\ J = 2.0$

(d) Comparison between different couplings J

Figure 4.1: Corrections to the flow of the scaling dimension

However the additional flow induced by the corrections cannot be fully studied by analyzing the flow of the scaling dimension. We will therefore focus on the analysis of the phase diagram.

4.2 Phase diagram

In the previous section we have analyzed the renormalization effect induced by a nontrivial density of states to the flow of the scaling dimension. We made predictions on the dependency of the Kondo scale on the additional coupling

functions $f_{\parallel/\perp}(p,q)$. But to analyze the full additional flow of the unperturbed system (constant density of states), we have to study the phase diagram.
We will derive the flow equations of the coupling functions analog to Section 2.3.

Again we use the ansatz

$$g_p(B) = \tilde{g}(B)e^{-Bp^2}, \tag{4.5}$$

Neglecting terms of $\mathcal{O}(g_p^3)$ we find in the low energy limit $|p| \ll 1$:

$$\begin{aligned}
\partial_B \tilde{g}(B) \;&=\; \frac{1}{4}\tilde{g}(B)\ln(B)\partial_B\lambda^2 - \tilde{g}(B)\frac{2\sqrt{2}\pi\lambda}{L} \times \\
&\times \sum_{q\neq 0}\sum_k f_\parallel(k+q,k)\frac{q}{|q|}\left[\Theta(-k-q)-\Theta(-k)\right]e^{-Bq^2},
\end{aligned} \tag{4.6}$$

where we again defined $a \equiv 1$. Introducing the logarithmic scale $x = \ln(B)$ leads to

$$\begin{aligned}
\partial_x \tilde{g}(x) \;&=\; \frac{1}{4}\tilde{g}(x)x\partial_x\lambda^2(x) - e^x\tilde{g}(x)\frac{2\sqrt{2}\pi\lambda(x)}{L} \times \\
&\times \sum_{q\neq 0}\sum_k f_\parallel(k+q,k,e^x)\frac{q}{|q|}\left[\Theta(-k-q)-\Theta(-k)\right]e^{-e^x q^2} \\
&\equiv\; \tilde{g}(x)\left(\frac{1}{4}x\partial_x\lambda^2(x) - f(x)\right),
\end{aligned} \tag{4.7}$$

which can be formally integrated:

$$\tilde{g}(x) = \tilde{g}_0 \exp\left(\frac{1}{4}x\lambda^2(x) - \frac{1}{4}\int_{x_0}^{x}\lambda^2(y)dy - \int_{x_0}^{x} f(y)dy\right). \tag{4.8}$$

Please note that the flow equation for λ^2 stays unchanged. Again defining

$$u(x) = \frac{1}{2}\left(1-\frac{\lambda^2(x)}{2}\right),\; u(0) = \frac{J_\parallel}{4\pi} + \mathcal{O}(J_\parallel^2) \tag{4.9}$$

and

$$v(x) = \sqrt{L}\tilde{g}(x)\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right),\; v(0) = \frac{J_\perp}{4\pi}, \tag{4.10}$$

we find in the limit of small couplings $\lambda^2 \to 2$

$$\partial_x u(x) = v^2(x) \tag{4.11}$$

and

$$\begin{aligned}
\partial_x v(x) &= \sqrt{L}\tilde{g}(x)\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right)\left(\frac{1}{2} - \frac{1}{4}\lambda^2(x)\right) + \\
&+\sqrt{L}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right)\left(-\frac{1}{4}\tilde{g}(x)x\partial_x\lambda^2(x)\right) + \\
&+\sqrt{L}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right)\partial_x\tilde{g}(x) \\
&= u(x)v(x) + \sqrt{L}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right)\left(-\frac{1}{4}\tilde{g}(x)x\partial_x\lambda^2(x)\right) + \\
&+\sqrt{L}\exp\left(\frac{1}{2}x - \frac{1}{4}x\lambda^2(x)\right)\tilde{g}(x)\left(\frac{1}{4}x\partial_x\lambda^2(x) - f(x)\right) \\
&= u(x)v(x) - v(x)e^x\frac{2\sqrt{2}\pi\sqrt{2-4u(x)}}{L}\times \\
&\times\sum_{q\neq 0}\sum_k f_\parallel(k+q,k,x)\frac{q}{|q|}\left[\Theta(-k-q) - \Theta(-k)\right]e^{-e^x q^2}. \qquad (4.12)
\end{aligned}$$

Summing up, we found the following set of flow equations for the couplings including the linear corrections due to a nontrivial density of states:

$$\boxed{\begin{aligned}
\partial_x u(x) &= v^2(x), \\
\partial_x v(x) &= u(x)v(x) - v(x)e^x\sum_{q\neq 0}\sum_k \frac{2\sqrt{2}\pi\sqrt{2-4u(x)}}{L}\times \\
&\times f_\parallel(k+q,k,x)\frac{q}{|q|}\left[\Theta(-k-q) - \Theta(-k)\right]e^{-e^x q^2}, \\
\partial_x f_\parallel(p,q,x) &= e^x\Bigg[-(p-q)^2 f_\parallel(p,q,x) + \sum_k A(k,p,q) + \\
&+\sum_k\sum_{m\neq 0} B(k,m,p,q) + \\
&+(1-\delta_{p,q})\sum_{k,m} C(k,m,p,q)\Bigg], \\
\partial_x f_\perp(p,q,x) &= -e^x(p-q)^2 f_\perp(p,q,x).
\end{aligned}} \qquad (4.13)$$

To check our approximations, we will calculate the effect of a constant correction

$$f_\parallel(p,q) \equiv f_\parallel^0\,(2L)^{-1}\,, \qquad (4.14)$$

which is equivalent to dividing the coupling $J_\parallel$ of the anisotropic Kondo model with a constant density of states into two parts, e.g.:

$$\frac{J_\parallel}{2\pi}\sum_{\alpha,\beta}\Psi_\alpha^\dagger(0)\sigma_{\alpha\beta}^z\Psi_\beta(0)S^z = \frac{1}{n}\frac{J_\parallel}{2\pi}\sum_{\alpha,\beta}\Psi_\alpha^\dagger(0)\sigma_{\alpha\beta}^z\Psi_\beta(0)S^z +$$

$$
\begin{aligned}
& + \left(1 - \frac{1}{n}\right) \frac{J_\parallel}{2\pi} \sum_{\alpha,\beta} \Psi^\dagger_\alpha(0)\sigma^z_{\alpha\beta}\Psi_\beta(0)S^z \\
\equiv \quad & \frac{\tilde{J}_\parallel}{2\pi} \sum_{\alpha,\beta} \Psi^\dagger_\alpha(0)\sigma^z_{\alpha\beta}\Psi_\beta(0)S^z + \\
& + \sum_{p,q} f^0_\parallel \,(2L)^{-1} \left(c^\dagger_{p\uparrow}c_{q\uparrow} - c^\dagger_{p\downarrow}c_{q\downarrow}\right) S^z. \quad (4.15)
\end{aligned}
$$

For simplicity we set $f_\perp(p,q) \equiv 0$. It is convenient to shift the initial value of x to $x_0 = 0$. The integration of the flow equation for $f_\parallel$ leads to

$$
f_\parallel(p,q,x) = f^0_\parallel \,(2L)^{-1} \exp\left[-(e^x - 1)(p-q)^2\right]. \quad (4.16)
$$

Calculating the sums in the $v(x)$ flow equation we find in the limit of small couplings $|u(x)| \ll 1$:

$$
\begin{aligned}
\partial_x v(x) &= u(x)v(x) + v(x)e^x \frac{2\pi}{L^2} \sum_{q>0} \sum_{-q}^{q} [1 - \delta(k)] f^0_\parallel \exp\left[-(e^x - 1)q^2\right] \\
&= u(x)v(x) + \frac{2}{L} v(x) e^x f^0_\parallel \sum_{q>0} q \exp\left[-(e^x - 1)q^2\right] \\
&= u(x)v(x) + 4v(x)e^x f^0_\parallel \frac{1}{4\pi} \int_0^{1/a \equiv 1} dq\, q \exp\left[-(e^x - 1)q^2\right] \\
&= u(x)v(x) + v(x) f^0_\parallel \frac{1}{4\pi} \frac{\exp(x)\Big(1 - \exp[-2\exp(x) - 1)]\Big)}{\exp(x) - 1}. \quad (4.17)
\end{aligned}
$$

Defining

$$
\tilde{u}(x) = u(x) + f^0_\parallel \frac{1}{4\pi} \quad (4.18)
$$

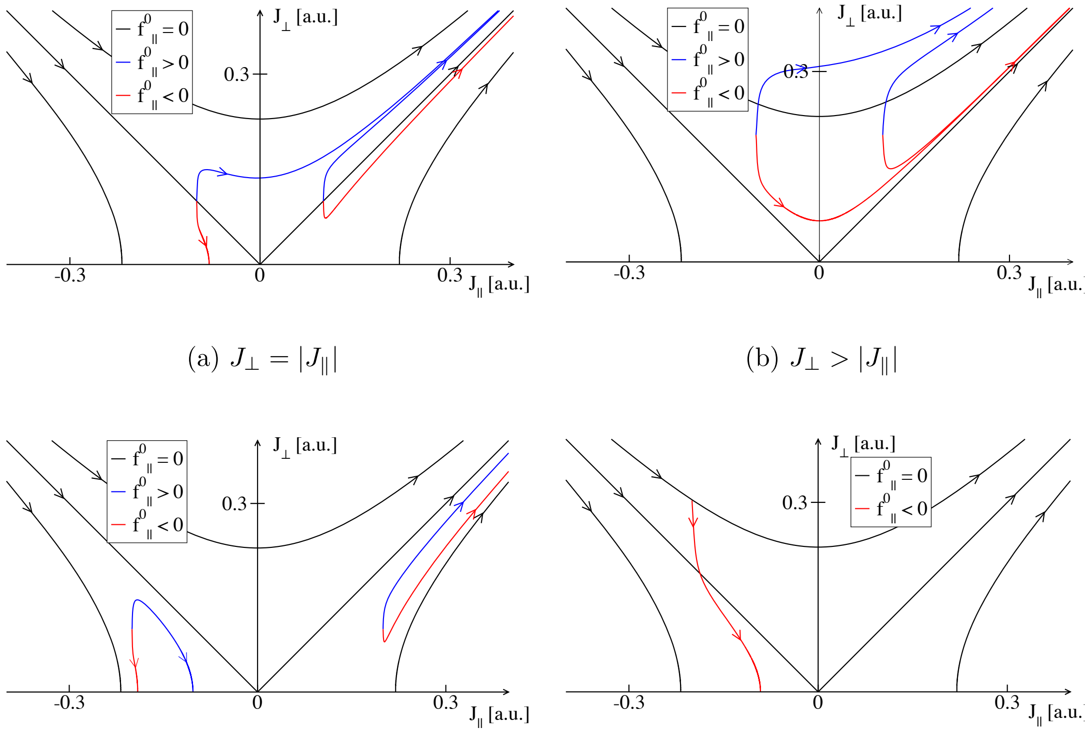
we find for $x \gg x_0$ the expected flow equations:

$$
\boxed{\begin{aligned} \partial_x \tilde{u}(x) &= v^2(x), \\ \partial_x v(x) &= \tilde{u}(x)v(x), \end{aligned}} \quad (4.19)
$$

where

$$
\tilde{u}(0) \equiv \frac{J_\parallel}{4\pi} \quad (4.20)
$$

is fulfilled. Please note that because of the structure of the flow induced by $f_\perp$ an equivalent calculation for the additional spin-flip scattering cannot be done as easily using analytic methods. However, by numerical investigation we found that also the spin-flip corrections lead to quite accurate results.



(a) $J_\perp = |J_\||$

(b) $J_\perp > |J_\||$

(c) $J_\perp < |J_\||$

(d) Strong- to weak coupling transition

Figure 4.2: Phase diagrams including corrections

Having checked the approximations, we now continue deriving the phase diagrams of the closed set of flow equations (4.13). For simplicity we again choose

$$f_\|(p, q, x = x_0) = f_\|^0 \sqrt{p^2 + q^2}(2L)^{-1}. \tag{4.21}$$

The correction $f_\perp(p, q, x)$ only enters the flow via $f_\|(p, q, x)$ and in the limit $f_\perp(p, q, x) \sim f_\|(p, q, x)$ its main actions are the slowdown of the exponential decay of the longitudinal correction and an enormous increase in computation time (scale: $N^2 \rightarrow N^4$). Since we are mainly interested in qualitative results, we will therefore set $f_\perp(p, q, x) \equiv 0$. Of course to derive quantitative results (or for anisotropic corrections), the spin-flip correction has to be taken into account. For convenience we define $J_{\|/\perp}(0, 0) \equiv J_{\|/\perp}$.

An example phase portrait with corrections to symmetric coupling constants $J_{\|/\perp}$ is plotted in Fig. 4.2(a). A positive (negative) $f_\|^0$ generates an immediate flow to larger (smaller) couplings $J_\perp$. After a very short "time" the correction vanishes (corresponding to the exponential decay) and the coupling functions continue their flow on universal trajectories of the anisotropic Kondo model with constant density of states. Starting with anisotropic coupling constants we find similar behaviour as can be seen in Figs. 4.2(b) and 4.2(c). Please note that for ferromagnetic couplings $J_{\|}$ also transitions between weak- and strong-coupling are possible (see Fig. 4.2(d)).

Summing up, we find that within our approximations the corrections generate the flow to a different point in the phase diagram of the original unperturbed system. Since they immediately vanish, they become effectively irrelevant for the low energy properties of the system. We are therefore able to map the Hamiltonian of the Kondo model with nontrivial density of states to an effective anisotropic Kondo Hamiltonian with constant density of states. The corrections only have to be taken into account by their renormalization effect on the coupling constants.

4.3 Large corrections

In the previous sections we studied the additional flow generated by terms linear in the corrections. But for large corrections also terms of higher orders have to be taken into account.

To get a better understanding of the additional terms we will first study only the fermionic part of the Hamiltonian by setting $J_{\|/\perp}(0,0) \equiv 0$. We are then left with the flow equations:

$$\boxed{\begin{aligned} \partial_B f_{\|}(p,q) &= -(p-q)^2 f_{\|}(p,q) + \\ &\quad + \sum_{k>0} 2(2k-p-q) f_{\perp}(k,q) f_{\perp}(p,k), \\ \partial_B f_{\perp}(p,q) &= -(p-q)^2 f_{\perp}(p,q) + \\ &\quad + \sum_{k} \frac{1}{2}(2k-p-q)\mathrm{sgn}(k)\big(f_{\|}(k,q) f_{\perp}(p,k) + \\ &\quad + f_{\|}(k,p) f_{\perp}(q,k)\big) - s_{\perp}(p-q). \end{aligned}} \tag{4.22}$$

Starting with the initial values

$$f_{\|/\perp}(p,q) = J_{\|/\perp}(2L)^{-1}, \tag{4.23}$$

which is equivalent to the Hamiltonian of the anisotropic Kondo model with a constant density of states, and using the ansatz

$$f_{\|/\perp}(p,q,B) = J_{\|/\perp} e^{-B(p-q)^2}(2L)^{-1}, \tag{4.24}$$

we find in the low energy limit $|p|, |q| \ll 1$:

$$\begin{aligned}\partial_B J_\parallel &= \frac{2}{L} J_\perp^2 \sum_{k>0} k e^{-2Bk^2} \\ &= \frac{1}{\pi} J_\perp^2 \int_0^\infty dk\; k e^{-2Bk^2} \\ &= \frac{J_\perp^2}{4\pi} \frac{1}{B}\end{aligned} \tag{4.25}$$

and analog

$$\partial_B J_\perp = \frac{J_\parallel J_\perp}{4\pi} \frac{1}{B}. \tag{4.26}$$

Introducing the couplings

$$u = \frac{J_\parallel}{4\pi} \text{ and } v = \frac{J_\perp}{4\pi} \tag{4.27}$$

and a logarithmic measure for the flow parameter

$$x = \ln(B), \tag{4.28}$$

we again find the scaling equations derived by Anderson [7]:

$$\boxed{\begin{aligned}\partial_x u(x) &= v^2(x), \\ \partial_x v(x) &= u(x)v(x).\end{aligned}} \tag{4.29}$$

As already mentioned above the solution of these differential equations diverges for a wide range of initial coupling constants (the trivial integration is left to the reader). Also for other densities of states we find the typical strong-coupling divergence.

By numerical investigation we found that these divergence also occur if the bosonized part of the Hamiltonian is included, leading to the breakdown of our approach for certain large corrections $f_{\parallel/\perp}(p, q)$. This is mainly an effect of the perturbative treatment of the corrections and the expansion of the fermionic many particle objects in Section 3.4 by using normal-ordering. A different approach in which also the momentum dependent part can be fully bosonized is currently in progress. Since also the solution of the Kondo model with a constant density of state has to be revised, the calculation would exceed this thesis.

In Appendix C we show a trial approach for bypassing the strong-coupling divergence for pseudogap-systems. Unfortunately it did not lead to satisfying results.

4.4 Summary

In this chapter we have analyzed the Kondo model with nonzero densities of states at the Fermi level and small changes in the density of states apart from it using the flow equations derived in Chapter 3. Within our approximations we were able to map the Hamiltonian of the Kondo model with nontrivial density of states (small corrections) to an effective anisotropic Kondo Hamiltonian with constant density of states and certainly larger (smaller) initial spin-flip coupling constants $J_\perp(0,0)$ for positive (negative) corrections. In the strong-coupling regime the latter Hamiltonian can be mapped to an effective RLM-Hamiltonian which can be solved exactly [13].

Though in principal also large corrections can be studied within our approach, this may not lead to accurate results due to its perturbative nature.

5 Conclusion

In this thesis the flow equation method has been applied to the Kondo model with nontrivial density of states. We first reviewed the solution of the anisotropic Kondo model with constant density of states. The interaction part of the corresponding Hamiltonian has been rewritten in terms of vertex operators by using bosonization. In contrast to earlier approaches in the fermionic representation the bosonized form allows an expansion that becomes exact during the flow to the strong-coupling regime. Thereby the typical strong-coupling divergence can be avoided. In the strong-coupling regime the bosonized Hamiltonian can mapped to an effective low energy Hamiltonian of the noninteracting resonant level model (RLM), which can be solved exactly.

In the second part we investigated the additional flow induced by corrections due to a nontrivial density of states. We separated the coupling functions into a momentum independent and a momentum dependent part. The latter can be considered as a small perturbation. While again bosonizing the first part we studied the second one in its fermionic representation. By this the flow equation solution of the anisotropic Kondo model with constant density of states can be reused and only the corrections due to the momentum dependent perturbation have to be evaluated. This can be easily done within the flow equation framework. The occurring mixed terms (bosonic and fermionic operators) and additional fermionic many-particle excitations were expanded using normal-ordering. In analogy to perturbation theory only the additional flow of the original "unperturbed" system (constant density of states) was investigated.

Within these approximations we were able to map the Hamiltonian of the Kondo model with nontrivial density of states to an effective low energy Hamiltonian with constant density of states and renormalized coupling constants. In the strong-coupling regime the latter can again be mapped to an effective RLM-Hamiltonian and thereby solved exactly.

We are thus able to give a systematic analytic description of the Kondo model with nontrivial density of states. Remarkably this thesis provides the *first analytic* description of this model including the correct low temperature properties.

The flow equation method provides a new powerful analytic tool for studying nonintegrable strong-coupling problems. Possible future developments include the application on other spin boson models with nontrivial coupling functions and also on a wide range of DMFT systems.

Appendix A

Useful operator identities

In the following we want to give a collection of operator identities used in this thesis. For rigorous proofs of these see e.g. [18].

In the following $f(A)$ is a function defined by its Taylor expansion

$$f(A) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) A^n. \tag{A.1}$$

The Baker-Hausdorff identity is given by

$$e^{-B} A e^{B} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_n, \tag{A.2}$$

where $[A, B]_{n+1} = [[A, B], B]_n$ and $[A, B]_0 = [A, B]$.

If $C = [A, B]$ satisfies $[A, C] = [B, C] = 0$ then the following relations are valid:

$$\begin{aligned}
e^{-B} A e^{B} &= A + C, && \text{(A.3)}\\
e^{A} e^{B} &= e^{A+B} e^{C/2}, && \text{(A.4)}\\
e^{-B} f(A) e^{B} &= f(A + C), && \text{(A.5)}\\
e^{A} e^{B} &= e^{B} e^{A} e^{C}. && \text{(A.6)}\\
& && \text{(A.7)}
\end{aligned}$$

If $[A, B] = DB$ and $[A, D] = [B, D] = 0$, then

$$f(A) B = B f(A + D). \tag{A.8}$$

Appendix B

Operator product expansions using Wick's theorem

Expansions used in Section 3.3:

$$
\begin{aligned}
c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha} \overset{\alpha\neq\beta}{=} \;& :c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha}: + \\
& +\langle 0|c^\dagger_{k\alpha}c_{q\alpha}|0\rangle :c_{k'\beta}c^\dagger_{p\beta}: + \\
& +\langle 0|c_{k'\beta}c^\dagger_{p\beta}|0\rangle :c^\dagger_{k\alpha}c_{q\alpha}: + \\
& +\langle 0|c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha}|0\rangle \\
= \;& :c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha}: + \\
& +\delta_{k,q}\Theta(-q)\left(c_{k'\beta}c^\dagger_{p\beta} - \langle 0|c_{k'\beta}c^\dagger_{p\beta}|0\rangle\right) + \\
& +\delta_{k',p}\Theta(p)\left(c^\dagger_{k\alpha}c_{q\alpha} - \langle 0|c^\dagger_{k\alpha}c_{q\alpha}|0\rangle\right) + \\
& +\delta_{k,q}\delta_{k',p}\Theta(-q)\Theta(p) \\
= \;& :c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha}: + \\
& +\delta_{k,q}\Theta(-q)(\delta_{k',p} - c^\dagger_{p\beta}c_{k'\beta}) - \delta_{k,q}\Theta(-q)\delta_{k',p}\Theta(p) + \\
& +\delta_{k',p}\Theta(p)c^\dagger_{k\alpha}c_{q\alpha} - \delta_{k',p}\Theta(p)\delta_{k,q}\Theta(-q) + \\
& +\delta_{k,q}\delta_{k',p}\Theta(-q)\Theta(p) \\
= \;& :c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha}: + \\
& +\delta_{k',p}\Theta(p)c^\dagger_{k\alpha}c_{q\alpha} - \delta_{k,q}\Theta(-q)c^\dagger_{p\beta}c_{k'\beta} + \\
& +\delta_{k,q}\delta_{k',p}\Theta(-q) - \delta_{k,q}\delta_{k',p}\Theta(-q)\Theta(p) \\
\approx \;& \delta_{k',p}\Theta(p)c^\dagger_{k\alpha}c_{q\alpha} - \delta_{k,q}\Theta(-q)c^\dagger_{p\beta}c_{k'\beta}
\end{aligned}
\tag{B.1}
$$

$$
\begin{aligned}
c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta}c_{q\alpha} \overset{\alpha\neq\beta, m\neq 0}{=} & :c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta}c_{q\alpha}: + \\
& +\langle 0|c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta}c_{q\alpha}|0\rangle + \\
& +\langle 0|c^\dagger_{k\alpha}c_{l\alpha}|0\rangle :c_{k'\beta}c^\dagger_{l+m\alpha}c^\dagger_{p\beta}c_{q\alpha}: +
\end{aligned}
$$

$$
\begin{aligned}
& +\langle 0|c^\dagger_{k\alpha}c_{q\alpha}|0\rangle : c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta} : + \\
& +\langle 0|c_{k'\beta}c^\dagger_{p\beta}|0\rangle : c^\dagger_{k\alpha}c^\dagger_{l+m\alpha}c_{l\alpha}c_{q\alpha} : + \\
& +\langle 0|c^\dagger_{l+m\alpha}c_{q\alpha}|0\rangle : c^\dagger_{k\alpha}c_{k'\beta}c_{l\alpha}c^\dagger_{p\beta} : + \\
& +\langle 0|c^\dagger_{k\alpha}c_{k'\beta}c_{l\alpha}c^\dagger_{p\beta}|0\rangle : c^\dagger_{l+m\alpha}c_{q\alpha} : + \\
& +\langle 0|c^\dagger_{k\alpha}c^\dagger_{l+m\alpha}c_{l\alpha}c_{q\alpha}|0\rangle : c_{k'\beta}c^\dagger_{p\beta} : + \\
& +\langle 0|c_{k'\beta}c^\dagger_{l+m\alpha}c^\dagger_{p\beta}c_{q\alpha}|0\rangle : c^\dagger_{k\alpha}c_{l\alpha} : \\
= \; & : c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta}c_{q\alpha} : + \\
& +\langle 0|c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta}c_{q\alpha}|0\rangle + \\
& +\langle 0|c^\dagger_{k\alpha}c_{l\alpha}|0\rangle : c_{k'\beta}c^\dagger_{l+m\alpha}c^\dagger_{p\beta}c_{q\alpha} : + \\
& +\langle 0|c^\dagger_{k\alpha}c_{q\alpha}|0\rangle : c_{k'\beta}c^\dagger_{l+m\alpha}c_{l\alpha}c^\dagger_{p\beta} : + \\
& +\langle 0|c_{k'\beta}c^\dagger_{p\beta}|0\rangle : c^\dagger_{k\alpha}c^\dagger_{l+m\alpha}c_{l\alpha}c_{q\alpha} : + \\
& +\langle 0|c^\dagger_{l+m\alpha}c_{q\alpha}|0\rangle : c^\dagger_{k\alpha}c_{k'\beta}c_{l\alpha}c^\dagger_{p\beta} : + \\
& +\delta_{k,l}\Theta(-l)\delta_{k',p}\Theta(p)\left(c^\dagger_{l+m\alpha}c_{q\alpha} - \langle 0|c^\dagger_{l+m\alpha}c_{q\alpha}|0\rangle\right) + \\
& +\delta_{k,l}\Theta(-l)\delta_{l+m,q}\Theta(-q)\left(\delta_{k',p} - c^\dagger_{p\beta}c_{k'\beta} - \langle 0|c_{k'\beta}c^\dagger_{p\beta}|0\rangle\right) + \\
& +\delta_{k',p}\Theta(p)\delta_{l+m,q}\Theta(-q)\left(c^\dagger_{k\alpha}c_{l\alpha} - \langle 0|c^\dagger_{k\alpha}c_{l\alpha}|0\rangle\right) \\
\approx \; & \delta_{k,l}\delta_{k',p}\Theta(-l)\Theta(p)c^\dagger_{l+m\alpha}c_{q\alpha} - \\
& -\delta_{k,l}\delta_{l+m,q}\Theta(-l)\Theta(-q)c^\dagger_{p\beta}c_{k'\beta} + \\
& +\delta_{k',p}\delta_{l+m,q}\Theta(p)\Theta(-q)c^\dagger_{k\alpha}c_{l\alpha}
\end{aligned} \tag{B.2}
$$

$$
\begin{aligned}
c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\beta}c_{l\beta}c^\dagger_{p\beta}c_{q\alpha} \quad & \overset{\alpha\neq\beta, m\neq 0}{=} \quad \ldots \\
& \approx \quad \langle 0|c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{l+m\beta}c_{q\alpha}|0\rangle : c_{l\beta}c^\dagger_{p\beta} : + \\
& \qquad +\langle 0|c^\dagger_{k\alpha}c_{k'\beta}c^\dagger_{p\beta}c_{q\alpha}|0\rangle : c^\dagger_{l+m\beta}c_{l\beta} : + \\
& \qquad +\langle 0|c^\dagger_{k\alpha}c_{l\beta}c^\dagger_{p\beta}c_{q\alpha}|0\rangle : c_{k'\beta}c^\dagger_{l+m\beta} : + \\
& \qquad +\langle 0|c_{k'\beta}c^\dagger_{l+m\beta}c_{l\beta}c^\dagger_{p\beta}|0\rangle : c^\dagger_{k\alpha}c_{q\alpha} : \\
& \approx \quad -\delta_{k,q}\delta_{k',l+m}\Theta(-q)\Theta(l+m)c^\dagger_{p\beta}c_{l\beta} + \\
& \qquad +\delta_{k,q}\delta_{k',p}\Theta(-q)\Theta(p)c^\dagger_{l+m\beta}c_{l\beta} - \\
& \qquad -\delta_{k,q}\delta_{l,p}\Theta(-q)\Theta(p)c^\dagger_{l+m\beta}c_{k'\beta} + \\
& \qquad +\delta_{k',l+m}\delta_{l,p}\Theta(l+m)\Theta(p)c^\dagger_{k\alpha}c_{q\alpha}
\end{aligned} \tag{B.3}
$$

$$
\begin{aligned}
c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{k'\alpha} c^\dagger_{l+m\alpha} c_{l\alpha} \quad & \overset{\alpha\neq\beta, m\neq 0}{=} \quad \ldots \\
& \approx \quad \langle 0| c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{k'\alpha} |0\rangle : c^\dagger_{l+m\alpha} c_{l\alpha} : + \\
& \quad\quad + \langle 0| c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{l\alpha} |0\rangle : c_{k'\alpha} c^\dagger_{l+m\alpha} : + \\
& \quad\quad + \langle 0| c^\dagger_{p\alpha} c_{k'\alpha} c^\dagger_{l+m\alpha} c_{l\alpha} |0\rangle : c_{q\beta} c^\dagger_{k\beta} : + \\
& \quad\quad + \langle 0| c_{q\beta} c^\dagger_{k\beta} c_{k'\alpha} c^\dagger_{l+m\alpha} |0\rangle : c^\dagger_{p\alpha} c_{l\alpha} : \\
& \approx \quad \delta_{p,k'} \delta_{q,k} \Theta(-p) \Theta(q) c^\dagger_{l+m\alpha} c_{l\alpha} - \\
& \quad\quad - \delta_{p,l} \delta_{q,k} \Theta(-p) \Theta(q) c^\dagger_{l+m\alpha} c_{k'\alpha} - \\
& \quad\quad - \delta_{p,l} \delta_{k',l+m} \Theta(-p) \Theta(l+m) c^\dagger_{k\beta} c_{q\beta} + \\
& \quad\quad + \delta_{q,k} \delta_{k',l+m} \Theta(q) \Theta(l+m) c^\dagger_{p\alpha} c_{l\alpha}
\end{aligned} \tag{B.4}
$$

$$
\begin{aligned}
c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{k'\alpha} c^\dagger_{l+m\beta} c_{l\beta} \quad & \overset{\alpha\neq\beta, m\neq 0}{=} \quad \ldots \\
& \approx \quad \langle 0| c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{k'\alpha} |0\rangle : c^\dagger_{l+m\beta} c_{l\beta} : + \\
& \quad\quad + \langle 0| c^\dagger_{p\alpha} c_{q\beta} c_{k'\alpha} c^\dagger_{l+m\beta} |0\rangle : c^\dagger_{k\beta} c_{l\beta} : + \\
& \quad\quad + \langle 0| c^\dagger_{p\alpha} c^\dagger_{k\beta} c_{k'\alpha} c_{l\beta} |0\rangle : c_{q\beta} c^\dagger_{l+m\beta} : + \\
& \quad\quad + \langle 0| c_{q\beta} c^\dagger_{k\beta} c^\dagger_{l+m\beta} c_{l\beta} |0\rangle : c^\dagger_{p\alpha} c_{k'\alpha} : \\
& \approx \quad \delta_{p,k'} \delta_{q,k} \Theta(-p) \Theta(q) c^\dagger_{l+m\beta} c_{l\beta} + \\
& \quad\quad + \delta_{p,k'} \delta_{q,l+m} \Theta(-p) \Theta(l+m) c^\dagger_{k\beta} c_{l\beta} - \\
& \quad\quad - \delta_{p,k'} \delta_{k,l} \Theta(-p) \Theta(-l) c^\dagger_{l+m\beta} c_{q\beta} + \\
& \quad\quad + \delta_{q,l+m} \delta_{k,l} \Theta(l+m) \Theta(-l) c^\dagger_{p\alpha} c_{k'\alpha}
\end{aligned} \tag{B.5}
$$

Expansion used in Section 3.4:

$$
\begin{aligned}
c^\dagger_{p\alpha} c_{q\alpha} c^\dagger_{k\alpha} c_{l\beta} \quad & \overset{\alpha\neq\beta}{=} \quad : c^\dagger_{p\alpha} c_{q\alpha} c^\dagger_{k\alpha} c_{l\beta} : + \\
& \quad\quad + \langle 0| c^\dagger_{p\alpha} c_{q\alpha} |0\rangle : c^\dagger_{k\alpha} c_{l\beta} : + \\
& \quad\quad + \langle 0| c_{q\alpha} c^\dagger_{k\alpha} |0\rangle : c^\dagger_{p\alpha} c_{l\beta} : + \\
& \quad\quad + \langle 0| c^\dagger_{p\alpha} c_{q\alpha} c^\dagger_{k\alpha} c_{l\beta} |0\rangle \\
& = \quad \delta_{p,q} \Theta(-q) c^\dagger_{k\alpha} c_{l\beta} + \delta_{k,q} \Theta(k) c^\dagger_{p\alpha} c_{l\beta} + \\
& \quad\quad + : c^\dagger_{p\alpha} c_{q\alpha} c^\dagger_{k\alpha} c_{l\beta} : + \text{const.} \\
& \approx \quad \delta_{p,q} \Theta(-q) c^\dagger_{k\alpha} c_{l\beta} + \delta_{k,q} \Theta(k) c^\dagger_{p\alpha} c_{l\beta}
\end{aligned} \tag{B.6}
$$

$$c^\dagger_{p\alpha} c_{q\alpha} c^\dagger_{k\beta} c_{l\alpha} \quad \overset{\alpha\neq\beta}{\approx} \quad \delta_{p,q}\Theta(-q) c^\dagger_{k\beta} c_{l\alpha} - \delta_{p,l}\Theta(-l) c^\dagger_{k\beta} c_{q\alpha} \tag{B.7}$$

$$\begin{aligned}
c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{l\alpha} &= \; : c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{l\alpha} : + \\
&\quad + \langle 0| c^\dagger_{p\alpha} c_{l\alpha} |0\rangle : c_{q\beta} c^\dagger_{k\beta} : + \\
&\quad + \langle 0| c_{q\beta} c^\dagger_{k\beta} |0\rangle : c^\dagger_{p\alpha} c_{l\alpha} : + \\
&\quad + \langle 0| c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{l\alpha} |0\rangle \\
&= \; : c^\dagger_{p\alpha} c_{q\beta} c^\dagger_{k\beta} c_{l\alpha} : - \delta_{p,l}\Theta(-l) c^\dagger_{k\beta} c_{q\beta} + \delta_{k,q}\Theta(k) c^\dagger_{p\alpha} c_{l\alpha} + \text{ const.} \\
&\approx \; \delta_{k,q}\Theta(k) c^\dagger_{p\alpha} c_{l\alpha} - \delta_{p,l}\Theta(-l) c^\dagger_{k\beta} c_{q\beta}
\end{aligned} \tag{B.8}$$

Appendix C

Pseudogap-systems

Most of the approximations used in Chapter 3 were based on the assumption that the varying density of states only leads to a small perturbation compared to the couplings at the Fermi level. But in systems with a power law density of states (3.1), the couplings at the Fermi level are zero and therefore every correction has to be considered as large. However applying only small changes we are able to derive similar results as Gonzales-Buxton and Ingersent [24].

C.1 Flow of the scaling dimension

For pseudogap-systems with a power law density of states (3.1) we assume couplings of the form

$$J_{\|/\perp}(p,q) = u_{\|/\perp}|p|^{x/2}|q|^{x/2},\ x>0. \tag{C.1}$$

Unfortunately the flow equations (3.52) cannot lead to a flow of the scaling dimension to the Toulouse point, since $J_\perp(0,0)$ is zero and consequently $g_p = 0 \rightarrow \partial_B\lambda^2 = 0$. Here the terms A, B and C can be neglected since they are proportional to $J_\perp(0,0)$ and we are left with the flow equations:

$$\boxed{\begin{array}{rcl} \partial_B f_\|(p,q) & = & -(p-q)^2 f_\|(p,q)+ \\ & & +\sum\limits_{k>0} 2(2k-p-q) f_\perp(k,q) f_\perp(p,k), \\ \partial_B f_\perp(p,q) & = & -(p-q)^2 f_\perp(p,q)+ \\ & & +\sum\limits_{k} \frac{1}{2}(2k-p-q)\mathrm{sgn}(k)\left(f_\|(k,q)f_\perp(p,k)+\right. \\ & & \left.+f_\|(k,p)f_\perp(q,k)\right). \end{array}} \tag{C.2}$$

As in Section 4.3 the corrections quadratic in the coupling functions can lead to a divergence. E.g. for symmetric couplings in the pseudogap-form (C.1) we find using the ansatz

$$f_\|(p,q,B) = f_\perp(p,q,B) = u(B)|p|^{x/2}|q|^{x/2}e^{-B(p-q)^2}(2L)^{-1} \tag{C.3}$$

that in the limit $|p|, |q| \ll 1$ both differential equations in (C.2) lead to

$$\begin{aligned}
\partial_B u(B) &= \frac{2}{L} \sum_{k>0} k|k|^x e^{-2Bk^2} u^2(B) \\
&= \frac{1}{2\pi} (2B)^{-(1+x/2)} \Gamma\left(\frac{x}{2}\right) u^2(B) \\
&\equiv h(x) B^{-(1+x/2)} u^2(B).
\end{aligned} \tag{C.4}$$

By integration we find

$$u(B) = \left(\frac{1}{u(B_0)} + \frac{2h(x)}{x} \left(B^{-x/2} - B_0^{-x/2} \right) \right)^{-1}, \tag{C.5}$$

where $B_0^{-1/2}$ is the initial bandwidth of the system. Obviously $u(B)$ is divergent for

$$\frac{1}{u(B_0)} \leq \frac{2h(x)}{x} B_0^{-x/2}, \tag{C.6}$$

implying a transition between weak- and strong-coupling. This will be discussed in the following section.
We will try to avoid this divergence by subtracting the arithmetic average (multiplied by a prefactor)

$$s_\perp(p) = \frac{2\pi}{L} \frac{1}{2 \frac{L}{2\pi} \frac{1}{a} + 1} \sum_{q=-1/a}^{1/a} f_\perp(q+p, q) \tag{C.7}$$

from the $f_\perp$ flow equation and adding it to the flow of g_p by using

$$\sum_k g_k \alpha_k C_k^\dagger \overset{(3.39)}{=} \sum_{p,q} g_q \frac{4\pi^2 a}{L\sqrt{L}} c_{p+q\uparrow}^\dagger c_{p\downarrow} + \mathcal{O}\left(J_\perp(0,0) \times J_\parallel(0,0)\right). \tag{C.8}$$

Please note that the resulting error of this expansion is of $\mathcal{O}(J_\parallel(0,0) \times J_\perp(0,0))$ and cannot be neglected for large initial couplings. Therefore one should not use the above approximation for systems with nonzero couplings at the Fermi level.

In other words we will add the terms

$$\sum_{p,q} s_\perp(p-q) \left(c_{p\uparrow}^\dagger c_{q\downarrow} S^- + c_{p\downarrow}^\dagger c_{q\uparrow} S^+ \right) \tag{C.9}$$

and

$$-\sum_{p,q} s_\perp(p-q) \left(c_{p\uparrow}^\dagger c_{q\downarrow} S^- + c_{p\downarrow}^\dagger c_{q\uparrow} S^+ \right) \tag{C.10}$$

to the right hand side of

$$\partial_B H(B) = [\eta(B), H(B)]. \tag{C.11}$$

While by using Eq. (C.8) the first term is identified to contribute to the flow of g_p, the second one will be added to the flow of $f_\perp(p,q)$.
Please note that with the choice of $s_\perp(p)$ in Eq. (C.7) the contribution to the flow of g_p is chosen as the average of the couplings $f_\perp(q+p,q)$ multiplied by $\sqrt{L}/(2\pi a)$ to measure $s_\perp(p)$ in the same units as g_p.

This leads to two corrected flow equations for pseudogap-systems:

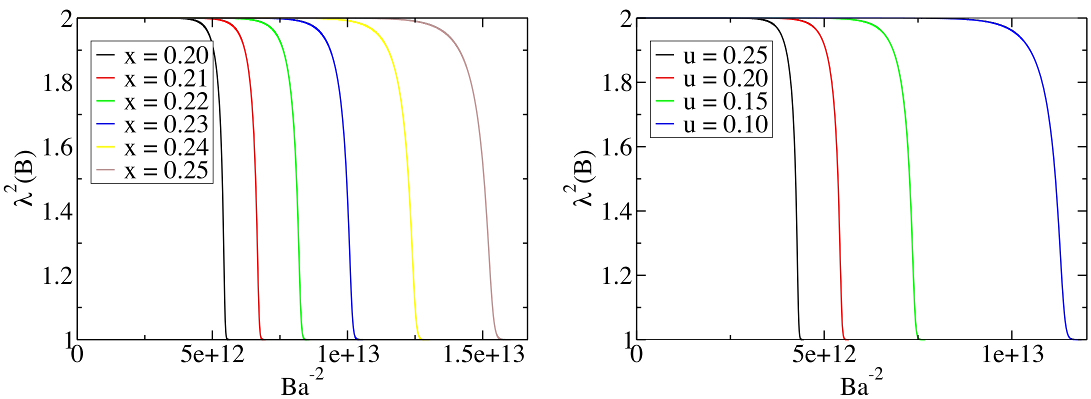
$$\boxed{\begin{aligned}
\partial_B g_p &= -p^2 g_p + 2\sum_{q\neq p}\frac{\alpha_q}{\alpha_p}\eta^{(2)}_{pq}g_q + \frac{1}{2}g_p\ln\left(\frac{B}{a^2}\right)\lambda\partial_B\lambda - \\
&\quad -\frac{\sqrt{2}\pi\lambda}{L}\sum_{q\neq 0}\sum_k g_{p+q}f_\parallel(k+q,k)\frac{p+2q}{|q|}e^{-a|q|/2}\times \\
&\quad \times\left(\Theta(-k-q)-\Theta(-k)\right) + \frac{L\sqrt{L}}{4\pi^2 a}s_\perp(p) - \\
&\quad -2pg_p\omega_p, \\
\partial_B f_\perp(p,q) &= -(p-q)^2 f_\perp(p,q) + \\
&\quad +\sum_k \frac{1}{2}(2k-p-q)\mathrm{sgn}(k)\left(f_\parallel(k,q)f_\perp(p,k)+\right. \\
&\quad \left.+f_\parallel(k,p)f_\perp(q,k)\right) - s_\perp(p-q).
\end{aligned}} \tag{C.12}$$

Since $s_\perp(p)$ couples the $f_\perp$ differential equations nontrivial, an analytic proof of the convergence of the complete set of flow equations is only hard to achieve. However by numerical investigation we did not find a divergence of the new flow equations (even far beyond the Toulouse point).

Figs. (C.1(a)) and (C.1(b)) show example plots for the flow of the scaling dimension using the revised flow equations (C.12). As expected from the initial values the flow starts only very slow. But due to the fact that g_p is no longer decreasing all the time, λ^2 reaches the Toulouse point quite fast after the flow finally started. As expected large couplings lead to a fast flow of the scaling dimension and therefore to a higher Kondo temperature as for smaller couplings.

C.2 Critical exponent

Examining again couplings of the form (C.1) it is clear that for finite parameters $u_{\parallel/\perp}$ the couplings for states close to the Fermi level vanish in the limit $x \to \infty$. Since the Kondo effect lives from the excitations of the latter it is very unlikely to find the strong-coupling regime for large values of the exponent x. On the other hand for $x = 0$ the system is equivalent to the anisotropic Kondo model with momentum independent couplings. So one can expect to find a transition



(a) u=0.2

(b) x=0.2

Figure C.1: Flow of the scaling dimension in pseudogap-systems

between weak- and strong-coupling in the exponent x. Of course this transition has to be continuous and cannot take place at a specific value of x. Nevertheless one can find regions where the strong-coupling regime is definitive unreachable.

NRG calculations (see e.g. [24]) show that in the limit of small couplings (compared to the bandwidth) the strong-coupling regime cannot be obtained for power law densities of states (3.1) with values of $x \gtrsim 0.5$. By the inequality (C.6) we already found the first evidence for such a transition. But actually the divergence of the solution is not required to find the Kondo effect. It is sufficient that the low energy couplings flow to values much larger than the hopping parameter (represented by the bandwidth of the system). Therefore the actual transition between strong- and weak-coupling will take place at certainly smaller initial couplings than the divergence.

Solving Eq. (C.6) numerically using *Maple* we find for $B_0 = 1$ and $u(B_0) = 0.1$ that the transition between the diverging and the finite solution takes place at $x \sim 0.17$. From Fig. C.1(a) we know that even small changes in the exponent x lead to drastic changes in the speed of the flow of the scaling dimension. Due to this strong influence of x on the flow - and therefore on the Kondo temperature - we do not expect to find the strong-coupling regime for exponents much larger than 0.17. However to get accurate results one has to solve the complete system of differential equations, which can only be done numerically.

The value of the flow parameter at which the scaling dimension reaches the Toulouse point B_c is (in first order) inverse proportional to the Kondo temperature. So one can obtain the "critical exponent" at which the transition takes place

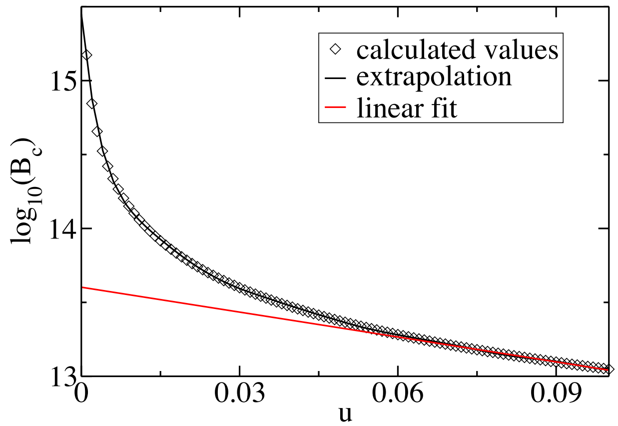


Figure C.2: B_c against u, $x = 0.2$

by determining $B_c(x)$, because B_c has to diverge if the Kondo temperature goes to zero. But due to numerical difficulties the exact point where λ^2 reaches the Toulouse can only hardly be obtained. Since in the pseudogap-case the scaling dimension always starts its flow at the same point, we can use any value between the starting point and the Toulouse point to obtain an equivalent relation. We therefore choose B_c to be the value of the flow parameter at which the square of the scaling dimension is $\lambda^2 = 1.5$.

To assure that we can find such a divergence, we first plotted B_c against u in Fig. (C.2) for one x-value, setting $a = 1$ throughout this section. Here B_c has to diverge in the limit $u \to 0$. Going from large to small u's, B_c seems to be increasing exponentially until it suddenly diverges, corresponding to the drop of the Kondo temperature to zero.

In Fig. (C.3) we plotted B_c against x for $u = 0.1$. Going from larger to smaller couplings (smaller to larger x) we again find an exponential increase of B_c, but at $x \approx 0.5$ it starts to diverge. From that we can conclude that for $x \gtrsim 0.5$ the crossover to the strong-coupling regime is only hard to achieve[1], which is in good analogy to the NRG results.

C.3 Summary

Summarizing this chapter we found that by rearranging the flow equations for systems with nonzero couplings at the Fermi level we are also able to solve them for pseudogap-systems. Analyzing systems with power law densities of states we

[1] Of course the point of the divergence is u-dependent and can be shifted to the right or to the left by using larger or smaller values for u. But since $a^{-1} = 1$ is the effective initial bandwidth of the system, only couplings $u \lesssim 0.1$ can be considered as small.

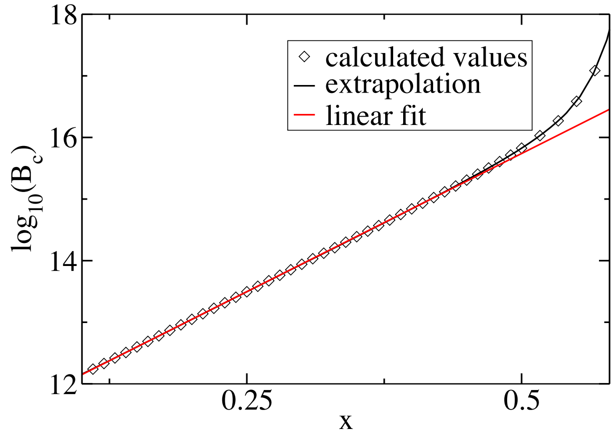


Figure C.3: B_c against x, $u = 0.1$

found that for exponents $x \gtrsim 0.5$ the Toulouse point can only be reached hard, which is in good agreement with previous NRG calculations.

But within our approximations we always map antiferromagnetic coupling functions of the form C.1 to an anisotropic Kondo Hamiltonian with a constant density of states with antiferromagnetic coupling constants. The latter will of course always show strong-coupling behaviour. Furthermore it is not clear that the rearrangement of the flow equations is a suitable way to remove the strong-coupling divergence, since the uniqueness of the coupled differential equations is abrogated and therefore also the solution is no longer unique. Therefore a different approach should be considered.

List of Figures

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