

Lattice path integral approach to the Kondo model

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Contents

Abstract/Zusammenfassung	1
1 Introduction	3
2 The Impurity Models	9
2.1 Lattice path integral formulation	9
2.1.1 Constituents of the model	9
2.1.2 Construction of the lattice model	14
2.1.3 Solution (NLIE)	28
2.2 Generalized models	45
2.2.1 Construction of the generalized models	45
2.2.2 Solution (NLIE)	51
3 Analytical Investigation	61
3.1 Low temperature evaluation	61
3.1.1 $2S = m$: Lowest orders	61
3.1.2 Linearization for $T = 0, h \neq 0$	64
3.1.3 Asymptotic linearization for $T, h \ll T_K, j < m$	76
3.2 High Temperature Evaluation	81
3.2.1 Isotropic case $\gamma = 0, h = 0$	81
3.2.2 High temperature expansion, $h \neq 0$	91
3.2.3 Low temperature evaluation in the under-screened case	93
3.2.4 Anisotropic case, $\gamma \neq 0$	94
3.3 Summary	95
4 Numerical Investigation	97
4.1 Thermodynamic quantities for $h = 0$	98
4.1.1 Under-screened and exactly screened cases	98
4.1.2 Over-screened cases	99
4.2 Thermodynamic quantities for $h \neq 0$	101
4.2.1 Under-screened and exactly screened cases	101
4.2.2 Over-screened case	102
5 Conclusion and Outlook	117

A	Appendix to Chapter 2	121
A.1	Eigenvalue of $\tau_I^{(Q)}$	121
A.2	Host Hamiltonian	129
A.2.1	$\mathfrak{gl}(2 1)$ invariance	131
A.3	Eigenvalue of $\tau_h^{(Q)}$	131
A.3.1	Diagonalization	132
A.3.2	Solution (NLIE)	138
A.4	Eigenvalue of $\tau_{eff}^{(l,m)}$	141
B	Appendix to Chapter 3	147
B.1	Calculation of $\hat{A}(k)$	147
B.2	Convolutions	149
B.2.1	Convolutions with algebraically decaying kernels	149
B.2.2	Convolutions with exponentially decaying kernels	150
C	Appendix to Chapter 4	151
C.1	Regularization schemes	151
C.1.1	Scheme I	152
C.1.2	Scheme II	153
C.1.3	Integrals	157
C.2	Algorithms	159
C.2.1	Recursive calculation of $\ln \mathfrak{B}_l$	159
C.2.2	Extended integration range	159
C.2.3	Smoothed functions for $h \neq 0$	159
C.3	Results	160
	Bibliography	163
	Acknowledgements/Danksagung	168

Abstract

A lattice regularization of the isotropic single channel spin-1/2 Kondo model is proposed. From symmetry arguments, effective models for the more general anisotropic m -channel spin- S case are given. By application of the Quantum Transfer Matrix formalism, the free energy and other thermodynamic equilibrium response functions are obtained exactly by a set of $\max(2S, m) + 1$ non-linear integral equations. These are studied analytically in certain limiting ranges of the external parameters (temperature and magnetic field) and numerically over wide parameter ranges. Both high- and low-temperature scales are calculated.

Zusammenfassung

Es wird eine Gitterregularisierung des isotropen Kondomodells (ein Kanal, Spin-1/2) vorgeschlagen. Mit Symmetrieargumenten werden effektive Modelle für den allgemeineren anisotropen, m -Kanal, Spin- S Fall angegeben. Durch die Anwendung des Quantentransfermatrixformalismus werden die freie Energie und andere thermodynamische Gleichgewichtsantwortfunktionen exakt durch einen Satz von $[\max(2S, m) + 1]$ nichtlinearen Integralgleichungen erhalten. Diese werden analytisch in gewissen Grenzfällen der externen Parameter (Temperatur, Magnetfeld) sowie numerisch über weite Parameterbereiche untersucht. Sowohl Hoch- als auch Tieftemperaturskalen werden berechnet.

Chapter 1

Introduction

Theoretical many particle physics develops tools and models to describe systems of interacting elementary particles. "Elementary" means that the particles are completely characterized by their properties and their states. A property cannot be changed, whereas the state is the ensemble of continuous and/or discrete variables which contain all information about the degrees of freedom. If a particle is free, its state will always be the same. The interaction with other particles causes the states to change. Indeed, the interaction is defined by the change of states of the interacting particles.

Let N identical particles, which interact in a pairwise manner, be in a d -dimensional volume V_d . N and V_d are auxiliary constructs for practical calculations. Each particle may be in one of $2S + 1$ states. The corresponding vector in $(2S + 1)^N$ dimensional Hilbert space evolves according to Schrödinger's equation. A thermodynamic description requires the knowledge of all eigenstates of the Hamiltonian with their corresponding eigenvalues. These functions depend analytically on the external parameters, since none of the underlying equations causes any divergence. However, singularities are observed, namely in phase transitions or critical points. These occur in the thermodynamic limit, $N, V_d \rightarrow \infty$ such that $N/V_d = \text{const.}$. The bulk behaviour is expected to be independent of N, V_d . The challenge is to find ways of describing the system which allow for the thermodynamic limit.

Once the system of N identical particles is understood, one further question is how an impurity is affected by such a homogeneous background (host) and how it influences the host. New phenomena only emerge if host and impurity are allowed to interact, that is, if a certain resonance condition is fulfilled. Then the impurity displays new characteristic features. On the other hand, its influence on the host is expected to be negligibly small, of the order $\mathcal{O}(1/N)$.

The subject of this work is the development of a lattice path integral approach to an exact evaluation of thermodynamic equilibrium response functions of the one-dimensional Kondo problem. Let us embed the method and the model into their respective backgrounds.

The spectrum of the isotropic Heisenberg chain of N sites was obtained by Bethe in 1931, [15]. In his work, the eigenvalues are given by $\mathcal{N} \leq N/2$ numbers, the Bethe ansatz numbers (BAN). The exact solvability relies on the factorization of the many body scattering matrix τ into a product of scattering matrices R between two adjacent particles. This factorization is equivalent to a self-consistency relation between scattering matrices of two particles, the Yang-Baxter-Equation (YBE). A review and bibliography are contained in the Baxter's book, [13].

Contrary to the coordinate approach initialized by Bethe, the algebraic Bethe ansatz (ABA) (see [62] for a review) provides an algebraic technique to diagonalize various one-dimensional quantum models. The scattering matrices are parametrized by a spectral parameter x , $R = R(x)$. R now is the representation of an operator, acting in the direct product of quantum and auxiliary space. A

product of R -operators in auxiliary space builds up a monodromy matrix T . τ , in this framework called transfer matrix, is the trace over the auxiliary space entries of the monodromy matrix. The logarithmic derivative of τ with respect to x , taken at a fixed value $x = x_0$, defines the Hamiltonian of the model. Since transfer matrices with different x commute due to the YBE, all eigenvalues of the model are obtained, again determined by BAN.

The next step is the calculation of thermodynamic equilibrium response functions. Takahashi (he reviews his work in [87]) made a hypothesis concerning the distribution of BAN in the complex plane, the so-called string hypothesis. With this hypothesis, he classifies the excitations and calculates the eigenvalues, without constructing the corresponding eigenstates. The eigenvalues known, one arrives at the free energy. It is encoded in a set of infinitely many coupled nonlinear integral equations.

Klümper pursues a different approach to the classification of the excitation spectra. He starts from analyticity arguments, [54]. Furthermore, he uses the Trotter-Suzuki mapping [88, 85, 86] of one-dimensional quantum models onto two-dimensional classical models. The latter previously had been solved by Baxter. This enables him to represent the free energy of the quantum models in terms of the leading eigenvalue of the corresponding quantum transfer matrix, QTM. The QTM itself is diagonalized by ABA. Furthermore, by analyticity arguments the unknown BAN are expressed through only two (for the spin-1/2 Heisenberg chain) auxiliary functions. These obey two non linear integral equations (NLIE) and give the free energy.

The application of this technique to fermionic models requires the translation of R -operators to fermionic annihilators and creators. By making use of the algebraic structure of the underlying super-algebras, Göhmann [36] develops a fermionization scheme, which avoids the cumbersome expressions appearing in Jordan-Wigner transformations.

The fermionization scheme, the QTM-approach, the ABA and the derivation of NLIE are the tools used in this work.

Let us now briefly review the background of the model we study, the Kondo model.

In 1934, de Haas et al [23] measured the resistivity of Au with 10^{-4} % Cu and found a minimum at a temperature of about 4 K. For nearly thirty years, this observation remained a puzzle. As a first guess, the impurity is thought of as an isotropic scatterer, any influence of the surrounding lattice symmetry is neglected. Thus the scattering is an effectively one-dimensional process, while the host itself is a free three-dimensional electron gas. Anderson [3] proposed a model of a localized impurity in a host of electrons with kinetic energy t and onsite Coulomb repulsion U . The impurity interacts with the host through a hybridization V . In the limit $|V|^2/U \ll 1$, a localized moment forms, and the Anderson model turns into the sd -model, [81]. The lesson to be learned from this limit is that a localized moment occurs if double occupation and hybridization with the environment on one lattice site are strongly suppressed. The sd -model describes a free host, interacting weakly with a localized magnetic moment via antiferromagnetic XXX spin exchange with an amplitude J . "Weak interaction" means that at high temperature, the coupling is negligible and the impurity spin shows Curie-Weiss behaviour. This model served as starting point for Kondo [61], who performed a perturbational calculation of the scattering amplitude between host and impurity up to third order in J . He discovered a $\ln T/\tilde{T}_k$ contribution to the resistivity and thus was able to explain the minimum observed by de Haas. \tilde{T}_k is the crossover temperature which indicates the limit of perturbation theory: A divergence occurs for $T \sim \tilde{T}_k$. This problem is termed "Kondo problem"; the XXX - sd model is henceforth called isotropic "Kondo model".

The method which overcomes the failure of perturbation theory is scaling. Using perturbational scaling arguments, Anderson [4] showed that the limit of low temperatures $T < \tilde{T}_k$ is connected with a divergent coupling constant J , but still a quantitative approach to this strong coupling limit was

missing. By the implementation of his numerical renormalization group, Wilson [94] realized a non-perturbative access to low temperatures down to $T = 0$. This contribution was recognized in the award of a Nobel prize in 1982. Wilson assumed a linear dispersion in the conduction band and calculated the impurity contributions to the magnetic susceptibility χ and the specific heat C at $T \ll \tilde{T}_k$. He found $\chi = \text{const.}$ and $C \propto T$, that is, Fermi liquid behaviour. Especially, the ratio χ/C is enhanced by a factor of 2 compared with free fermions, and χ is inversely proportional to \tilde{T}_k , a high temperature scale. Let us call the low temperature ratio χ/C the "low temperature Wilson ratio" and the constant $\chi(T = 0) \cdot \tilde{T}_k$ the "high temperature Wilson ratio". These two numbers contain the whole physics of equilibrium response functions in the Kondo model.

The Fermi liquid signatures of the many body bound state at low temperatures incited Nozières [69, 70] to formulate a phenomenological Fermi liquid theory. He also proposed a generalization, including m electronic species, each with spin 1/2, instead of one. The physical background is the orbital degeneracy of 3d electrons. This model is known as the multichannel Kondo model.

Wilson realized the first non-perturbative approach to the Kondo model. Andrei [5] and Wiegmann [93] succeeded in applying the Bethe Ansatz (BA) to the Kondo model and thus obtained the spectrum exactly. In their works, the host is reduced to one dimension. Since the scattering process itself is one-dimensional, this is a natural approximation. Two particle-functions of the host are factorized in a charge and a spin contribution. Only the antisymmetric charge function and the symmetric spin function is accounted for in order to set up two-particle scattering matrices which obey the YBE. Although this construction is justified for linear dispersion in the host, "half" of the host degrees of freedom is rejected. Thermodynamic equilibrium response functions were calculated in the following by employing TBA techniques, [27, 28, 73, 6, 7, 90]. These works include the generalization to the spin- S Kondo model, with an impurity of spin S interacting with a host of $m = 1$ spin-1/2-electrons. Furthermore, an anisotropic XXZ -like spin exchange for $S = 1/2$, $m = 1$ has been explored. Finally, Tselvick and Wiegmann [91, 92, 89] paved the way for the exact description of the isotropic m -channel, spin- S model. In these works, the impurity contribution to the free energy is encoded in a set of infinitely many coupled NLIE. These contain the whole information about equilibrium response functions. Especially, the asymptotic high-temperature expansion due to Kondo and the Wilson ratios are supposed to be encoded therein. As to the low temperature Wilson ratio and the high temperature expansion, it was confirmed in the cited works. However, care had to be taken when calculating the host contributions. In the isotropic $m = 1 = 2S$ case, for example, the susceptibility was correctly reproduced, but only half of the specific heat of spin-1/2 fermions was obtained. This artefact is due to the special way the host was included: The magnetic field does not couple to the antisymmetric (singlet) spin part; but the symmetric part of the charge function contributes as much to the specific heat as the antisymmetric part. With this prescription in mind, the low-temperature result by Wilson was obtained exactly by TBA-techniques. To evaluate the high-temperature Wilson ratio, a perturbational expansion of the free energy by Andrei [8] confirms Wilson's result. Its derivation in the framework of the exact solution is still lacking.

Very recently, Schlottmann [79, 80] has generalized the exact solution to the multichannel, anisotropic spin- S Kondo model for special values of anisotropy. He finds evidence for a quantum critical point at $T = 0$, $h = 0$ in the XXZ -case. Affleck [2] considered the isotropic $m > 2S$ Kondo problem by conformal field theory, and gives analytical expressions of Wilson ratios. These have only partially been confirmed by an exact solution yet.

The TBA method yields exact results of thermodynamic equilibrium response functions. In principle, all information necessary to calculate these quantities is available. Nevertheless, questions remain open:

- i) Is it possible to include the host such that the restriction to two-particle functions with even spin-, and uneven charge-functions is lifted?
- ii) Can Wilson's high temperature ratio be extracted? Are Affleck's results accessible by the exact solution?
- iii) Is it possible to include an arbitrary XXZ -like anisotropy?
- iv) How to calculate dynamical response functions?

Probably, question ii) was not answered yet since it requires the numerical evaluation of the infinitely many NLIE, an impossible task. Numerical studies of TBA results demand some cutoff scheme, which inevitably leads to errors. Question iii) is answered with "no" in the TBA approach. At the very fundamentals of this technique is the string-hypothesis. This hypothesis only works for special cases of the anisotropy parameter. The last question is, since excitation energies are known without their corresponding eigenstates, out of reach in the TBA. It requires the evaluation of correlation functions between impurity and host operators.

In this work, questions i), ii) and iii) are answered positively. The door to the answer to question iv) is opened a little in so far that principally, all eigenvalues *and* the eigenstates are known.

We shall develop a lattice path integral representation of the free energy of the entire system, host and impurity, in one dimension. This model can be viewed as a lattice-regularized version of the continuous Kondo model. A regularized Hamiltonian on a lattice is proposed, which yields the Kondo model in a certain scaling limit of external parameters. The host relies on a four-dimensional representation of the Lie superalgebra $\mathfrak{gl}(2|1)$. The corresponding four states per lattice site are zero, single (with spin up or down) and double occupation. The impurity degrees of freedom are described by a three-dimensional representation of $\mathfrak{gl}(2|1)$. Double occupation on the impurity site is excluded from the beginning. According to the work by Schrieffer and Wolf [81], one thus expects a localized moment to occur. In order to regularize the continuous Kondo model, it is quite natural to choose the superalgebra $\mathfrak{gl}(2|1)$. Its even subalgebra is $\mathfrak{u}(1) \otimes \mathfrak{su}(2)$, encoding charge and spin degrees of freedom, respectively. Spin-charge separation occurs in one dimension for interacting electron systems [41], and the impurity is supposed to possess exclusively spin degrees of freedom. Indeed, in the impurity space, $\mathfrak{gl}(2|1)$ is reduced to one of its subalgebras, $\mathfrak{su}(2)$, in the scaling limit. Only the spin degrees of freedom rest on the impurity site. The fact that the same algebra for the host and the impurity is used can be considered as the resonance condition for interactions of both. Then the free energy of the host and of the impurity are encoded in eigenvalues of distinct quantum transfer matrices and can therefore be separated.

It is not our aim to justify the models themselves from physical arguments deeper than the rather intuitive ideas given in this introduction. Such considerations are of vital importance, since any theory must be built up on experiments and must find its way back to experiments by predicting measurable phenomena. As far as the spin-1/2, channel $m = 1, 2$ models are concerned, this issue is elucidated in [70, 90]. Furthermore, one model may serve as a benchmark for many theories, and it is of no less importance to understand the structure, the benefits and the failure of each to estimate their respective potentials in predicting new phenomena. The subject of this work is the latter challenge.

This work consists of five parts. The first chapter contains the introduction. The next chapter sets up the models we want to analyse. A $\mathfrak{gl}(2|1)$ symmetric lattice model with an impurity is given, and the isotropic $m = 1 = 2S$ Kondo model is recovered therefrom by a canonical transformation in the limit of a singly occupied impurity site. The free energy is derived and expressed in terms of

two auxiliary functions, obeying two NLIE formally identical to the analogous equations leading to the free energy of the XXX -Heisenberg chain. This motivates us to propose a $U_q(\mathfrak{su}(2))$ symmetric effective transfer matrix which yields the free energy of the impurity of the generalized models. It is given through a set of $[\max(2S, m) + 1]$ NLIE.

In the third chapter, the NLIE are studied analytically in the limits of low and high temperatures. The fourth chapter is dedicated to numerical studies over the whole range of temperatures and magnetic field. Wilson's two ratios are calculated and Affleck's results are confirmed within some numerical errors. Qualitative agreement is found with Schlottmann, however his results differ by constant prefactors from ours.

Concluding remarks form the last chapter.

To keep the work readable for non-experts of ABA-techniques, the corresponding algebraic manipulations are relegated to the appendix. In the main part, only the results, that is the eigenvalues of the transfer matrices, are given. Equally, details of the numerical procedure have been excluded from the main part.

In the whole work we set $k_B = 1$ and $g\mu_B = 1$, where k_B is Boltzmann's constant, g is the gyromagnetic factor and μ_B is the Bohr magneton. The inverse temperature $1/T$ is denoted by β and the external magnetic field by h .

Chapter 2

The Impurity Models

We construct Kondo-like impurity models in two steps: In the first part, a spin-1/2-impurity site is embedded in a host of spin-1/2 fermions. The second part is dedicated to generalizations of this model. Thermodynamic equilibrium functions are derived from the grand canonical potential $\Omega = \Omega(\mu, T, h)$. Since we will give the models in second quantization, it is natural to start in the grand canonical formalism. However, once Ω is calculated, we will restrict $T, h \ll D$, where D is the bandwidth of the host. Then $\mu = \text{const.}$ is readily expressed by the particle number $N = \text{const.}$, which effectively is equivalent to the canonical description. The corresponding potential is denoted by $f = f(T, h)$; following custom, we call it the "free energy" - although strictly speaking, it is the free enthalpy. In the ongoing, no distinction is made between Ω and f , only the latter symbol is used for the thermodynamic potential.

2.1 Lattice path integral formulation

2.1.1 Constituents of the model

This section provides the tools which are used to construct the impurity model on the lattice. Essentially, these are $\mathfrak{gl}(2|1)$ -invariant R matrices which satisfy the Yang-Baxter-Equation (YBE). Based on these matrices, a transfer matrix is constructed, from which the Hamilton operator is derived. Since the super-algebra $\mathfrak{gl}(2|1)$ admits both a three-dimensional irreducible representation (irrep) as well as a one-parameter family of inequivalent four-dimensional irreps, several YBEs intertwining the different irreps are fulfilled.

Let $V^{(d)}$ be the module giving rise to the d -dimensional irrep of $\mathfrak{gl}(2|1)$, $d = 3, 4$. A grading is assigned to the basis vectors through the parity function p ,

$$\begin{aligned} d = 4 : \quad & p[1] = p[4] = 0; \quad p[2] = p[3] = 1 \\ d = 3 : \quad & p[1] = p[2] = 0; \quad p[3] = 1. \end{aligned} \tag{2.1}$$

Note the different parities in three and four dimensions. Then $R_{i,j}^{(d,d')}(u) \in \text{End}(V_i^{(d)} \otimes V_j^{(d')})$ satisfies the graded Yang-Baxter-Equation (YBE),

$$\begin{aligned} & \left[R_{2,3}^{(d,d')}(u) \right]_{\beta',\gamma'}^{\beta,\gamma} \left[R_{1,2}^{(d'',d')}(v) \right]_{\alpha',\gamma''}^{\alpha,\gamma'} \left[R_{1,3}^{(d'',d)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} (-1)^{(p[\alpha]+p[\alpha'])p[\beta']} \\ = & \left[R_{1,3}^{(d'',d)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[R_{1,2}^{(d'',d')}(v) \right]_{\alpha'',\gamma''}^{\alpha',\gamma'} \left[R_{2,3}^{(d,d')}(u) \right]_{\beta'',\gamma''}^{\beta',\gamma'} (-1)^{(p[\alpha']+p[\alpha''])p[\beta']}. \end{aligned} \tag{2.2}$$

Summation over doubly occurring indices is implied in the foregoing equation and in all what follows. Since the compatibility condition

$$\left[R_{i,j}^{(d,d')}(u) \right]_{\gamma,\delta}^{\alpha,\beta} = (-1)^{p[\alpha]+p[\beta]+p[\gamma]+p[\delta]} \left[R_{i,j}^{(d,d')}(u) \right]_{\gamma,\delta}^{\alpha,\beta}$$

is satisfied, the redefinition

$$\left[\tilde{R}_{i,j}^{(d,d')}(u) \right]_{\gamma,\delta}^{\alpha,\beta} = (-1)^{p[\alpha]p[\beta]} \left[R_{i,j}^{(d,d')}(u) \right]_{\gamma,\delta}^{\alpha,\beta}$$

makes disappear the minus-signs in eq. (2.2), resulting in the non-graded YBE.

Explicit expressions of the R matrices are given in the following.

$$R^{(3,3)}(u) = \frac{1}{u+1} \left(u + (-1)^{p[a]p[b]} e_a^b \otimes e_b^a \right) \quad (2.3)$$

$$R^{(3,4)}(u) = \frac{1}{u + \frac{\alpha}{2} + 1} \left(u + \frac{\alpha}{2} + 1 + (-1)^{p[a]p[b]} e_a^b \otimes E_b^a \right) \quad (2.4)$$

$$R^{(4,4)}(u) = - \left(1 + \frac{2\alpha}{u-\alpha} \check{P}_1 - \frac{2\alpha+2}{u+\alpha+1} \check{P}_3 \right). \quad (2.5)$$

e_a^b (E_a^b) are the nine three- (four-) dimensional generators of $\mathfrak{gl}(2|1)$, obeying

$$\begin{aligned} [e_b^a, e_d^c]_{\pm} &:= e_b^a e_d^c - (-1)^{(p[a]+p[b])(p[c]+p[d])} e_d^c e_b^a \\ &= \delta_d^a e_b^c - (-1)^{(p[a]+p[b])(p[c]+p[d])} \delta_b^c e_d^a, \end{aligned} \quad (2.6)$$

and the same for the E_b^a . In the four-dimensional case, the generators depend on the extra free parameter α , which also enters the definition of $R^{(4,4)}$. The latter involves the projectors \check{P}_1, \check{P}_3 .¹ For a matrix representation of e_b^a , choose the basis

$$|\bar{1}\rangle = (1, 0, 0), \quad |\bar{2}\rangle = (0, 1, 0), \quad |\bar{3}\rangle = (0, 0, 1).$$

Then $e_b^a := |\bar{b}\rangle\langle\bar{a}|$ provides the common matrix representation of projectors in three dimensional space.

As to the E_b^a , we choose a basis in $V^{(4)}$,

$$|1\rangle = (1, 0, 0, 0), \quad |2\rangle = (0, 1, 0, 0), \quad |3\rangle = (0, 0, 1, 0), \quad |4\rangle = (0, 0, 0, 1).$$

Then one verifies that the set

$$\begin{aligned} E_1^1 &= -|3\rangle\langle 3| - |4\rangle\langle 4|, & E_2^2 &= -|2\rangle\langle 2| - |4\rangle\langle 4|, \\ E_3^3 &= \alpha|1\rangle\langle 1| + (\alpha+1)(|2\rangle\langle 2| + |3\rangle\langle 3|) + (\alpha+2)|4\rangle\langle 4|, \\ E_1^2 &= |2\rangle\langle 3|, & E_2^1 &= |3\rangle\langle 2|, \\ E_2^3 &= \sqrt{\alpha}|1\rangle\langle 2| + \sqrt{\alpha+1}|3\rangle\langle 4|, & E_3^2 &= \sqrt{\alpha}|2\rangle\langle 1| + \sqrt{\alpha+1}|4\rangle\langle 3|, \\ E_1^3 &= -\sqrt{\alpha}|1\rangle\langle 3| + \sqrt{\alpha+1}|2\rangle\langle 4|, & E_3^1 &= -\sqrt{\alpha}|3\rangle\langle 1| + \sqrt{\alpha+1}|4\rangle\langle 2|, \end{aligned}$$

¹As mentioned above, the $R^{(d,d')}$ -matrices act in $V^{(d)} \otimes V^{(d')}$. Generally, $V^{(d)} \otimes V^{(d')} = \sum_k^{\oplus} V_k^{(d_k)}$, where the direct sum is over K modules of d_k -dimensional irreps of the underlying symmetry algebra, in this case $\mathfrak{gl}(2|1)$, [78]. The R matrices reflect this structure by their spectral decomposition, as shown by Jimbo [44], $R^{(d,d')}(u) = \sum_k \rho_k(u) \check{P}_k$. The $\rho_k(u)$ are polynomials of degree $K-1$, and the \check{P}_k are projectors from $V^{(d)} \otimes V^{(d')}$ onto $V_k^{(d_k)}$. For $d=3=d'$ and $d=3=d'-1$, $K=2$, whereas in the case $d=4=d'$, $K=3$, explaining the different structure of eq. (2.5) in comparison with eqs. (2.3), (2.4). These rather qualitative statements are made more profound and quantitative by arguments of group theory, see [19, 25].

satisfies eq. (2.6). It is well known in the literature [18,14,67,71]. Depending on the sign of α , different types of unitary representations follow, [38]. In the sequel, the real parameter α is restricted to $\alpha > 0$.

We quote the expressions for \check{P}_1, \check{P}_3 as they occur in the literature [18,71,77]

$$\check{P}_1 = \sum_{\nu=1}^4 |\Psi_\nu^1\rangle \langle \Psi_\nu^1| \quad (2.7)$$

$$\check{P}_3 = \sum_{\nu=1}^4 |\Psi_\nu^3\rangle \langle \Psi_\nu^3| \quad (2.8)$$

$$|\Psi_1^1\rangle = |1\rangle \otimes |1\rangle, \quad |\Psi_2^1\rangle = \frac{1}{\sqrt{2}}(|2\rangle \otimes |1\rangle + |1\rangle \otimes |2\rangle), \quad |\Psi_3^1\rangle = \frac{1}{\sqrt{2}}(|3\rangle \otimes |1\rangle + |1\rangle \otimes |3\rangle)$$

$$|\Psi_4^1\rangle = \frac{1}{\sqrt{2(2\alpha+1)}} [\sqrt{\alpha+1}(|4\rangle \otimes |1\rangle + |1\rangle \otimes |4\rangle) + \sqrt{\alpha}(|2\rangle \otimes |3\rangle - |3\rangle \otimes |2\rangle)]$$

$$|\Psi_1^3\rangle = \frac{1}{\sqrt{2(2\alpha+1)}} [\sqrt{\alpha}(|4\rangle \otimes |1\rangle + |1\rangle \otimes |4\rangle) + \sqrt{\alpha+1}(-|2\rangle \otimes |3\rangle + |3\rangle \otimes |2\rangle)]$$

$$|\Psi_2^3\rangle = \frac{1}{\sqrt{2}}(|2\rangle \otimes |4\rangle + |4\rangle \otimes |2\rangle), \quad |\Psi_3^3\rangle = \frac{1}{\sqrt{2}}(|3\rangle \otimes |4\rangle + |4\rangle \otimes |3\rangle), \quad |\Psi_4^3\rangle = |4\rangle \otimes |4\rangle$$

These states are orthonormal, so that

$$\begin{aligned} \langle \Psi_\nu^j | &= (|\Psi_\nu^j\rangle)^\dagger, \quad \nu = 1, 2, 3, 4; \quad j = 1, 3 \\ (|a\rangle \otimes |b\rangle)^\dagger &= (-1)^{p[a]p[b]} (|a\rangle)^\dagger \otimes (|b\rangle)^\dagger, \\ (|a\rangle)^\dagger &= \langle a|; \quad a, b = 1, 2, 3, 4 \\ (|a\rangle \otimes |b\rangle)(|c\rangle \otimes |d\rangle)^\dagger &= (-1)^{p[c]p[d]} (|a\rangle \otimes |b\rangle)(\langle c| \otimes \langle d|) \\ &= (-1)^{p[c](p[b]+p[d])} |a\rangle \langle c| \otimes |b\rangle \langle d|. \end{aligned} \quad (2.9)$$

In the last identity, the multiplication rule for the tensor product has been used,

$$(a \otimes b)(c \otimes d) = (-1)^{p[b]p[c]}(ac \otimes bd).$$

Eq. (2.9) is the prescription how to obtain explicit expressions for $\check{P}_{1,3}$ from their definitions. Details are given in appendix A.3.

Apart from the matrices (2.3)-(2.5), which obey eq. (2.2), a further set of matrices is obtained.

$$\left[\overline{R}^{(d',d)}(u) \right]_{\gamma,\delta}^{\alpha,\beta} = (-1)^{p[\delta](p[\gamma]+p[\alpha])} \left[R^{(d,d')}(u) \right]_{\delta,\alpha}^{\beta,\gamma}. \quad (2.10)$$

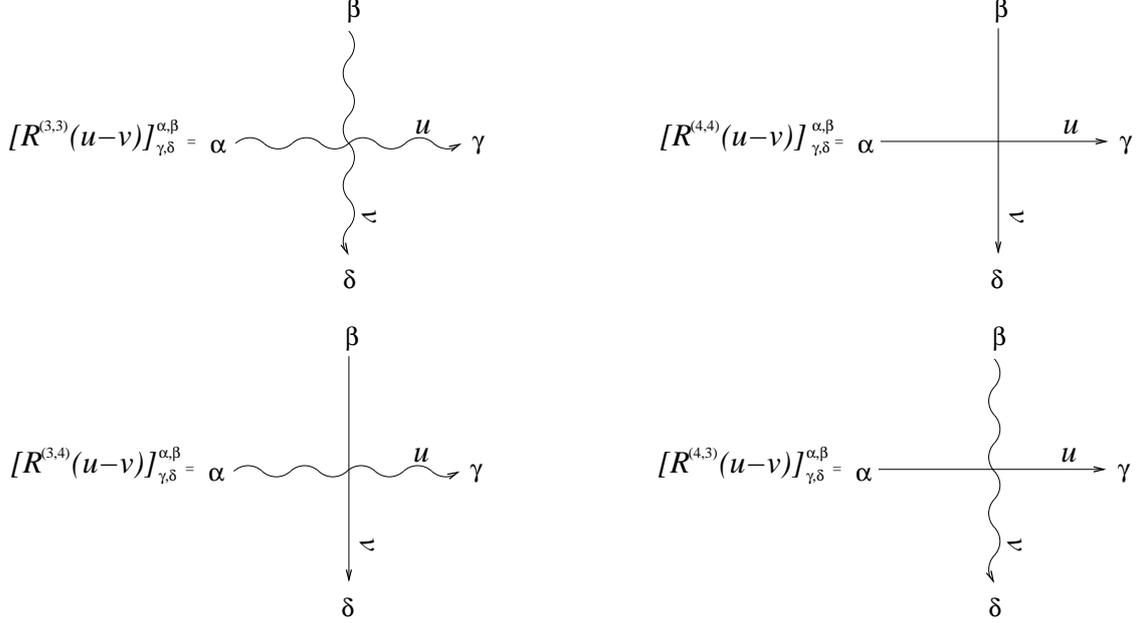
The permutation of the indices means exchanging creators and annihilators in the quantum space of R , while simultaneously permuting the spaces. For $d = 3 = d'$ and $d = 3 = d' - 1$, one may exchange the spaces once more,

$$\begin{aligned} \left[\overline{R}^{(d,d')}(u) \right]_{\gamma,\delta}^{\alpha,\beta} &= \left[\overline{R}^{(d',d)}(u) \right]_{\delta,\gamma}^{\beta,\alpha}, \quad d = 3, \quad d' = 3, 4 \\ &= (-1)^{p[\gamma](p[\delta]+p[\beta])} \left[R^{(d,d')}(u) \right]_{\gamma,\beta}^{\alpha,\delta} \end{aligned}$$

To get from R to \overline{R} , annihilator and creators are exchanged in the quantum space of R . These \overline{R} -matrices satisfy

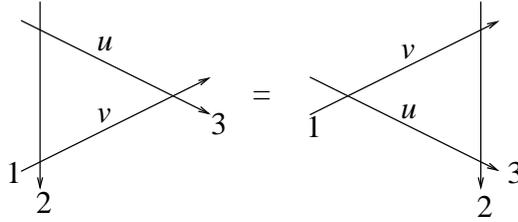
$$\begin{aligned} &\left[\overline{R}^{(d,d')}(-u) \right]_{\beta',\gamma'}^{\beta,\gamma} \left[\overline{R}^{(d'',d')}(-v) \right]_{\alpha',\gamma''}^{\alpha,\gamma'} \left[R^{(d'',d)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} (-1)^{p[\alpha]+p[\alpha']p[\beta']} \\ &= \left[R^{(d'',d)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[\overline{R}^{(d'',d')}(-v) \right]_{\alpha'',\gamma''}^{\alpha',\gamma'} \left[\overline{R}^{(d,d')}(-u) \right]_{\beta',\gamma''}^{\beta',\gamma'} (-1)^{p[\alpha']+p[\alpha'']p[\beta']}. \end{aligned} \quad (2.11)$$

The R -matrices can be translated into a graphical language. Straight lines denote the 4-dim. space, wavy lines symbolize three-dimensional space.



The two bonds symbolize the two spaces intertwined by $R_{i,j}$. Each bond carries a direction indicated by an arrow; both the vertical and horizontal bonds carry spectral parameters. The argument of R is given by the difference between the right and the left "incoming" parameters. The replacement $R \rightarrow \bar{R}$ means flipping the arrow on the vertical bond. The arrows on the vertex representing R give the "direction" of its action: They point towards the out-coming states.

The YBE eq. (2.2) in graphical language reads:



"Other" YBEs are obtained by flipping arrows (that means replacing $R \rightarrow \bar{R}$) and/or substituting straight by wavy lines (that is, changing the dimension in one of the spaces).

"Unitarity" is a further property of the R -matrices.

$$\left[R^{(d,d')}(u) \right]_{\delta,\alpha}^{\beta,\gamma} \left[R^{(d',d)}(-u) \right]_{\gamma',\beta'}^{\alpha,\delta} = \delta_{\beta'}^{\beta} \delta_{\gamma'}^{\gamma}, \quad (2.12)$$

and the same for \bar{R} . The unitarity property fixes normalizing constants of the R -matrices. In the following, we will speak of "normalized" R -matrices when they satisfy eq. (2.12); non-normalized R -matrices differ from those by constant pre-factors, but still fulfill the YBE. Eq. (2.12) is verified for $d = d' = 3$ ($d = d' = 4$) by using the projection properties

$$\begin{aligned} e_b^a e_d^c &= \delta_d^a e_b^c \\ \tilde{P}_i \tilde{P}_j &= \delta_{i,j} \tilde{P}_i. \end{aligned} \quad (2.13)$$

On the contrary, for $d = 3 = d' - 1$ in eq. (2.12), one should employ

$$E_\beta^\alpha E_\delta^\beta (-1)^{p[\beta](p[\alpha]+p[\delta])} = -(\alpha + 2)(-1)^{p[\alpha]p[\delta]} E_\delta^\alpha .$$

In order to construct a lattice model, one has to "localize" the R matrices. It is sufficient to define $[e_j]_b^a$, since all matrix entries are combinations of $e_b^a \otimes e_d^c$ (here $e_b^a = |a\rangle\langle b|$, $a, b = 1, 2, 3, 4$ or $e_b^a = |\bar{a}\rangle\langle \bar{b}|$, $\bar{a}, \bar{b} = 1, 2, 3$; for simplicity of notation, a common symbol is used for both cases). Following [36], define

$$\begin{aligned} [e_j]_b^a &= I_d^{\otimes s(j-1)} \otimes_s e_b^a \otimes_s I_d^{\otimes s(L-j)} \\ &= (-1)^{(p[a]+p[b])\sum_{k=j+1}^L p[c_k]} I_d^{\otimes(j-1)} \otimes e_b^a \otimes e_{c_{j+1}}^{c_{j+1}} \otimes \cdots \otimes e_{c_L}^{c_L} , \end{aligned}$$

with $d = 3, 4$. Then

$$[e_j]_b^a [e_j]_d^c = \delta_d^a [e_j]_b^c \quad (2.14a)$$

$$[e_j]_b^a [e_k]_d^c = (-1)^{(p[a]+p[b])(p[c]+p[d])} [e_k]_d^c [e_j]_b^a \quad (2.14b)$$

$$(-1)^{p[a]} [e_j]_b^a [e_{j+1}]_a^b = (-1)^{p[a]p[b]} e_b^a \otimes e_a^b . \quad (2.14c)$$

The direct product on the rhs of eq. (2.14c) is taken between spaces V_j, V_{j+1} . Eq. (2.14c) serves to "localize" the R -matrices $R^{(3,3)}, R^{(3,4)}$, eqs. (2.3), (2.4). $R^{(4,4)}$, eq. (2.5), is "localized" by eq. (2.9), where the direct product acts between spaces V_j, V_{j+1} .

Principally, one could calculate at this point the Hamiltonian. However, it is more convenient to "fermionize" the R matrices in order to use the more common language of fermionic field operators $c_{\tau,j}^\dagger, c_{\tau,j}$, acting on the spin directions $\tau = \uparrow, \downarrow$ and on the lattice site j . This is done by employing the technique of G6hmann [35, 36], which consists in identifying the $[e_j]_b^a$ with certain combinations of fermionic operators.

The entries $[X_j^\downarrow]_b^a$ of the matrix

$$X_j^\downarrow = \begin{pmatrix} n_{j\downarrow} & c_{j\downarrow}^\dagger \\ c_{j\downarrow} & 1 - n_{j\downarrow} \end{pmatrix} ,$$

satisfy projection and commutation properties formally identical to eqs. (2.14a), (2.14b) with grading $p[1] = 0, p[2] = 1$. Going one step further, one defines projection operators for both spin species,

$$\begin{aligned} X_j &= X_j^\downarrow \otimes_s X_j^\uparrow \\ &= \begin{pmatrix} n_{j\downarrow}n_{j\uparrow} & n_{j\downarrow}c_{j\uparrow}^\dagger & c_{j\downarrow}^\dagger n_{j\uparrow} & c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger \\ n_{j\downarrow}c_{j\uparrow} & n_{j\downarrow}(1 - n_{j\uparrow}) & -c_{j\downarrow}^\dagger c_{j\uparrow} & -c_{j\downarrow}^\dagger(1 - n_{j\uparrow}) \\ c_{j\downarrow}n_{j\uparrow} & c_{j\downarrow}c_{j\uparrow}^\dagger & (1 - n_{j\downarrow})n_{j\uparrow} & (1 - n_{j\downarrow})c_{j\uparrow}^\dagger \\ -c_{j\downarrow}c_{j\uparrow} & -c_{j\downarrow}(1 - n_{j\uparrow}) & (1 - n_{j\downarrow})c_{j\uparrow} & (1 - n_{j\downarrow})(1 - n_{j\uparrow}) \end{pmatrix} . \end{aligned} \quad (2.15)$$

The super-product \otimes_s is defined by

$$[A \otimes_s B]_{\beta,\delta}^{\alpha,\gamma} := (-1)^{(p[\alpha]+p[\beta])p[\gamma]} [A]_\beta^\alpha [B]_\delta^\gamma . \quad (2.16)$$

Eqs. (2.14a), (2.14b) are satisfied by the $[X_j]_b^a$ with grading $p[1] = p[4] = 0, p[2] = p[3] = 1$, in accordance with eq. (2.1) for $d = 4$. This is the only constraint on $[e_j]_b^a$, so that we identify

$$[X_j]_b^a \equiv [e_j]_b^a , \quad (2.17)$$

and Fermi operators are given by linear combinations of $[X_j]_b^a$. Let us shortly comment on the three- and four-dimensional generators of $\mathfrak{gl}(2|1)$. By deleting the j th row and column in the matrix X_j , one gets four possible fermionizations of $[e_j]_b^a = [X_j]_b^a$, the e_j being three-dimensional generators of $\mathfrak{gl}(2|1)$ with the grading resulting without the j th element of the ordered list $\{0, 1, 1, 0\}$. To make contact with eq. (2.1) for $d = 3$, let us delete the first row and column. In order to get the corresponding four-dimensional representation E_j , one makes the ansatz [34]

$$\begin{aligned} E_1^3 &= -a^* X_1^3 + b^* X_2^4, & E_3^1 &= -a X_3^1 + b X_4^2 \\ E_2^1 &= X_3^2 & E_1^2 &= X_2^3 \\ E_2^3 &= a^* X_1^2 + b^* X_3^4, & E_3^2 &= a X_2^1 + b X_4^3 \end{aligned}$$

The commutators eq. (2.6) are obeyed under the condition

$$|b|^2 - |a|^2 = 1,$$

which is accounted for by the parameterization $b = \sqrt{\alpha+1}$, $a = \sqrt{\alpha}$, $\alpha \in \mathbb{R}^+$.² The "diagonal" generators can also be deduced from the above ansatz and eq. (2.6). Note that the limit $\alpha \rightarrow \infty$ leads to $a = b$. The whole set reads

$$\begin{aligned} E_3^3 &= |b|^2 - X_1^1 + X_4^4 = \alpha + 2 - (n_\downarrow + n_\uparrow) & E_2^2 &= -X_2^2 - X_4^4 = n_\uparrow - 1 \\ E_1^1 &= -X_3^3 - X_4^4 = n_\downarrow - 1 & E_1^2 &= -c_\downarrow^\dagger c_\uparrow \\ E_2^1 &= -c_\uparrow^\dagger c_\downarrow & E_1^3 &= -\sqrt{\alpha} n_\uparrow c_\downarrow^\dagger - \sqrt{\alpha+1} (1 - n_\uparrow) c_\downarrow^\dagger \\ E_3^1 &= -\sqrt{\alpha} n_\uparrow c_\downarrow - \sqrt{\alpha+1} (1 - n_\uparrow) c_\downarrow & E_2^3 &= \sqrt{\alpha} n_\downarrow c_\uparrow^\dagger - \sqrt{\alpha+1} (1 - n_\downarrow) c_\uparrow^\dagger \\ E_3^2 &= \sqrt{\alpha} n_\downarrow c_\uparrow - \sqrt{\alpha+1} (1 - n_\downarrow) c_\uparrow \end{aligned} \quad (2.18)$$

The even sub-algebras are manifest: E_3^3 is the $\mathfrak{u}(1)$ -generator, and $E_{1,2}^{1,2}$ are the $\mathfrak{su}(2)$ generators.

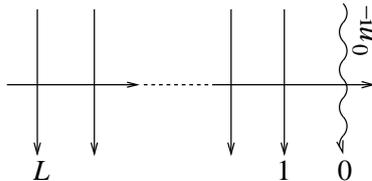
2.1.2 Construction of the lattice model

Having the relevant properties of the R -matrices at hand, one proceeds with the definition of a transfer matrix, from which the Hamiltonian is calculated as a logarithmic derivative.

The monodromy matrices

$$\begin{aligned} T(u) &= R_{a,L}^{(4,4)}(u) R_{a,L-1}^{(4,4)}(u) \dots R_{a,1}^{(4,4)}(u) R_{a,0}^{(4,3)}(u + iu_0) \\ \bar{T}(u) &= \bar{R}_{a,L}^{(4,4)}(u) \bar{R}_{a,L-1}^{(4,4)}(u) \dots \bar{R}_{a,1}^{(4,4)}(u) \bar{R}_{a,0}^{(4,3)}(u + iu_0) \end{aligned} \quad (2.19)$$

consist of sequences of R matrices, multiplied in (horizontal) auxiliary space. Note the shift by iu_0 on the zeroth lattice site, where the dimension of the (vertical) quantum space is reduced by one. This site shall be denoted as "impurity site". The shift is done by $iu_0 \in \mathbb{C}$, for reasons which will become clear later. Graphically, $T(u)$ is schematically depicted as



²The most general parameterization is $b = e^{i\phi_1} \cosh \gamma$, $a = e^{i\phi_2} \sinh \gamma$. However, the α -parameterization is convenient to distinguish different orders in the limit $\alpha \gg 1$.

The super-trace is called transfer matrix

$$\tau(u) = \text{str}_a T(u), \quad \bar{\tau}(u) = \text{str}_a \bar{T}(u) \quad (2.20)$$

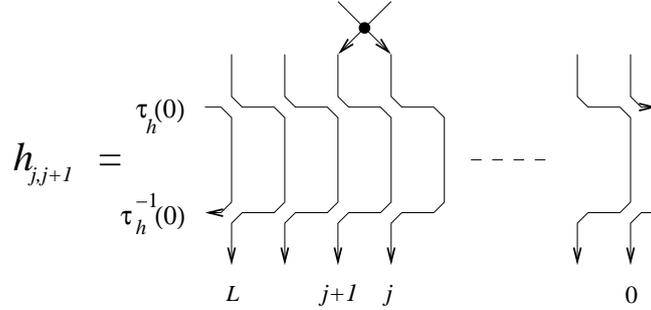
$$\ln[\tau\bar{\tau}](u) = \ln[\tau\bar{\tau}](0) + u \underbrace{[\tau^{-1}(0)\tau'(u) + \bar{\tau}^{-1}(0)\bar{\tau}'(u)]_{u=0}}_{=: \text{const. } H} + \mathcal{O}(u^2). \quad (2.21)$$

In the last line, the Hamiltonian was defined as logarithmic derivative of the two transfer matrices at zero spectral parameter. By scaling u , one is free to multiply the Hamiltonian by a constant factor.

Before evaluating eq. (2.21), let us shortly comment on the case $R_{a,0}^{(4,3)}(u) = 1_{a,0}$, ie. the absence of any impurity; we denote the corresponding quantities with a subscript h . This model has been extensively studied in [10, 18, 37]. $\tau_h(0)$ ($\bar{\tau}_h(0)$) is the right (left) shift operator, and

$$\ln \tau_h(0) = iP = -\ln \bar{\tau}_h(0), \quad (2.22)$$

where P is the generator of translations to the right. Following a nice trick due to [54], the Hamiltonian is derived graphically:



The figure shows the j th term of $[\tau_h^{-1}(0)\tau_h'(u)]_{u=0}$. For $u = 0$, the vertices decouple and, by taking the trace, give rise to the right shift operator $\tau_h(0)$. Upon taking the derivative with respect to u , a sum of L terms emerges, each one containing $R'_{j,j+1}$ for some j , $j = 1, \dots, L$. They are supplemented with $R_{j,j+1}(0)R_{j,j+1}(0) = 1$. One of these factors completes $\tau_h(0)$, the other "twists" $R'_{j,j+1}$. The dot in the figure symbolizes the derivative of $R_{j,j+1}$ with respect to u . Thus

$$H_h = \sum_{j=1}^L h_{j,j+1} \quad (2.23)$$

$$h_{j,j+1} = (\alpha + 1)D \frac{d}{du} \ln [R^{(4,4)}(u)]_{j,j+1}$$

In eq. (2.23), periodic boundary conditions $L + 1 \equiv 1$ are assumed. H_h is scaled by $D(\alpha + 1)$, D is a bandwidth parameter whose significance will become clear later.

In appendix A.2, we find:

$$\begin{aligned} h_{j,j+1} &= (\alpha + 1)D \left(\frac{2}{\alpha} (\check{P}_1)_{j,j+1} - \frac{2}{\alpha + 1} (\check{P}_3)_{j,j+1} \right) \\ &= -D \sum_{\tau} (c_{j,\tau}^\dagger c_{j+1,\tau} + c_{j+1,\tau}^\dagger c_{j,\tau}) e^{-\frac{\eta}{2}(n_{j,\bar{\tau}} + n_{j+1,\bar{\tau}})} \\ &\quad + U (n_{j,\uparrow} n_{j,\downarrow} + n_{j+1,\uparrow} n_{j+1,\downarrow}) + t_p \left(c_{j+1,\uparrow}^\dagger c_{j+1,\downarrow}^\dagger c_{j,\uparrow} c_{j,\downarrow} + c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger c_{j+1,\uparrow} c_{j+1,\downarrow} \right) \\ &\quad + D(n_j + n_{j+1}) - 2D, \quad (2.24) \\ U &= \frac{D}{\alpha} = t_p, \quad e^{-\eta} = \frac{\alpha + 1}{\alpha}; \quad \bar{\tau} = -\tau. \end{aligned}$$

This expression agrees with [10, 18, 37]. The dispersion relation of the free fermions is $|\epsilon(k)| \leq 4D$, such that the bandwidth is $4D$.

In the limit $\alpha \rightarrow \infty$,

$$\lim_{\alpha \rightarrow \infty} h_{j,j+1} =: h_{j,j+1}^{(ff)} = -D \sum_{\sigma} (c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger} c_{j,\sigma}) + D(n_j + n_{j+1} - 2), \quad (2.25)$$

which is the free-fermion hopping between sites j and $j+1$, including a shifted chemical potential and a shifted zero energy point. On the other hand one can show by a canonical transformation [10] that

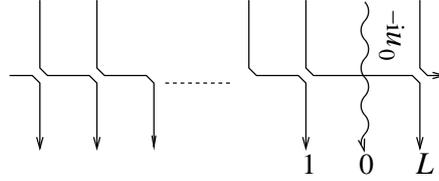
$$\lim_{\alpha \rightarrow 0} h_{j,j+1} = h_{j,j+1}^{tJ}$$

leads to the $t - J$ -model. In this work, we are interested in the weak coupling limit $\alpha \gg 1$.

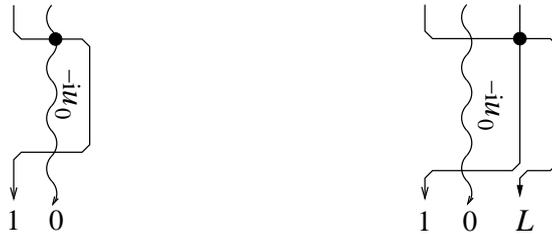
Due to $R_{a,0}^{(4,3)}$, H_h receives an impurity contribution H_I . It can be derived graphically. First observe that eq. (2.22) does no longer hold; but because of unitarity (2.12), one still has

$$\tau(0) = \bar{\tau}^{-1}(0).$$

The graphical translation of $\tau(0)$ is:



The changes induced by the impurity in comparison with the free host stemming from $\ln \tau'(0)$ are depicted as:



A vertex with a dot symbolizes the derivative with respect to the spectral parameter. The first term,

$$\sim R_{1,0}^{(3,4)}(-iu_0) \left[R_{1,0}^{(4,3)} \right]'(iu_0) = R_{1,0}^{-1(4,3)}(iu_0) \left[R_{1,0}^{(4,3)} \right]'(iu_0),$$

couple the impurity to the left neighboring site. The second term,

$$\sim R_{1,0}^{(3,4)}(-iu_0) \frac{h_{0L,1}}{D(\alpha+1)} R_{1,0}^{(4,3)}(iu_0) = R_{1,0}^{-1(4,3)}(iu_0) \left[R_{1,L}^{(4,4)} \right]'(0) R_{1,0}^{(4,3)}(iu_0),$$

is a three site coupling. Analogous terms, with L and 1 interchanged, are provided by $\ln \bar{\tau}'(0)$. The

inverse matrix $R^{-1(4,3)}$ is found by eq. (2.12). Thus the impurity contribution reads:

$$H_I = \frac{D(\alpha+1)}{2} \left[R_{1,0}^{-1(4,3)}(iu_0) \left[R_{1,0}^{(4,3)} \right]'(iu_0) + R_{1,0}^{-1(4,3)}(iu_0) \frac{h_{L,1}}{D(\alpha+1)} R_{1,0}^{(4,3)}(iu_0) - \frac{h_{L,1}}{D(\alpha+1)} + (L \leftrightarrow 1) \right] \quad (2.26)$$

$$= \frac{D(\alpha+1)}{2(u_0^2 + (\alpha/2 + 1)^2)} (-1)^{p[a]} [e_0]_b^a \left[[E_1]_a^b + (\alpha/2 + 1) \left(\frac{h_{1,L}}{D(\alpha+1)} [E_1]_a^b + [E_1]_a^b \frac{h_{1,L}}{D(\alpha+1)} \right) - iu_0 \left[[E_1]_a^b, \frac{h_{1,L}}{D(\alpha+1)} \right] + (-1)^{p[g](p[a]+p[b])+p[a]p[b]} [E_1]_g^b \frac{h_{1,L}}{D(\alpha+1)} [E_1]_a^g + (1 \leftrightarrow L) \right] \quad (2.27)$$

Note that in eq. (2.26), the host-contribution between sites L and 1 is subtracted; however, it is contained in the rest. In analogy to the host Hamiltonian, the spectral parameter u has been scaled by $D(\alpha+1)$, where D is a bandwidth parameter. Since H_I is derived from $\tau(u)$ and $\bar{\tau}(u)$, a factor $1/2$ has to be included.

Eq. (2.27) is conveniently evaluated upon fermionizing the $E_{1,L}$, e_0 . The fermionization of $[e_0]_b^a$ is done with the matrix Y , resulting from X , eq. (2.15) by deleting the first row and column,

$$Y = \left(\begin{array}{cc|cc} n_{d,\downarrow}(1-n_{d,\uparrow}) & -d_{\downarrow}^{\dagger}d_{\uparrow} & -d_{\downarrow}^{\dagger}(1-n_{d,\uparrow}) & \\ d_{\downarrow}d_{\uparrow}^{\dagger} & (1-n_{d,\downarrow})n_{d,\uparrow} & (1-n_{d,\downarrow})d_{\uparrow}^{\dagger} & \\ \hline -d_{\downarrow}(1-n_{d,\uparrow}) & (1-n_{d,\downarrow})d_{\uparrow} & (1-n_{d,\downarrow})(1-n_{d,\uparrow}) & \end{array} \right). \quad (2.28)$$

Horizontal and vertical lines separate fermionic and bosonic sectors. The boxes on the diagonal of Y contain the generators of $\mathfrak{su}(2)$, $\mathfrak{u}(1)$. Set $e_a^b = Y_a^b$, such that eqs. (2.14a), (2.14b) hold with grading $\{1, 1, 0\}$. As to the algebraic relations eq. (2.14a), (2.14b), that grading is equivalent to $\{0, 0, 1\}$, given by eq. (2.1).

The two matrices X , Y give the impurity Hamiltonian in the conventional, fermionized form. It contains the free fermion hopping in the host, host-host correlations and a host-impurity coupling. This coupling contains essentially two terms: A hybridization (i.e. particle hopping onto or off the impurity), due to $E_{1,2}^3 e_3^{1,2} + \text{h.c.}$, and a spin exchange, going back to $E_1^2 e_2^1 + \text{h.c.}$. These are the "leading" contributions in terms of powers of α . They are discussed in the ongoing.

Before, add external fields μ , h , by

$$H_{ex} = \frac{h}{2} \left[\sum_{j=1}^L (n_{j,\uparrow} - n_{j,\downarrow}) + (n_{d,\uparrow} - n_{d,\downarrow}) \right] - \mu \left[\sum_{j=1}^L n_j + \sum_{\tau} n_{d,\tau} (1 - n_{d,\bar{\tau}}) \right]. \quad (2.29)$$

Eqs. (2.23), (2.26), (2.29) define the whole Hamiltonian of the impurity model. In appendix A.2.1, it is shown that $H_h + H_I$ displays $\mathfrak{gl}(2|1)$ symmetry. H_{ex} breaks this symmetry.

Instead of being interested in the explicit form of the entire Hamiltonian, we want to simplify the problem along the following lines:

- i) α can be viewed as a coupling-parameter which tunes the correlations in the host and the host-impurity coupling. Our strategy is an asymptotical development for $\alpha \rightarrow \infty$, both of the Hamiltonian and of the resulting equations for the free energy. This means that we give all physical quantities f depending parametrically on α as

$$f(\alpha) = g(\alpha) + o(1/\alpha^{1+2\epsilon}) \Leftrightarrow \lim_{\alpha \rightarrow \infty} \alpha^{1+2\epsilon} [f(\alpha) - g(\alpha)] = 0. \quad (2.30)$$

$\epsilon \geq 0$ is restricted later. Instead of eq. (2.30) the notation $[f(\alpha) - g(\alpha)] \sim 1/\alpha^{1+2\epsilon}$ is common. Especially, eq. (2.30) permits to neglect contributions $\mathcal{O}(D/\alpha^{3/2})$. In this limit of weak coupling one distinguishes orders $\mathcal{O}(D)$ (free fermion hopping), $\mathcal{O}(D\alpha^{3/2}/(u_0^2 + \alpha^2))$ (hybridization), $\mathcal{O}(D/\alpha)$ (electron-electron-interaction in the host) and $\mathcal{O}(D\alpha/(u_0^2 + \alpha^2))$ (spin-spin-interaction between the impurity and the host),

$$D > D \frac{\alpha^{3/2}}{u_0^2 + \alpha^2} > \frac{D}{\alpha} \geq D \frac{\alpha}{u_0^2 + \alpha^2} > D \frac{\alpha^{1/2}}{u_0^2 + \alpha^2} > \frac{D}{\alpha^2}. \quad (2.31)$$

The bandwidth D is absorbed by introducing electronic density operators of the host (rather than particle operators, see item iv)). The last two orders in eq. (2.31) are next-leading contributions of the impurity and the host, respectively. They are neglected. The relation between the third and fourth term in eq. (2.31) is not given uniquely, it depends on u_0 : One expects $u_0 \sim \alpha^{1+\epsilon}$, with $1/4 > \epsilon \geq 0$. If $\epsilon < 0$, u_0 would be dominated by α and its introduction is meaningless. For $\epsilon = 0$, host-host-correlations are exactly of the same order as spin-spin-interaction on the impurity site. In any case, from eq. (2.30) it ensues that the leading order of spin-exchange between host and impurity is retained. So it is sufficient to include only the leading terms of the $E_{1,L}$, eqs. (2.18). The resulting Hamiltonian will be given explicitly below.

- ii) The non-occupied sector of the impurity has a weight $\sim 4D\alpha^{-2\epsilon}$. This gives the one particle-energy of the impurity $\sim 4D - \mu$. The host's one-particle energy is $\sim 2D(\cos k + 1) - \mu$. Consequently, $0 < \mu < 4D$, $\mu \sim D$, is restricted such that the band is neither completely empty nor completely filled. On the other hand, zero occupation of the impurity is not suppressed (as would be the case for $\mu > 4D$). However, one finds a canonical transformation which eliminates hybridization, i.e. the operators which cause transitions between single and zero occupation. Therefore, the Hamiltonian is written in Fourier space. The canonical transformation induces correction terms to the original Hamiltonian of order $\mathcal{O}(1/\alpha^{1+4\epsilon})$. $\epsilon = 0$ yields a renormalized spin exchange coupling, $\epsilon > 0$ implies that these terms can be neglected. Furthermore, the fifth order in eq. (2.31) is also given by particle-hopping between the impurity and the host. Principally, it may equally be eliminated by a suitable transformation (not given explicitly), which would yield corrections $\mathcal{O}(1/\alpha^{3+4\epsilon})$. Thus $0 \leq \epsilon < 1/2$ is the permitted range of ϵ . Excitations (i.e. spin-flipping) of the impurity solely arise for single occupation (otherwise, the impurity contribution is constant). Our aim is to separate this excitation spectrum of $\mathcal{O}(1/\alpha^{1+2\epsilon})$ from the zero occupation constant $\sim D$.
- iii) From the exact solution presented in the next section it follows that D is arbitrarily large: It is much larger than the spin exchange coupling and $T \ll D$ always is implicit. This prescription is meaningful only for a linearized host spectrum.
- iv) The linear dispersion approximation involves arbitrary wavelengths in Fourier space. It thus goes in hand with the continuum limit, which blurs the microscopic details of the impurity-host interaction and yields a point-like spin exchange. The continuum limit gives a meaning to the *a priori* arbitrary scale D . It is found that $D \sim 1/a_0$, where a_0 is the lattice constant.
- v) u_0, D, α are auxiliary parameters to construct the lattice model; in the equations for physical quantities (here thermodynamic equilibrium functions), it is possible to combine them to a scale-invariant constant. This constant is found from the exact solution. It cannot be derived from the Hamiltonian, but only in the equation for the free energy.

Actually, the discovery of the constant mentioned in item v) motivates steps i)-iv). In the rest of this section, items i)-iv) are carried out successively. Item v) is elucidated in the next section.

Let us calculate the different terms in eq. (2.27), consequently neglecting terms of higher order than $D \cdot \mathcal{O}(1/\alpha^{1+2\epsilon})$, in the sense of eq. (2.30). For the ease of notation, use the shorthand

$$h_{1,L}^{(ff)} =: D\hat{h} \quad (2.32)$$

The following relations are helpful to evaluate eq. (2.27):

$$\begin{aligned} \hat{h}c_{1,\uparrow} &= -c_{1,\downarrow}^\dagger c_{L,\downarrow} c_{1,\uparrow} - c_{L,\downarrow}^\dagger c_{1,\downarrow} c_{1,\uparrow} - c_{1,\uparrow}^\dagger c_{L,\uparrow} c_{1,\uparrow} - 2c_{1,\uparrow} + n_L c_{1,\uparrow} + n_{1,\downarrow} c_{1,\uparrow} \\ c_{1,\uparrow} \hat{h} &= \hat{h}c_{1,\uparrow} - c_{L,\uparrow} + c_{1,\uparrow} \\ \hat{h}c_{1,\downarrow}^\dagger c_{1,\uparrow} &= -c_{L,\downarrow}^\dagger c_{1,\downarrow} c_{1,\uparrow} - c_{1,\uparrow}^\dagger c_{L,\uparrow} c_{1,\downarrow}^\dagger c_{1,\uparrow} - c_{1,\downarrow}^\dagger c_{1,\uparrow} + n_L c_{1,\downarrow}^\dagger c_{1,\uparrow} \\ c_{1,\downarrow}^\dagger c_{1,\uparrow} \hat{h} &= \hat{h}c_{1,\downarrow}^\dagger c_{1,\uparrow} + c_{L,\downarrow}^\dagger c_{1,\uparrow} - c_{1,\downarrow}^\dagger c_{L,\uparrow} \\ c_{1,\uparrow} \hat{h} c_{1,\downarrow}^\dagger &= -\hat{h}c_{1,\downarrow}^\dagger c_{1,\uparrow} - c_{1,\downarrow}^\dagger c_{1,\uparrow} \\ \hat{h}n_{\uparrow,1} &= -c_{1,\downarrow}^\dagger c_{L,\downarrow} c_{1,\uparrow}^\dagger c_{1,\uparrow} - c_{L,\downarrow}^\dagger c_{1,\downarrow} c_{1,\uparrow}^\dagger c_{1,\uparrow} - c_{L,\uparrow}^\dagger c_{\uparrow,1} - n_{\uparrow,1} + n_L n_{\uparrow,1} + n_{\uparrow,1} n_{\downarrow,1} \\ n_{\uparrow,1} \hat{h} &= \hat{h}n_{\uparrow,1} + c_{L,\uparrow}^\dagger c_{\uparrow,1} - c_{\uparrow,1}^\dagger c_{L,\uparrow} \\ c_{\uparrow,1} \hat{h} c_{\uparrow,1}^\dagger &= -\hat{h}n_{1,\uparrow} + \hat{h} + c_{1,\uparrow}^\dagger c_{L,\uparrow} - n_{\uparrow,1} + 1 \\ c_{1,\uparrow}^\dagger \hat{h} c_{1,\uparrow} &= n_{1,\uparrow} \hat{h} - n_{1,\uparrow} + c_{1,\uparrow}^\dagger c_{L,\uparrow} . \end{aligned}$$

First note that the commutator $\left[[E_1]_a^b, \hat{h}_{1,L} \right] + (1 \leftrightarrow L)$ in eq. (2.27) vanishes. Set

$$u_0 := v_0/2, v_0 \in \mathbb{R} . \quad (2.33)$$

It is convenient to define a coupling constant

$$J_\alpha = \frac{2\alpha}{v_0^2 + \alpha^2} > 0 . \quad (2.34)$$

The leading order in H_I is given by the coefficient of $[e_0]_3^3$, since it involves

$$E_3^3 = \alpha + 2 - n .$$

Then the coefficient of $[e_0]_3^3$ is given by

$$\begin{aligned} &-DJ_\alpha \left(\alpha + 2 - n_1 + (\alpha + 2)\hat{h} - \frac{1}{2} \left(\hat{h}n_1 + n_1\hat{h} \right) \right. \\ &\quad \left. - [E_1]_3^3 \frac{\hat{h}}{\alpha + 1} [E_1]_3^3 - [E_1]_2^3 \frac{\hat{h}}{\alpha + 1} [E_1]_3^2 - [E_1]_1^3 \frac{\hat{h}}{\alpha + 1} [E_1]_3^1 + (1 \leftrightarrow L) \right) \\ &= -DJ_\alpha \left(\alpha + 2 - n_1 - 2\hat{h} + \frac{1}{2} \left(\hat{h}n_1 + n_L\hat{h} \right) - c_{\uparrow,L}^\dagger \hat{h}c_{\uparrow,L} - c_{\downarrow,L}^\dagger \hat{h}c_{\downarrow,L} + (1 \leftrightarrow L) \right) \\ &= -DJ_\alpha 2 \left(\alpha + 2 - 2\hat{h} - c_{1,\uparrow}^\dagger c_{L,\uparrow} - c_{1,\downarrow}^\dagger c_{L,\downarrow} - c_{L,\uparrow}^\dagger c_{1,\uparrow} - c_{L,\downarrow}^\dagger c_{1,\downarrow} \right) \\ &=: -DJ_\alpha 2 (\alpha + F_{1,L}) . \end{aligned}$$

In the last equation, all terms $\mathcal{O}(1)$ in the bracket on the rhs have been summarized in an operator $F_{1,L}$.

Consider the coefficient of $[e_0]_1^1 = n_{d,\downarrow}(1 - n_{d,\uparrow})$ in eq. (2.27).

$$\begin{aligned} DJ_\alpha \left([E_1]_1^1 + \frac{1}{2} \left(\hat{h} [E_1]_1^1 + [E_1]_1^1 \hat{h} \right) + [E_1]_3^1 \frac{\hat{h}}{\alpha+1} [E_1]_1^3 + (1 \leftrightarrow L) \right) \\ = DJ_\alpha \left(c_{\downarrow,1}^\dagger c_{\downarrow,L} + c_{\downarrow,L}^\dagger c_{\downarrow,1} \right) \end{aligned}$$

The term with $[e_0]_2^2$ is obtained from the preceding one by the spin-flip operation.

Concentrating on the off-diagonal elements, one finds for the contribution of $[e_0]_1^3 = -d_{d,\downarrow}^\dagger (1 - n_{d,\uparrow})$:

$$\begin{aligned} DJ_\alpha \sqrt{\alpha} \left[[E_1]_3^1 + \frac{1}{2} \left(\hat{h} [E_1]_3^1 + [E_1]_3^1 \hat{h} \right) - [E_1]_3^1 \frac{\hat{h}}{\alpha+1} [E_1]_3^3 + (1 \leftrightarrow L) \right] \\ = -DJ_\alpha \sqrt{\alpha} (c_{1,\downarrow} + c_{L,\downarrow}) \end{aligned}$$

The analogous expression for $[e_0]_2^3 = -d_{d,\uparrow}^\dagger (1 - n_{d,\downarrow})$ follows from spin-flipping.

Finally, consider the coefficient of $[e_0]_1^2 = -d_{\downarrow}^\dagger d_{\uparrow}$.

$$\begin{aligned} DJ_\alpha \left[[E_1]_2^1 + \frac{1}{2} \left(\hat{h} [E_1]_2^1 + [E_1]_2^1 \hat{h} \right) + [E_1]_3^1 \frac{\hat{h}}{\alpha+1} [E_1]_2^3 + (1 \leftrightarrow L) \right] \\ = -DJ_\alpha \left(c_{1,\downarrow}^\dagger c_{L,\uparrow} + c_{L,\downarrow}^\dagger c_{1,\uparrow} \right) \end{aligned}$$

All remaining terms are obtained by hermitian conjugating the off-diagonal elements.

The entire impurity contribution reads explicitly up to the relevant order:

$$\begin{aligned} H_I = & -\mu \sum_{\tau} n_{d,\tau} (1 - n_{d,\bar{\tau}}) + \frac{\hbar}{2} (n_{d,\uparrow} - n_{d,\downarrow}) - 2DJ_\alpha (1 - n_d + n_{d,\uparrow} n_{d,\downarrow}) (\alpha + F_{1,L}) \\ & - DJ_\alpha \sqrt{\alpha} \sum_{\tau} \left[d_{\tau}^\dagger (1 - n_{d,\bar{\tau}}) (c_{L,\tau} + c_{1,\tau}) - d_{\tau} (1 - n_{d,\bar{\tau}}) (c_{L,\tau}^\dagger + c_{1,\tau}^\dagger) \right] \\ & + DJ_\alpha \sum_{\tau} n_{d,\tau} (1 - n_{d,\bar{\tau}}) \left(c_{L,\tau}^\dagger c_{1,\tau} + c_{1,\tau}^\dagger c_{L,\tau} \right) \\ & + DJ_\alpha \sum_{\tau} d_{\tau}^\dagger d_{\bar{\tau}} \left(c_{L,\bar{\tau}}^\dagger c_{1,\tau} + c_{1,\bar{\tau}}^\dagger c_{L,\tau} \right) + \mathcal{O}(D/\alpha^{3/2}) . \end{aligned} \quad (2.35)$$

Spin exchange occurs only across the impurity, upon hopping $L \leftrightarrow 1$. For completeness, the host Hamiltonian is given neglecting orders $\mathcal{O}(D/\alpha^{3/2})$.

$$\begin{aligned} H_h/D = & 2 \sum_{j=1}^L n_j - 2 - \sum_{j=1}^L \sum_{\tau} \left(c_{j,\tau}^\dagger c_{j+1,\tau} + c_{j+1,\tau}^\dagger c_{j,\tau} \right) \left[1 + \frac{1}{2\alpha} (n_{j,\bar{\tau}} + n_{j+1,\bar{\tau}}) \right] \\ & + \frac{2}{\alpha} \sum_{j=1}^L n_{j,\uparrow} n_{j,\downarrow} + \frac{1}{\alpha} \sum_{j=1}^L \left(c_{j+1,\uparrow}^\dagger c_{j+1,\downarrow}^\dagger c_{j,\uparrow} c_{j,\downarrow} + c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger c_{j+1,\uparrow} c_{j+1,\downarrow} \right) + \mathcal{O}(D/\alpha^{3/2}) . \end{aligned} \quad (2.36)$$

The whole Hamiltonian

$$H = H_h + H_I + H_{ex} \quad (2.37)$$

describes a correlated host interacting with an impurity spin via anti-ferromagnetic spin exchange and hybridization with the host. In the host, particle hopping $\mathcal{O}(D)$ dominates the electron-electron

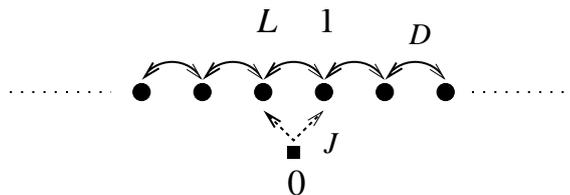


Figure 2.1: The host interacting with the impurity. The impurity site 0 is not included in the hopping of the host. D and J are the hopping amplitude and coupling strength, respectively.

interaction $\mathcal{O}(D/\alpha)$ by a factor of α ; the latter will be seen to be absorbed in a rescaled one-particle spectrum. On the impurity site, there is one $\mathcal{O}(D)$ contribution $\propto (1 - n_d + n_{d,\uparrow}n_{d,\downarrow})$. Next-leading terms cause the host-impurity-coupling. The model eq. (2.37) is already of interest on its own. It is the sum of the Fano-Anderson model

$$H_F = H_h^{(ff)} + \sum_{k,\tau} V_k (d_\tau^\dagger c_{k,\tau} + c_{k,\tau}^\dagger d_\tau) \quad (2.38)$$

with a spin exchange term (in eq. (2.38) host operators are Fourier transformed). We will show that by suppressing charge fluctuations on the impurity site, the Kondo model results.

The operators acting on the impurity site have been fermionized using the matrix eq. (2.28). These operators are annihilated by the doubly occupied state. That is, double occupation on the impurity site is excluded from the beginning.

By a canonical transformation, transitions between the singly and not occupied sectors can be eliminated. This transformation is very similar to the Schrieffer-Wolf transformation [81] connecting the Anderson model H_A (that is Fano-Anderson model with on-site Coulomb repulsion U on the impurity site) to the Kondo model,

$$H_A = H_h^{(ff)} + \epsilon_d n_d + \sum_{k,\tau} V_k (d_\tau^\dagger c_{k,\tau} + c_{k,\tau}^\dagger d_\tau) - U n_{d,\uparrow} n_{d,\downarrow}, \quad U > 0. \quad (2.39)$$

The essential lesson to be learned is that in the limit $U \gg |V_k|$, a localized magnetic moment occurs on the impurity site. Since in our approach, double occupation of the impurity site is excluded from the beginning, it is quite natural to discover a "bare" spin exchange between host and impurity; the canonical transformation is expected to "dress" the value of the coupling constant.

The transformation which eliminates zero occupation is conveniently done in Fourier space; the chemical potential terms are included in H_h , H_I and $h = 0$ is set for the moment. The discrete Fourier variable k takes L discrete values

$$k = -\pi + n \frac{2\pi}{L}, \quad n = 1, \dots, L. \quad (2.40)$$

The Fourier representation of the Hamiltonian is found to be:

$$\begin{aligned}
c_{j,\tau}^\dagger &= \frac{1}{\sqrt{L}} \sum_{k=-\pi}^{\pi} c_{k,\tau}^\dagger e^{ikj} \\
H_h &= D \left\{ \sum_k \sum_{\tau} \epsilon_k c_{k,\tau}^\dagger c_{k,\tau} - 2 \right. \\
&\quad + \frac{2}{L\alpha} \sum_{Q,q,q'} \left[\sum_{\tau} \cos \frac{Q}{2} \cos \left(q + \frac{Q}{2} \right) c_{q+Q,\tau}^\dagger c_{q,\tau} c_{q'-Q,\bar{\tau}}^\dagger c_{q',\bar{\tau}} \right. \\
&\quad \left. \left. + c_{q,\uparrow}^\dagger c_{q+Q,\uparrow} c_{q'-Q,\downarrow}^\dagger c_{q',\downarrow} - \cos(q+q') c_{q+Q,\uparrow}^\dagger c_{q,\uparrow} c_{q'-Q,\downarrow}^\dagger c_{q',\downarrow} \right] \right\} \quad (2.41)
\end{aligned}$$

$$D\epsilon_k = 2D(\cos k + 1) - \mu \quad (2.42)$$

$$\begin{aligned}
H_I &= -2DJ_\alpha(1 - n_{d,\downarrow})(1 - n_{d,\uparrow})(\alpha + F_{1,L}) - \mu \sum_{\tau} n_{d,\tau}(1 - n_{d,\bar{\tau}}) \\
&\quad + J_\alpha \alpha^{1/2} \frac{D}{\sqrt{L}} \sum_{k,\tau} \sqrt{l} (M_k d_\tau^\dagger c_{k,\tau} + M_k^* c_{k,\tau}^\dagger d_\tau) (1 - n_{d,\bar{\tau}}) \\
&\quad + J_\alpha \frac{D}{L} \sum_{\tau,k,k'} l N_{k,k'} \left[n_{d,\tau}(1 - n_{d,\bar{\tau}}) c_{k,\tau}^\dagger c_{k',\tau} + d_\tau^\dagger d_{\bar{\tau}} c_{k,\bar{\tau}}^\dagger c_{k',\tau} \right] \quad (2.43)
\end{aligned}$$

$$M_k = -\frac{1}{\sqrt{l}} (1 + e^{ik})$$

$$N_{k,k'} = \frac{1}{l} (e^{-ik'} + e^{ik}) .$$

The k -dependence of the coupling parameters M, N results from periodic boundary conditions:

$$c_L^\dagger c_1 + c_1^\dagger c_L = \frac{1}{L} \sum_{k,k'} (e^{-ik'} + e^{ik}) c_k^\dagger c_{k'} . \quad (2.44)$$

Without the impurity, there are L lattice sites, separated by unit spacing 1. The impurity alters the corresponding k values, eq. (2.40), but in the limit $L \rightarrow \infty$, this change is negligible. Furthermore, one more lattice site (the impurity) is introduced, without being included in the hopping of the host, fig. 2.1.

The periodic boundary condition $L + 1 \equiv 1$ is kept. The leading term in eq. (2.43) is

$$H_I^{(0)} = -\mu \sum_{\tau} n_{d,\tau}(1 - n_{d,\bar{\tau}}) - 2J_\alpha \alpha (1 - n_{d,\downarrow})(1 - n_{d,\uparrow}) . \quad (2.45)$$

This Hamiltonian does not couple the impurity to the host, only a free spin rests. The challenge in the thermodynamic description is to separate the impurity's contribution from the bulk and to keep the spin-flip terms, while at the same time realizing a free host.

In view of the continuum limit which is done later, one introduces the lattice spacing a_0 , so that $l = L \cdot a_0 = \text{const}$. Let $D = 1/a_0$, so that the chemical potential scales as $D, \mu \sim D$.

Denote the hybridization term in eq. (2.43) by $H^{(1)}$.

$$H^{(1)} := J_\alpha \sqrt{\alpha D} \sum_{k,\tau} (M_k d_\tau^\dagger c_{k,\tau} + M_k^* c_{k,\tau}^\dagger d_\tau) . \quad (2.46)$$

The rest $H - H^{(1)} =: H^{(0)}$. The canonical transformation consists in finding an operator A such that

$$[H^{(0)}, A] = H^{(1)} . \quad (2.47)$$

Then the transformed Hamiltonian $\bar{H} = e^A H e^{-A}$ does not contain linear terms in A :

$$\bar{H} = e^A H e^{-A} = H^{(0)} + \frac{1}{2} [A, H^{(1)}] + \frac{1}{3} [A, [A, H^{(1)}]] + \frac{1}{8} [A, [A, [A, H^{(1)}]]] \dots \quad (2.48)$$

Before writing A explicitly, consider orders of magnitude.

$$\begin{aligned} H^{(0)} &\sim D \left(\epsilon_k + \epsilon_d + \frac{1}{\alpha} \right), \quad D\epsilon_d = -\mu + 2\alpha J_\alpha D \\ H^{(1)} &\sim J_\alpha \sqrt{\alpha D} \\ \Rightarrow A &\sim J_\alpha \sqrt{\frac{\alpha}{D}} \frac{1}{\epsilon_k - \epsilon_d + 1/\alpha} \\ \Rightarrow [A, H^{(1)}] &\sim \frac{J_\alpha^2 \alpha}{(\epsilon_k - \epsilon_d)} \end{aligned} \quad (2.49)$$

Use has been made of eq. (2.47). Eq. (2.49) constitutes the first correction to $H^{(0)}$. It depends crucially on the relation between v_0 and α . At this stage, this relation is undetermined; one expects $v_0 \sim \alpha^{1+\epsilon}$. For $\epsilon > 0$, eq. (2.49) is $\mathcal{O}(1/\alpha^{1+4\epsilon})$ and negligible, if only terms $\mathcal{O}(1/\alpha^{1+2\epsilon})$ are retained in the Hamiltonian. For $\epsilon = 0$, eq. (2.49) is of the same order as the "bare" spin exchange. ϵ undetermined here, we proceed with the evaluation of the canonical transformation.

Higher orders in eq. (2.49) are not accounted for in the definition of A , since they give corrections $\mathcal{O}(J_\alpha^2) = \mathcal{O}(1/\alpha^{2+4\epsilon})$ to $H^{(0)}$. Thus the definition (2.47) can be simplified further,

$$[H_h^{(ff)} + H_I^{(0)}, A] = H^{(1)}. \quad (2.50)$$

This defining property of A does neither involve correlations in the host nor the spin exchange interaction. Furthermore, it suffices to include the first correction to $H^{(0)}$ in eq. (2.48),

$$\bar{H} = e^A H e^{-A} \approx H^{(0)} + \underbrace{\frac{1}{2} [A, H^{(1)}]}_{=: H^{(2)}}. \quad (2.51)$$

The problem of finding A from eq. (2.50) has been solved by Schrieffer and Wolf, [81], in the Anderson model eq. (2.39). In our case, A has a similar form to that given in [81]:

$$A = J_\alpha \sqrt{\frac{\alpha}{D}} \sum_{k,\tau} \frac{1}{\epsilon_d - \epsilon_k} (M_k d_\tau^\dagger c_{k,\tau} - M_k^* c_{k,\tau}^\dagger d_\tau) (1 - n_{d,\bar{\tau}}).$$

This is the operator we are looking for, because

$$\begin{aligned} \left[\sum_{k,\tau} D \epsilon_k c_{k,\tau}^\dagger c_{k,\tau}, A \right] &= J_\alpha \sqrt{D\alpha} \sum_{k,\tau} \frac{-\epsilon_k}{\epsilon_d - \epsilon_k} (1 - n_{d,\bar{\tau}}) \left(M_k d_\tau^\dagger c_{k,\tau} + M_k^* c_{k,\tau}^\dagger d_\tau \right) \\ \left[\sum_{\tau} D \epsilon_d n_{d,\tau}, A \right] &= J_\alpha \sqrt{D\alpha} \sum_{k,\tau} \frac{\epsilon_d}{\epsilon_d - \epsilon_k} (1 - n_{d,\bar{\tau}}) \left(M_k d_\tau^\dagger c_{k,\tau} + M_k^* c_{k,\tau}^\dagger d_\tau \right) \\ [n_{d,\uparrow} n_{d,\downarrow}, A] &= 0. \end{aligned}$$

The sum gives $H^{(1)}$.

The resultant Hamiltonian is $H = H^{(0)} + H^{(2)}$, $H^{(2)}$ being defined in eq. (2.51). The commutator

$$\begin{aligned} & \left[(1 - n_{d,\bar{\tau}}) d_{\tau}^{\dagger} c_{k,\tau} - c_{k,\tau}^{\dagger} (1 - n_{d,\bar{\tau}}) d_{\tau}, (1 - n_{d,\bar{\tau}'}) d_{\tau'}^{\dagger} c_{k',\tau} + c_{k',\tau'}^{\dagger} (1 - n_{d,\bar{\tau}'}) d_{\tau'} \right] \\ & = 2\delta_{k,k'} \delta_{\tau,\tau'} (1 - n_{d,\bar{\tau}}) n_{d,\tau} - (1 - n_{d,\bar{\tau}}) \delta_{\tau,\tau'} \left(c_{k',\tau}^{\dagger} c_{k,\tau} + c_{k,\tau}^{\dagger} c_{k',\tau'} \right) \\ & \quad - (1 - \delta_{\tau,\tau'}) d_{\tau}^{\dagger} d_{\bar{\tau}} \left(c_{k',\tau}^{\dagger} c_{k,\bar{\tau}} + c_{k,\bar{\tau}}^{\dagger} c_{k',\tau'} \right). \end{aligned}$$

Thus three contributions are identified (note the factor 1/2 in eq. (2.51)):

$$H^{(2)} = H_d + H_{fm} + H_{pot} \quad (2.52a)$$

$$H_d = J_{\alpha}^2 \alpha \epsilon_d^{(2)} \sum_{\tau} (1 - n_{d,\bar{\tau}}) n_{d,\tau}, \quad \epsilon_d^{(2)} := \sum_k \frac{|M_k|^2}{\epsilon_d - \epsilon_k} \quad (2.52b)$$

$$H_{sp} = -\frac{J_{\alpha}^2 \alpha}{2} \sum_{\tau, k, k'} d_{\tau}^{\dagger} d_{\bar{\tau}} J_{k,k'} c_{k',\bar{\tau}}^{\dagger} c_{k,\tau} \quad (2.52c)$$

$$H_{pot} = -\frac{J_{\alpha}^2 \alpha}{2} \sum_{k, k', \tau} J_{k,k'} (1 - n_{d,\bar{\tau}}) c_{k',\tau}^{\dagger} c_{k,\tau} \quad (2.52d)$$

$$J_{k,k'} = \frac{M_k M_{k'}^*}{\epsilon_d - \epsilon_k} + \frac{M_k^* M_{k'}}{\epsilon_d - \epsilon_{k'}}.$$

$H^{(2)} \sim J_{\alpha}^2 \alpha$, as expected. Estimate $\epsilon_d^{(2)}$:

$$\epsilon_d^{(2)} = (v_0^2 + \alpha^2) \sum_k \frac{2 \cos k + 2}{4\alpha^2 - (v_0^2 + \alpha^2)(2 \cos k + 2)} \quad (2.53)$$

Consider the case $\epsilon = 0$ and assume

$$v_0^2 \sim \alpha^2 (1 - \delta) \lesssim \alpha^2, \quad 0 < \delta < 1. \quad (2.54)$$

Then one continues by writing eq. (2.53) as an integral over the energy ($\epsilon(k) = 2 \cos k + 2$):

$$\begin{aligned} \epsilon_d^{(2)} & = -\frac{L}{\pi} (2 - \delta) \int_{-2}^2 \frac{\epsilon}{4 - (2 - \delta)\epsilon} \frac{1}{\sqrt{1 - \epsilon^2/4}} d\epsilon \\ & = L \frac{1}{4 - \delta} \left(1 - \frac{2}{\sqrt{\delta(4 - \delta)}} \right) < 0 \end{aligned} \quad (2.55)$$

The integral can be done since v_0 is restricted by eq. (2.54). It is negative and finite. The pre-factor L in eq. (2.55) is absorbed in the continuum limit, see below.

H_d shifts ϵ_d by $\epsilon_d^{(2)}$. It can be absorbed by a redefinition of μ , which is small: μ itself is $\mathcal{O}(D)$, and D may be arbitrarily large, so H_d will not be mentioned in the following. H_{pot} introduces a potential scattering of host particles only. It is of the same order as correlations in the host. In the next section we will see that these correlations can be summarized in order $\mathcal{O}(1/\alpha)$ into a redefinition of the Fermi velocity, a one-particle quantity. So neither H_{pot} is written down in the ongoing. Finally, eq. (2.52c) constitutes an anti-ferromagnetic spin exchange term, according to the sign of $\epsilon_d^{(2)}$. It enhances the coupling which is present from the beginning. The renormalized spin exchange constant differs from the bare exchange constant merely by a pre-factor.

Note that if $v_0 \sim \alpha^{1+\epsilon}$, the sum in eq. (2.53) would become a sum over unity. However, the pre-factor $J_\alpha^2 \sim 1/\alpha^{1+4\epsilon}$ of the corrections eq. (2.52) is subleading in the sense of eq. (2.30).

In the following, the coupling - either J_α multiplied by some number if $\epsilon = 0$ or J_α itself if $\epsilon > 0$ - is denoted by J .

Once the transformation has been carried out, the impurity operator does not contain any hybridization in the relevant order between the singly and not occupied impurity site. Single occupation on the impurity site gets a weight comparable to zero occupation by scaling $\mu \sim D$ without filling the conduction band completely, $0 < \mu < 4D$. Thus zero occupation cannot be eliminated, but there are no transitions between zero and single occupation on the impurity site.

In the ongoing, only the subspace with $\langle n_d \rangle = 1$ is considered, since the subspace with $\langle n_d \rangle = 0$ only yields an additive constant contribution.

Spin exchange between host and impurity is $\mathcal{O}(J) \ll D$. This interaction is important for electrons with energy near the Fermi edge, $k = k_F + \Delta k$. It is most important if the Fermi sea is well populated,

$$T, h \ll D. \quad (2.56)$$

The linearization of the conduction band is worked out in the following, continuing with eq. (2.42).

The Fermi point $k_F = \frac{\pi}{2}N/L$ is taken away from half-filling, zero and complete band occupation (in the two latter cases a linearization would be meaningless). In the ground state, linearizing the dispersion $\epsilon(k) = 2 \cos k$,

$$\langle c_{k,\tau}^\dagger c_{k,\tau} \rangle_0 = \theta(-\nu k_\nu - k_F), \nu = \pm. \quad (2.57)$$

$\langle \dots \rangle_0$ is the expectation in the ground state. The handedness ν is plus (minus) for particles moving to the right (left). Note that ν and k are independent variables in the summations, and Q may take values $Q = 0, \pm 2k_F$. To avoid divergences due to the unbounded linear spectrum, operator products are normal ordered:

$$:c_{k,\nu,\tau}^\dagger c_{k,\nu',\tau'}: = c_{k,\nu,\tau}^\dagger c_{k,\nu',\tau'} - \langle c_{k,\nu,\tau}^\dagger c_{k,\nu',\tau'} \rangle_0.$$

Furthermore, let $f(q)$, $g(q')$ be operator-valued functions of the c^\dagger , c . Then

$$\sum_{q,q'} f(q)g(q') = \sum_{q,q'} f(\pm k_F)g(\pm k_F) + \mathcal{O}((q - k_F)^2).$$

The linear terms in $(q - k_F)$, $(q' - k_F)$ cancel since the q, q' -summations are independent. The quadratic order is neglected.

Apart from the chemical potential term, eqs. (2.41), (2.43) are written as

$$\begin{aligned} H_h/(2D) &= \sum_{\nu,k,\tau} (\cos k_F + 1 + \nu k \sin k_F) :c_{k,\nu,\tau}^\dagger c_{k,\nu,\tau}: \\ &+ \frac{1}{L\alpha} \sum_{q,q',\nu} \left[\sum_{\tau} \cos k_F \left(:n_{q,\nu,\tau} n_{q',\nu,\bar{\tau}}: + :n_{q,\nu,\tau} n_{q',\bar{\nu},\bar{\tau}}: + :c_{q,\bar{\nu},\tau}^\dagger c_{q,\nu,\tau} c_{q',\nu,\bar{\tau}}^\dagger c_{q',\bar{\nu},\bar{\tau}}: \right) \right. \\ &+ :n_{q,\nu,\uparrow} n_{q',\nu,\downarrow}: + :n_{q,\nu,\uparrow} n_{q',\bar{\nu},\downarrow}: + :c_{q,\bar{\nu},\uparrow}^\dagger c_{q,\nu,\uparrow} c_{q',\bar{\nu},\downarrow}^\dagger c_{q',\nu,\downarrow}: + :c_{q,\bar{\nu},\uparrow}^\dagger c_{q,\nu,\uparrow} c_{q',\nu,\downarrow}^\dagger c_{q',\bar{\nu},\downarrow}: \\ &- \cos 2k_F (:n_{q,\nu,\uparrow} n_{q',\nu,\downarrow}: + :c_{q,\bar{\nu},\uparrow}^\dagger c_{q,\nu,\uparrow} c_{q',\bar{\nu},\downarrow}^\dagger c_{q',\nu,\downarrow}:) - :n_{q,\nu,\uparrow} n_{q',\bar{\nu},\downarrow}: \\ &\left. - :c_{q,\bar{\nu},\uparrow}^\dagger c_{q,\nu,\uparrow} c_{q',\nu,\downarrow}^\dagger c_{q',\bar{\nu},\downarrow}: \right] \quad (2.58a) \end{aligned}$$

$$\begin{aligned} H_I &= \frac{J}{l} \sum_{q,q',\nu,\tau} 2 \cos k_F \left[\left(:c_{k,\nu,\tau}^\dagger c_{k',\nu,\bar{\tau}}: + :c_{k,\nu,\tau}^\dagger c_{k',\bar{\nu},\bar{\tau}}: \right) d_\tau^\dagger d_\tau \right. \\ &\left. + \left(:c_{k,\nu,\tau}^\dagger c_{k',\nu,\tau}: + :c_{k,\nu,\tau}^\dagger c_{k',\bar{\nu},\bar{\tau}}: \right) n_{d,\tau} (1 - n_{d,\bar{\tau}}) \right]. \quad (2.58b) \end{aligned}$$

$\bar{\nu} = -\nu$ and $\bar{\tau} = -\tau$. Terms of the form $i \sum_{q,q',\nu,\tau,\tau'} \nu \sin k_F \left(c_{k,\nu,\tau}^\dagger c_{k',\nu,\tau'} + c_{k,\nu,\tau}^\dagger c_{k',\nu,\tau'} \right)$ are omitted; these are current-like contributions which are negligible in the linear-dispersion-limit considered here. The potential scattering eq. (2.52d) can be treated in a similar manner; this is not done explicitly since it does not give more insight.

Generally speaking, the interaction terms are of forward and backward scattering type. Umklapp scattering is not allowed since k_F is chosen away from half filling. The Hubbard- and correlated pair hopping contributions in H_h cancel except for two-particle excitations at the same Fermi point. The bond-charge interaction completely remains. Nevertheless, the Hamiltonian eq. (2.58a) is suited to correctly model the bulk of the "ordinary" Kondo model, with free fermions. Since $D \gg 1$, the leading bulk behaviour at $\beta \gg 1$ is that of a Fermi liquid. The impurity is influenced by the bulk-bulk interaction indirectly, with an effective coupling $\sim 1/\alpha^2$. Such terms will vanish in the scaling limit, carried out later.³ Furthermore, $1/\alpha$ -correlations in the host can be cast into a renormalized Fermi velocity, which is demonstrated in the next section. Right- and left-moving electrons couple with equal amplitudes to the impurity, both backward and forward scattering appear in the same fashion. In an analogous manner, $H^{(2)}$ can be approximated.

By carrying out the linear dispersion limit, formally infinitely many more k -states are involved than originally allowed (the restriction eq. (2.56) rejects most of them afterwards). They probe the lattice in direct space at arbitrary wavelengths. However, the system's properties should not depend on the lattice's properties. One is thus lead to pass to a continuous description [34]:

$$\begin{aligned} c_{k,\nu,\tau}^\dagger &= \frac{1}{\sqrt{L}} \sum_{n=1}^L e^{ik_\nu n} c_{n,\nu,\tau}^\dagger \\ &= \frac{1}{\sqrt{L}a_0} \sum_{n=1}^L e^{i\frac{k\nu}{a_0} na_0} \frac{c_{n,\nu,\tau}^\dagger}{\sqrt{a_0}} a_0 \\ &= \frac{1}{\sqrt{l}} \int_0^l e^{iq_{k,\nu} x} \psi_{\nu,\tau}^\dagger(x) dx , \end{aligned}$$

with a_0 the lattice constant, $l = L \cdot a_0$ is the (constant) length of the chain, $x = n \cdot a_0$, $\psi_{\nu,\tau}^\dagger(x) = \lim_{a_0 \rightarrow 0} \frac{c_{n,\nu,\tau}^\dagger}{\sqrt{a_0}}$, $q_k = k/a_0$. ψ^\dagger , ψ are now fermionic *density* (or field) operators. Note that

$$\left\{ \psi_{\nu,\tau}(x), \psi_{\nu',\tau'}^\dagger(x') \right\} = \delta(x - x') \delta_{\nu,\nu'} \delta_{\tau,\tau'} .$$

With these prescriptions, one goes back to eqs. (2.58a), (2.58b), and considers the free fermion contribution of the host and the impurity-host exchange, as well as the external fields. Again normal ordering is imposed,

$$:\psi_{\nu,\tau}^\dagger(x) \psi_{\nu',\tau'}(x): = \lim_{\epsilon \rightarrow 0} \left[\psi_{\nu,\tau}^\dagger(x + \epsilon) \psi_{\nu',\tau'}(x) - \langle \psi_{\nu,\tau}^\dagger(x + \epsilon) \psi_{\nu',\tau'}(x) \rangle_0 \right] ,$$

where $\langle \cdots \rangle_0$ is the expectation value in the ground state. Let us summarize the external fields again

³Studies of conformal field theory on a Kondo impurity in a Luttinger liquid [29,30] stress that the stable fixed point for $g = 0$ at $T = 0$ must survive for $g \neq 0$, otherwise the theory would become non-critical.

in an operator H_{ex} . Then

$$H_h/(2D) = \int_0^l \sum_{\nu, \nu', \tau} \left[(\cos k_F + 1) :n_{\nu}: - \mathbb{1}_{\nu} + i\nu a_0 \sin k_F : \psi_{\tau, \nu}^{\dagger}(x) \frac{d}{dx} \psi_{\tau, \nu'}(x) : \right] dx \quad (2.59a)$$

$$H_I = 2 \cos k_F J \int_0^l \delta(x) \sum_{\nu, \nu', \tau} \left[n_{d, \tau} (1 - n_{d, \bar{\tau}}) :n_{\nu, \tau}(x): + d_{\tau}^{\dagger} d_{\bar{\tau}} : \psi_{\nu, \bar{\tau}}^{\dagger}(x) \psi_{\nu', \tau}(x) : \right] dx \quad (2.59b)$$

$$H_{ex} = \int_0^l -\mu \left[n(x) + \delta(x) \sum_{\tau} n_{d, \tau} (1 - n_{d, \bar{\tau}}) \right] + \frac{\hbar}{2} [\delta(x)(n_{d, \uparrow} - n_{d, \downarrow}) + (n_{\uparrow}(x) - n_{\downarrow}(x))] dx \quad (2.59c)$$

$n_{\tau, \nu} = : \psi_{\tau, \nu}^{\dagger} \psi_{\tau, \nu} :$, $n_{\nu} = \sum_{\tau} n_{\nu, \tau}$, $n_{\tau} = \sum_{\nu} n_{\tau, \nu}$. Since $D = 1/a_0$, the linear dispersion term in the host is kept.

As far as the terms eqs. (2.59a), (2.59b) are concerned, one may pass to a Weyl basis by the canonical transformation

$$\begin{aligned} \phi_{\pm, \tau}(x) &= \frac{1}{\sqrt{2}} [\psi_{-, \tau}(x) \pm \psi_{+, \tau}(-x)] \\ \{ \phi_{\nu, \tau}(x), \phi_{\nu', \tau'}^{\dagger}(x') \} &= \delta(x - x') \delta_{\nu, \nu'} \delta_{\tau, \tau'} . \end{aligned}$$

Interaction terms in the host are non-local in the $\phi_{\pm}(x)$; however, it has been argued that these are accounted for later by a redefinition of the Fermi velocity v_F , $\sin k_F = v_F \rightarrow \tilde{v}_F = v_F(1 + \mathcal{O}(1/\alpha))$. The Weyl basis is useful to recognize that the host actually consists of two channels, but the impurity couples only to the symmetric channel; we give the Hamiltonian density with $D = 1/a_0$:

$$\mathcal{H}_h = 2 \sum_{\tau, \nu = \pm} \left[i\tilde{v}_F : \phi_{\nu, \tau}^{\dagger}(x) \frac{d}{dx} \phi_{\nu, \tau}(x) : + D(\cos k_F + 1) :n_{\nu}(x): - D \mathbb{1}_{\nu} \right] \quad (2.60)$$

$$\mathcal{H}_I = 4J \cos k_F \sum_{\tau} \delta(x) \left[: \phi_{+, \tau}^{\dagger}(x) \phi_{+, \tau}(x) : n_{d, \tau} (1 - n_{d, \bar{\tau}}) + : \phi_{+, \tau}^{\dagger}(x) \phi_{+, \bar{\tau}}(x) : d_{\bar{\tau}}^{\dagger} d_{\tau} \right]$$

$$\mathcal{H}_{ex} = -\mu \left[n(x) + \delta(x) \sum_{\tau} n_{d, \tau} (1 - n_{d, \bar{\tau}}) \right] + \frac{\hbar}{2} [\delta(x)(n_{d, \uparrow} - n_{d, \downarrow}) + n_{\uparrow}(x) - n_{\downarrow}(x)] .$$

Zero occupation of the impurity site is dropped. The impurity contribution is trivial if $n(0) = 0, 2$: The impurity is fixed in one single state, no excitations are possible. If these trivial configurations are excluded, the operator of unity $\mathbb{1}_{0,+}$ of the impurity site can be expressed solely in terms of occupation operators, and the exchange operator can be completed to the XXX -exchange operator,

$$\begin{aligned} \mathbb{1}_{0,+} &= (n_{d, \uparrow}(1 - n_{d, \downarrow}) + n_{d, \downarrow}(1 - n_{d, \uparrow})) :n_+(0): \\ \sigma_I^z &= n_{d, \uparrow} - n_{d, \downarrow}, \quad \sigma_I^+ = d_{\uparrow}^{\dagger} d_{\downarrow}, \quad \sigma_I^- = d_{\downarrow}^{\dagger} d_{\uparrow} \\ \mathcal{H}_I &= 2J \delta(x) \sum_{\tau, \tau'} : \phi_{+, \tau}^{\dagger}(x) \sigma_{\tau, \tau'} \phi_{+, \tau'}(x) : \sigma_I + 2J \delta(x) \mathbb{1}_{0,+} . \end{aligned} \quad (2.61)$$

$n_+(x) = \sum_{\tau} \phi_{+, \tau}^{\dagger}(x) \phi_{+, \tau}(x)$, $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)^T$ and $2 \cos k_F J \rightarrow J$ is redefined. The fermionic operators of the impurity have been expressed in terms of spin operators with index I ,

$$\sigma_I^z = n_{d, \uparrow} - n_{d, \downarrow}, \quad \sigma_I^+ = d_{\uparrow}^{\dagger} d_{\downarrow}, \quad \sigma_I^- = d_{\downarrow}^{\dagger} d_{\uparrow} .$$

Eqs. (2.60), (2.61) define the isotropic Kondo model. It describes a free host with a linear dispersion and an interaction between a localized spin and the spin *density* of the host. Note that fermionic $+$, $-$ -operators do not interact among each other and the impurity couples only to one of both. Therefore, one may conceive the model (2.60), (2.61) as one-half dimensional, with fermionic operators stemming only from one Fermi point. This is the model which has been solved by coordinate BA techniques, cf. eq. (4.2.5) in [90]. The parameter $u_0 = v_0/2$ is still free in eq. (2.61); as shown later in the equations for the free energy, it ensures that the "universal limit" $D \gg 1$ can be carried out, such that D, α, u_0 are combined to a constant.

2.1.3 Solution (NLIE)

In this section, the impurity contribution to the free energy of the regularized model is derived in terms of non-linear integral equations, (NLIE).

Taking account of eq. (2.21),

$$\begin{aligned} e^{-\beta H_h^{(ff)}} &= \lim_{N \rightarrow \infty} [\bar{\tau}_0(u_N) \tau_0(u_N)]^{N/2}, \quad u_N = -\frac{\beta D(\alpha + 1)}{N} \\ e^{-\beta H} &= \lim_{N \rightarrow \infty} [\bar{\tau}(u_N) \tau(u_N)]^{N/2} e^{-\beta H_{ex}} \\ e^{-\beta H_{ex}} &= \prod_{j=1}^L e^{-\beta[h/2(n_{j,\uparrow} - n_{j,\downarrow}) - \mu n_j]} e^{-\beta[h/2(n_{d,\uparrow} - n_{d,\downarrow}) - \mu \sum_{\tau} n_{d,\tau}(1 - n_{d,\bar{\tau}})]} =: e^{-\beta \sum_{j=1}^L h_{ex,j}} e^{-\beta H_{ex,I}}, \end{aligned}$$

where the factor $D(\alpha + 1)$ is contained in u_N . The even integer N is referred to as Trotter number and is the height of the fictitious underlying square lattice. The impurity contribution to the free energy is

$$f_I = - \lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{\beta} \left\{ \ln \text{tr} \left[[\bar{\tau}(u_N) \tau(u_N)]^{N/2} e^{-\beta H_{ex}} \right] - \ln \text{tr} \left[[\bar{\tau}_h(u_N) \tau_h(u_N)]^{N/2} e^{-\beta H_{ex,h}} \right] \right\}, \quad (2.62)$$

where $H_{ex,h} = \sum_{j=1}^L h_{ex,j}$. The crucial idea in calculating eq. (2.62) is to exchange tr and str in the expression

$$\begin{aligned} \text{tr} \left\{ [\bar{\tau}(u_N) \tau(u_N)]^{N/2} e^{-\beta H_{ex}} \right\} &= \text{tr} e^{-\beta H_{ex}} \prod_{k=1}^{N/2} \text{str}_{a_{2k} a_{2k-1}} \left[\bar{R}_{a_{2k} L}^{(4,4)}(u_N) \dots \bar{R}_{a_{2k-1} 1}^{(4,4)}(u_N) \right. \\ &\quad \left. \times \bar{R}_{a_{2k} 0}^{(4,3)}(u_N - iu_0) R_{a_{2k-1} L}^{(4,4)}(u_N) \dots R_{a_{2k-1} 1}^{(4,4)}(u_N) R_{a_{2k-1} 0}^{(4,3)}(u_N + iu_0) \right]. \end{aligned}$$

This leads to

$$\begin{aligned} \text{str} \prod_{j=1}^L \left[\text{tr}_j e^{-\beta h_{ex,j}} \prod_{k=1}^{N/2} \bar{R}_{a_{2k} j}^{(4,4)}(u_N) R_{a_{2k-1} j}^{(4,4)}(u_N) \right] &= \left[\text{tr}_0 e^{-\beta H_{ex,I}} \prod_{k=1}^{N/2} \bar{R}_{a_{2k} 0}^{(4,3)}(u_N - iu_0) R_{a_{2k-1} 0}^{(4,3)}(u_N + iu_0) \right] \\ &=: \text{str} \left[\tau_h^{(Q)}(0) \right]^L \tau_I^{(Q)}(iu_0) \end{aligned}$$

$$\tau_h^{(Q)}(v) := \text{tr}_j e^{-\beta h_{ex,j}} \prod_{k=1}^{N/2} \bar{R}_{a_{2k} j}^{(4,4)}(u_N - v) R_{a_{2k-1} j}^{(4,4)}(u_N + v) =: \text{tr}_j T_h^{(Q)}(v) \quad (2.63)$$

$$\tau_I^{(Q)}(v) := \text{tr}_0 e^{-\beta H_{ex,I}} \prod_{k=1}^{N/2} \bar{R}_{0, a_{2k}}^{(3,4)}(u_N - v) R_{0, a_{2k-1} j}^{(3,4)}(u_N + v) =: \text{tr}_0 T_I^{(Q)}(v) \quad (2.64)$$

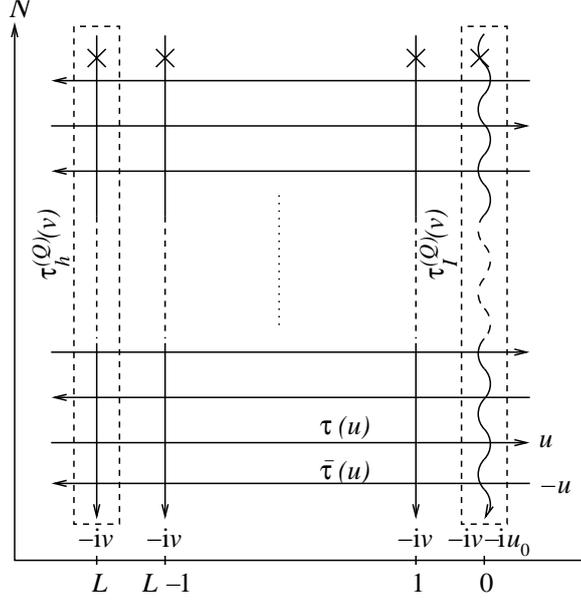


Figure 2.2: Classical lattice representing the free energy of the impurity model. L is the physical, N the Trotter direction. The dimension in the impurity quantum space (wavy line) is reduced by one. Crosses stand for twisted boundary conditions, induced by external fields h and μ .

Eqs. (2.63), (2.64) define the Quantum Transfer Matrix (QTM) $\tau_h^{(Q)}$ of the host and the QTM $\tau_I^{(Q)}$ of the impurity, respectively. Note that the host matrix is independent of the lattice site j . Each QTM is the trace over the auxiliary space of a Quantum Monodromy Matrix $T^{(Q)}$ (QMM). The auxiliary space of $\tau_h^{(Q)}$ is four-dimensional, of $\tau_I^{(Q)}$ three-dimensional. Fig. 2.2 depicts this "rotation" from auxiliary space into quantum space. Due to eqs. (2.2), (2.11),

$$\left[\tau_\nu^{(Q)}(v), \tau_{\nu'}^{(Q)}(v') \right] = 0, \quad (2.65)$$

where the symbolical indices ν, ν' may take values h, I . The auxiliary spectral parameter is essential for the diagonalization of $\tau^{(Q)}$, the u_N are inhomogeneities with alternating signs. Especially, eq. (2.65) holds for $\nu \neq \nu'$: The impurity and host QTM's share the same set of eigenvectors. The largest eigenvalue of $\tau_\nu^{(Q)}$ is separated by a gap from the rest of the spectrum for any N . The eigenstate $|\Phi_{\max}^{(Q)}\rangle$ leading to the largest eigenvalue $\Lambda_I^{\max}(v)$ of $\tau_I^{(Q)}(v)$ also leads to the largest eigenvalue $\Lambda_h^{\max}(v)$ of $\tau_h^{(Q)}(v)$. This is shown in appendices A.1, A.3. Although interesting, this is not essential: The host automatically gives the "correct" eigenvalue of $\tau_I^{(Q)}$ with respect to $|\Phi_{\max}^{(Q)}\rangle$.

$$\begin{aligned} & \ln \left[\text{str} \left(\tau_h^{(Q)}(0) \right)^L \tau_0^{(Q)}(0) \right] \\ &= \ln \left[(-1)^{p[\max]} (\Lambda_h^{\max}(0))^L \Lambda_I^{\max}(u_0) + \sum_{k \neq \max} (-1)^{p[k]} \left(\Lambda_h^{(k)}(0) \right)^L \Lambda_I^{(k)}(u_0) \right] \end{aligned} \quad (2.66a)$$

$$= \ln \left[(\Lambda_h^{\max}(0))^L \Lambda_I^{\max}(u_0) \right] + \sum_{k \neq \max} (-1)^{p[k]} \left(\frac{\Lambda_h^{(k)}(0)}{\Lambda_h^{\max}(0)} \right)^L \frac{\Lambda_I^{(k)}(u_0)}{\Lambda_I^{\max}(u_0)}. \quad (2.66b)$$

Generally, the eigenstate of the $k \neq \text{max}$ -largest eigenvalue of $\tau_h^{(Q)}$ does not lead to the $k \neq \text{max}$ -largest eigenvalue of $\tau_I^{(Q)}$. So with respect to $\tau_I^{(Q)}$, k does not label the eigenvalues according their order. The supertrace requires to include the parity of the projector on the eigenstate k . In appendix A.1, it is shown that $p[\text{max}] = N/2$. One is free to chose $N/2$ even, so that $p[\text{max}] = 0$. Suzuki [86] proves that the two limits $N \rightarrow \infty$, $L \rightarrow \infty$ may be interchanged. Then the thermodynamic limit $L \rightarrow \infty$ in eq. (2.66b) can be carried out by observing that only the largest eigenvalues $\Lambda_{h,I}^{\text{max}}$ survive.

One concludes that the impurity and host contribution to the free energy per lattice site are given by

$$f_I = - \lim_{N \rightarrow \infty} \frac{1}{\beta} \ln \Lambda_I^{\text{max}}(u_0) \quad (2.67)$$

$$f_h = - \lim_{N \rightarrow \infty} \frac{1}{\beta} \ln \Lambda_h^{\text{max}}(0) \quad (2.68)$$

Eqs. (2.67), (2.68) summarize the enormous advantage of considering the QTM: The calculation of the free energy is reduced to the evaluation of a single eigenvalue.

It is convenient to set $v \rightarrow iv$. For this reason, the shift has been done by iu_0 in eq. (2.19), with $u_0 = v_0/2$, eq. (2.33).

f_h has already been calculated in this approach, [47, 77], with the underlying algebra being $U_q(\mathfrak{gl}(2|1))$. In this work, the rational limit is treated explicitly. In the ongoing, we will concentrate on f_I and defer the analogous calculation of f_h to appendix A.3. The diagonalization of $\tau_h^{(Q)}$ is done by applying techniques of the nested Algebraic Bethe Ansatz (NABA) [26, 33, 82]. Some details of the calculation are given in appendix A.1. There, eigenvalues of the non-normalized QTM are calculated. In the ongoing, $\tau_I^{(Q)}$ and Λ_I denote the non-normalized quantities.

$$\Lambda_I(v) = \lambda_-(v) + \lambda_+(v) + \lambda_0(v) \quad (2.69)$$

$$\lambda_-(v) = \frac{q_-(v+i)}{q_-(v)} \phi_+(v+i\alpha/2) \phi_-(v-i\alpha/2-i) e^{\beta(\mu+h/2)}$$

$$\lambda_+(v) = \frac{q_+(v-i)}{q_+(v)} \phi_-(v-i\alpha/2) \phi_+(v+i\alpha/2+i) e^{\beta(\mu-h/2)}$$

$$\lambda_0(v) = \frac{q_-(v+i)q_+(v-i)}{q_-(v)q_+(v)} \phi_+(v-i\alpha/2) \phi_-(v+i\alpha/2)$$

$$q_+(v) = \prod_{j=1}^M (v - v_j), \quad q_-(v) = \prod_{k=1}^{\widetilde{M}} (v - \widetilde{v}_k).$$

An external magnetic field h and a chemical potential μ have been introduced. The roots $\{v_j\}$, $\{\widetilde{v}_k\}$ are determined by the analyticity of the eigenvalue:

$$\frac{\lambda_+(v_j)}{\lambda_0(v_j)} = \frac{q_-(v)}{q_-(v+i)} \frac{\phi_-(v-i\alpha/2) \phi_+(v+i+i\alpha/2)}{\phi_+(v-i\alpha/2) \phi_-(v+i\alpha/2)} e^{\beta(\mu-h/2)} \Big|_{v=v_j} = -1 \quad (2.70a)$$

$$\frac{\lambda_-(\widetilde{v}_k)}{\lambda_0(\widetilde{v}_k)} = \frac{q_+(v)}{q_+(v-i)} \frac{\phi_+(v+i\alpha/2) \phi_-(v-i-i\alpha/2)}{\phi_+(v-i\alpha/2) \phi_-(v+i\alpha/2)} e^{\beta(\mu+h/2)} \Big|_{v=\widetilde{v}_k} = -1. \quad (2.70b)$$

These are $M + \widetilde{M}$ many nonlinear coupled algebraic equations for the unknown roots. The largest eigenvalue is obtained for $M = \widetilde{M} = N/2$. Then, for $h = 0$, $\{v_j\} = \{\widetilde{v}_k^*\}$. A finite magnetic field breaks this symmetry. From numerical studies for finite N , we know that in the largest eigenvalue case, these

"particle solutions" obey $\text{Im}[v_j] > 0$, $\text{Im}[\tilde{v}_k] < 0 \forall j, k$. Additionally, eqs. (2.70a) and (2.70b) are solved by sets $\{v_j^{(h)}\}$, $\{\tilde{v}_k^{(h)}\}$, respectively, called "hole" solutions, contrary to the "particle" solutions. They are considered in more detail in appendix A.1. From a numerical solution of the BAE for finite N , one finds that they are distributed in the complex plane as $\text{Im}[v_j^{(h)}] < 1$, $\text{Im}[\tilde{v}_k^{(h)}] > 1, \forall j, k$. The particle and hole solutions accumulate at points on the imaginary axis with vanishing real part. That's why a formulation in terms of densities is not possible. Results of numerical solutions of eqs. (2.70a), (2.70b) are presented in figs. 2.3, 2.4 at the end of this section.

Let us now formulate non-linear integral equations (NLIE) along arguments similar to the $t - J$ -model, [45]. Generally speaking, there are six unknown functions in eq. (2.69):

$$\begin{aligned} q_+ & , & q_- , \\ q_-^{(h)}(v) & := & \prod_{j=1}^{N-M+\tilde{M}} (v - v_j^{(h)}) \\ q_+^{(h)}(v) & := & \prod_{k=1}^{\tilde{N}-\tilde{M}+M} (v - \tilde{v}_k^{(h)}) \\ \Lambda_{I,+} & , & \Lambda_{I,-} . \end{aligned}$$

The index denotes the part of the complex plane where these functions have zeroes: If a $q-$ function carries an index $+$ ($-$), it has zeroes in the upper (lower) half plane. For the degrees of the polynomials $q_+^{(h)}$, $q_-^{(h)}$, see appendix A.1. One can eliminate these unknowns by appropriate auxiliary functions.

$$\begin{aligned} \frac{1}{\mathfrak{b}(v)} & := \frac{\lambda_+(v)}{\lambda_-(v)} \left(1 + \frac{\lambda_0(v)}{\lambda_+(v)} \right) \\ & = \frac{q_+(v-i) \phi_-(v-i\alpha/2) \phi_+(v+i+i\alpha/2)}{q_-(v+i) \phi_+(v+i\alpha/2) \phi_-(v-i-i\alpha/2)} e^{-\beta h} \\ & \quad \times \underbrace{\frac{q_-(v)}{q_+(v)} \left(1 + \frac{q_-(v+i)}{q_-(v)} \frac{\phi_+(v-i\alpha/2) \phi_-(v+i\alpha/2)}{\phi_-(v-i\alpha/2) \phi_+(v+i+i\alpha/2)} e^{-\beta(\mu-h/2)} \right)}_{\equiv \frac{q_-^{(h)}(v)}{\phi_-(v-i\alpha/2) \phi_+(v+i+i\alpha/2)}} \\ & = \frac{1}{\phi_+(v+i\alpha/2) \phi_-(v-i-i\alpha/2)} \frac{q_+(v-i)}{q_-(v+i)} q_-^{(h)}(v) e^{-\beta h} \end{aligned} \quad (2.71)$$

The term denoted as $q_-^{(h)}$ has been identified by reasons of analyticity: The zeroes of nominator and denominator cancel as far as the particle solutions are concerned, the hole solutions rest as zeroes of the nominator. The polynomials in the denominator are the same as the ϕ -terms in λ_0/λ_+ . Along the same reasoning (or simply by taking the complex conjugate and $h \rightarrow -h$), we find another function $\bar{\mathfrak{b}}$:

$$\begin{aligned} \frac{1}{\bar{\mathfrak{b}}(v)} & := \frac{\lambda_-(v)}{\lambda_+(v)} \left(1 + \frac{\lambda_0(v)}{\lambda_-(v)} \right) \\ & = \frac{1}{\phi_-(v-i\alpha/2) \phi_+(v+i+i\alpha/2)} \frac{q_-(v+i)}{q_+(v-i)} q_+^{(h)}(v) e^{\beta h} . \end{aligned}$$

A third function \mathfrak{c} is introduced,

$$\begin{aligned} \frac{1}{\mathfrak{c}(v)} & := \frac{\lambda_0(v)}{\lambda_+(v) \lambda_-(v)} \Lambda_I(v) \\ & = \frac{\phi_+(v-i\alpha/2) \phi_-(v+i\alpha/2) e^{-2\beta\mu}}{\phi_-(v-i\alpha/2) \phi_+(v+i+i\alpha/2) \phi_+(v+i\alpha/2) \phi_-(v-i\alpha/2-i)} \Lambda_I(v) . \end{aligned} \quad (2.72)$$

Consider $\mathfrak{B} := \mathfrak{b} + 1$, $\overline{\mathfrak{B}} := \overline{\mathfrak{b}} + 1$, $\mathfrak{C} := \mathfrak{c} + 1$.

$$\begin{aligned}\mathfrak{B}(v) &= \frac{1}{\lambda_-(v)} \mathfrak{b}(v) \Lambda_I(v) = \frac{q_-(v)}{q_+(v-i) q_-^{(h)}(v)} \Lambda_I(v) e^{-\beta(\mu-h/2)} \\ \overline{\mathfrak{B}}(v) &= \frac{1}{\lambda_+(v)} \overline{\mathfrak{b}}(v) \Lambda_I(v) = \frac{q_+(v)}{q_-(v+i) q_+^{(h)}(v)} \Lambda_I(v) e^{-\beta(\mu+h/2)} \\ \mathfrak{C}(v) &= \frac{1}{\mathfrak{b}(v) \overline{\mathfrak{b}}(v)} \mathfrak{c}(v) = \frac{q_+^{(h)}(v) q_-^{(h)}(v)}{\phi_+(v-i\alpha/2) \phi_-(v+i\alpha/2)} \frac{1}{\Lambda_I(v)} e^{2\beta\mu}.\end{aligned}$$

In the following, the largest eigenvalue case is studied. Let us take the logarithmic derivative of these auxiliary functions. Then constant terms vanish. Since we know the analyticity properties of all functions in the complex v -plane, we can calculate their Fourier-transforms,

$$\hat{f} = \int_{-\infty}^{\infty} [\ln f(v)]' e^{-ikv} \frac{dv}{2\pi}. \quad (2.73)$$

The integration contour is taken along the real axis. This is allowed as long as $|\alpha/2| > |u_N|$, which certainly is the case for N and α sufficiently large. The final results are independent of this assumption, the limit $\alpha \rightarrow 0$ is contained and may be carried out after application of the Fourier transform and its inverse. \hat{f} vanishes for $k < 0$ ($k > 0$) for $f(v)$ analytic in \mathbb{C}^+ (\mathbb{C}^-). Thus it is convenient to calculate the Fourier transforms separately for $k < 0$, $k > 0$. For the moment, concentrate on $k < 0$.

$$-\hat{\mathfrak{b}}(k) = -e^{(\alpha/2+1)k} \hat{\phi}_-(k) + e^k \hat{q}_+(k) \quad (2.74a)$$

$$-\hat{\overline{\mathfrak{b}}}(k) = -e^{k\alpha/2} \hat{\phi}_-(k) - e^k \hat{q}_+ + \hat{q}_+^{(h)} \quad (2.74b)$$

$$-\hat{\mathfrak{c}}(k) = e^{\alpha/2k} (\hat{\phi}_+(k) - \hat{\phi}_-(k)) - e^{(\alpha/2+1)k} \phi_-(k) + \hat{\Lambda}_{I,+}(k) \quad (2.74c)$$

$$\hat{\mathfrak{B}}(k) = -e^k \hat{q}_+(k) + \hat{\Lambda}_{I,+}(k) \quad (2.74d)$$

$$\hat{\overline{\mathfrak{B}}}(k) = \hat{q}_+(k) - \hat{q}_+^{(h)}(k) + \hat{\Lambda}_{I,+}(k) \quad (2.74e)$$

$$\hat{\mathfrak{C}}(k) = -e^{\alpha/2k} \hat{\phi}_+(k) + \hat{q}_+^{(h)}(k) - \hat{\Lambda}_{I,+}(k). \quad (2.74f)$$

The essential observation is that in eqs. (2.74a)-(2.74f), there appear the three unknowns, namely \hat{q}_+ , $\hat{q}_+^{(h)}$ and $\hat{\Lambda}_{I,+}$, and the three auxiliary functions $\hat{\mathfrak{b}}$, $\hat{\overline{\mathfrak{b}}}$ and $\hat{\mathfrak{c}}$. This means that one may eliminate the unknowns through the auxiliary functions, resulting in a set of three algebraic equations coupling the latter. This avoids the detailed knowledge of q_{\pm} , $q_{\pm}^{(h)}$ and makes it possible to carry out the limit $N \rightarrow \infty$ analytically. Add eqs. (2.74e), (2.74f) and combine this sum with eq. (2.74a):

$$\hat{\mathfrak{b}}(k) = e^{(\alpha/2+1)k} (\hat{\phi}_-(k) - \phi_+(k)) - e^k (\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)). \quad (2.75)$$

Combine eqs. (2.74d) with (2.74a) and these two with eq. (2.75). An expression for $\hat{\Lambda}_{I,+}$ results,

$$\hat{\Lambda}_{I,+}(k) = \hat{\mathfrak{B}}(k) + e^k (\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)) + e^{(\alpha/2+1)k} \hat{\phi}_+(k),$$

which is inserted into eq. (2.74c):

$$\hat{\mathfrak{c}}(k) = -e^{\alpha/2k} (\hat{\phi}_+(k) - \hat{\phi}_-(k)) + e^{(\alpha/2+1)k} (\hat{\phi}_-(k) - \hat{\phi}_+(k)) - \hat{\mathfrak{B}}(k) - e^k (\hat{\overline{\mathfrak{B}}}(k) + \hat{\mathfrak{C}}(k)).$$

Finally, eqs. (2.74d) and (2.74f) give $\hat{q}_+^{(h)}(k)$, which is inserted into eq. (2.74b),

$$\hat{\overline{\mathfrak{b}}}(k) = e^{\alpha/2k} (\hat{\phi}_-(k) - \hat{\phi}_+(k)) - (\hat{\mathfrak{C}}(k) + \hat{\mathfrak{B}}(k)). \quad (2.76)$$

The case $k > 0$ is obtained by exchanging $\hat{\mathbf{b}}, \hat{\bar{\mathbf{b}}}$, switching $k \rightarrow -k$ in the exponential terms and replacing $\phi_- \leftrightarrow \phi_+$. The result is summarized:

$$\hat{\mathbf{b}}(k) = \begin{cases} e^{-\alpha/2k}(\hat{\phi}_+(k) - \hat{\phi}_-(k)) - (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \\ e^{(\alpha/2+1)k}(\hat{\phi}_-(k) - \hat{\phi}_+(k)) - e^k(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k < 0 \end{cases} \quad (2.77a)$$

$$\hat{\bar{\mathbf{b}}}(k) = \begin{cases} e^{-(\alpha/2+1)k}(\hat{\phi}_+(k) - \hat{\phi}_-(k)) - e^{-k}(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \\ e^{\alpha/2k}(\hat{\phi}_-(k) - \hat{\phi}_+(k)) - (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k < 0 \end{cases} \quad (2.77b)$$

$$\hat{\mathbf{c}}(k) = \begin{cases} (e^{-(\alpha/2+1)k} + e^{-\alpha/2k})(\hat{\phi}_+(k) - \hat{\phi}_-(k)) - \hat{\mathfrak{B}}(k) - e^{-k}(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k > 0 \\ -\hat{\mathfrak{B}}(k) - (\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k = 0 \\ (e^{(\alpha/2+1)k} + e^{\alpha/2k})(\hat{\phi}_-(k) - \hat{\phi}_+(k)) - \hat{\mathfrak{B}}(k) - e^k(\hat{\mathfrak{B}}(k) + \hat{\mathfrak{C}}(k)) & k < 0 \end{cases} \quad (2.77c)$$

Application of the inverse Fourier transform and integration leads to a system of non-linear integral equations.

$$\ln \mathbf{b}(v) = \phi_{\mathbf{b}}^{(N)}(v + i\delta) - [k_{\mathbf{b}} * \ln \bar{\mathfrak{B}}](v + 2i\delta) - [k_{\mathbf{b}} * \ln \mathfrak{C}](v + i\delta) + \beta(\mu + h/2) \quad (2.78a)$$

$$\ln \bar{\mathbf{b}}(v) = \phi_{\bar{\mathbf{b}}}^{(N)}(v - i\delta) - [k_{\bar{\mathbf{b}}} * \ln \mathfrak{B}](v - 2i\delta) - [k_{\bar{\mathbf{b}}} * \ln \mathfrak{C}](v + i\delta) + \beta(\mu - h/2) \quad (2.78b)$$

$$\ln \mathbf{c}(v) = \phi_{\mathbf{c}}^{(N)}(v) - [k_{\mathbf{b}} * \ln \bar{\mathfrak{B}}](v + i\delta) - [k_{\bar{\mathbf{b}}} * \ln \mathfrak{B}](v - i\delta) - [k_{\mathbf{c}} * \ln \mathfrak{C}](v) + 2\beta\mu \quad (2.78c)$$

The convolution

$$[f * g](x) := \int_{-\infty}^{\infty} f(x)g(x-y)dy \quad (2.79)$$

is done with local kernels:

$$k_{\mathbf{b}}(v) = \frac{1}{2\pi v(v-i)}, \quad k_{\bar{\mathbf{b}}}(v) = k_{\mathbf{b}}(v)^*, \quad k_{\mathbf{c}}(v) = k_{\mathbf{b}}(v) + k_{\bar{\mathbf{b}}}(v) = \frac{2}{2\pi(v^2+1)}.$$

In order to achieve convergence, the equation for $\ln \mathbf{b}$ ($\ln \bar{\mathbf{b}}$), eq. (2.78a) (eq. (2.78b)), is taken for $v + i\delta$, ($v - i\delta$). The argument of $\ln \mathbf{c}$, eq. (2.78c), can be moved to the real axis upon replacing $\alpha \rightarrow \alpha - \epsilon$.

The constant terms are integration constants derived from the asymptotic behaviour of the auxiliary functions for large $|v|$.

$$\lim_{|v| \rightarrow \infty} \mathbf{b} = \frac{a}{1+a}, \quad \lim_{|v| \rightarrow \infty} \bar{\mathbf{b}} = \frac{\bar{a}}{1+a}, \quad \lim_{|v| \rightarrow \infty} \mathbf{c} = \frac{a\bar{a}}{1+a+\bar{a}} \quad (2.80)$$

$$a = e^{\beta(\mu+h/2)}, \quad \bar{a} = e^{\beta(\mu-h/2)}. \quad (2.81)$$

In this limit, convolutions reduce to simple multiplications,

$$\lim_{|v| \rightarrow \infty} [k * f](v) = f(\infty) \int_{-\infty}^{\infty} k(v)dv,$$

where f is one of the auxiliary functions $\ln \mathfrak{B}$, $\ln \bar{\mathfrak{B}}$, $\ln \mathfrak{C}$. The norms of the kernels are

$$\begin{aligned} \int_{-\infty}^{\infty} k_{\mathbf{b}}(v + i\delta)dv &= 1 = \int_{-\infty}^{\infty} k_{\bar{\mathbf{b}}}(v - i\delta)dv \\ \int_{-\infty}^{\infty} k_{\mathbf{c}}(v)dv &= 1. \end{aligned}$$

The $\phi^{(N)}$ -terms are v -dependent,

$$\begin{aligned}\phi_{\mathfrak{b}}^{(N)}(v) &= \ln \frac{\phi_+(v + i\frac{\alpha}{2}) \phi_-(v - i\frac{\alpha}{2} - i)}{\phi_-(v + i\frac{\alpha}{2}) \phi_+(v - i\frac{\alpha}{2} - i)} \\ \phi_{\bar{\mathfrak{b}}}^{(N)} &= [\phi_{\mathfrak{b}}^{(N)}]^* \\ \phi_{\mathfrak{c}}^{(N)} &= \phi_{\mathfrak{b}}^{(N)} + \phi_{\bar{\mathfrak{b}}}^{(N)}\end{aligned}$$

Once the auxiliary functions are known, the eigenvalue can be calculated from eq. (2.72):

$$-\ln \mathfrak{c}(v) = \frac{\beta D(\alpha + 1)\alpha}{v^2 + \alpha^2/4} - 2\beta\mu + \ln \frac{\Lambda_I(v)}{\phi_+(v + i + i\alpha/2)\phi_-(v - i\alpha/2 - i)}. \quad (2.82)$$

The denominator of the last term is the norm of $\tau_I^{(Q)}$. The free energy, eq. (2.67), is given by the eigenvalue of the normalized QTM. Furthermore, one identifies the coupling constant J_α , eq. (2.34).

$$-\beta f_I(T, h) = -\ln \mathfrak{c}(v_0/2) - 2\beta(\alpha + 1)J_\alpha + 2\beta\mu. \quad (2.83)$$

Let us shortly comment on an approximate solution of the Bethe Ansatz equations (2.70a), (2.70b). Set $\mathfrak{a} := \lambda_0/\lambda_+$. Then a root v_j yields

$$\begin{aligned}\mathfrak{a}(v_j) &= -1 \\ \ln \mathfrak{a}(v_j) &= (2j + 1)\pi i.\end{aligned}$$

For large β and without external fields, $\mu = 0 = h$, the driving terms dominate the integral equations, permitting for the approximate solution

$$\begin{aligned}\ln \mathfrak{a}(v_j) &\approx [\phi_{\mathfrak{b}}^{(N)}(v_j^*)]^* \\ v_j &\approx -\frac{i}{2} + i\sqrt{\frac{(\alpha + 1)^2}{4} + u^2 + iu(\alpha + 1) \cot \frac{2k + 1}{N}\pi} \\ \lim_{N \rightarrow \infty} v_j &\approx -\frac{i}{2} + i\sqrt{\frac{(\alpha + 1)^2}{4} - i\frac{\beta D(\alpha + 1)^2}{(2k + 1)\pi}}.\end{aligned} \quad (2.84)$$

Values from eq. (2.84) are used as initial values for μ, h finite with finite N . Initial values for hole solutions $v_j^{(h)}$ are also given by eq. (2.84), with a negative sign in front of the square root. Note that the Trotter limit $N \rightarrow \infty$ could be taken.

Obviously, the limit $N \rightarrow \infty$ can be carried out analytically also in the integral equations, resulting in terms $\lim_{N \rightarrow \infty} \phi^{(N)} =: \phi$:

$$\phi_{\mathfrak{b}}(v) = -\beta D(\alpha + 1) \frac{\alpha + 1}{(v + i\alpha/2)(v - i\alpha/2 - i)}, \quad \phi_{\bar{\mathfrak{b}}} = \phi_{\mathfrak{b}}^* \quad (2.85)$$

$$\begin{aligned}\phi_{\mathfrak{c}}(v) &= -\beta D(\alpha + 1) \left(\frac{\alpha}{v^2 + \alpha^2/4} + \frac{2 + \alpha}{v^2 + (\alpha/2 + 1)^2} \right) \\ &= \phi_{\mathfrak{b}}(v) + \phi_{\bar{\mathfrak{b}}}(v).\end{aligned} \quad (2.86)$$

Let us write the NLIE (2.78) with these terms once more:

$$\ln \mathfrak{b}(v) = \phi_{\mathfrak{b}}(v + i\delta) - [k_{\mathfrak{b}} * \ln \bar{\mathfrak{B}}](v + 2i\delta) - [k_{\mathfrak{b}} * \ln \mathfrak{C}](v + i\delta) + \beta(\mu + h/2) \quad (2.87a)$$

$$\ln \bar{\mathfrak{b}}(v) = \phi_{\bar{\mathfrak{b}}}(v - i\delta) - [k_{\bar{\mathfrak{b}}} * \ln \mathfrak{B}](v - 2i\delta) - [k_{\bar{\mathfrak{b}}} * \ln \mathfrak{C}](v + i\delta) + \beta(\mu - h/2) \quad (2.87b)$$

$$\ln \mathfrak{c}(v) = \phi_{\mathfrak{c}}(v) - [k_{\mathfrak{b}} * \ln \bar{\mathfrak{B}}](v + i\delta) - [k_{\bar{\mathfrak{b}}} * \ln \mathfrak{B}](v - i\delta) - [k_{\mathfrak{c}} * \ln \mathfrak{C}](v) + 2\beta\mu \quad (2.87c)$$

In close analogy to the treatment of the Hamiltonian in the preceding section, we are interested in an asymptotic expansion of the free energy in the limit $\alpha \rightarrow \infty$. The essential observation from the study of the Hamiltonian was that after the canonical transformation, excitations of the impurity stem exclusively from the singly occupied state. However, this spectrum is sub-leading by an order of α compared to the constant contribution from zero occupation. So our strategy is again to perform an asymptotic expansion in the spirit of eq. (2.30), now in the framework of the NLIE.

Let us scale $v \rightarrow \alpha v$. The kernels decay algebraically in v , they shrink to δ -functions, with corrections $\mathcal{O}(1/\alpha^2)$. The leading correction $\mathcal{O}(1/\alpha)$ thus solely stems from the driving terms $\phi_{\mathfrak{b}, \bar{\mathfrak{b}}, \mathfrak{c}}$:

$$\begin{aligned} \phi_{\mathfrak{c}}(\alpha v) &= \frac{1}{v^2 + 1/4} + \frac{1}{\alpha} \left[\frac{3}{v^2 + \frac{1}{4}} - \frac{1}{(v^2 + \frac{1}{4})^2} \right] + \mathcal{O}(1/\alpha^2) \\ &=: \frac{1}{v^2 + 1/4} + 2R_{\alpha}(\alpha v) \end{aligned} \quad (2.88)$$

Eq. (2.88) summarizes corrections $\mathcal{O}(1/\alpha)$ in a function R_{α} . Higher orders $\mathcal{O}(1/\alpha^2)$ are omitted, consistently with the approximations in the Hamiltonian realized in the preceding section. We end up with algebraic equations for the auxiliary functions:

$$\begin{aligned} \ln \mathfrak{b}(v) &= -\frac{\beta D}{v^2 + 1/4} + R_{\alpha}(\alpha v) + \beta(\mu + h/2) - [\ln \bar{\mathfrak{B}}\mathfrak{C}](v) \\ \ln \bar{\mathfrak{b}}(v) &= -\frac{\beta D}{v^2 + 1/4} + R_{\alpha}(\alpha v) + \beta(\mu - h/2) - [\ln \mathfrak{B}\mathfrak{C}](v) \\ \ln \mathfrak{c}(v) &= -\frac{2\beta D}{v^2 + 1/4} + 2R_{\alpha}(\alpha v) + 2\beta\mu - [\ln \mathfrak{B}\bar{\mathfrak{B}}\mathfrak{C}](v) \end{aligned}$$

These equations are solved by

$$\mathfrak{b}(v) = \frac{a(v)}{1 + \bar{a}(v)}, \quad \bar{\mathfrak{b}}(v) = \frac{\bar{a}(v)}{1 + a(v)}, \quad \mathfrak{c}(v) = \frac{a(v)\bar{a}(v)}{1 + a(v) + \bar{a}(v)} \quad (2.89a)$$

$$\begin{aligned} a(v) &= \exp \left[-\frac{\beta D}{v^2 + 1/4} + R_{\alpha}(\alpha v) + \beta(\mu + h/2) \right] \\ \bar{a}(v) &= \exp \left[-\frac{\beta D}{v^2 + 1/4} + R_{\alpha}(\alpha v) + \beta(\mu - h/2) \right]. \end{aligned} \quad (2.89b)$$

Note the formal identity to eqs. (2.80), (2.81) (in fact, $a = \lim_{|v| \rightarrow \infty} a(v)$). As to J_{α} , scale $v_0 \rightarrow \alpha v_0$, so that

$$\lim_{\alpha \rightarrow \infty} (\alpha + 1)J_{\alpha} = \frac{2}{v_0^2 + 1} =: J_0.$$

From the expression of f_I , eq. (2.83) it follows that the free energy is that of an uncoupled impurity,

$$\begin{aligned} \lim_{\alpha \rightarrow \infty} f_I(T, h) &= -T \ln [(a\bar{a})^{-1}(v_0/2) + a^{-1}(v_0/2) + \bar{a}^{-1}(v_0/2)] + 2DJ_0 - 2\mu \\ &= -T \ln \left[e^{\beta 2DJ_0} + e^{\beta(\mu+h/2)} + e^{\beta(\mu-h/2)} \right]. \end{aligned} \quad (2.90)$$

The free energy reflects the three possible impurity states, namely empty and singly occupied with up or down spin. This result corresponds to the Hamiltonian which would result from the limit $\alpha \rightarrow \infty$ before the canonical transformation, eq. (2.45).

The more interesting case is to eliminate charge fluctuations on the impurity site, so that the spectrum of a localized moment is recovered. This is done by performing an asymptotic expansion defined by eq. (2.30). The auxiliary functions exhibit a crossover from $\mathfrak{b}, \bar{\mathfrak{b}}, \mathfrak{c} \ll 1$ to $\mathfrak{b}, \bar{\mathfrak{b}}, \mathfrak{c} > 1$ in regions around "Fermi points" $\pm\Lambda_{\mathfrak{c}}$ defined by

$$\begin{aligned} -\phi_{\mathfrak{c}}(\Lambda_{\mathfrak{c}}) &\sim 2\beta\mu \\ \Lambda_{\mathfrak{c}} &= \pm\alpha\sqrt{\frac{D}{\mu} - \frac{1}{4}}. \end{aligned} \quad (2.91)$$

Set $h \ll \mu$. The influence of h on the Fermi points is neglected, since it enters quadratically.

The more common parameterization is

$$\frac{v}{\alpha} = \frac{1}{2} \tan \frac{k}{2}, \quad (2.92)$$

where k is the wave-vector used in the Fourier representation of the Hamiltonian in the preceding section (and not the Fourier variable conjugate to v). At $v = \Lambda_{\mathfrak{c}}$, eq. (2.91) is equivalent to

$$2D(\cos k_F + 1) = \mu, \quad (2.93)$$

which defines k_F at constant μ at $T \ll D$, such that $\mu = \epsilon_F$ (μ in turn is defined by the particle number N such that $k_F = \pi N/(2L)$). Then eq. (2.93) yields a relation between μ and N - this demonstrates that the formally grand-canonical description is effectively canonical, because $T \ll D$. The analysis of the NLIE is most conveniently done in the grand-canonical formalism and in v -parameterization, rather than in k -space).

The energy-dependent density of states for the dispersion $\epsilon(k) = 2D(\cos k + 1)$ is

$$\varrho(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k) = \frac{l}{\pi\sqrt{1 - \left(\frac{\epsilon}{2D} - 1\right)^2}}.$$

For $T \ll D$, the Fermi energy equals the chemical potential, $\mu = \epsilon_F$, so that

$$\varrho(\epsilon_F) =: \varrho_0 = \frac{l}{\pi\sqrt{1 - \left(\frac{\mu}{2D} - 1\right)^2}}.$$

Without loss of generality, one may set $l = \pi$.

The crossover at $\pm\Lambda_{\mathfrak{c}}$ becomes pronounced in the low-temperature limit, very similar to the behaviour of the corresponding functions in the $t - J$ -model, [45]. Consider [57]

$$\ln \mathfrak{C} = \ln \mathfrak{c} + \ln \frac{\mathfrak{C}}{\mathfrak{c}}. \quad (2.94)$$

The second term gives its leading contribution for $|v| < \Lambda_{\mathfrak{c}}$, since in the asymptotic regime, $\mathfrak{c} = \mathfrak{C} + \mathcal{O}(1, e^{\beta h})$, cf. eqs. (2.80), (2.81). This statement is made quantitative by the observation that asymptotically, including terms $\mathcal{O}(1/\alpha)$,

$$\frac{\mathfrak{C}}{\mathfrak{c}} = \frac{1}{a\bar{a}}(1+a)(1+\bar{a}) = \mathcal{O}\left(\frac{1}{\mathfrak{b}\bar{\mathfrak{b}}}\right) \quad (2.95)$$

$$\ln \frac{\mathfrak{C}(v)}{\mathfrak{c}(v)} = \ln [(1+a(v))(1+\bar{a}(v))]_{|v|<\Lambda_{\mathfrak{c}}} + \left[2\beta D \frac{\alpha^2}{v^2 + \alpha^2/4} - 2\beta\mu + 2R_{\alpha}(v) \right]_{|v|<\Lambda_{\mathfrak{c}}}. \quad (2.96)$$

The first term in eq. (2.96) is exponentially small, the second term dominates. The second summand in eq. (2.94) is of the same order as \mathfrak{b} , $\bar{\mathfrak{b}}$, eq. (2.95). The convolution of eq. (2.94) with the relevant kernels becomes

$$k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{C}(v) = k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{c}(v) + \int_{|w| < \Lambda_{\mathfrak{c}}} k_{\mathfrak{c},\mathfrak{b}}(v-w) \ln \frac{\mathfrak{C}(w)}{\mathfrak{c}(w)} dw. \quad (2.97)$$

f_I is determined by $\ln \mathfrak{c}(u_0)$. The second term in eq. (2.97) shall be considered as a next-leading correction compared to the driving terms in eq. (2.87). Set

$$|u_0| = |v_0/2| = \frac{b}{2} \alpha^{1+\epsilon} > \Lambda_{\mathfrak{c}} \sim \alpha, \quad (2.98)$$

with some constant of proportionality b . Then $|v_0| > \Lambda_{\mathfrak{c}}$. (2.98) gives a lower bound on the scaling of v_0 with α . $\epsilon = 0$ is allowed if factors are chosen such that the inequality (2.98) is fulfilled, which is possible. We rather choose $0 < \epsilon < 1/4$. This choice is not of crucial importance, but justifies *a posteriori* that the canonical transformation performed in the preceding section does not dress the bare coupling

$$J = 2 \cos k_F J_{\alpha} \sim 4 \cos k_F \alpha^{-1-2\epsilon} / b^2 = \frac{4 \cos k_F}{bv_0} \alpha^{-\epsilon}.$$

From the preceding equation, $\alpha^{-\epsilon} = \left(\frac{Jb^2}{4 \cos k_F} \right)^{\epsilon/(1+2\epsilon)}$. Choose $b = 2\pi \varrho_0 \cos k_F$. Then

$$\frac{\pi v_0}{2} = \frac{1}{J \varrho_0} (J \pi^2 \cos k_F \varrho_0^2)^{\frac{\epsilon}{1+2\epsilon}}. \quad (2.99)$$

The reason for the choice of b , which leads to eq. (2.99), will become clear below.

We proceed with eq. (2.97)

$$k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{C}(v) \stackrel{v > w}{\approx} k_{\mathfrak{c},\mathfrak{b}} * \ln \mathfrak{c}(v) + k_{\mathfrak{c},\mathfrak{b}}(v) \int_{|w| < \Lambda_{\mathfrak{c}}} \ln \frac{\mathfrak{C}(w)}{\mathfrak{c}(w)} dw + \mathcal{O}(1/v^4).$$

Since the free energy is to be taken for $v_0 \sim \alpha^{1+\epsilon}$, higher orders in approximating the convolution are neglected. As an estimate for the integral, one uses the leading term of eq. (2.96):

$$\begin{aligned} \ln \frac{\mathfrak{C}(v)}{\mathfrak{c}(v)} &= 2\beta \left[\frac{D\alpha^2}{v^2 + \alpha^2/4} + R_{\alpha}(v) - \mu \right] + \mathcal{O}(\exp[-\beta D]) \\ \int_{|w| < \Lambda_{\mathfrak{c}}} \ln \frac{\mathfrak{C}(w)}{\mathfrak{c}(w)} dw &\approx 4\beta\alpha D [2 \arctan 2\Lambda_{\mathfrak{c}} - \mu\Lambda_{\mathfrak{c}}/D + \mathcal{O}(1/\alpha)] =: \beta\kappa > 0. \end{aligned} \quad (2.100)$$

The sub-leading order $\mathcal{O}(1/\alpha)$ originates in R_{α} ; it is neglected in the following (which is justified rigorously below). The factor in brackets in eq. (2.100) takes values between π and 0. It is a monotonously decreasing function of $r := \mu/(4D)$, since $\Lambda_{\mathfrak{c}}$ and k_F are defined by r , eqs. (2.91), (2.93) (note that by virtue of eq. (2.92), $\kappa = 4\alpha D \left[k_F - \frac{\mu}{4D} \tan \frac{k_F}{2} \right]$). Summarizing,

$$k_{\mathfrak{b},\mathfrak{c}} * \ln \mathfrak{C} = k_{\mathfrak{b},\mathfrak{c}} * \ln \mathfrak{c} + \beta\kappa k_{\mathfrak{b},\mathfrak{c}}. \quad (2.101)$$

The Fourier transforms of $\phi_{\mathfrak{b}}$, $\phi_{\bar{\mathfrak{b}}}$, $\phi_{\mathfrak{c}}$, eqs. (2.85), (2.86) are:

$$\begin{aligned} \hat{\phi}_{\mathfrak{b}}(k) &= -\beta D(\alpha + 1) \begin{cases} e^{-\alpha/2k}, & k \geq 0 \\ e^{(\alpha/2+1)k}, & k < 0 \end{cases} \\ \hat{\phi}_{\bar{\mathfrak{b}}}(k) &= -\beta D(\alpha + 1) \begin{cases} e^{-(\alpha/2+1)k}, & k \geq 0 \\ e^{\alpha/2k}, & k < 0 \end{cases} \\ \hat{\phi}_{\mathfrak{c}}(k) &= \hat{\phi}_{\mathfrak{b}}(k) + \hat{\phi}_{\bar{\mathfrak{b}}}(k) = -\beta D(\alpha + 1) \begin{cases} e^{-\alpha/2k} (1 + e^{-k}), & k \geq 0 \\ e^{\alpha/2k} (1 + e^k), & k < 0 \end{cases} \end{aligned} \quad (2.102)$$

Inserting eq. (2.101) gives, using eq. (2.87):

$$\hat{c}(k) = \begin{cases} \frac{\hat{\phi}_c}{1+e^{-k}} - \frac{1}{1+e^k} \beta \kappa - \frac{\hat{\mathfrak{B}}+e^{-k} \mathfrak{B}}{1+e^{-k}} & k \geq 0 \\ \frac{\hat{\phi}_c}{1+e^k} - \frac{1}{1+e^{-k}} \beta \kappa - \frac{\hat{\mathfrak{B}}+e^k \mathfrak{B}}{1+e^k} & k < 0 \end{cases} \quad (2.103a)$$

$$\hat{\mathfrak{b}}(k) = -\frac{1}{1+e^{-k}} \beta \kappa + \frac{1}{1+e^{|k|}} (\hat{\mathfrak{B}} - \mathfrak{B}) \quad (2.103b)$$

$$\hat{\bar{\mathfrak{b}}}(k) = -\frac{1}{1+e^k} \beta \kappa + \frac{1}{1+e^{|k|}} (\hat{\mathfrak{B}} - \mathfrak{B}) \quad (2.103c)$$

The careful analysis in eq. (2.97) is of vital importance to retain a non-zero driving term: Otherwise, the resulting equations are trivially solved; $\ln \mathfrak{b} = \beta h = -\ln \bar{\mathfrak{b}}$, and $\mathfrak{B} = 1 + \exp(\beta h)$, $\bar{\mathfrak{B}} = 1 + \exp(-\beta h)$,

$$f_I = \text{const.} + \ln \left(e^{\beta h/2} + e^{-\beta h/2} \right). \quad (2.104)$$

This is the free energy of a free, uncoupled spin. No strong coupling fixed point would occur at low temperatures. This situation corresponds to the limit $\mu \rightarrow \infty$, such that $\mathfrak{C}(v) = \mathfrak{c}(v) \forall v$. Then the band is filled completely, and single occupation is enforced on the impurity site.

The NLIE eq. (2.103) are transformed back to direct space,

$$\ln \mathfrak{b}(v) = -\Phi(v + i\delta) + \beta h/2 + [k * \ln \mathfrak{B}](v) - [k * \ln \bar{\mathfrak{B}}](v + 2i\delta) \quad (2.105a)$$

$$\ln \bar{\mathfrak{b}}(v) = \Phi(v - i\delta) - \beta h/2 + [k * \ln \bar{\mathfrak{B}}](v) - [k * \ln \mathfrak{B}](v - 2i\delta) \quad (2.105b)$$

$$\begin{aligned} \ln \mathfrak{c}(v) &= -\beta D(\alpha + 1) \frac{\alpha}{v^2 + \alpha^2/4} - k(v) \beta \kappa + \beta \mu \\ &+ [\Phi * \ln \mathfrak{B}](v - i\delta) - [\Phi * \ln \bar{\mathfrak{B}}](v + i\delta). \end{aligned} \quad (2.105c)$$

The driving term and integration kernel read:

$$\begin{aligned} \Phi(v) &= \frac{i\pi}{\sinh \pi v} \beta \kappa \\ k(v) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-|k|/2}}{2 \cosh k/2} e^{ikv} dk. \end{aligned}$$

Choose $\delta = 1/2$, to remove the divergence in $\Phi(v)$ and scale v by $1/\pi$. Since Φ decays exponentially, it is possible to absorb κ and v_0 in a new constant. Substitute

$$v = x - \ln(2\pi\kappa) \quad (2.106)$$

and remember that κ scales with αD , eq. (2.100) and therefore may be arbitrarily large. All parameters can be combined in the free energy such that T_K remains constant,

$$\begin{aligned} -\ln(2\pi\kappa) - \pi v_0/2 &= -\ln T_K \\ T_K &= 2\pi\kappa e^{\pi v_0/2}. \end{aligned} \quad (2.107)$$

The range of $|v_0|$ has been identified in eq. (2.98), we take $v_0 = -|v_0|$. This is no restriction as will be seen below. From the definition (2.99):

$$T_K \sim 2\pi D \exp \left[-\frac{1}{J\varrho_0} \left(1 - \frac{\epsilon}{1+2\epsilon} \ln J + \dots \right) - \ln(J\varrho_0) \right] \quad (2.108)$$

$$D \sim e^\alpha / \alpha. \quad (2.109)$$

Starting directly from eq. (2.61) (without the constant) and a three-dimensional host whose dispersion relation is not specified, one finds [1]

$$\tilde{T}_K = \tilde{D}e^{-1/(J\tilde{\varrho}_0)+\frac{1}{2}\ln(J\tilde{\varrho}_0)+\dots} \quad (2.110)$$

\tilde{D} is the bandwidth of a *three*-dimensional host and $\tilde{\varrho}_0$ the density of states at the Fermi edge. Eqs. (2.108), (2.110) differ, but they have been derived from different assumptions. The cut-off schemes are not the same: The one-dimensional density of states $\varrho(\epsilon)$ diverges at the band edges contrary to the three-dimensional case. Furthermore, our model still contains the constant for zero occupation (which is omitted in eq. (2.61)). In the derivation of eq. (2.107), it was vital not to fill the system completely, so that the non-occupied sector still is finite. We do not want to dwell on the comparison between eqs. (2.108), (2.110) at this point. Rather, it is possible to extract the ratio T_K/\tilde{T}_K from the NLIE, which is done in section 3.2.1. This shows that $T_K \propto \tilde{T}_K$. Thus both the models underlying perturbation theory and our derivation of the NLIE are equivalent in the scaling limit.

The shift eq. (2.106) scales the driving term $\Phi(v + i/2)$:

$$\begin{aligned} -\Phi(v/\pi + i/2) &= -\frac{\beta\pi\kappa}{\cosh v} & (2.111) \\ &= -\frac{2\beta\pi\kappa}{e^{x-\ln(2\pi\kappa)} + e^{-x+\ln(2\pi\kappa)}} \\ &\stackrel{\kappa \rightarrow \infty}{=} -\beta e^x. \end{aligned}$$

In the second line, eq. (2.106) has been employed. At this point it is clear that sub-leading orders in eq. (2.100) can safely be neglected. This scaling opens the door to understand the impurity behaviour for all temperatures: The driving term $\propto \kappa/\cosh v$ is bounded for each finite D ; only in the limit $\kappa \rightarrow \infty$ it is scaled to the unbounded exponential $\propto e^x$. This alters the auxiliary functions such that at low temperatures, $\ln \mathfrak{B}$, $\ln \overline{\mathfrak{B}}$ decay exponentially fast towards zero. Such a behaviour is neither predictable heuristically on the basis of the Hamiltonian, nor from the definition of the auxiliary functions. One needs the exact solution of the problem, which incorporates the many-particle physics, to discover the strong coupling fixed point at low temperatures. This discovery has first been made by Wilson, necessitating a non-perturbative solution.

We rewrite the equations in the scaling limit:

$$\ln \mathfrak{b}(x) = -\beta e^x + \beta h/2 + [k * \ln \mathfrak{B}](x) - [k * \ln \overline{\mathfrak{B}}](x - i\pi + i\epsilon) \quad (2.112a)$$

$$\ln \overline{\mathfrak{b}}(x) = -\beta e^x - \beta h/2 + [k * \ln \overline{\mathfrak{B}}](x) - [k * \ln \mathfrak{B}](x + i\pi - i\epsilon) \quad (2.112b)$$

$$-\beta f_I = \beta\mu + \beta\kappa k(v_0/2) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{[\ln \mathfrak{B}\overline{\mathfrak{B}}](x)}{\cosh(x - \ln T_K)} dx, \quad (2.112c)$$

with

$$k(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-\pi/2|k|}}{2 \cosh \pi/2k} e^{ikx} dk. \quad (2.113)$$

Shifts by $\pm i\epsilon$ ensure integrability. These shifts will not be mentioned explicitly in the ongoing. Note that the shift in the ground state energy due to the non-occupied state has vanished in eq. (2.112c). The chemical potential contributes a constant to f_I , it is dropped in the following. The term $\propto \kappa$ in eq. (2.112c) is of order $\mathcal{O}(D/\alpha)$. It originates in the ground state energy and also is omitted, since excitations are exclusively contained in $\ln \mathfrak{B}\overline{\mathfrak{B}}$. Eqs. (2.112a)-(2.112c) are similar to the equations for the isotropic anti-ferromagnetic spin-1/2 Heisenberg chain, [55]. They result from scaling these equations in the high-temperature regime [56].

Furthermore, a factor β can be absorbed by shifting $x \rightarrow x - \ln \beta$. Let us write the NLIE once more:

$$\ln \mathfrak{b}(x) = -e^x + \beta h/2 + [k * \ln \mathfrak{B}](x) - [k * \ln \overline{\mathfrak{B}}](x - i\pi) \quad (2.114a)$$

$$\ln \overline{\mathfrak{b}}(x) = -e^x - \beta h/2 + [k * \ln \overline{\mathfrak{B}}](x) - [k * \ln \mathfrak{B}](x + i\pi) \quad (2.114b)$$

$$-\beta f_I = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{[\ln \mathfrak{B} \overline{\mathfrak{B}}](x)}{\cosh\left(x + \ln \frac{T}{T_K}\right)} dx. \quad (2.114c)$$

These are the NLIE of the single channel isotropic spin-1/2 Kondo model, where the impurity contribution to the free energy has been identified with the largest eigenvalue of the impurity QTM, eq. (2.67). Note that without a careful asymptotic expansion for $\alpha \rightarrow \infty$, the end of the impurity's story would have been eq. (2.104). This is the high-temperature limit $T \gg T_K$ of eqs. (2.114a)-(2.114c). Eqs. (2.114a), (2.114b) do neither depend on α nor on D . Eq. (2.114c) is the free energy of the impurity site - a quantity which is infinitesimally small in the continuous limit $a_0 \rightarrow 0$. This is not visible in the scaled equations, they are independent from any parameters of the model. Also note that the shift in the integral of the free energy is now temperature-dependent.

The system eq. (2.114) involves two auxiliary functions \mathfrak{B} , $\overline{\mathfrak{B}}$ in comparison to three in eq. (2.87). The function \mathfrak{C} encoding charge fluctuations could be eliminated by an asymptotic expansion, so that the excitations described by \mathfrak{B} , $\overline{\mathfrak{B}}$ are retained. This is conceptually analogous to the canonical transformation of the Hamiltonian.

The choice $v_0 = |v_0|$ leads to the same result: Instead of eq. (2.106), one would substitute $v = x + \ln(2\pi\kappa)$, resulting in a driving term $-e^{-x}$ and $T_K = 2\pi\kappa e^{-\pi v_0/2}$. The shift in the convolution of the free energy would be $-\ln T/T_K$ instead of $+\ln T/T_K$ in eq. (2.114c). However, by the substitution $x \rightarrow -x$ one recovers eqs. (2.114). The restriction of v_0 to one of the two Fermi points occurs naturally and does not mean any loss of generality. This is consistent with the observation that the Hamiltonian eqs. (2.60), (2.61) can be viewed as one-half dimensional, as explained in the sequel of eq. (2.61).

u_0 enables one to attain the limit $T \ll T_K$, the regime of "strong coupling". The way how D, α, u_0 are scaled (eq. (2.107)) is, despite simple, by no means obvious. Apparently, it does not make sense to reinsert v_0 from eq. (2.107) into J_α , eq. (2.34), and realize rigorously the limits $D, u_0, \alpha \rightarrow \infty$ (mathematically speaking, this is due to J_α decaying algebraically with v_0 - the driving term in eq. (2.111) decays exponentially in the spectral parameter). We will come back to this point in chapter 5.

Let us now turn our attention to the host. The problem of finding the largest eigenvalue, eq. (2.68), is solved in an analogous manner as above. In appendix A.3, it is shown that:

$$\begin{aligned} \ln \Lambda_h(v) &= \eta(v) + [\zeta * \ln \mathfrak{B}](v) + [\bar{\zeta} * \ln \overline{\mathfrak{B}}](v) + [(\zeta + \bar{\zeta}) * \ln \mathfrak{C}](v) \quad (2.115) \\ 2\pi\zeta(v) &= -\frac{\phi_{\mathfrak{b}}(-v)}{D\beta(\alpha+1)}, \quad \eta(v) = 2\beta D \frac{(\alpha+1)^2}{v^2 + (\alpha+1)^2}. \end{aligned}$$

The $\ln \mathfrak{B}$, $\ln \overline{\mathfrak{B}}$, $\ln \mathfrak{C}$ are given by eqs. (2.78a)-(2.78c) (!), with driving terms (2.85), (2.86). The technical differences on this level between host and impurity are the functional dependence of the eigenvalue on the auxiliary functions and the lack of a free parameter u_0 ; the auxiliary functions themselves are the same. Note that the limit $\mu \rightarrow \infty$ would lead to $f_h = 2\mu$, the contribution of a fully occupied band. Instead, one rather employs eq. (2.94) in eq. (2.115). The $\ln \mathfrak{C}/c$ -term is given by (2.96). Now it is vital to use the full expression of eq. (2.96) (otherwise, the free energy would be a trivial constant - as is expected for the host in the limit $T \rightarrow 0$, since a crossover T_K is missing). These manipulations are conveniently done in Fourier space. The result for the eigenvalue $\Lambda_h(0)$ is

given in direct space:

$$\ln \Lambda_h(0) = \eta(0) + \frac{1}{2\pi} \int_{-\Lambda_c}^{\Lambda_c} \frac{1}{v^2 + 1/4} \ln [(1 + a(v))(1 + \bar{a}(v))] dv .$$

The functions a, \bar{a} are defined in eq. (2.89).

Observe the relation between the elementary excitation energy $\epsilon(v)$ and the momentum $k(v)$ as functions of the spectral parameter v (cf. eq. (2.92)),

$$\epsilon(v) = \frac{d}{dv} k(v) . \quad (2.116)$$

Then one confirms that $\lim_{\alpha \rightarrow \infty} \ln \Lambda_h(0) = -\beta f^{(ff)}$ contains the free-fermion contribution to the free energy per lattice site:

$$\begin{aligned} \epsilon(v) &= \frac{1}{v^2 + 1/4} \rightarrow k(v) = 2 \arctan 2v \\ \epsilon(k) &= 4 \cos^2 \frac{k}{2} = 2 \cos k + 2 \\ -\beta f_h &= 2\beta D + \frac{1}{2\pi} \int_{-k_F}^{k_F} \ln \left[1 + e^{-\beta(D(1+3/\alpha)\epsilon(k) - D\epsilon^2(k)/\alpha - h/2 - \mu)} \right] \\ &\quad \times \left[1 + e^{-\beta(D(1+3/\alpha)\epsilon(k) - D\epsilon^2(k)/\alpha + h/2 - \mu)} \right] dk . \end{aligned} \quad (2.117)$$

$$(2.118)$$

The function $k(v)$ in the first line is given by eq. (2.116). This is the free energy per site of the host, corresponding to eq. (2.42). From eq. (2.109), D gets arbitrarily large. This makes sense only for a linear dispersion in the host, while $\beta D \gg 1$. Then it suffices to keep only the leading orders in T^2, h^2 in f_h . The constant shift in the ground state energy is dropped. The linear dispersion approximation and the continuum limit are realized by a procedure similar to the analogous transformation of the Hamiltonian. Substitute $q_k = k/a_0, D = 1/a_0$. Then the *entire* free energy of the host, $F_h = L \cdot f_h$, results:

$$\begin{aligned} F_h &= -La_0 \lim_{\beta \gg 1} \frac{T}{2\pi} \int_{-k_F/a_0}^{k_F/a_0} \ln \left[1 + e^{-\beta(D' + \tilde{v}_F |q_k| - h/2 - \mu)} \right] \left[1 + e^{-\beta(D' + \tilde{v}_F |q_k| + h/2 - \mu)} \right] dq_k \quad (2.119) \\ D' &:= 2D \left(\left(1 + \frac{3}{\alpha} \right) (\cos k_F + 1) - \frac{2}{\alpha} (\cos k_F + 1)^2 \right) \\ \tilde{v}_F &= 2 \left(1 + \frac{3}{\alpha} - \frac{4}{\alpha} (\cos k_F + 1) \right) \sin k_F . \end{aligned}$$

$k_F \neq 0, \pi/2, \pi$. $La_0 = l$ is the length of the chain, it is kept constant. F_h/l then is the free energy density in the host. The diverging constant D' vanishes upon taking the derivative of eq. (2.119) in order to calculate static response functions. Note that interactions in the host of order $\mathcal{O}(1/\alpha)$ can be absorbed into a redefinition of $v_F = 2 \sin k_F$, resulting in effectively free fermions. This rescaling of the one-particle spectrum is very important: Including the order of spin-exchange coupling between impurity and host, the host is indeed free.

Strictly speaking, the Fermi sea separates into two parts for spin up and spin down particles, giving rise to four Fermi points $\pm k_F^{(\uparrow, \downarrow)}$. However, this modification is negligible in eq. (2.118): The Fermi points are scaled by $1/a_0$ in the continuum limit, eq. (2.119). The first contribution to the free energy is quadratic in h . More generally, we were justified to neglect $h \ll \mu$ in eq. (2.91): The leading order which enters the impurity equations is the second term in eq. (2.96), where h also enters quadratically.

The leading orders of the specific heat and magnetic susceptibility are

$$C_h(T) = T \frac{\pi^2}{3} \frac{2}{\pi \tilde{v}_F} =: T \frac{\pi^2}{3} \tilde{\rho}_h \quad (2.120)$$

$$\chi_h(T) = \frac{1}{4} \frac{2}{\pi \tilde{v}_F} =: \frac{1}{4} \tilde{\rho}_h. \quad (2.121)$$

An effective density of states per spin degree of freedom in the host, $\tilde{\rho}_h$, has been defined.

One may speculate whether a localized magnetic moment also shows up in the host, if at one lattice site the spectral parameter is shifted by iu_0 . Without calculating the corresponding Hamiltonian, we can exclude such a scenario: Insert eq. (2.105c) into (2.115). Then the leading orders of $\ln \mathfrak{B}$, $\ln \overline{\mathfrak{B}}$ cancel. This agrees with the intuitive picture that with four states per lattice site available in the host, a localized moment cannot form unless the doubly occupied state is suppressed.

Let us throw a view back and forward. Using four- and three-dimensional representations of $\mathfrak{gl}(2|1)$, an impurity model has been constructed on a lattice. The impurity site is realized by dimension three, whereas each host site has dimension four, thereby excluding double occupation on the former. The Hamiltonian contains four parameters, D, α, u_0, μ (and h , but this is not scaled). $0 < \mu < 4D$, so there are three independent parameters.

The model describes spin-1/2-fermions with a Hubbard and bond-charge interaction, interacting with the impurity site via hybridization and spin exchange. The hybridization can be suppressed in first order by a canonical transformation. The spin-exchange coupling J is much smaller than the bandwidth, $J \ll D$. Consistently, the dispersion relation of the host particles is linearized. This linearization is directly connected to the continuum limit. The result is the well known Kondo model: It describes an effectively free host with linear dispersion, interacting with a localized spin via spin exchange. The underlying symmetry of this model is $\mathfrak{su}(2)$, a sub-algebra of $\mathfrak{gl}(2|1)$. So one may view the Kondo model as an effective $\mathfrak{su}(2)$ continuum model of the underlying $\mathfrak{gl}(2|1)$ lattice model.

The exact solution reveals a scaling law which combines the parameters of the Hamiltonian in such a way that only T_K is constant, eq. (2.107). This means that only two of the three parameters are independent. In the solution, a relation between v_0 and α had to be required, $v_0 \sim \alpha^{1+\epsilon}$, which implies that D and α are independent. D is a scale of the whole Hamiltonian, and α tunes the interactions on the host. In other words, interactions in the host (which can be absorbed by a rescaling of the one-particle spectrum in the interesting order) and the spin-exchange coupling between impurity and host are determined by the same parameter. We postpone speculations about this issue to chapter 5.

The free energy both of the host and the impurity depend on two external parameters, T, h . Both are restricted by eq. (2.56), where T, h are small compared to the bandwidth D , a quantity induced by the host. This reduces the host to free fermions with linear dispersion, showing the common Fermi liquid properties. However, a crossover scale T_K is found which characterizes the behaviour of the impurity. Referring to this scale, $T, h \ll T_K$ and $T, h \gg T_K$ are to be distinguished, while eq. (2.56) is still obeyed. In the rest of this work, we will concentrate on the impurity; $T, h \ll T_K$ is denoted the regime of "low" temperatures/fields and $T, h \gg T_K$ is the range of "high" temperatures/fields.

Generalizations of that Kondo model have been proposed:

- i) The spin exchange may be generalized to XXZ type, of $U_q(\mathfrak{su}(2|1))$ symmetry, [90].
- ii) The localized impurity may a S -spin, corresponding to $2S + 1$ -dimensional representations of $U_q(\mathfrak{su}(2|1))$, [90].
- iii) The host may consist of m types of mutually non-interacting fermions, [91,92]. These m degrees of freedom are called "flavors" or "channels".

We suppose that it is possible to find an underlying lattice model to all these generalizations principally in a somehow similar manner as above. Item i) may be solved by considering $U_q(\mathfrak{gl}(2|1))$ as a possible symmetry instead of $\mathfrak{gl}(2|1)$ as for the isotropic case. The challenge of items ii) and iii) is the realization of higher dimensions in the impurity and host spaces. We leave these questions open as a playground for further work.

Nevertheless, we are able to treat the generalized models i)-iii) in the QTM framework, by setting up an effective $U_q(\mathfrak{su}(2))$ -symmetric QTM, without caring about the regularized underlying lattice. This approach results in NLIE for the impurity's degrees of freedom alone. This is shown in the next section.

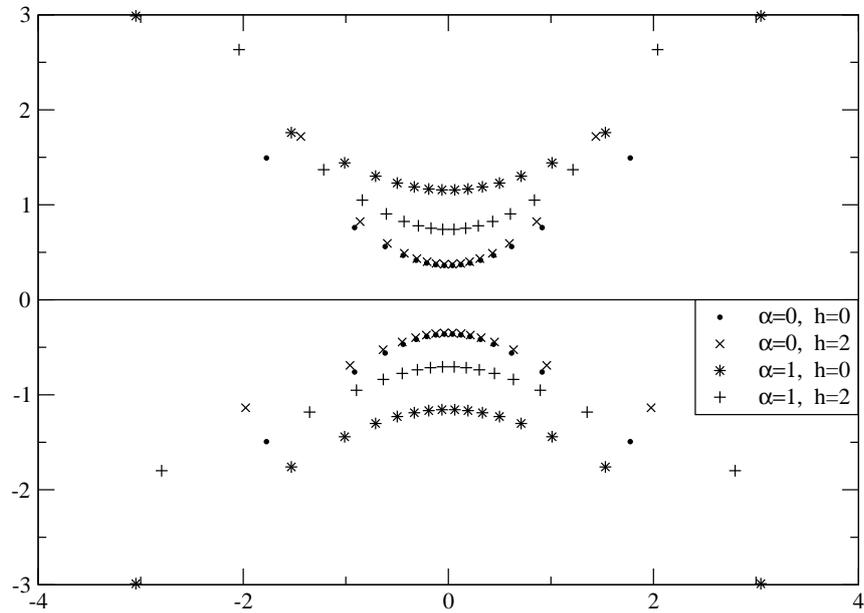


Figure 2.3: Particle solutions for two values of h and $\alpha > 0$ in the complex plane.

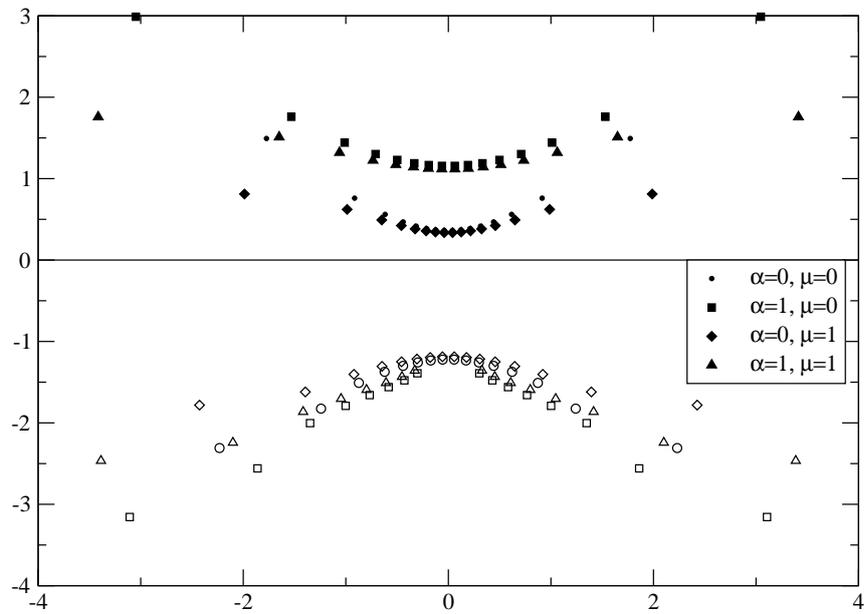


Figure 2.4: Particle (filled symbols) and hole (open symbols) solutions for two values of μ and $\alpha > 0$ in the complex plane.

2.2 Generalized models

The striking feature of eqs. (2.114a)-(2.114c) is that they can be obtained from the corresponding NLIE of the isotropic $S = 1/2$ Heisenberg model. Let us appreciate this delightful connection in detail. It allows to formulate the thermodynamics of the generalized models presented at the end of the preceding section in terms of a system of NLIE.

We proceed in two steps: The first part contains the explicit construction of the generalized models. Their free energy is obtained by diagonalizing a certain transfer matrix. This diagonalization is done in appendix A.4. NLIE are formulated in the second part.

2.2.1 Construction of the generalized models

The super-algebra $\mathfrak{gl}(1|2)$ possesses two even sub-algebras, $\mathfrak{u}(1)$ and $\mathfrak{su}(2)$. In the three-dimensional representation, these correspond - roughly speaking - to charge and spin degrees of freedom. The R -matrix belonging to the $S = 1/2$ representation of $\mathfrak{su}(2)$ reads

$$\begin{aligned} R^{(2,2)}(u) &= \frac{1}{u+1} \left(u + f_a^b \otimes f_b^a \right) \\ &= \frac{1}{u+1} \left(u + \frac{1}{2} (1 + 2\vec{S} \cdot \vec{\sigma}) \right). \end{aligned}$$

It acts in the direct product of 2-dimensional auxiliary and quantum spaces. $f_b^a = |b\rangle\langle a|$, $a, b \in \{1, 2\}$ denote the four non-vanishing matrix elements in the $S = 1/2$ representation of the three generators of $\mathfrak{su}(2)$

$$\begin{aligned} [S^z, S^\pm] &= \pm S^\pm & [S^+, S^-] &= 2S^z \\ [\sigma^z, \sigma^\pm] &= \pm 2\sigma^\pm & [\sigma^+, \sigma^-] &= \sigma^z. \end{aligned}$$

Note that the eigenvalues of S^z , σ^z are $\pm 1/2, \pm 1$. In the ongoing, we will express R by these operators rather than by the f_b^a . Applying the QTM-formalism to this model, one has to diagonalize the matrix defined in eq. (2.64), with $R^{(4,3)}$ interchanged by $R^{(2,2)}$ and an external field h coupling to the spin degree of freedom. Let us call this matrix $\tau_{xxx}(x)$; the spectral parameter is denoted by x . In appendix A.4, it is shown that the corresponding eigenvalue reads:

$$\begin{aligned} \Lambda_{xxx}(x) &= \lambda_-(x) + \lambda_+(x) & (2.122) \\ \lambda_-(x) &= \frac{q(x+i)}{q(x)} \phi_+(x) \phi_-(x-i) e^{\beta h/2} \\ \lambda_+(x) &= \frac{q(x-i)}{q(x)} \phi_-(x) \phi_+(x+i) e^{-\beta h/2} \\ \frac{q(x_k+i)}{q(x_k-i)} e^{-\beta h} &= -\frac{\phi_-(x_k) \phi_+(x_k+i)}{\phi_+(x_k) \phi_-(x_k-i)} \\ q(x) &= \prod_{j=1}^M (x - x_j), \quad \phi_\pm(x) = (x \pm iu)^{N/2}. \end{aligned}$$

$u = J\beta/N$, with the coupling constant J . The eigenvalue is the sum of two terms, corresponding to spin down and up. These are determined by one set of (real) BAN, guaranteeing analyticity. It is interesting to observe that eq. (2.122) follows from eq. (2.69) by $\mu \rightarrow \infty$: Then in eq. (2.69) the terms with $e^{\beta\mu}$ dominate exponentially, and the two (conjugate) sets of particle BAN shrink together

to only one, placed on the real axis. Applying techniques similar to section 2.1.3, one finds NLIE for the largest eigenvalue ($M = N/2$),

$$\begin{aligned}\ln \Lambda_{xxx}(x_0) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\cosh \pi(x-x_0)} \ln \mathfrak{A} \overline{\mathfrak{A}}(x) dx \\ \ln \mathfrak{a}(x) &= -\frac{J_{xxx}\beta}{\cosh \pi x} + \frac{\beta h}{2} + [k * \ln \mathfrak{A} - k_- * \ln \overline{\mathfrak{A}}](x).\end{aligned}\quad (2.123)$$

$k(x)$ is the kernel defined in eq. (2.113), and $k_{\pm} = k(x \pm i\pi)$. J_{xxx} is the coupling constant, and $\ln \overline{\mathfrak{A}}$ results from $\ln \mathfrak{A}$ by complex conjugation and $h \rightarrow -h$. One sees that we again arrived at eqs. (2.112a)-(2.112b), which can be scaled $x \rightarrow x - \frac{1}{\pi} \ln(2J_{xxx}\beta)$, $J_{xxx} \rightarrow \infty$ analogously, resulting in eqs. (2.114a)-(2.114c). Then $T_K = 2J_{xxx}e^{-\pi x_0}$ and $-\beta f_I = \ln \Lambda_{xxx}(x_0)$.

Thus it has been demonstrated that the NLIE of the $\text{su}(2)$ Heisenberg model can be mapped onto those of the impurity in the Kondo model. This relation was discovered heuristically in [60]. Since we did not employ any special features of the $S = 1/2$ representation, this mapping holds for general $\text{su}(2)$ symmetric matrices $R^{(d,d')}$ with arbitrary dimensions in auxiliary and quantum space. This will be exploited below. Without the background which leads to eqs. (2.114a)-(2.114c), this mapping is somehow unsatisfactory: The shift x_0 in Λ_{xxx} is introduced a posteriori. Neither the scaling of J_{xxx} , x_0 is justified by an underlying model.

This puzzle becomes even more exciting when one tries to map the TBA-equations by Tsvetick et al., [90], onto NLIE. In [90], a monodromy matrix is considered:

$$\begin{aligned}T^{(2,2)}(x, x_0) &= \hat{R}_{a,N}^{(2,2)}(x) \hat{R}_{a,N-1}^{(2,2)}(x) \dots \hat{R}_{a,1}^{(2,2)}(x) \\ \hat{R}_{a,j}^{(2,2)}(x) &= \rho \left(x + \frac{i}{2} \left(1 + 2\vec{S} \cdot \vec{\sigma} \right) \right).\end{aligned}\quad (2.124)$$

$\hat{R}^{(2,2)}$ differs from $R^{(2,2)}$ by the pre-factor. If ρ and x_0 are chosen appropriately,

$$\rho = e^{-iJ} \cos 2J, \quad x_0 = 1/g = 1/(\tan 2J), \quad (2.125)$$

then

$$\hat{R}_{a,j}^{(2,2)}(1/g) = e^{iJ\vec{\sigma}_a \otimes \vec{\sigma}_j}. \quad (2.126)$$

This is just the exponential of the impurity contribution to the Kondo Hamiltonian eq. (2.61), with an exchange constant J . In [90], it is shown by a coordinate BA that the logarithm of $T(x, x_0)$, eq. (2.124), includes the spectrum of the whole Hamiltonian in the linear dispersion approximation, eqs. (2.60), (2.61), under a further restriction on the host: The two-particle wave function of two host particles is factorizable in a charge-function f_c and a spin-function f_s . The product of both must be antisymmetric, such that (a : antisymmetric, s : symmetric) $f_c^{(a)} \cdot f_s^{(s)}$ and $f_c^{(s)} \cdot f_s^{(a)}$ are the two allowed combinations. In the coordinate BA, only the former combination is accounted for. Consequently, only half of the specific heat of the host is found; the susceptibility is reproduced correctly (because the symmetric spin function couples in the same way to the magnetic field as two separate spin-1/2-functions).

The spectrum can be calculated by BA techniques, and therefore also the thermodynamics by applying the TBA. One finally separates the impurity contribution from the host. The corresponding equations are formally equal to the TBA equations of the $S = 1/2$ $\text{su}(2)$ model, for a review, see [87]. The only difference is the spectral parameter dependent driving term: Instead of $-J\beta/\cosh x$, one finds $-2\mathcal{D}\beta \arctan e^x$. \mathcal{D} is some cutoff, related in an unknown manner to the bandwidth of the host.

Let us ask the question: What is the corresponding transfer matrix whose largest eigenvalue is given by the NLIE with precisely this driving term, $-2\mathcal{D}\beta \arctan e^x$, i.e.

$$-\beta f_I = \ln \hat{\Lambda}(x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\cosh(x+x_0)} \ln[\mathfrak{D}\overline{\mathfrak{D}}](x) dx \quad (2.127)$$

$$\ln \mathfrak{d}(x) = -2\mathcal{D}\beta \arctan e^x + \frac{\beta h}{2} + [k * \ln \mathfrak{D} - k_- * \ln \overline{\mathfrak{D}}](x). \quad (2.128)$$

The answer (to be derived later) is

$$\tau_{eff}^{(2,2)}(x=1/g) := \text{tr} \left\{ e^{-\beta h S_I^z / 2} \hat{R}_{I,N}^{(2,2)}(x) \dots \hat{R}_{I,1}^{(2,2)}(x) \Big|_{x=1/g} \right\}. \quad (2.129)$$

The external field h is included in the form of an imaginary twist angle, depending on the spin of the auxiliary space. The auxiliary space a is now the quantum space of the impurity. If one chooses $N = i\mathcal{D}\beta \in \mathbb{C}$, one arrives at eq. (2.128). These relations are quite appealing and suggest an intuitive path integral representation of the impurity. However, the host is by no means included in the effective matrix eq. (2.129). It is contained implicitly in a crucial manner: The prescription of taking the largest eigenvalue of τ_{eff} . To discover its real presence in the form of a linearized spectrum, the "detour" of section 2.1.2 is necessary. This is confirmed by the \mathcal{D} -cutoff scheme, in contrast to the D -scheme. Both are related non-trivially, as shown in section (3.2.1). τ defined in eq. (2.129) carries a subscript *eff* to make clear that it is an effective matrix, whose largest eigenvalue leads to the impurity contribution of the free energy.

At this point, it is well worth commenting on the formal equivalence of the NLIE for $\ln \mathfrak{a}$, $\ln \mathfrak{b}$, $\ln \mathfrak{d}$, which differ from each other only in the functional form of their x -dependent driving terms. This is not too surprising when remembering the functional form of the eigenvalue, resulting from ABA: It is the sum of terms λ_j , each one being a product of ϕ - and q -functions. The ϕ -functions are the vacuum eigenvalues, they are known. The q -functions originate in the creation operators acting on the vacuum, which are necessary to create the largest eigenvalue. They are unknown. The ϕ -functions lead to the driving terms, the q -functions to the convolutions. The convolutions provide the "dressing" of the driving terms. The contributions from ϕ - and q -functions separate because one treats the logarithms of the relevant equations. These become algebraic equations for the unknowns. The functional dependence of the eigenvalue on the q functions is exclusively determined by the underlying algebra, in the form of the YBE. The conclusion to be drawn is that within the same representation of the same algebra, the NLIE are formally identical, and different vacuum eigenvalues can be directly translated into different driving terms. Take eq. (2.128) as starting point. Then the driving term in the NLIE for the eigenvalue of $\tau_{xxx}(x)$ is

$$-N \arctan e^{x+u} + N \arctan e^{x-u} = -uN \frac{1}{\cosh x} + \mathcal{O}(Nu^2).$$

With $u = \beta/N$, next leading order terms vanish in the limit $N \rightarrow \infty$ and one is back at eq. (2.123).

Next we want to reveal that the mapping includes also the q -deformed algebra $U_q(\text{su}(2))$ with commutators

$$\begin{aligned} [S^z, S^\pm] &= \pm S^\pm; & [S^+, S^-] &= [2S^z] \\ [u] &= \frac{\sinh i\gamma u}{\sinh i\gamma}, \end{aligned} \quad (2.130)$$

The $S = 1/2$ dimensional $U_q(\text{su}(2))$ symmetric R -matrix reads with these operators

$$\hat{R}^{(2,2)}(x) = \rho \left[\sinh \left(x + i\frac{\gamma}{2} (1 + 2S^z \otimes \sigma^z) \right) + i \sin \gamma (S^- \otimes \sigma^+ + S^+ \otimes \sigma^-) \right].$$

$T(x)$ is defined as in eq. (2.124). Now

$$\begin{aligned}
\hat{R}_{I,j}^{(2,2)}(x_0) &= \exp \left[i \left(J_{\parallel} \sigma_I^z \otimes \sigma_j^z + 2J_{\perp} \left(\sigma_I^- \otimes \sigma_j^+ + \sigma_I^+ \otimes \sigma_j^- \right) \right) \right] \\
\cos \gamma &= \frac{\cos 2J_{\parallel}}{\cos 2J_{\perp}} \\
(\coth x_0)^2 &= \frac{\sin^2 2J_{\parallel}}{\sin 2(J_{\parallel} + J_{\perp}) \sin 2(J_{\parallel} - J_{\perp})} \\
\rho &= e^{-iJ_{\parallel}} \frac{\sinh x_0}{(\cosh^2 x_0 \cos^2 \gamma + \sinh^2 x_0 \sin^2 \gamma)^{1/2}}.
\end{aligned} \tag{2.131}$$

Eq. (2.131) induces an Ising like anisotropy. Without any further ado, we give the corresponding NLIE for $\gamma \leq \pi/2$, citing results for similar $U_q(\mathfrak{su}(2))$ models, [55]:

$$\begin{aligned}
-\beta f_I = \ln \hat{\Lambda}(x_0) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\cosh(x + \pi x_0/\gamma)} \ln \mathfrak{D} \overline{\mathfrak{D}}(x) dx \\
\ln \mathfrak{d}(x) &= -2\mathcal{D}\beta \arctan e^x + \frac{\beta h}{2(1 - \gamma/\pi)} + [k * \ln \mathfrak{D} - k_- * \ln \overline{\mathfrak{D}}](x) \\
\mathcal{F}_k[k(x)] &= \frac{\sinh \frac{\pi}{2} \left(\frac{\pi}{\gamma} - 2 \right) k}{2 \cosh \frac{\pi}{2} k \sinh \frac{\pi}{2} \left(\frac{\pi}{\gamma} - 1 \right) k}.
\end{aligned}$$

The crucial difference is the modified kernel, which is now γ -dependent and decays exponentially in direct space.

Generalizations of the $S = 1/2$ model are to include an arbitrary impurity spin S and an arbitrary "channel number" m of electronic channels. Mathematically speaking, this means to allow for arbitrary dimensions $l + 1, m + 1$ in the auxiliary and quantum spaces of \hat{R} , preserving $U_q(\mathfrak{su}(2))$ symmetry (which contains the isotropic case $\mathfrak{su}(2)$ through the limit $q \rightarrow 0$) and the YBE. The isotropic l, m models have been solved in the TBA approach, [90, 91, 92, 89]. The rest of this chapter is dedicated with the generalization of these models to the anisotropic case with $\gamma \leq \frac{\pi}{2\max(l,m)}$.

The R -operator, which is $U_q(\mathfrak{su}(2))$ symmetric with dimensions $l + 1, l = 2S$ of the auxiliary space and $m + 1$ of the quantum space is denoted by $\hat{R}^{(l,m)}(x)$. Let $\hat{R}^{(1,1)}$ act in $V_a \otimes V_q$, the direct product of auxiliary and quantum space. $V_q \simeq V_a \simeq \mathbb{C}^2$. Then $\hat{R}^{(l,m)}$ is constructed to fulfill the YBE with arbitrary dimensions in the involved spaces, eq. (2.2). This goal is achieved by fusing a lattice of $m \times l$ operators $\hat{R}^{(1,1)}$, by projectors P_a, P_q onto the subspaces of completely symmetric tensors in $V_{a_1} \otimes \dots \otimes V_{a_l}$ and $V_{q_1} \otimes V_{q_m}$. The result is [52]:

$$\begin{aligned}
\hat{R}^{(l,m)}(x) &= \rho(x) \left(A^{(l)} \otimes A^{(m)} \right) (P_a \otimes P_q) \prod_{j=1}^l \prod_{k=1}^m R_{a_j q_k}^{(1,1)}(x + i\gamma(1/2 + l - m - k - j)) \\
&\quad \times (P_a \otimes P_q) \left(A^{(l)-1} \otimes A^{(m)-1} \right) \\
A^{(l)} &= \sum_a |R_a|^{1/2} \mathcal{P}^{(a)} \\
\prod_{k < j} R_{a_k q_j}(i\gamma(k - j)) &=: \sum_a R_a \mathcal{P}^{(a)}.
\end{aligned} \tag{2.132}$$

The last equation defines R_a and $\mathcal{P}^{(a)}$. For $l = 1$, $\hat{R}^{(1,m)}$ is expressed through the generators of

$U_q(\mathfrak{su}(2))$,

$$\hat{R}^{(1,m)}(x) = \rho \left[\sinh \left(x + \frac{i\gamma}{2} (1 + 2S^z \otimes \sigma^z) \right) + i \sin \gamma (S^+ \otimes \sigma^- + S^- \otimes \sigma^+) \right]. \quad (2.133)$$

The algebra (2.130) implies the following explicit representations of S^- , S^+ , S^z :

$$S^- |k-1\rangle = \sqrt{[m-k+2][k-1]} |k\rangle, \quad k = 2, \dots, m+1 \quad (2.134a)$$

$$S^+ |k+1\rangle = \sqrt{[m-k+1][k]} |k\rangle, \quad k = 1, \dots, m \quad (2.134b)$$

$$S^z |k\rangle = \left(\frac{m}{2} - k + 1 \right) |k\rangle, \quad k = 1, m+1 \quad (2.134c)$$

In the isotropic case $\gamma = 0$,

$$\hat{R}^{(1,m)}(1/g) = \exp \left[i2J\vec{S} \otimes \vec{\sigma} \right] \quad (2.135)$$

$$\rho = e^{-iJ} \cos J(l+1), \quad g = \frac{2}{l+1} \tan J(l+1).$$

In eq. (2.135), one recognizes the spin-scattering between the impurity with spin $S = l/2$ and one electron. Unfortunately, one is, up to now, not able to write the general case, eq. (2.132), analogously. So we give a formal expression for the Hamiltonian density in analogy to the $l = m = 1$ case, namely

$$\mathcal{H} = \mathcal{H}_h + \mathcal{H}_{sd} + \mathcal{H}_{ex}$$

$$\mathcal{H}_h = -iDv_f \sum_{\nu, \sigma = \pm 1/2} \sum_{k=1}^m : \psi_{\nu, \sigma, k}^\dagger(x) \frac{d}{dx} \psi_{\nu, \sigma, k}(x) : \quad (2.136a)$$

$$\mathcal{H}_{sd} = -i\delta(x) \sum_{\nu, \sigma, \sigma'} : \psi_{\nu, \sigma}^\dagger(x) \left[\ln \hat{R}^{(l,m)}(x_0) \right]_{\sigma}^{\sigma'} \psi_{\nu, \sigma'}(x) : \quad (2.136b)$$

$$\begin{aligned} \mathcal{H}_{ex} = & -\mu \left[\sum_{\nu} \sum_{k=1}^m n_{\nu, k}(x) + \sum_{\tau=-S}^S n_{d, \tau} (1 - n_{d, \bar{\tau}}) \right] \\ & + \frac{\hbar}{2} \left[\sum_{\nu} \sum_{\sigma=-m/2}^{m/2} \sigma n_{\nu, \sigma}(x) + \sum_{\tau=-S}^S \tau n_{d, \tau} (1 - n_{d, \bar{\tau}}) \right] \end{aligned} \quad (2.136c)$$

$$n_{\nu, \sigma, k} := : \psi_{\nu, \sigma, k}^\dagger \psi_{\nu, \sigma, k} : , \quad n_{\nu, k} = \sum_{\sigma} n_{\nu, \sigma, k} , \quad n_{\nu, \sigma} = \sum_k n_{\nu, \sigma, k} .$$

$\nu = \pm$ denotes the handedness of host operators stemming from the right and left Fermi points respectively. $\sigma, \sigma' = -m/2, \dots, m/2$ in eqs. (2.136a), (2.136b). In eq. (2.136b), $\hat{R}^{(l,m)}$ is a matrix in auxiliary space with operator-valued entries in the (quantum) impurity space. Eqs. (2.136a), (2.136b) are unsatisfactory, in several regards:

- The details of spin exchange do not show up explicitly for $m > 1$, neither for $\gamma \neq 0$.
- The host is not understood at all. In the bulk, the m species, each of spin-1/2, are free. However, they form a totally symmetric fused state when interacting with the impurity, somehow glued together with an effective spin $m/2$: The quantum numbers σ, k are combined to a new "spin" number $\sigma \in [-m/2, m/2]$. This is justified mathematically to keep integrability; the physical reason (if there is one) is unclear up to now. Possibly, the indirect coupling between the electrons mediated by the impurity is so large at low temperatures that they are fused together. These

compound objects also couple with their effective spins to the magnetic field. This makes no difference in the susceptibility, but reduces the specific heat in comparison to free particles in m independent channels.

These questions are known since long [92] and as long remained open. To answer them, one should find a lattice path integral formulation in analogy to the $S = 1/2$, $m = 1$, $\gamma = 0$ case in section 2.1.2. We leave this task as a future challenge.

In the ongoing, eqs. (2.136a) and (2.136b) are taken as definitions of the S -spin, m -channel, anisotropic Kondo model. The chemical potential has no influence on the impurity's behaviour, so it is dropped. We will not bother about the normalizing factor $\rho(x)$ and omit it in the sequel, while keeping the same symbols for the non-normalized quantities. Fortunately, in order to diagonalize the corresponding transfer matrix

$$\begin{aligned} T_{eff}^{(l,m)}(x) &= e^{-\beta S^z/2} \hat{R}_{a,N}^{(l,m)}(x) \hat{R}_{a,N-1}^{(l,m)}(x) \dots \hat{R}_{a,1}^{(l,m)}(x) \\ \tau_{eff}^{(l,m)}(x) &= \text{tr}_a T^{(l,m)}(x), \end{aligned} \quad (2.137)$$

the full expression eq. (2.132) is not needed. Details of the diagonalization, which is done by ABA, can be found in appendix A.4.

In the ongoing discussion, we replace, for reasons of symmetry, x and each member in the set $\{x_\nu\}$ by

$$x - i\gamma/2. \quad (2.138)$$

This shift will be reversed after the calculation of the largest eigenvalue. In appendix A.4, it is shown that:

$$\begin{aligned} \Lambda^{(l)}(x) &= \sum_{j=1}^{l+1} \lambda_j^{(l)}(x) \\ &:= \sum_{j=1}^{l+1} e^{-\beta h(l+2-2j)/2} \prod_{p=1}^{j-1} \phi\left(x + \frac{i\gamma}{2}(1+l-m-2p)\right) \prod_{p=1}^{l-j+1} \phi\left(x + \frac{i\gamma}{2}(3+l+m-2p-2j)\right) \\ &\quad \times \frac{q\left(x + \frac{i\gamma}{2}(l+1)\right) q\left(x - \frac{i\gamma}{2}(l+1)\right)}{q\left(x + \frac{i\gamma}{2}(1+l-2j)\right) q\left(x + \frac{i\gamma}{2}(3+l-2j)\right)} \end{aligned} \quad (2.139)$$

With

$$\begin{aligned} \phi(x) &= \sinh^N(x) \\ q(x) &= \prod_{\nu=1}^{\mathcal{N}} \sinh(x - x_\nu) \\ \frac{\phi\left(x_\nu + \frac{i\gamma}{2}m\right)}{\phi\left(x_\nu - \frac{i\gamma}{2}m\right)} &= e^{\beta h} \prod_{\mu \neq \nu}^{\mathcal{N}} \frac{\sinh(x_\nu - x_\mu + i\gamma)}{\sinh(x_\nu - x_\mu - i\gamma)}. \end{aligned} \quad (2.140)$$

It is crucial to observe that $\Lambda^{(l)}(x)$ is analytic if the BAE (2.140) are fulfilled. To see this, set $x = x_\nu - i\gamma(l+1-2j)/2$. Then the j -th and the $j+1$ -st summand show poles, due to $q(x_\nu)$ in the denominator. The requirement that these poles cancel each other leads to eq. (2.140).

Before proceeding further, let us make three remarks:

- $\Lambda^{(l)}(x)$ is real-valued. Therefore observe that

$$\lambda_j^{(l)}(x) = \left[\lambda_{l-j+2}^{(l)} \right]^* ,$$

where * denotes complex conjugation.

- The ϕ -factors cause a zero of Λ in the strip of interest: It occurs for $m = l - 1$ at $x = 0$ and is of order N . Then all $\lambda_j^{(l)}$ have one factor in common, $\phi(x)$. Thus for $m = l - 1$,

$$\tilde{\Lambda}^{(l)}(x) := \Lambda^{(l)}(x)/\phi(x) \quad (2.141)$$

is analytic and non-zero (ANZ) for $\text{Im}x \in [-i\gamma/2, i\gamma/2]$. For $m \neq l - 1$, $\Lambda^{(l)}$ is ANZ for $\text{Im}x \in [-i\gamma/2, i\gamma/2]$. In the ongoing, $\tilde{\Lambda}^{(l)}$ denotes the zero-free eigenvalue.

- For the ongoing, it is important to define strips in the complex plane where the functions are ANZ.

$$\begin{array}{lll} \phi(x) & \text{ANZ} & -\pi < \text{Im}x < 0 \\ q(x) & \text{ANZ} & -\pi + \frac{\gamma}{2}(l-1) < \text{Im}x < -\frac{\gamma}{2}(l-1) \\ \tilde{\Lambda}^{(l)} & \text{ANZ} & -\frac{\gamma}{2} < \text{Im}x < \frac{\gamma}{2} \end{array}$$

The anisotropy parameter is restricted to

$$\gamma < \frac{\pi}{2 \max(m, l)} . \quad (2.142)$$

Then $q(x)$ is ANZ in a strip of maximal (minimal) width π ($\pi/2$), and centered symmetrically around $\text{Im}x = -\pi/2$.

2.2.2 Solution (NLIE)

One is interested in calculating the largest eigenvalue of the transfer matrix; it is given by $\mathcal{N} = N/2$ Bethe-*Ansatz* numbers $\{x_\nu\}$. As in the preceding section, it is possible to derive functional equations between certain auxiliary functions which, together with the analyticity properties of $\Lambda(x)$ itself, make it possible to set up non-linear integral equations, determining the largest eigenvalue.

In the following, the index m and the dependence on $\{x_\nu\}$ are not noted explicitly. By inserting explicit expressions, one shows that

$$\begin{aligned} \Lambda^{(1)}\left(x - \frac{i\gamma}{2}(l+1)\right) \Lambda^{(l)}(x) &= g^{(l)}(x) \Lambda^{(l-1)}\left(x + \frac{i\gamma}{2}\right) + \Lambda^{(l+1)}\left(x - \frac{i\gamma}{2}\right) \\ g^{(l)} &= \phi\left(x - \frac{i\gamma}{2}(l-m-1)\right) \phi\left(x - \frac{i\gamma}{2}(l+m+1)\right) . \end{aligned} \quad (2.143)$$

In [59], a similar case has been treated by complete induction. We borrow this idea and deduce from eq. (2.143) by complete induction the conversion relation

$$\begin{aligned} \Lambda^{(l)}\left(x + \frac{i\gamma}{2}\right) \Lambda^{(l)}\left(x - \frac{i\gamma}{2}\right) &= f^{(l)}(x) + \Lambda^{(l-1)} \Lambda^{(l+1)}(x) \\ f^{(l)} &= \lambda_1^{(l)}\left(x + \frac{i\gamma}{2}\right) \lambda_{l+1}^{(l)}\left(x - \frac{i\gamma}{2}\right) \\ &= \prod_{p=1}^l \phi\left(x + \frac{i\gamma}{2}(2+l+m-2p)\right) \phi\left(x + \frac{i\gamma}{2}(l-m-2p)\right) , \end{aligned} \quad (2.144)$$

where $f^{(l)}$ has the property that

$$f^{(l)}\left(x - \frac{i\gamma}{2}\right) f^{(l)}\left(x + \frac{i\gamma}{2}\right) = f^{(l-1)}(x) f^{(l+1)}(x).$$

Eq. (2.144) is proved by complete induction, following [59]. Consider the identity

$$\Lambda^{(l)}\left(x + \frac{i\gamma}{2}\right) \left[\Lambda^{(l-1)}(x) \Lambda^{(1)}\left(x - \frac{i\gamma}{2}\right) \right] = \left[\Lambda^{(l)}\left(x + \frac{i\gamma}{2}\right) \Lambda^{(l-1)}(x) \right] \Lambda^{(1)}\left(x - \frac{i\gamma}{2}\right).$$

The products in brackets can be treated by eq. (2.143), then one isolates $\Lambda^{(l)}\left(x + \frac{i\gamma}{2}\right) \Lambda^{(l)}\left(x - \frac{i\gamma}{2}\right)$ and substitutes eq. (2.144) with the shift $l \rightarrow l - 1$. Eventually, one ends up with eq. (2.144) itself. Note that these relations between the eigenvalues are equally valid for the corresponding matrices, since they commute, m being fixed.

The conversion relation converts shifts in l , that is the dimension of the auxiliary space, into shifts of the spectral parameter. It permits to formulate successively coupled functional equations for suitably chosen auxiliary functions y_l , Y_l , [63, 84].

$$\begin{aligned} y_l(x) &:= \frac{\Lambda^{(l-1)}(x) \Lambda^{(l+1)}(x)}{f^{(l)}(x)} \\ Y_l(x) &:= 1 + y_l(x) = \frac{\Lambda^{(l)}\left(x - \frac{i\gamma}{2}\right) \Lambda^{(l)}\left(x + \frac{i\gamma}{2}\right)}{f^{(l)}(x)} \end{aligned} \quad (2.145)$$

$$\Rightarrow Y_{l+1}(x) Y_{l-1}(x) = y_l\left(x - \frac{i\gamma}{2}\right) y_l\left(x + \frac{i\gamma}{2}\right) \quad (2.146)$$

It is crucial to observe that this Y -hierarchy can be closed. This was first done by Suzuki for the isotropic S -spin Heisenberg model, [84]. Closing the Y -hierarchy means that we can find convenient functions $\mathfrak{B}_l, \overline{\mathfrak{B}}_l$ and functionals F and G , such that $F[\mathfrak{B}_l, \overline{\mathfrak{B}}_l] = Y_l$ and $G[\mathfrak{B}_l, \overline{\mathfrak{B}}_l] = Y_{l-1}$. Then the equation

$$y_{l-1}(x - i\gamma/2) y_{l-1}(x + i\gamma/2) = F[\mathfrak{B}_l, \overline{\mathfrak{B}}_l] Y_{l-2}$$

is the last one in the Y -hierarchy. We show that

$$\begin{aligned} F[\mathfrak{B}_l, \overline{\mathfrak{B}}_l](x) &:= \mathfrak{B}_l(x) \cdot \overline{\mathfrak{B}}_l(x) \\ G[\mathfrak{B}_l, \overline{\mathfrak{B}}_l](x) &= \mathfrak{b}_l\left(x + \frac{i\gamma}{2}\right) \overline{\mathfrak{b}}_l\left(x - \frac{i\gamma}{2}\right) \end{aligned}$$

$\mathfrak{B}_l = 1 + \mathfrak{b}_l$, are suitable with

$$\mathfrak{B}_l(x) = \frac{\Lambda^{(l)}\left(x - \frac{i\gamma}{2}\right)}{\lambda_{l+1}^{(l)}\left(x - \frac{i\gamma}{2}\right)}, \quad \overline{\mathfrak{B}}_l(x) = \frac{\Lambda^{(l)}\left(x + \frac{i\gamma}{2}\right)}{\lambda_1^{(l)}\left(x + \frac{i\gamma}{2}\right)} \quad (2.147)$$

$$\mathfrak{B}_l \overline{\mathfrak{B}}_l = Y_l \quad (2.148)$$

Eq. (2.148) follows from eq. (2.147) by definition. It is this identity, eq. (2.148), which contains the closure of the Y -hierarchy. One should be aware of the analyticity properties of the different functions: The zero caused by the ϕ -functions in $\text{Im}x \in [-\gamma/2, \gamma/2]$ of $y_k(x)$ is located at $x = 0$, if $k = m$, and of order $2N$. Similarly, \mathfrak{b}_l possesses a zero of order N at $x = 0$, if $m = l$. Let us distinguish three cases:

- $m < l$: "Under-screening" of the impurity by the host. There are $l + 1$ unknown functions; the free energy results from the eigenvalue $\Lambda^{(l)}$.
- $m = l$: "Exact screening" with as many unknowns as in the under-screened case.
- $m > l$: "Over-screening". $m + 1$ auxiliary functions are needed. The equations are identical to the exactly screened case with $m + 1$ unknowns as shown later. The functional dependence of the eigenvalue on the auxiliary functions is different: The free energy is given by $\Lambda^{(l)}$, resulting from Y_l , eq. (2.145).

This means that we can close the Y -hierarchy with at least $\max(l, m) + 1$ functions. In the following, we set

$$l := \max(l, m) ,$$

so that we do not need to introduce a further index. Then the preceding derivation and analysis of $\Lambda^{(l)}$ holds for the general case.

Our choice to close the hierarchy after $l + 1$ equations is optimal in our approach, but it is not the only possibility. Indeed, the hierarchy may be closed after arbitrary many equations $l' > l$. Especially, $l' = \infty$ is permitted. In the isotropic case, this is just the set of TBA equations by [90]. In other words, fusion proves the equivalence of the NLIE approach with TBA results for $\gamma = 0$; for further details, cf. [46]. For $\gamma \neq 0$, the equivalence is not shown as easily: TBA is restricted to the "root of unity" case $2\gamma/\pi = \text{integer}$. At least for the spin- $\frac{1}{2}$ XXZ model, the equivalence has been shown in [64].

By inserting explicit expressions one furthermore finds

$$\begin{aligned} \mathfrak{b}_l(x) &= e^{\frac{\beta h}{2}(l+1)} \frac{q\left(x - \frac{i\gamma}{2}(l+2)\right)}{q\left(x + \frac{i\gamma}{2}l\right)} \frac{\phi\left(x - \frac{i\gamma}{2}(l-m)\right)}{\prod_{p=1}^l \phi\left(x + \frac{i\gamma}{2}(l-m-2p)\right)} \Lambda^{(l-1)}(x) \\ \bar{\mathfrak{b}}_l(x) &= e^{-\frac{\beta h}{2}(l+1)} \frac{q\left(x + \frac{i\gamma}{2}(l+2)\right)}{q\left(x - \frac{i\gamma}{2}l\right)} \frac{\phi\left(x + \frac{i\gamma}{2}(l-m)\right)}{\prod_{p=1}^l \phi\left(x + \frac{i\gamma}{2}(2+l+m-2p)\right)} \Lambda^{(l-1)}(x) \end{aligned}$$

\mathfrak{b}_l and $\bar{\mathfrak{b}}_l$ are related to Y_{l-1} by

$$\mathfrak{b}_l\left(x + \frac{i\gamma}{2}\right) \bar{\mathfrak{b}}_l\left(x - \frac{i\gamma}{2}\right) = Y_{l-1}(x) . \quad (2.149)$$

Employing the ANZ-property of $\Lambda^{(l)}$, it is possible to convert the functional relations into integral equations for the auxiliary functions, eliminating the unknown q -function. We list some properties of the auxiliary functions.

- \mathfrak{b}_l and $\bar{\mathfrak{b}}_l$ are related by complex conjugation and the substitution $\beta h \rightarrow -\beta h$. They approach constant values for $|x| \rightarrow \infty$:

$$\lim_{|x| \rightarrow \infty} \mathfrak{b}_l(x) = e^{\frac{\beta h}{2}(l+1)} \frac{\sinh \frac{\beta h l}{2}}{\sinh \frac{\beta h}{2}} \quad \lim_{|x| \rightarrow \infty} \bar{\mathfrak{b}}_l(x) = e^{-\frac{\beta h}{2}(l+1)} \frac{\sinh \frac{\beta h l}{2}}{\sinh \frac{\beta h}{2}} .$$

Therefore

$$\begin{aligned} \lim_{|x| \rightarrow \infty} \mathfrak{B}_l(x) &= e^{\frac{\beta h}{2}l} \frac{\sinh \frac{\beta h}{2}(l+1)}{\sinh \frac{\beta h}{2}} \\ \lim_{|x| \rightarrow \infty} Y_l(x) &= \lim_{|x| \rightarrow \infty} y_l(x) - 1 = \left[\frac{\sinh \frac{\beta h}{2}(l+1)}{\sinh \frac{\beta h}{2}} \right]^2 . \end{aligned}$$

- With a glance to eqs. (2.146), (2.149), it is possible to extract the functional form of the zeros in y_k , \mathfrak{b}_l , $\bar{\mathfrak{b}}_l$. Make use of

$$\tanh\left(ax - i\frac{\pi}{4}\right) \tanh\left(ax + i\frac{\pi}{4}\right) = 1, a \in \mathbb{R}. \quad (2.150)$$

By comparing with eq. (2.150), one recognizes that eqs. (2.146), (2.149) determine the functional form of the zeros uniquely:

$$y_k(x) =: \tanh^{2N}\left(\frac{\pi}{2\gamma}x\right) \tilde{y}_k(x), \mathfrak{b}_l(x) =: \tanh^N\left(\frac{\pi}{2\gamma}x\right) \tilde{\mathfrak{b}}_l(x) \quad (2.151)$$

\tilde{y}_k and $\tilde{\mathfrak{b}}_l$ are then free of zeroes in the strip of interest. One proceeds similarly with $\bar{\mathfrak{b}}_l$.

We now want to convert the functional relations into integral equations. Therefore, the logarithmic derivatives of the zero-free auxiliary functions and the eigenvalue are Fourier transformed (note that these display zero asymptotes for $|x| \rightarrow \infty$). The shifts in the arguments of the functions appear then as exponential pre-factors in Fourier-space, resulting into convolutions with exponentially decaying kernels in the direct space after transforming back and integrating twice, taking account of the known asymptotes. Explicitly, for the y -hierarchy one finds

$$\begin{aligned} \ln y_k(x) &= \delta_{k,m} 2N \ln \tanh\left(\frac{\pi}{2\gamma}x\right) + [s * (\ln Y_{k-1} + \ln Y_{k+1})](x), \quad k \leq l-2 \\ \ln y_k(x) &= \delta_{k,m} 2N \ln \tanh\left(\frac{\pi}{2\gamma}x\right) + [s * (\ln Y_{k-1} + \ln \mathfrak{B}_l \bar{\mathfrak{B}}_l)](x), \quad k = l-1 \\ s(x) &= \mathcal{F}_k \left[\frac{1}{2 \cosh \gamma k} \right] \end{aligned}$$

Next, remember the analyticity of $\tilde{\Lambda}^{(l)}(x)$ in the strip $\text{Im}x \in [-\gamma/2, \gamma/2]$. This means that $\ln \Lambda^{(l)}$ can equally be Fourier transformed along the two paths $x \pm i\gamma/2$,

$$e^{-\frac{\gamma}{2}k} \mathcal{F}_k \left[\ln \tilde{\Lambda}(x - i\gamma/2)' \right] = e^{\frac{\gamma}{2}k} \mathcal{F}_k \left[\ln \tilde{\Lambda}(x + i\gamma/2)' \right]. \quad (2.152)$$

Care has to be taken that the transforms of the different functions are done in their respective ANZ-domains. $q(x - i\gamma l/2)$, $q(x + i\gamma l/2)$ are ANZ in

$$\begin{aligned} -\pi + \gamma \left(l - \frac{1}{2} \right) &< x < \frac{\gamma}{2} \\ -\pi - \frac{\gamma}{2} &< x < -\gamma \left(l - \frac{1}{2} \right), \end{aligned}$$

respectively. To obtain a common ANZ strip with $\Lambda^{(l)}$, one shifts the argument $x + i\gamma l/2$ in the q -functions to $x + i(\gamma l/2 - \pi)$.

One expresses the brackets on the left-hand and right-hand site of eq. (2.152) in terms of $\mathcal{F}_k[\ln \mathfrak{B}'_l]$, $\mathcal{F}_k[\ln \bar{\mathfrak{B}}'_l]$, $\mathcal{F}_k[\ln \lambda']$ according to eqs. (2.147). In the resulting equation, the q functions are isolated and written in terms of $\mathcal{F}_k[\ln \mathfrak{B}'_l]$, $\mathcal{F}_k[\ln \bar{\mathfrak{B}}'_l]$, $\mathcal{F}_k[\ln \phi']$. One then takes the Fourier transform of the logarithmic derivative of \mathfrak{b}_l and inserts the expression for $\mathcal{F}_k[\ln q']$. One is left with

$$\mathcal{F}_k[\ln \mathfrak{b}'_l] = \frac{\sinh \frac{\pi - \gamma(l+1)}{2} k}{2 \cosh \frac{\gamma}{2} k \sinh \frac{\pi - \gamma l}{2} k} \left[\mathcal{F}_k[\ln \mathfrak{B}'_l] - e^{-\gamma k} \mathcal{F}_k[\ln \bar{\mathfrak{B}}'_l] \right] + \frac{1}{2 \cosh \frac{\gamma}{2} k} \mathcal{F}_k[\ln Y'_{l-1}] + \mathcal{F}_k[d'_\phi],$$

and similarly for $\ln \bar{\mathfrak{b}}_l$. The driving term $\mathcal{F}_k[d'_\phi]$ consists of the Fourier transforms of all ϕ -factors which appear in the above expression. They account for the zero of $\ln \mathfrak{b}_l$ and for the poles of the different functions. Being aware of the common strip of analyticity, they are contracted to $\mathcal{F}_k[\ln \tanh^{2N}(\pi/(2\gamma)x)]$. This result can be anticipated by eq. (2.151): The functional form of the zeroes is known. Thus

$$\begin{aligned} \ln \mathfrak{b}_l(x) &= \ln \tanh^N(\pi/(2\gamma)x) + \frac{\beta h}{2(1-l\gamma/\pi)} + [s * \ln Y_{l-1}](x) \\ &\quad + [k * \ln \mathfrak{B}_l](x) - [k * \ln \bar{\mathfrak{B}}_l](x - i\gamma + i\epsilon) \\ \ln \bar{\mathfrak{b}}_l(x) &= \ln \tanh^N(\pi/(2\gamma)x) - \frac{\beta h}{2(1-l\gamma/\pi)} + [s * \ln Y_{l-1}](x) \\ &\quad + [k * \ln \bar{\mathfrak{B}}_l](x) - [k * \ln \mathfrak{B}_l](x + i\gamma - i\epsilon) \\ k(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh \frac{\pi-\gamma(l+1)}{2}k}{2 \cosh \frac{\gamma}{2}k \sinh \frac{\pi-\gamma l}{2}k} e^{ikx} dk . \end{aligned}$$

Shifts by $\pm i\epsilon$ ensure integrability. They shall not be written down explicitly in the ongoing. The βh -dependent constant has been determined such that the asymptotes $x \rightarrow \infty$ are the same on both sides. These are discussed later. Finally, the largest eigenvalue is given by the regular part of the functions $\mathfrak{B}_l, \bar{\mathfrak{B}}_l$, (see eq. (2.147)). The non-regular terms are traced back to the fact that we operated with the non-normalized eigenvalue. So

$$\ln \Lambda(x) = [s * \ln \mathfrak{B}_l \bar{\mathfrak{B}}_l](x)$$

One now performs the shift $x \rightarrow x + i\gamma/2$ which reverses eq. (2.138). It is done simultaneously with the replacement $N = i\beta\mathcal{D}$. The equations rest the same, except the driving-term, which is converted to

$$\ln \tanh^N(\pi/(2\gamma)x) \rightarrow -2\mathcal{D}\beta \arctan e^{-\frac{\pi}{\gamma}x} .$$

Then the logarithm of the largest eigenvalue represents the free energy of the impurity f ,

$$\begin{aligned} \ln \Lambda(x_0) &= -\beta f_I \\ f_I &= -T \int_{-\infty}^{\infty} \frac{\ln[Y_{2S}](x)}{2\gamma \cosh \pi/\gamma(x-x_0)} dx . \end{aligned}$$

Lastly, rescale $x \rightarrow \gamma/\pi x$. After this substitution, the isotropic limit $\gamma \rightarrow 0$ can be directly carried out. Finally, by translation of the spectral parameter the bandwidth D can be absorbed. Substitute

$$x \rightarrow -x - \ln(2\mathcal{D}\beta) .$$

Then the limit $\mathcal{D} \rightarrow \infty$ can be taken, leaving $-e^x$ as spectral dependent driving term. Defining the temperature scale

$$T_K = 2\mathcal{D}e^{-\pi x_0/\gamma} , \tag{2.153}$$

one is left with the following system of NLIE ($l = \max(l, m)$):

$$\mathbf{y}(x) = \mathbf{d}(x) + [\hat{\mathbf{k}} * \mathbf{Y}](x) \quad (2.154)$$

$$\mathbf{y} := (\ln y_1, \ln y_2, \dots, \ln y_{l-1}, \ln \mathfrak{b}_l, \ln \bar{\mathfrak{b}}_l)^T$$

$$\mathbf{Y} := (\ln Y_1, \ln Y_2, \dots, \ln \mathfrak{B}_l, \ln \bar{\mathfrak{B}}_l)^T$$

$$\mathbf{d}(x) := \left(\begin{array}{cccccc} 0, 0, \dots, 0, & \underbrace{-e^x}_{m^{\text{th entry}}}, & 0, \dots, 0, & c\beta h, & -c\beta h & \end{array} \right)^T$$

$$\hat{\mathbf{k}}(x) = \left(\begin{array}{cccccc} 0 & s(x) & 0 & \dots & \dots & 0 \\ s(x) & 0 & s(x) & \dots & & \vdots \\ 0 & \ddots & \ddots & \ddots & & \dots 0 \\ 0 & \dots & s(x) & 0 & s(x) & s(x) \\ 0 & \dots & 0 & s(x) & k(x) & -k(x - i\pi) \\ 0 & \dots & 0 & s(x) & -k(x + i\pi) & k(x) \end{array} \right) \quad (2.155)$$

$$k(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh \frac{\pi}{2} k \left(\frac{\pi}{\gamma} - (l+1) \right)}{2 \cosh \frac{\pi k}{2} \sinh \frac{\pi}{2} k \left(\frac{\pi}{\gamma} - l \right)} e^{ikx} dk$$

$$\stackrel{\gamma \rightarrow 0}{=} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-\frac{\pi}{2} |k|}}{2 \cosh \frac{\pi k}{2}} e^{ikx} dk \quad (2.156)$$

$$s(x) = \frac{1}{2 \cosh x}$$

$$c = \frac{1}{2(1 - l\gamma/\pi)}$$

$$\stackrel{\gamma \rightarrow 0}{=} \frac{1}{2}.$$

The integration kernel k depends on the entire system size via l if $\gamma \neq 0$. The asymmetric driving term $-e^x$ in the m -th equation gives rise to different asymptotes in the limits $x \rightarrow \infty$, $x \rightarrow -\infty$. The $x \rightarrow -\infty$ asymptotes of the auxiliary functions can be read of their definition eqs. (2.145), (2.147). For $x \rightarrow \infty$, however, the exponentially large driving term in the m -th equation decouples the first $m-1$ equations from the last $l-m+1$ ones. Denote $\lim_{x \rightarrow \infty} \ln Y_j$ by $\ln Y_j^{(\infty)}$. The resulting system for the first $m-1$ functions

$$\ln y_j^{(\infty)} = \frac{1}{2} \ln Y_{j-1}^{(\infty)} Y_{j+1}^{(\infty)}$$

$$\ln y_1^{(\infty)} = \frac{1}{2} \ln Y_2^{(\infty)} \quad (2.157)$$

$$\ln y_{m-1}^{(\infty)} = \frac{1}{2} \ln Y_{m-2}^{(\infty)} \quad (2.158)$$

is solved by

$$Y_j^{(\infty)} = \left[\frac{\sinh(ja + b)}{\sinh a} \right]^2; \quad (2.159)$$

The constants a, b are determined by the boundary conditions eqs. (2.157), (2.158): $a = b = \frac{i\pi}{m+2}$.

Thus

$$Y_{j < m}^{(\infty)} = \left[\frac{\sin \frac{\pi}{m+2}(j+1)}{\sin \frac{\pi}{m+2}} \right]^2 \quad (2.160)$$

As to $j \geq m$, the system reads

$$\ln y_j^{(\infty)} = \frac{1}{2} \ln Y_{j-1}^{(\infty)} Y_{j+1}^{(\infty)} \quad (2.161a)$$

$$\ln Y_m^{(\infty)} = 0 \quad (2.161b)$$

$$\ln \mathfrak{b}_l^{(\infty)} = \frac{\beta h}{2(1 - \frac{\gamma}{\pi} l)} + \frac{1}{2} \ln Y_{l-1} + \frac{\ln \mathfrak{B}_l^{(\infty)} - \ln \overline{\mathfrak{B}}_l^{(\infty)}}{2} \frac{1 - \frac{\gamma}{\pi}(l+1)}{1 - \frac{\gamma}{\pi} l}. \quad (2.161c)$$

One remarks that there are $l - m + 1$ equations, formally identical to the $l + 1$ equations in the limit $x \rightarrow -\infty$. The Y -hierarchy, eq. (2.161a), is again solved by eq. (2.159), with different boundary conditions. Eq. (2.161b) leads to $b = a(1 - m)$. As to $\ln \mathfrak{B}_l$, we make the *ansatz*

$$\begin{aligned} \ln \mathfrak{B}_l^{(\infty)} &= \ln \left[e^{a(l-m)} \frac{\sinh a(l-m+1)}{\sinh a} \right] \\ \ln \mathfrak{b}_l^{(\infty)} &= \ln \left[e^{a(l-m+1)} \frac{\sinh a(l-m)}{\sinh a} \right], \end{aligned}$$

allowing for an effective rescaling of the magnetic field. Eq. (2.161c) is solved provided that

$$a = \frac{\beta h}{2(1 - \frac{\gamma}{\pi} m)}. \quad (2.162)$$

Note that since a depends on m and not on l , the relation $\mathfrak{B}_l \overline{\mathfrak{B}}_l = Y_l$, $l \geq m$, originating in the closure of the fusion hierarchy (eq. (2.148)) still holds. In the isotropic limit, the expressions reduce to:

$$\begin{aligned} Y_{j \geq m}^{(\infty)} &= \left[\frac{\sinh \frac{\beta h}{2}(j-m+1)}{\sinh \frac{\beta h}{2}} \right]_{h=0}^2 (j-m+1)^2 \\ \mathfrak{B}_{j \geq m}^{(\infty)} &= e^{\frac{\beta h}{2}(l-m)} \frac{\sinh \frac{\beta h}{2}(l-m+1)}{\sinh \frac{\beta h}{2}} \Big|_{h=0} l-m+1. \end{aligned}$$

The result implied by eq. (2.162) is a unique solution of the system (2.161a)-(2.161c), determining the only free parameter a . This is in contradiction with findings of Schlottmann, [79, 80].

The asymptotes are summarized in the following:

$$\begin{aligned}
\ln Y_j^{(-\infty)} &= 2 \ln \frac{\sinh \frac{\beta h}{2} (j+1)}{\sinh \frac{\beta h}{2}} \xrightarrow{\beta \rightarrow \infty} j \beta h & \ln Y_{j < m}^{(\infty)} &= 2 \ln \frac{\sin \frac{\pi}{m+2} (j+1)}{\sin \frac{\pi}{m+2}} \\
\ln \mathfrak{B}_l^{(-\infty)} &= \ln \left[e^{\frac{\beta h}{2} l} \frac{\sinh \frac{\beta h}{2} (l+1)}{\sinh \frac{\beta h}{2}} \right] \xrightarrow{\beta \rightarrow \infty} l \beta h & \ln Y_{j \geq m}^{(\infty)} &= 2 \ln \frac{\sinh \frac{\beta h}{2} (j-m+1)}{\sinh \frac{\alpha \beta h}{2}} \xrightarrow{\beta \rightarrow \infty} (j-m) \alpha \beta h \\
\ln \overline{\mathfrak{B}}_l^{(-\infty)} &= \ln \left[e^{-\frac{\beta h}{2} l} \frac{\sinh \frac{\beta h}{2} (l+1)}{\sinh \frac{\beta h}{2}} \right] \xrightarrow{\beta \rightarrow \infty} 0 & \ln \mathfrak{B}_l^{(\infty)} &= \ln \left[e^{\frac{\alpha \beta h}{2} (l-m)} \frac{\sinh \frac{\alpha \beta h}{2} (l-m+1)}{\sinh \frac{\alpha \beta h}{2}} \right] \\
\ln y_j^{(-\infty)} &= \ln \left(e^{\ln Y_j^{(-\infty)}} - 1 \right) \xrightarrow{\beta \rightarrow \infty} j \beta h & & \xrightarrow{\beta \rightarrow \infty} (l-m) \alpha \beta h \\
\ln \mathfrak{b}_l^{(-\infty)} &= \ln \left[e^{\frac{\beta h}{2} (l+1)} \frac{\sinh \frac{\beta h}{2} l}{\sinh \frac{\beta h}{2}} \right] \xrightarrow{\beta \rightarrow \infty} l \beta h & \ln \overline{\mathfrak{B}}_l^{(\infty)} &= \ln \left[e^{-\frac{\alpha \beta h}{2} (l-m)} \frac{\alpha \sinh \frac{\alpha \beta h}{2} (l-m+1)}{\sinh \frac{\alpha \beta h}{2}} \right] \xrightarrow{\beta \rightarrow \infty} 0 \\
\ln \overline{\mathfrak{b}}_l^{(-\infty)} &= \ln \left[e^{-\frac{\beta h}{2} (l+1)} \frac{\sinh \frac{\beta h}{2} l}{\sinh \frac{\beta h}{2}} \right] \xrightarrow{\beta \rightarrow \infty} -\beta h & \ln y_{j < m}^{(\infty)} &= \ln \left(e^{\ln Y_{j < m}^{(\infty)}} - 1 \right) \\
& & \ln y_{j \geq m}^{(\infty)} &= \ln \left(e^{\ln Y_{j \geq m}^{(\infty)}} - 1 \right) \xrightarrow{\beta \rightarrow \infty} (j-m) \alpha \beta h \\
& & \ln \mathfrak{b}_l^{(\infty)} &= \ln \left[e^{\frac{\alpha \beta h}{2} (l-m+1)} \frac{\sinh \frac{\alpha \beta h}{2} (l-m)}{\sinh \frac{\alpha \beta h}{2}} \right] \\
& & & \xrightarrow{\beta \rightarrow \infty} (l-m) \alpha \beta h \\
& & \ln \overline{\mathfrak{b}}_l^{(\infty)} &= \ln \left[e^{-\frac{\alpha \beta h}{2} (l-m+1)} \frac{\sinh \frac{\alpha \beta h}{2} (l-m)}{\sinh \frac{\alpha \beta h}{2}} \right] \\
& & & \xrightarrow{\beta \rightarrow \infty} -\alpha \beta h
\end{aligned} \tag{2.163}$$

with $\alpha = (1 - m\gamma/\pi)^{-1}$.

One is allowed to close the hierarchy after $l + n$ equations, n arbitrary, as was argued above. Especially, $n \rightarrow \infty$ is allowed. In the isotropic limit, this results in

$$\begin{aligned}
\ln Y_0 &= 0 \\
\ln y_j &= -\delta_{j,m} e^x + [s * \ln Y_{j-1} Y_{j+1}] (x) \\
\lim_{j \rightarrow \infty} \frac{\ln y_j}{j} &= \beta h \\
-\beta f_I &= \int_{-\infty}^{\infty} \frac{1}{2\pi \cosh \left(x + \ln \frac{T}{T_K} \right)} \ln Y_{2S}(x) dx .
\end{aligned} \tag{2.164}$$

These are the TBA equations, found by Tsvetick [89] for the isotropic spin- S , m -channel Kondo model. In contrast to the TBA approach, the system of NLIE comprises the same information in a finite set, namely $\max(l, m) + 1$ many, equations. This makes the latter formulation particularly useful for numerical calculations. As will be seen, also analytical investigations can be compactly performed.

Numerical calculations of the entropy, magnetization, specific heat and magnetic susceptibility are based on systems of NLIE for these quantities themselves - rather than taking numerical derivatives

of the free energy with respect to temperature or the magnetic field.

$$\begin{aligned} \mathbf{y}_\kappa^{(\nu)} &:= \left(y_{1,\kappa}^{(\nu)}, y_{2,\kappa}^{(\nu)}, \dots, y_{l-1,\kappa}^{(\nu)}, b_{l,\kappa}^{(\nu)}, \bar{b}_{l,\kappa}^{(\nu)} \right)^T \\ \mathbf{Y}_\kappa^{(\nu)} &:= \left(Y_{1,\kappa}^{(\nu)}, Y_{2,\kappa}^{(\nu)}, \dots, Y_{l-1,\kappa}^{(\nu)}, B_{l,\kappa}^{(\nu)}, \bar{B}_{l,\kappa}^{(\nu)} \right)^T \\ Y_{j,\kappa}^{(1)} &= \frac{y_j}{1+y_j} y_{j,\kappa}^{(1)} \end{aligned} \quad (2.165)$$

$$\begin{aligned} Y_{j,\kappa}^{(2)} &= \frac{y_j}{1+y_j} y_{j,\kappa}^{(2)} + \frac{y_j}{(1+y_j)^2} \left(y_{j,\kappa}^{(1)} \right)^2 \\ \mathbf{y}^{(\nu)} &= \mathbf{d}_\kappa^{(\nu)} + \hat{\mathbf{k}} * \mathbf{Y}^{(\nu)} \end{aligned} \quad (2.166)$$

The index κ stands for one of the symbols S, m, C, χ , abbreviating entropy, magnetization, specific heat, susceptibility, respectively. $f^{(\nu)}$ denotes the ν -th derivation of f with respect to the relevant parameter. $\nu = 1$ for $\kappa = S, m$ and $\nu = 2$ for $\kappa = C, \chi$.

$$\begin{aligned} \mathbf{d}_S^{(1)} &= (0, \dots, 0, \underbrace{-e^x}_{m^{\text{th entry}}}, 0, \dots, ch, -ch)^T \\ \mathbf{d}_m^{(1)} &= (0, \dots, 0, c, -c)^T \\ \mathbf{d}_C^{(2)} &= (0, \dots, 0)^T \\ \mathbf{d}_\chi^{(2)} &= (0, \dots, 0)^T \\ f(T, h) &= -T \int_{-\infty}^{\infty} \frac{1}{2\pi \cosh\left(x + \ln \frac{T}{T_K}\right)} \ln Y_{2S}(x) dx \\ S(T, h) &= \int_{-\infty}^{\infty} \frac{1}{2\pi \cosh\left(x + \ln \frac{T}{T_K}\right)} \left[\ln Y_{2S} - \beta Y_{2S,S}^{(1)} \right] (x) dx \\ m(T, h) &= \int_{-\infty}^{\infty} \frac{1}{2\pi \cosh\left(x + \ln \frac{T}{T_K}\right)} Y_{2S,m}^{(1)}(x) dx \\ C(T, h) &= \int_{-\infty}^{\infty} \frac{1}{2\pi \cosh\left(x + \ln \frac{T}{T_K}\right)} Y_{2S,C}^{(2)}(x) dx \\ \chi(T, h) &= \frac{1}{T} \int_{-\infty}^{\infty} \frac{1}{2\pi \cosh\left(x + \ln \frac{T}{T_K}\right)} Y_{2S,\chi}^{(2)}(x) dx \end{aligned} \quad (2.167)$$

Let us ask the question: Are the sets of NLIE (2.78a)-(2.78c) and (2.154) minimal in the sense that there does not exist a set containing less equations which exactly describes the thermodynamics?

Consider first eqs. (2.78a)-(2.78c). Eqs. (2.78a), (2.78b) are redundant: Eq. (2.78b) results from eq. (2.78a) by complex conjugation and negating $h \rightarrow -h$; there are only two independent NLIE. On the other hand, there are two independent sets of BAN, and therefore two unknown q -functions, namely q_+ and $q_+^{(h)}$. The two others, q_- and $q_-^{(h)}$, also result upon complex conjugation and $h \rightarrow -h$ from the former. So the set of eqs. (2.78a)-(2.78c) is minimal.

In the same spirit, eq. (2.154) constitutes a set of l seemingly independent equations. On the other hand, there is only one set of BAN, composed of l subsets. Each subset is characterized by the imaginary part of its members, eq. (A.78). Consequently, it should be possible to find only one equation which contains all information of the set eq. (2.154). This does not mean that such an

equation is better conditioned, especially for numerical investigations. Further exploration of this statement may be the task of future research.

For the time being, we will be content with the set of eqs. (2.154), obtained from closing the fusion hierarchy. These are as many equations as the maximum of the impurity's and host's degrees of freedom. In the next two chapters, they will be solved analytically in some limiting regions of the external parameters and numerically over the full parameter range.

Chapter 3

Analytical Investigation

The system of NLIE eq. (2.154) is analytically solvable in certain limiting ranges of the external parameters β , h . The natural scale for T given by eq. (2.167) is T_K . One expects a similar scale $T_h \propto T_K$, $T_h = \mathcal{O}(T_K)$ for h . These scales provide the reference points for high energies ($T, h \gg T_K$) or low energies ($T, h \ll T_K$).

The analytical investigations are carried out in two steps. The first part contains the discussion of low temperatures. In the second part, the limit of high temperatures is dealt with.

3.1 Low temperature evaluation

3.1.1 $2S = m$: Lowest orders

The first non-vanishing order in a low temperature, low field expansion of the free energy in the exactly screened case can be obtained by approximating the corresponding integral

$$\begin{aligned} \lim_{T, h \ll T_K} f_I(T, h) &= - \lim_{T, h \ll T_K} \frac{T}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\cosh\left(x + \ln \frac{T}{T_K}\right)} \ln [\mathfrak{B}_l \overline{\mathfrak{B}}_l](x) dx \\ &= - \frac{T^2}{\pi T_K} \int_{-\infty}^{\infty} e^x \ln [\mathfrak{B}_l \overline{\mathfrak{B}}_l](x) dx + \mathcal{O}\left(\frac{T^3}{T_K}\right) \end{aligned} \quad (3.1)$$

The temperature and the field are supposed to be small compared to T_K . The integral in eq. (3.1) exists if $\lim_{|x| \rightarrow \infty} \ln [\mathfrak{B}_l \overline{\mathfrak{B}}_l](x) = \mathcal{O}(e^{-x-\delta|x|})$, $\delta > 0$. Since $\ln \mathfrak{B}_l \overline{\mathfrak{B}}_l$ approaches a constant for $x \rightarrow -\infty$, this is a restriction on the behaviour in the region $x \rightarrow \infty$: An exponential decay only occurs for $l = m$, so that the validity of eq. (3.1) is restricted to the exactly screened case. The above approximation makes sense if $T \ll T_K$ (so that higher-order contributions can be neglected) and $h \ll T_K$. The latter condition follows since the largest error is certainly made in the region $x < 0$ of the integrand, where the constant asymptotes of $\ln \mathfrak{B}_l, \ln \overline{\mathfrak{B}}_l$ increase monotonously with βh . It is exciting to observe that with these approximations, the integral in eq. (3.1) can be done exactly, by a generalization of the method discovered in [58] and applied to the isotropic spin- S Heisenberg chain in [84].

In the notation of eq. (2.154), consider the integral

$$I(T, h) := \int_{-\infty}^{\infty} \left(\frac{d}{dx} \mathbf{y}(x) \right) \cdot \mathbf{Y}(x) - \mathbf{y}(x) \cdot \left(\frac{d}{dx} \mathbf{Y}(x) \right) dx. \quad (3.2)$$

First use the fact that the kernels are local and the auxiliary functions (symbolically denoted by f in

the following equation) have constant asymptotes:

$$\frac{d}{dx}[s * f](x) = [s * f'](x).$$

Secondly, one employs the symmetry of the integration kernels in the matrix \hat{k} , namely $\hat{k}(x - ia) = \hat{k}(-x + ia)$, $a \in \mathbb{R}$. It leads to the cancellation of all the convolutions in the integral eq. (3.2):

$$\begin{aligned} \int_{-\infty}^{\infty} \ln Y_j(x) [s * \ln Y_k'](x) dx &= \int_{-\infty}^{\infty} [s * \ln Y_j](x) (\ln Y_k)'(x) dx \\ \Rightarrow I(T, h) &= -2 \int_{-\infty}^{\infty} e^x \ln [\mathfrak{B}_m \bar{\mathfrak{B}}_m](x) dx - c\beta h (\ln \mathfrak{B}_m - \ln \bar{\mathfrak{B}}_m)_{-\infty}^{\infty} \\ &= -2 \int_{-\infty}^{\infty} e^x \ln [\mathfrak{B}_m \bar{\mathfrak{B}}_m](x) dx + c(\beta h)^2 m \end{aligned} \quad (3.3)$$

Thus

$$\lim_{T, h \ll T_K} f_I(T, h) = \frac{T^2}{2\pi T_K} I(T, h) - \frac{c}{2\pi T_K} h^2 l. \quad (3.4)$$

From eq. (3.2), it follows that $I(T, h) = I(T, -h)$. Here we restrict ourselves on the first non-vanishing orders in T, h , so that we set $I(T, h) = I(T, 0) + \mathcal{O}(h^2)$ in eq. (3.4) and neglect the term $\mathcal{O}(T^2 h^2)$. Then one finds a closed expression of the integral $I(T, 0) \equiv I(T)$, exploiting that the asymptotes of the auxiliary functions do not depend on βh : substitute $y := y_k(x)$, $b := \mathfrak{b}_m(x)$, $b := \bar{\mathfrak{b}}_m(x)$ in eq. (3.2), leading to

$$\begin{aligned} I(T) &= \sum_{k=1}^{m-1} \int_{y_k(-\infty)}^{y_k(\infty)} \frac{\ln(1+y)}{y} - \frac{\ln y}{1+y} dy + \int_{\mathfrak{b}_m(-\infty)}^{\mathfrak{b}_m(\infty)} \frac{\ln(1+b)}{b} - \frac{\ln b}{1+b} db \\ &\quad + \int_{\bar{\mathfrak{b}}_m(-\infty)}^{\bar{\mathfrak{b}}_m(\infty)} \frac{\ln(1+b)}{b} - \frac{\ln b}{1+b} db \\ &= \sum_{k=1}^{m-1} \left[\int_0^{y_k(\infty)} \frac{\ln(1+y)}{y} - \frac{\ln y}{1+y} dy - \int_0^{y_k(-\infty)} \frac{\ln(1+y)}{y} - \frac{\ln y}{1+y} dy \right] \\ &\quad - 2 \int_0^{\mathfrak{b}_m(-\infty)} \frac{\ln(1+b)}{b} - \frac{\ln b}{1+b} db. \end{aligned}$$

Since $h = 0$ here, $\mathfrak{b}_m(\pm\infty) = \bar{\mathfrak{b}}_m(\pm\infty)$. The crucial observation at this point is that

$$I(T) = 2 \cdot \sum_{k=1}^{m-1} [L_+(y_k(\infty)) - L_+(y_k(-\infty))] - 4L_+(\mathfrak{b}_m(-\infty)) \quad (3.5)$$

$$= -2 \cdot \sum_{k=1}^{m-1} \left[L\left(\frac{k(k+2)}{(k+1)^2}\right) - L\left(\frac{\sin \frac{\pi k}{m+2} \sin \frac{\pi(k+2)}{m+2}}{\sin^2 \frac{\pi(k+1)}{m+2}}\right) \right] - 4L\left(\frac{m}{1+m}\right). \quad (3.6)$$

Dilogarithm functions were identified; a good account is Lewin's book, [65]. $L_+(x)$ is related to Rogers' dilogarithm function by $L_+(x) = L\left(\frac{x}{1+x}\right)$,

$$\begin{aligned} L_+(x) &:= \frac{1}{2} \int_0^x \frac{\ln(1+y)}{y} - \frac{\ln y}{1+y} dy \\ L(x) &:= -\frac{1}{2} \int_0^x \frac{\ln(1-y)}{y} + \frac{\ln y}{1-y} dy \end{aligned}$$

In eq. (3.6), the asymptotic values $y_k(\pm\infty)$ and $\mathfrak{b}_m(\pm\infty)$ have been inserted explicitly. Ref. [51] contains a collection of relations satisfied by L , among which the following three are most useful in the present case:

$$\begin{aligned} L(x) + L(1-x) &= \frac{\pi^2}{6} \\ 2L\left(\frac{1}{m+1}\right) + \sum_k^{m-1} L\left(\frac{1}{(1+k)^2}\right) &= \frac{\pi^2}{6} \\ \sum_{k=1}^{m-1} L\left(\frac{\sin^2 \frac{\pi}{m+2}}{\sin^2 \frac{\pi(k+1)}{m+2}}\right) + \frac{\pi^2}{6} &= \frac{\pi^2}{6} \frac{3m}{m+2} \end{aligned}$$

Consequently,

$$I = -2\pi^2 \frac{m}{m+2}. \quad (3.7)$$

Combining results (3.3), (3.7), one gets the first term in an expansion of the free energy for low fields and temperatures:

$$\lim_{T,h \ll T_K} f(T, h) = -\frac{T^2}{\pi T_K} \int_{-\infty}^{\infty} e^x \ln [\mathfrak{B}_m \overline{\mathfrak{B}}_m](x) dx = -\frac{T^2}{2T_K} \frac{\pi m}{m+2} - \frac{m}{4(\pi - m\gamma)} \frac{h^2}{T_K}. \quad (3.8)$$

The anisotropy γ only enters through the βh -dependent driving terms in eq. (2.154).

From eq. (3.8),

$$\lim_{T,h \ll T_K} C(T) = \frac{T}{T_K} \frac{\pi m}{m+2} \quad \lim_{T,h \ll T_K} \chi(h) = \frac{1}{T_K} \frac{m}{2(\pi - m\gamma)}. \quad (3.9)$$

T_K is seen to be a normalized to the single-channel low temperature susceptibility, up to a factor of 2π . That's why it is referred to as "low temperature scale".¹

According to eq. (3.9), the impurity's contribution to the specific heat and magnetic susceptibility are Fermi liquid like at $T, h \ll T_K$ in the exactly screened case. This is the regime of "strong coupling": The anti-ferromagnetic spin exchange leads to the formation of a many particle state between the impurity and the host electrons, which screens the impurity's magnetic moment. Elementary excitations of this bound state are Fermi like. Nozières [69, 70] built up a phenomenological Fermi liquid theory to describe this regime.

This Fermi liquid behaviour is to be compared with the host, eqs. (2.120), (2.121). Since in the present context, the host consists of spin-1/2-fermions of m non-interacting channels (or of m flavors), the density of states is enhanced by a factor of m .

$$\lim_{T,h \rightarrow 0} C_h(T) = T \frac{m\pi^2}{3} \rho_h \quad \lim_{T,h \rightarrow 0} \chi_h(h) = \frac{m \rho_h}{4}. \quad (3.10)$$

Define the coefficient of the linear T -dependence of C_0 by δ_0 . The low-temperature Wilson ratio R is defined and calculated as

$$R := \lim_{T \rightarrow 0} \frac{\chi}{\chi_h} \frac{\delta_h}{\delta} = \frac{2(m+2)}{3(1 - m\frac{\gamma}{\pi})} \geq 2. \quad (3.11)$$

The lower bound 2 is reached for $m = 1$, $\gamma = 0$. The striking feature in comparing eqs. (3.9), (3.10) is that C is reduced by a factor of $3/(2m+4)$ in comparison to C_h , if the constant ρ_h is chosen such that $\chi = \chi_h$ for $\gamma = 0$. This may be interpreted by the localization of the impurity: Contrary to the host electrons, it does not move, so that the specific heat is reduced.

¹ T_K , defined by eqs. (2.107), (2.153), could have been found by scaling the (non-scaled) NLIE in the low-temperature limit and taking eq. (3.9) as definition.

3.1.2 Linearization for $T = 0$, $h \neq 0$

The limit $T \rightarrow 0$ can be performed by linearizing the NLIE for $h \neq 0$. From eqs. (2.163) one observes that if $h \neq 0$, in the limit $\beta \rightarrow \infty$ the asymptotic values in the limit $x \rightarrow -\infty$ of the auxiliary functions scale with βh , with one exception, namely $\ln \overline{\mathfrak{B}}_l$. In the limit $\beta \rightarrow \infty$, $\ln \overline{\mathfrak{b}}_l \ll 0$, so that

$$\lim_{\beta \gg 1} \ln \overline{\mathfrak{B}}_l = 0 + \mathcal{O}\left(e^{-\beta h}\right).$$

Thus one can neglect $\ln \overline{\mathfrak{B}}_l$ with exponential accuracy.

One introduces the scaling functions ϵ_j ,

$$\begin{aligned} \ln y_j(x) &=: \beta h K_m \epsilon_j(-x + \ln \beta h K_m) & j = 1, \dots, l-1 \\ \ln \mathfrak{b}_l(x) &=: \beta h K_m \epsilon_l(-x + \ln \beta h K_m). \end{aligned}$$

$\ln K_m$ is defined by the zero of $\ln y_m$,

$$\ln y_m(\ln \beta h K_m) = 0.$$

The shift in the spectral parameter is performed in order to deal with functions which have a zero in the origin,

$$\epsilon_m(0) = 0. \quad (3.12)$$

The ϵ -functions are inserted into the original set of NLIE. It is convenient to define a matrix \hat{A}^{-1} by its Fourier transform

$$\hat{A}_{i,j}^{-1}(k) := \begin{cases} 1 - \mathcal{F}_k[k] & i = j = l \\ \delta_{i,j} - \mathcal{F}_k[s](\delta_{i,j+1} + \delta_{i,j-1}) & \text{otherwise} \end{cases}. \quad (3.13)$$

In order to write the NLIE solely in terms of ϵ -functions, manipulate

$$\ln y = (\ln y - \ln Y) + \ln Y = -\ln\left(1 + e^{-\ln y}\right) + \ln\left(1 + e^{\ln y}\right).$$

Then the ϵ functions fulfill the equations

$$\begin{aligned} \left[\hat{A}_{ij}^{-1} * \frac{1}{\beta h K_m} \ln\left(1 + e^{\beta h K_m \epsilon_j}\right) \right] (x) &= -e^{-x} \delta_{i,m} + \frac{c}{K_m} \delta_{i,l} + \frac{1}{\beta h K_m} \ln\left(1 + e^{-\beta h K_m \epsilon_i(x)}\right) \\ c &= \frac{1}{2(1 - l\gamma/\pi)}. \end{aligned} \quad (3.14)$$

The logarithms can be linearized by noting that

$$\epsilon_j(x) \begin{cases} > 0, & x > \ln K_m; & j = m \\ < 0, & x < \ln K_m; & j = m \\ > 0; & & \text{otherwise} \end{cases}. \quad (3.15)$$

First consider the case $j > m$. Both asymptotic values of $\ln Y_j$ scale linearly with βh , such that one expects the whole function to do so. Explicitly, in the limit $\beta \rightarrow \infty$,

$$\lim_{\beta \gg 1} \ln\left(1 + e^{\beta h K_m \epsilon_{m < j \leq l}}\right) = \beta h K_m \epsilon_{m < j \leq l} + \mathcal{O}\left(e^{-\beta h}\right).$$

Because of the zero of ϵ_m ,

$$\begin{aligned} \ln \left(1 + e^{\beta h K_m \epsilon_m(x)} \right) &= \beta h K_m \epsilon_m(x) \theta(x) + \ln \left(1 + e^{-\beta h |\epsilon_m(x)|} \right) \\ &= \beta h K_m \epsilon_m(x) \theta(x) + \ln \left(1 + e^{-\beta h \epsilon'_m(0) |x|} \right) + \mathcal{O} \left(e^{-\beta h \epsilon''_m(0) x^2} \right) \\ &=: \beta h K_m \theta(x) \left(\epsilon_{m,0}(x) + \tilde{U}_m(x) \right) + \frac{\pi^2}{6} \frac{1}{\beta h K_m \epsilon'_m(0)} \delta(x). \end{aligned} \quad (3.16)$$

In the region around $x = 0$, the leading behaviour of $\epsilon_m(x)$ is expected to be given by its tangent,

$$\epsilon_m(x) = x \epsilon'_m(0) + \mathcal{O}(x^2 \epsilon''_m).$$

In eq. (3.16), a formal saddle-point approximation of the sharply peaked "integrand" $\left(1 + e^{-\beta h \epsilon'_m(0) |x|} \right)$ has been made, since it will be seen to occur exclusively in convolutions with local kernels. Lastly, $\epsilon_m = \epsilon_{m,0} + \tilde{U}_m$ is split into two functions. It has to be determined iteratively: First, the linearization

$$\ln \left(1 + e^{\beta h K_m \epsilon_m(x)} \right) = \beta h K_m \theta(x) \epsilon_{m,0}(x)$$

is made; in a second step, \tilde{U}_m is derived from the known $\epsilon_{m,0}$. We will see below that the first T -dependent correction to $\epsilon_{m,0}$ is of order $\mathcal{O}(T)$, such that it gives a contribution of $\mathcal{O}(T^2)$ in the free energy. The physical picture behind this formalism is intuitive: $\ln K_m$ is the "Fermi-point" which limits the "Fermi sea", completely filled for $T = 0$. Then the system is described by the "bare" energy function $\epsilon_{m,0}$. The sharp cutoff is softened with increasing temperature, the "bare" functions becoming "dressed" to ϵ_m . This dressed energy picture is common in the low-temperature description of integrable models, see [45, 48].

If $j < m$, one proceeds somehow similarly,

$$\begin{aligned} \ln \left(1 + e^{\beta h K_m \epsilon_j(x)} \right) &= \beta h K_m \epsilon_j(x) \theta(x) + \ln \left(1 + e^{-\beta h K_m \epsilon'_j(0) x} \right) \theta(x) + \ln \left(1 + e^{\beta h K_m \epsilon_j(x)} \right) \theta(-x) \\ &= \beta h K_m \theta(x) \left(\epsilon_{j,0}(x) + \tilde{U}_j(x) \right) + \ln Y_m^{(\infty)} \theta(-x). \end{aligned} \quad (3.17)$$

However, the last summand does not scale with βh , but is rather constant in the limit $x \rightarrow -\infty$. Contrary to $\epsilon_m(x)$, which has a zero at $x = 0$ with known derivative, the $\beta h \epsilon_{j < m}(x)$ show step-like behaviour, with constant, i.e. non βh -dependent asymptotes at $-\infty$. In order to consistently linearize the whole system of auxiliary functions, let us set

$$\lim_{x \ll 0} \epsilon_{j < m,0}(x) \equiv 0. \quad (3.18)$$

By doing so, one has to accept that for the function $\epsilon_{j < m}$, the first correction to $\epsilon_{j,0}$ is of constant order, giving a contribution $\mathcal{O}(T)$ to the free energy. Higher orders for $j < m$ need the knowledge of the functions around the origin (especially $\epsilon'_j(0^+)$), where the "crossover" from constant behaviour to βh -scaling takes place. The analysis of this nonlinear dependence is beyond the scope of this work and will not pursued further here. Nonetheless, one can treat the first T -dependent contribution to the specific heat for $2S \geq m$ by formally dealing with the second derivative of the NLIE with respect to T .

For further calculations, we introduce the shorthand-notations

$$\epsilon_j(x) \theta(x) =: \epsilon_j^+(x), \quad \epsilon_j(x) \theta(-x) =: \epsilon_j^-(x)$$

for functions in direct space. Their Fourier transforms are denoted as

$$\begin{aligned}\mathcal{F}_k[\epsilon_j^+] &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \epsilon_j^+(x) e^{ikx} dx \\ &=: \epsilon_j^+(k),\end{aligned}$$

where the index $+$ denotes analyticity in the upper half of the complex k -plane. Note that the Fourier transform is defined with changed "-"-signs compared to eq. (2.73). Then the system (3.14) is, up to the indicated orders, written as

$$\begin{aligned}j < m : \quad & \epsilon_{j,0}^+(k) + \tilde{U}_j^+(k) + \hat{A}_{j,m}(k) \left(\epsilon_{m,0}^-(k) + \tilde{U}_m^-(k) \right) + \frac{\ln Y_j^{(\infty)}}{\beta h K_m} \mathcal{F}_k[\theta(-x)] \\ &= \hat{A}_{j,m}(k) d_m(k) + \hat{A}_{j,l}(k) \frac{c}{K_m} + \frac{1}{\beta h K_m} \sum_{p=1}^{m-1} \hat{A}_{jp}(k) \ln Y_p^{(\infty)} \mathcal{F}_k[\theta(-x)] \\ j \geq m : \quad & \epsilon_{j,0}^+(k) + \epsilon_{j,0}^-(k) \delta_{j>m} + \tilde{U}_m^+(k) \delta_{j,m} + \hat{A}_{j,m}(k) \left(\epsilon_{m,0}^-(k) + \tilde{U}_m^-(k) \right) + \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} \delta(k) \\ &= \hat{A}_{j,m}(k) d_m(k) + \hat{A}_{j,l}(k) \frac{c}{K_m} + \hat{A}_{j,m}(k) \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} \\ &+ \frac{1}{\beta h K_m} \sum_{p=1}^{m-1} \hat{A}_{jp}(k) \ln Y_p^{(\infty)} \mathcal{F}_k[\theta(-x)] \quad .\end{aligned}\tag{3.19}$$

$d_m(k) := \mathcal{F}_k[-e^{-x}]$ has been defined, the inverse of \hat{A}^{-1} is calculated below.

Define a new energy scale

$$T_h := \frac{T_K}{K_m}.\tag{3.20}$$

Then in complete analogy, the free energy is given by

$$\lim_{\beta \rightarrow \infty} f(\beta, h) = -\frac{h K_m}{2\pi} \int_0^{\infty} \frac{1}{\cosh\left(x + \ln \frac{h}{T_h}\right)} \epsilon_{l,0}(x) dx + \Delta f_l(T, h) \delta_{l \geq m}.$$

By the same reasons as described previously, we are able to calculate the first T -correction to $f(T=0, h)$ only for $l \geq m$.

We begin with the calculation of $\epsilon_{j,0}$. Until the calculation of $\tilde{U}_m(x)$, the index 0 is suppressed, $\epsilon_{j,0} =: \epsilon_j$.

The free energy is only h -dependent,

$$\begin{aligned}f(h) &= -\frac{h K_m}{2} \int_{-\infty}^{\infty} \frac{1}{\cosh \frac{\pi k}{2}} \epsilon_l(k) e^{-ik \ln \frac{h}{T_h}} dk \\ M(h) &= -\frac{\partial f(h)}{\partial h} \\ &= \frac{K_m}{2} \int_{-\infty}^{\infty} \frac{1 - ik}{\cosh \frac{\pi k}{2}} \epsilon_l(k) e^{-ik \ln \frac{h}{T_h}} dk.\end{aligned}\tag{3.21}$$

We aim at calculating the magnetization.

Under-screened and exactly screened cases, $l \geq m$

First consider the case $l > m$. The resulting linear system is written in a compact form:

$$\begin{aligned}\bar{\epsilon}(k) &:= (\mathcal{F}_k[\epsilon_1^+], \dots, \mathcal{F}_k[\epsilon_m^+], \mathcal{F}_k[\epsilon_{m+1}], \dots, \mathcal{F}_k[\epsilon_l])^T \\ &=: (\epsilon_1^+(k), \dots, \epsilon_m^+(k), \dots, \epsilon_l(k))^T \\ \vec{d}(k) &:= \left(0, \dots, 0, \underbrace{d_m(k) - \mathcal{F}_k[\epsilon_m^-]}_{m^{\text{th}} \text{entry}}, 0, \dots, \frac{c}{K_m} \delta(k) \right) \\ \bar{\epsilon}(k) &= \hat{A}(k) \cdot \vec{d}(k).\end{aligned}\tag{3.22}$$

All $\epsilon_j^{(+)}$ now can be expressed in terms of ϵ_m^- and the driving terms. The matrix $\hat{A}^{-1}(k)$ is inverted to give a matrix $\hat{A}(k)$ with elements

$$[\hat{A}(k)]_{i,j} = \frac{1}{\det \hat{A}^{-1}(k)} \alpha_{i,j}(k),\tag{3.23}$$

$\alpha_{i,j}$ being the adjunct to $[\hat{A}^{-1}]_{i,j}$ in $\det \hat{A}^{-1}$. Both quantities are seen to satisfy recursion relations, which can be solved by applying the Z -transformation. In appendix B.1, one finds:

$$\begin{aligned}\det \hat{A}(k) &= \frac{\sinh \frac{\pi}{\gamma} \frac{\pi k}{2}}{(2 \cosh \frac{\pi k}{2})^l \sinh \left(\frac{\pi}{\gamma} - l \right) \frac{\pi k}{2}} \\ \hat{A}_{j,j}(k) &= \frac{2 \cosh \frac{\pi k}{2} \sinh j \frac{\pi k}{2} \sinh \left(\frac{\pi}{\gamma} - l \right) \frac{\pi k}{2}}{\sinh \frac{\pi k}{2} \sinh \left(\frac{\pi}{\gamma} - (l - j) \right) \frac{\pi k}{2}}, \quad j < l \\ \hat{A}_{j,l}(k) &= \frac{2 \cosh \frac{\pi k}{2} \sinh j \frac{\pi k}{2} \sinh \left(\frac{\pi}{\gamma} - l \right) \frac{\pi k}{2}}{\sinh \frac{\pi k}{2} \sinh \frac{\pi}{\gamma} \frac{\pi k}{2}}\end{aligned}\tag{3.24}$$

Other matrix elements are not needed. Then

$$\frac{\epsilon_m^+(k)}{\hat{A}_{m,m}(k)} = -\epsilon_m^-(k) + d_m(k) + \frac{\hat{A}_{m,l}(k)}{\hat{A}_{m,m}(k)} \frac{c}{K_m} \delta(k)\tag{3.25}$$

$$\epsilon_l(k) = \frac{\hat{A}_{m,l}(k)}{\hat{A}_{m,m}(k)} \epsilon_m^+(k) + \left(\hat{A}_{l,l}(k) - \frac{\hat{A}_{m,l}^2(k)}{\hat{A}_{m,m}(k)} \right) \frac{c}{K_m} \delta(k).\tag{3.26}$$

Eq. (3.25) is solved by observing that $\hat{A}_{m,m}$ can be factorized into two functions G_{\pm} , G_+ (G_-) being analytic in the upper (lower) half of the complex k -plane. This factorization is done using

$$\begin{aligned}\Gamma\left(\frac{1}{2} + ik\right) \Gamma\left(\frac{1}{2} - ik\right) &= \frac{\pi}{\cosh \pi k} \\ \Gamma(1 + ik) \Gamma(1 - ik) &= \frac{\pi k}{\sinh \pi k}.\end{aligned}$$

Then one finds

$$\begin{aligned}\hat{A}_{m,m}(k) &= G_+(k) G_-(k) \\ G_+(k) &= \left(\frac{2\pi m \left(1 - \frac{\gamma}{\pi} l\right)}{1 - \frac{\gamma}{\pi} (l - m)} \right)^{\frac{1}{2}} \frac{\Gamma\left(1 - i\frac{k}{2}\right) \Gamma\left(1 - i\frac{k}{2} \left(\frac{\pi}{\gamma} - (l - m)\right)\right)}{\Gamma\left(\frac{1}{2} - i\frac{k}{2}\right) \Gamma\left(1 - im\frac{k}{2}\right) \Gamma\left(1 - i\frac{k}{2} \left(\frac{\pi}{\gamma} - l\right)\right)} e^{-iak} \\ G_-(k) &= G_+(-k).\end{aligned}\tag{3.27}$$

The constant a is chosen such that $\lim_{|k| \rightarrow \infty} G_{\pm}(k) = 1$. It is not explicitly determined here, but later in the isotropic limit $\gamma \rightarrow 0$. Consider the derivative of eq. (3.25) with respect to the spectral parameter in direct space (the constant then vanishes). We find

$$\mathcal{F}_k [(\epsilon_m^+)]' = -\frac{1}{2\pi i} \frac{G_+(k) G_-(-i)}{k + i}\tag{3.28}$$

$$\epsilon_m^+(x) = \int_0^x (\epsilon_m^+)'(x') dx'\tag{3.29}$$

$$\epsilon_m^+(k) = \frac{1}{2\pi} \frac{G_+(k) G_-(-i)}{(k + i0^+)(k + i)}.$$

Eq. (3.29) follows since $\epsilon_m(x = 0) = 0$. The constant K_m can be determined from its defining property $\epsilon_m(x = 0) = 0$ in direct space. From eq. (3.25), one calculates $\epsilon_m(x = 0) = \int_{-\infty}^{\infty} \epsilon_m(k) dk$.

$$\begin{aligned}0 &= \int_{-\infty}^{\infty} \frac{\epsilon_m^+(k)}{\hat{A}_{m,m}(k)} dk - \int_{-\infty}^{\infty} \epsilon_m^+(k) dk - \int_{-\infty}^{\infty} d_m(k) dk - \frac{\hat{A}_{m,l}(0)}{\hat{A}_{m,m}(0)} \frac{c}{K_m} \\ \int_{\mathcal{C}_-} \frac{\epsilon_m^+(k)}{\hat{A}_{m,m}(k)} dk &= -1 + \frac{G_-(-i)}{G_-(0)} \int_{\mathcal{C}_+} \epsilon_m^+(k) dk = 0 \quad \int_{\mathcal{C}_-} d_m(k) dk = 1 \\ K_m &= c \frac{\hat{A}_{m,l}(0)}{\hat{A}_{m,m}(0)} \frac{G_-(0)}{G_-(-i)}.\end{aligned}\tag{3.30}$$

The integrals are done by closing the integration contour over the upper (\mathcal{C}_+) or lower (\mathcal{C}_-) half plane. One is now ready to compute ϵ_l in Fourier space, by inserting ϵ_m in eq. (3.26).

$$\epsilon_l(k) = \frac{\sinh \frac{\pi k}{2} \left(\frac{\pi}{\gamma} - (l - m)\right)}{\sinh \frac{\pi k}{2} \frac{\pi}{\gamma}} \epsilon_m^+(k) + \left(A_{ll}(0) - \frac{A_{m,l}^2(0)}{A_{m,m}(0)} \right) \frac{c}{K_m}$$

The magnetization is written down from eq. (3.21),

$$\begin{aligned}M(h) &= \frac{K_m}{2} \frac{G_-(-i)}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh \frac{\pi k}{2} \left(\frac{\pi}{\gamma} - (l - m)\right)}{\cosh \frac{\pi k}{2} \sinh \frac{\pi k}{2} \frac{\pi}{\gamma}} \frac{iG_+(k)}{k + i0^+} e^{-ik \ln \frac{h}{T_h}} dk \\ &\quad + \frac{c}{2} \left(\hat{A}_{ll}(0) - \frac{\hat{A}_{m,l}^2(0)}{\hat{A}_{m,m}(0)} \right) \\ &= \frac{m}{4\pi^{3/2}} \left(1 - \frac{\gamma}{\pi} (l - m) \right) \int_{-\infty}^{\infty} i \frac{\Gamma\left(\frac{1}{2} + i\frac{k}{2}\right) \Gamma\left(1 + i\frac{\pi k}{2\gamma}\right) \Gamma\left(1 - i\frac{k}{2}\right) \Gamma\left(1 - i\frac{\pi k}{2\gamma}\right)}{\Gamma\left(1 + i\frac{k}{2} \left(\frac{\pi}{\gamma} - (l - m)\right)\right) \Gamma\left(1 - i\frac{mk}{2}\right) \Gamma\left(1 - i\frac{k}{2} \left(\frac{\pi}{\gamma} - l\right)\right)} \\ &\quad \times e^{-iak} \frac{e^{-ik \ln \frac{h}{T_h}}}{k + i0^+} dk + \frac{l - m}{2} \left(1 + m \frac{\gamma}{\pi} \right).\end{aligned}\tag{3.31}$$

$$\tag{3.32}$$

The integral can be calculated by closing the contour in the lower ($h > T_h$) or in the upper ($h < T_h$) half plane. This results in two power series in T_h/h for $h > T_h$ and in h/T_h for $h < T_h$ with integer and non-integer powers, depending on the poles of the integrand. Although the determination of the residuals is straightforward, we do not write down the power series here; it is quite lengthy and does not give more physical insight. It is interesting however to extract the asymptotic behaviour for $h \ll T_h$, $h \gg T_h$. In the latter case, the pole at $k_0 := -i0^+$ contributes,

$$M(h) \rightarrow \begin{cases} \frac{l-m}{2} (1 + m\frac{\gamma}{\pi}) + \mathcal{O}\left(\left(\frac{h}{T_h}\right)^{2\gamma/\pi}\right), & h \ll T_h \\ \frac{l}{2} + \mathcal{O}\left(\left(\frac{h}{T_h}\right)^{-2\gamma/\pi}\right), & h \gg T_h \end{cases} \quad (3.33)$$

Thus for $h = 0$, a non-integer rest-spin remains in the case $\gamma \neq 0$, $l > m$ and h -dependent corrections are of non-integer powers of h . This is in qualitative agreement with [79,80], who investigated the same model by TBA-techniques. However, there is quantitative disagreement in the non-integer pre-factor. It remains to be explored how this disagreement, which already appeared in the asymptotes of the auxiliary functions, eq. (2.163), is solved. In [79,80], the non-integer rest spin is traced back to a quantum critical point at $T = 0$, $H = 0$ for the anisotropic over-screened model. We will come back to this picture later.

In the isotropic limit $\gamma \rightarrow 0$

$$\begin{aligned} \lim_{\gamma \rightarrow 0} G_+(k) &= \sqrt{2\pi m} \frac{\Gamma(1 - i\frac{k}{2})}{\Gamma(\frac{1}{2} - i\frac{k}{2}) \Gamma(1 - i\frac{km}{2})} \left(\frac{-ikl}{2e}\right)^{-i\frac{kl}{2}} \left(\frac{-ik(l-m)}{2e}\right)^{\frac{ik(l-m)}{2}} e^{-iak} \\ a &= \frac{1}{2} (m \ln m - l \ln l + (l-m) \ln(l-m) - m) < 0 \\ \lim_{\gamma \rightarrow 0} \frac{A_{ml}(k)}{A_{mm}(k)} &= e^{-\frac{\pi|k|}{2}(l-m)} = \left(\frac{-ik(l-m)}{2e}\right)^{-\frac{ik(l-m)}{2}} \left(\frac{ik(l-m)}{2e}\right)^{\frac{ik(l-m)}{2}} \\ M(h) &= \frac{m}{4\pi^{3/2}} \int_{-\infty}^{\infty} i \frac{\Gamma(\frac{1}{2} + i\frac{k}{2}) \Gamma(1 - i\frac{k}{2})}{\Gamma(1 - i\frac{mk}{2})} \left(\frac{-ikl}{2e}\right)^{-i\frac{kl}{2}} \left(\frac{ik(l-m)}{2e}\right)^{\frac{ik(l-m)}{2}} \frac{e^{-ik(a + \ln \frac{h}{T_h})}}{k + i0^+} dk \\ &\quad + \frac{l-m}{2} \\ &\rightarrow \begin{cases} \frac{l-m}{2}, & h \ll T_h \\ \frac{l}{2}, & h \gg T_h \end{cases}. \end{aligned} \quad (3.34)$$

In the last line, only the leading behaviour due to the simple pole at $-i0^+$ for high fields has been included. The integral in eq. (3.34) has already been found by Tselvick and Wiegmann, [92]. We want to evaluate it explicitly, since it reveals exciting physical insight. First of all, distinguish between the following cases of the analyticity properties of the integrand eq. (3.34) in the complex k -plane:

- i) $m = 1$, $l = 1$: Simple poles occur in the upper half plane and a cut along the negative imaginary axis. This case is illustrated in figure 3.1.
- ii) $m = 1$, $l > 1$: The cut along the whole imaginary axis dominates the poles in the upper half plane (the latter give power law contributions $\sim (h/T_h)^n$, whereas the cut leads to $\sim (\ln h/T_h)^{-m}$, as will be shown below).
- iii) $m = l \neq 1$: Poles are distributed in the upper and lower plane, in the latter case dominated by a cut along the negative imaginary axis.

- iv) $1 \neq m < l \neq 1$: A cut along the whole imaginary axis goes along with sub-leading poles in both the upper and lower half planes.

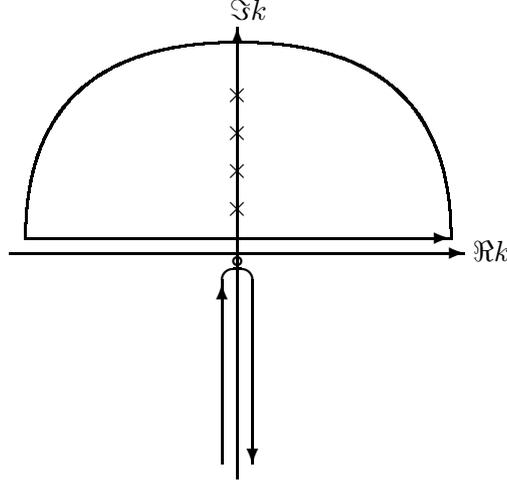


Figure 3.1: Integration contours in the exactly screened case $l = m = 1$. For $h < T_h$, poles in the upper half plane are encircled, for $h > T_h$, one encounters a cut in the lower half plane and a pole near the real axis.

Singularities in the lower (upper) half plane are relevant for $h > T_h$ ($h < T_h$). Poles $k_n = i(2n+1)$, $n = 0, 1, \dots$ in the upper half plane only give a contribution in the exactly screened case. They have residuals $-(-1)^n 2i/n!$, such that the magnetization is a series

$$M(h < T_h) \stackrel{m=l}{=} \frac{m}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)n!} \frac{\Gamma(n+\frac{1}{2})}{\Gamma(m(n+\frac{1}{2}))} \left(\frac{m(n+\frac{1}{2})}{e} \right)^{m(n+\frac{1}{2})} e^{(2n+1)a} \left(\frac{h}{T_h} \right)^{2n+1}.$$

One recognizes the signature of a Fermi liquid in the first order : $M(h) \propto h$ and $\chi(h=0) = \text{const.}$ Upon inserting explicit values, one finds agreement with eq. (3.9). We shall establish this agreement explicitly for arbitrary γ in section 3.1.2, eqs. (3.59), (3.60).

Let us draw our attention to the cut in the lower half plane, for values $l \geq m$. The contour is deformed in a way depicted in figure (3.1). Only the paths next to the cut give a non-zero contribution, so the integral can be written

$$M(h > T_h) - \frac{l}{2} \stackrel{l \geq m}{=} -\frac{m}{2\pi^{3/2}} \int_0^{\infty} \frac{\Gamma(\frac{1}{2} + \frac{p}{2}) \Gamma(1 - \frac{p}{2})}{\Gamma(1 - \frac{mp}{2})} \left(\frac{pl}{2e} \right)^{-\frac{pl}{2}} \left(\frac{p(l-m)}{2e} \right)^{\frac{p(l-m)}{2}} \frac{\sin \pi \frac{pl}{2}}{p-0^+} e^{-(p+a) \ln \frac{h}{T_h}} dp.$$

Substitute $p \ln h/T_h =: q$ and expand the integrand in a Taylor series. All terms can be integrated. We will content ourselves with a linearization of the integrand, using

$$\frac{\Gamma(\frac{1}{2} + \frac{p}{2}) \Gamma(1 - \frac{p}{2})}{\Gamma(1 - \frac{mp}{2})} = \sqrt{\pi} \left(1 - \frac{1}{2}(Cm + 2 \ln 2)p \right),$$

and $C \approx 0.5772$ is the Euler constant. We find

$$\begin{aligned} M(h > T_h) - \frac{l}{2} &\stackrel{l \geq m}{=} -\frac{ml}{4} \left(\frac{1}{\ln \frac{h}{T_h}} + \frac{m}{2} \frac{\ln \ln \frac{h}{T_h}}{\ln^2 \frac{h}{T_h}} + \frac{A}{\ln^2 \frac{h}{T_h}} + \mathcal{O}(\ln^{-3} h/T_h) \right) \\ A &= \frac{1}{2} [-m \ln m + (m-2) \ln 2 - m] . \end{aligned} \quad (3.35)$$

The contribution $\mathcal{O}(\ln^{-2} h/T_h)$ is absorbed by the definition

$$T_h = e^{-A} \tilde{T}_h \quad (3.36)$$

$$M(h > \tilde{T}_h) - \frac{l}{2} \stackrel{l \geq m}{=} -\frac{ml}{4} \left(\frac{1}{\ln \frac{h}{\tilde{T}_h}} + \frac{m}{2} \frac{\ln \ln \frac{h}{\tilde{T}_h}}{\ln^2 \frac{h}{\tilde{T}_h}} + \mathcal{O}(\ln^{-3} h/\tilde{T}_h) \right) \quad (3.37)$$

Note that the ratio \tilde{T}_h/T_K does not depend on l .

Finally, upon "encircling" the cut in the upper half plane, one only replaces the pre-factor l in eq. (3.37) by $l - m$ and sets $-\ln h/T_h = \ln T_h/h$:

$$M(h < \tilde{T}_h) - \frac{l-m}{2} \stackrel{l \geq m}{=} \frac{m(l-m)}{4} \left(\frac{1}{\ln \frac{\tilde{T}_h}{h}} - \frac{m}{2} \frac{\ln \ln \frac{\tilde{T}_h}{h}}{\ln^2 \frac{\tilde{T}_h}{h}} + \mathcal{O}(\ln^{-3} T_h/h) \right) \quad (3.38)$$

Note that this simple replacement does not hold for $\gamma \neq 0$, as can already be seen from the lowest order, eq. (3.33).

The free spin value of the magnetization is approached logarithmically at high fields. This "asymptotical freedom" in the "low coupling limit" is a genuine feature of the Kondo model. An analogous effect occurs for low fields in the under-screened case; however, the first correction is of opposite sign compared to the high-temperature case, cf. eqs. (3.37), (3.38). Classical Fermi liquid behaviour appears at low temperatures if the impurity is exactly screened. The physics quantified by these results has been given by Nozières [70] already before the exact solution of the Kondo model was known: At high fields, corrections to the asymptotical freedom of the impurity spin are due to the weak antiferromagnetic coupling with the host particles. At low fields, the impurity spin is partially screened due to strong antiferromagnetic exchange. Two kinds of interactions with this impurity-electron system may occur: On the one hand, a weak *ferromagnetic* coupling of the residual spin $S - m/2$ with the host, due to the Pauli principle (this explains the change of sign in the leading order on the rhs of eqs. (3.37), (3.38)). On the other hand, a polarization of the bound complex by host electrons, analogously to the Fermi liquid excitations at $S = m/2$. The latter are given by the poles and dominated by the asymptotic Kondo interactions, reflected by the the cuts in the complex plane.

After the calculation of $\epsilon_{j,0}$, one proceeds with \tilde{U}_j . As pointed out above, corrections to $\epsilon_{j>m,0}$ are of exponentially small order $\mathcal{O}(e^{-\beta h})$, which are negligible in comparison with corrections to $\epsilon_{j \leq m}$. Since ϵ_l is essentially given by ϵ_m , consider the equation for ϵ_m . One defines a kernel $\tilde{k}_m(k)$

$$1 - \tilde{k}_m := \hat{A}_{mm}^{-1}(k) .$$

For $m = 1$, $\tilde{k}_1 \equiv \tilde{k}$ is the integration kernel from eq. (2.156), with $l = 1$ there. Consider the case $j = m$ in eq. (3.19):

$$\begin{aligned} \epsilon_{m,0}^+ + \epsilon_{m,0}^- + \tilde{U}_m^+ + \tilde{U}_m^- &= d_m + \frac{\hat{A}_{m,l}}{\hat{A}_{m,m}} \frac{c}{K_m} \delta(k) + \tilde{k}_m \epsilon_{m,0}^+ + \tilde{k}_m \tilde{U}_m^+ + \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} \tilde{k}_m \\ &+ \frac{1}{\hat{A}_{mm}(k)} \frac{1}{\beta h K_m} \sum_{p=1}^{m-1} \hat{A}_{mp} \ln Y_p^{(\infty)} \mathcal{F}_k[\theta(-x)] . \end{aligned} \quad (3.39)$$

The contribution of the bare function $\epsilon_{m,0}$ is identified by eq. (3.25). Then eq. (3.39) determines \tilde{U}_m ,

$$\tilde{U}_m^+ + \tilde{U}_m^- = \tilde{k}_m \tilde{U}_m^+ + \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} \tilde{k}_m + \frac{1}{\hat{A}_{mm}(k)} \frac{1}{\beta h K_m} \sum_{p=1}^{m-1} \hat{A}_{mp} \ln Y_p^{(\infty)} \mathcal{F}_k[\theta(-x)]. \quad (3.40)$$

Corrections to $\epsilon_{l,0}$ are given by corrections to $\epsilon_{m,0}$ and result from inserting eq. (3.39) into eq. (3.26):

$$\begin{aligned} \epsilon_l = & \epsilon_{l,0} + \frac{\hat{A}_{m,l}}{\hat{A}_{m,m}} \left(\tilde{U}_m^+ + \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} \delta(k) + \frac{1}{\beta h K_m} \sum_{p=1}^{m-1} \hat{A}_{mp} \ln Y_p^{(\infty)} \mathcal{F}_k[\theta(-x)] \right) \\ & + \sum_{p=1}^{m-1} \hat{A}_{lp} \frac{1}{\beta h K_m} \ln Y_p^{(\infty)} \mathcal{F}_k[\theta(-x)]. \end{aligned} \quad (3.41)$$

Since there are two different orders of magnitude in the corrections (namely $\mathcal{O}(1/\beta)$ and $\mathcal{O}(1/\beta^2)$), we split \tilde{U}_m into two parts:

$$\tilde{U}_m(x) = \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} U_m(x) + \frac{1}{\beta h K_m} \hat{U}_m(x). \quad (3.42)$$

The order $\mathcal{O}(T)$ is not accessible analytically: The calculation of \tilde{U} should be done by the Wiener-Hopf-technique, which requires the splitting of the inhomogeneity into a sum of functions analytic in the upper- and lower part of the complex plane. We could not solve this problem for $\sum_k \hat{A}_{mk}(k)$, occurring in eq. (3.40) for $m > 1$.

The best we can do at this stage is to restrict ourselves to the determination of U_m , that is to contributions $\mathcal{O}(T^2)$ to the free energy. Formally, this restriction is justified by forming the second derivative of eq. (3.41) with respect to T . The order $\mathcal{O}(T)$ thus is omitted in the following. Then one expects the leading low-temperature contribution to the specific heat. From eq. (3.9), the low-temperature specific heat is related to the low-field magnetic susceptibility for $m = l$. At least for low fields, the $\mathcal{O}(T^2)$ -correction to $\epsilon_{m=l}$ is expected to confirm eq. (3.9). The lhs of eq. (3.41) is written as

$$\epsilon_l = \epsilon_{l,0} + \frac{\pi^2}{6(\beta h K_m)^2 \epsilon'_m(0)} U_m,$$

where $\epsilon_{l,0}$ is the function ϵ_l calculated in the preceding paragraph. Let us drop the index m and set

$$U_m \equiv U \quad (3.43)$$

From eqs. (3.39) and (3.42) it follows that

$$\begin{aligned} U(x) &= \tilde{k}(x) + \int_0^\infty \tilde{k}(x-y) U(y) dy \\ &= [\tilde{k} * (U_+ + \delta)](x), \end{aligned} \quad (3.44)$$

and $\delta(x)$ is Dirac's δ -distribution. From eq. (3.41), one finds for the free energy

$$\begin{aligned} \lim_{T \ll T_K} f(T, h) &= -\frac{h K_m}{2\pi} \int_0^\infty \frac{1}{\cosh(x - \ln h/T_h)} \epsilon_{m,0}(x) dx \\ &\quad - \frac{\pi^2}{12\pi K_1 h \beta^2 \epsilon'_m(x=0)} \left[\int_0^\infty \mathcal{S}_l(x - \ln h/T_h) U(x) dx + \mathcal{S}_l(\ln h/T_h) \right] \\ &=: f_0(h) + \Delta f_l(T, h) \\ \mathcal{F}_k[\mathcal{S}_l] &:= s(k) \frac{\hat{A}_{ml}(k)}{\hat{A}_{mm}(k)}. \end{aligned} \quad (3.45)$$

A function $V(x)$ is introduced which describes the T -dependent correction $\Delta f_l(T, h)$ (note that $\mathcal{S}_l(x) = \mathcal{S}_l(-x)$),

$$\begin{aligned} V(x) &:= \int_0^\infty \mathcal{S}_l(x-y) U(y) dy + \mathcal{S}_l(x) \\ &= [\mathcal{S}_l * (U_+ + \delta)](x) \end{aligned} \quad (3.46)$$

$$-\frac{\pi^2}{12\pi K_m h \beta^2 \epsilon'_m(x=0)} V(\ln h/T_h) \equiv \Delta f_l(T, h). \quad (3.47)$$

From eq. (3.46) one recognizes that it suffices to know $[U_+(x) + \delta(x)]$, which can be calculated from eq. (3.44) in Fourier representation. Let us consider

$$\begin{aligned} u(x) &:= \int_x^\infty U(x') dx', & u(k) &= \frac{iU(k)}{k + i0^+} \\ v(x) &:= \int_x^\infty V(x') dx', & v(k) &= \frac{iV(k)}{k + i0^+}, \end{aligned}$$

where the k -dependent functions denote as usual the Fourier transforms. The reason for considering u, v instead of U, V is merely technical; the integrated functions are preferred for the application of the Wiener-Hopf-technique. The kernel is separated as

$$\tilde{k} = 1 - \hat{A}_{mm}^{-1} = 1 - \frac{1}{G_+ G_-}.$$

This is the factorization of eq. (3.27). Then eq. (3.44) can be written as

$$u_+(k) + \frac{i}{k + i0^+} = \frac{i}{k + i0^+} G_-(0) G_+(k). \quad (3.48)$$

The lhs of eq. (3.48) is $\mathcal{F}_k[f(U_+ + \delta)]$. From the definition of $v(k)$ one deduces

$$\begin{aligned} v(k) &= \frac{i}{k + i0^+} G_-(0) \mathcal{S}_l(k) G_+(k) \\ v(x) &= \frac{G_-(0)}{2} \int_{-\infty}^\infty \frac{1}{2 \cosh \frac{\pi k}{2}} \frac{\hat{A}_{ml}(k)}{\hat{A}_{mm}(k)} \frac{iG_+(k)}{k + i0} e^{-ikx} dk \\ v(\ln h/T_h) &= \frac{2\pi G_-(0)}{K_m G_-(-i)} M(h/T_h) \end{aligned} \quad (3.49)$$

$$V(\ln h/T_h) = \frac{2\pi G_-(0) h}{K_m G_-(-i)} \tilde{\chi}(h/T_h) = \frac{2\pi G_-(0) h}{G_-(-i)} \chi(h/T_K). \quad (3.50)$$

$\tilde{\chi}(h/T_h) := K_m \chi(h/T_K)$. In the exactly screened case for low energies, $\tilde{\chi} \equiv \chi$. In order to arrive at eq. (3.49), use has been made of eq. (3.31). The result of eq. (3.50) is remarkable: It states that for all fields, the low-temperature specific heat is proportional to the low temperature magnetic susceptibility. This relation holds in the under-screened and exactly screened cases, $2S \geq m$. Note that in eq. (3.50), we included the constant K_m in the definition of χ since it scales T_h , eq. (3.20). From eqs. (3.47), (3.50), the specific heat results:

$$\lim_{T \ll T_K} C(T, h) = T \frac{\pi^2}{3} \frac{G_-(0)}{K_m G_-(-i) \epsilon'_m(0)} \chi(\ln h/T_h). \quad (3.51)$$

Finally, go back to eq. (3.39) to determine $\epsilon'_m(0)$ (this cannot be done with eq. (3.28), since there $\epsilon'_{m,0}(0)$ is dealt with). Consider $k \cdot \epsilon_m$, (ϵ_m denotes the Fourier transform of $\epsilon_m(x)$), by multiplying

eq. (3.39) with the variable k . Upon accomplishing the inverse transform, only the driving term rests, and

$$\epsilon'_m(0) = 1 .$$

Insert K_m from eq. (3.30) into eq. (3.51),

$$\lim_{T \ll T_K} C(T) = T \frac{2\pi^2}{3} \frac{1 - \frac{\gamma l}{\pi}}{1 - \frac{\gamma}{\pi}(l - m)} \chi(T_K, h) \quad (3.52)$$

This relation is valid for arbitrary fields. It gives the low-temperature Wilson-ratio for $l \geq m$, which is partially accessible (namely $m = l$) by the trick using dilogarithms. Formally, eq. (3.52) is of Fermi liquid type. However, $\chi(h \ll T_h)$ is finite only for $S = m/2$, otherwise it diverges as shown in eqs. (3.37), (3.38):

$$\lim_{T \ll T_K} C(T) = T \frac{2\pi^2}{3} \frac{1 - \frac{\gamma l}{\pi}}{1 - \frac{\gamma}{\pi}(l - m)} \frac{m}{4} \begin{cases} \frac{l-m}{K_m h \ln^2 \frac{T_h}{h}} & h < \tilde{T}_h \\ \frac{m}{K_m h \ln^2 \frac{h}{T_h}} & h > \tilde{T}_h \end{cases} . \quad (3.53)$$

One may consider the field h as the Fermi temperature, so that such a behaviour is called a "field tuned Fermi liquid" in [20]. In the ongoing, we rather prefer to speak of a "formal Fermi liquid".

Over-screened and exactly screened cases, $l \leq m$

If $l \leq m$, there are m equations, the last one being

$$\epsilon_m(x) = -e^{-x} + \frac{c}{K_m} + [s * \epsilon_{m-1} + k * \epsilon_m](x) .$$

In the driving vector $\vec{d}(k)$ on the right-hand site of eq. (3.22), only the last entry is different from zero, $[\vec{d}(k)]_m = d_m(k) + c/K_m \delta(k)$. Consequently,

$$\frac{\epsilon_m^+}{\hat{A}_{m,m}} = -\epsilon_m^- + d_m + \frac{c}{K_m} \delta(k) \quad (3.54)$$

$$\epsilon_l = \left[\frac{\hat{A}_{l,m}}{\hat{A}_{m,m}} \right] \epsilon_m^+ \quad (3.55)$$

Eqs. (3.25), (3.54) are solved by the Wiener-Hopf method, afterwards ϵ_m^+ is inserted in eqs. (3.26), (3.55). The relevant matrix entries read

$$\hat{A}_{m,m}(k) = 2 \cosh \frac{\pi k}{2} \frac{\sinh \frac{\pi k}{2} m \sinh \frac{\pi k}{2} \left(\frac{\pi}{\gamma} - m \right)}{\sinh \frac{\pi k}{2} \sinh \frac{\pi k}{2} \frac{\pi}{\gamma}}$$

$$\hat{A}_{l,m}(k) = 2 \cosh \frac{\pi k}{2} \frac{\sinh \frac{\pi k}{2} l \sinh \frac{\pi k}{2} \left(\frac{\pi}{\gamma} - m \right)}{\sinh \frac{\pi k}{2} \sinh \frac{\pi k}{2} \frac{\pi}{\gamma}} .$$

The auxiliary functions are then given by

$$\begin{aligned}\epsilon_m^+(k) &= \frac{G_+(k) G_-(-i)}{-2\pi(k + i0^+)(k + i)} \\ \hat{A}_{m,m}(k) &= G_+(k) G_-(k) \\ G_+(k) &= \left(2m\pi \left(1 - m\frac{\gamma}{\pi}\right)\right)^{\frac{1}{2}} \frac{\Gamma(1 - i\frac{k}{2}) \Gamma\left(1 - i\frac{\pi}{\gamma}\frac{k}{2}\right)}{\Gamma\left(\frac{1}{2} - i\frac{k}{2}\right) \Gamma(1 - im\frac{k}{2}) \Gamma\left(1 - i\frac{k}{2}\left(\frac{\pi}{\gamma} - m\right)\right)} \\ K_m &= c \frac{G_-(0)}{G_-(-i)}\end{aligned}$$

Note that $c = \frac{1}{2(1-\gamma/\pi m)}$ here. Remember eq. (3.18): The linearization can be fully exploited only in the regime of high fields $h \gg T_h$. In this limit, the magnetization reads

$$\begin{aligned}M(h) &= \frac{l}{4\pi^{3/2}} \int_{-\infty}^{\infty} i \frac{\Gamma\left(\frac{1}{2} + i\frac{k}{2}\right) \Gamma(1 + im\frac{k}{2}) \Gamma(1 - i\frac{k}{2}) \Gamma\left(1 - i\frac{k}{2}\frac{\pi}{\gamma}\right) e^{-ik \ln \frac{h}{T_h}}}{\Gamma\left(1 - i\frac{k}{2}\left(\frac{\pi}{\gamma} - m\right)\right) \Gamma(1 - il\frac{k}{2}) \Gamma(1 + il\frac{k}{2})} \frac{dk}{k + i0^+} \quad (3.56) \\ &\xrightarrow{h \gg T_h} \frac{l}{2}.\end{aligned}$$

The isotropic limit $\gamma \rightarrow 0$ yields

$$\begin{aligned}\lim_{\gamma \rightarrow 0} G_+(k) &= \sqrt{2m\pi} \frac{\Gamma(1 - i\frac{k}{2})}{\Gamma\left(\frac{1}{2} - i\frac{k}{2}\right) \Gamma(1 - im\frac{k}{2})} \left(-\frac{ikm}{2e}\right)^{-i\frac{mk}{2}} \\ M(h) &= \frac{l}{4\pi^{3/2}} \int_{-\infty}^{\infty} i \frac{\Gamma\left(\frac{1}{2} + i\frac{k}{2}\right) \Gamma(1 + im\frac{k}{2}) \Gamma(1 - i\frac{k}{2})}{\Gamma(1 - il\frac{k}{2}) \Gamma(1 + il\frac{k}{2})} \left(-\frac{ikm}{2e}\right)^{-i\frac{mk}{2}} \frac{e^{-ik \ln \frac{h}{T_h}}}{k + i0^+} dk\end{aligned}$$

Note that for $\gamma = 0$, a cut along the negative half of the imaginary axis occurs. It dominates the poles in the lower half of the complex plane, and one is faced with the expected Kondo behaviour for $h > T_h$.

A novel characteristic appears for $h < T_h$. Care has to be taken in this case, so that we only extract the leading behaviour. It is given by the poles with smallest positive imaginary part.

$$M(h \ll T_K) \propto \left(\frac{h}{T_K}\right)^{2/m} \quad (3.57)$$

$$\chi(h \ll T_K) \propto \left(\frac{h}{T_K}\right)^{2/m-1}. \quad (3.58)$$

The constants of proportionality are not of importance here. In words: Over-screening induces non-integer exponents, independent of γ , at low energies. We will see in section 3.2 that this is true also for low temperatures at $h = 0$, as to the specific heat and susceptibility.

Finally note that for $l = m$, the two expressions eqs. (3.34), (3.56) coincide. It is shown that the first non-vanishing order linear in h of the magnetization leads to the $T = 0$, $h = 0$ susceptibility, calculated in eq. (3.9). For $l = m$, the magnetization reads

$$M(h) = \frac{m}{4\pi^{3/2}} \int_{-\infty}^{\infty} i \frac{\Gamma\left(\frac{1}{2} + i\frac{k}{2}\right) \Gamma(1 - i\frac{k}{2}) \Gamma\left(1 - i\frac{\pi k}{2\gamma}\right) e^{-ik \ln \frac{h}{T_h}}}{\Gamma\left(1 - i\frac{mk}{2}\right) \Gamma\left(1 - i\frac{k}{2}\left(\frac{\pi}{\gamma} - m\right)\right)} \frac{dk}{k + i0^+}.$$

Being interested in fields $h < T_h$, one takes account of the poles at $k_n := i(2n + 1)$ with residuals $-2i(-1)^n/n!$. These result in the series

$$M(h) = \frac{1}{\pi^{1/2} \left(1 - \frac{\gamma}{\pi} m\right)} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)n!} \frac{\Gamma\left(\frac{1}{2} + n\right) \Gamma\left(\frac{\pi}{\gamma} \left(n + \frac{1}{2}\right)\right)}{\Gamma\left(m \left(\frac{1}{2} + n\right)\right) \Gamma\left(\left(\frac{\pi}{\gamma} - m\right) \left(n + \frac{1}{2}\right)\right)} \left(\frac{h}{T_h}\right)^{2n+1}.$$

The constant K_m is, for $l = m$, determined to be

$$K_m = \frac{m \Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{1}{2} \left(\frac{\pi}{\gamma} - m\right)\right)}{2\pi \Gamma\left(\frac{\pi}{2\gamma}\right)}.$$

From the definition of T_h , eq. (3.20), one gets to first order in h :

$$\lim_{h \ll T_h} M(h) = \frac{m}{2\pi \left(1 - \frac{\gamma}{\pi} m\right)} \frac{h}{T_K} \quad (3.59)$$

$$\chi(T = 0, h = 0) = \frac{m}{2\pi \left(1 - \frac{\gamma}{\pi} m\right)} \frac{1}{T_K}. \quad (3.60)$$

This result is expected from eq. (3.9).

3.1.3 Asymptotic linearization for $T, h \ll T_K, j < m$

As pointed out in the preceding section, we are not able to account for corrections of the linearized functions $\epsilon_{j < m}$, $m > 1$ in the framework above. Such corrections essentially concern the region around the origin, where for large magnetic fields, we have set $\epsilon_{j < m}(x) \equiv \epsilon_{j < m}(x)\theta(x)$. In the following, we consider the case $j < m$ for small magnetic fields and low temperatures. This case was treated previously in [92] by the TBA-equations. Corrections to $\ln Y_j^{(\infty)}$ are expressed through a correction function $D_j(x)$,

$$\ln Y_j(x) = \ln Y_j^{(\infty)} + D_j(x), \quad \lim_{x \rightarrow \infty} D_j(x) = 0.$$

Linearizing $\ln y_j$ to first order in D_j ,

$$\begin{aligned} \ln y_j(x) &= \frac{1}{2} \ln Y_{j-1}^{(\infty)} Y_{j+1}^{(\infty)} + \frac{f_j^2}{f_{j-1} f_{j+1}} D_j(x) + \mathcal{O}(D_j^2) \\ f_j &:= \left(Y_j^{(\infty)}\right)^{1/2} = \frac{\sin \frac{\pi}{m+2} (j+1)}{\sin \frac{\pi}{m+2}} \\ \lim_{x \gg 0} \frac{f_j^2}{f_{j-1} f_{j+1}} D_j(x) &= [s * (D_{j-1} - D_{j+1})](x), \quad j = 1, \dots, m-1 \\ D_m &\equiv \ln \mathfrak{B}_m \overline{\mathfrak{B}}_m. \end{aligned} \quad (3.61)$$

It is emphasized that this approximation gets not automatically better by taking into account higher order terms $\mathcal{O}(D_j^2)$, but rather with increasing x . Eq. (3.61) has been derived for $x \gg 0$. This is approximately accounted for by writing $D_j(x) \equiv D_j(x)\theta(x)$. The linearized equations form an

algebraic system by Fourier transforming. Each unknown function $D_j(x)$ can be expressed in terms of D_m ,

$$\begin{aligned} D_j(x) &= [t_j * D_m](x) \\ t_j(k) &:= \frac{f_{j-1} \sinh(j+2) \frac{\pi k}{2} - f_{j+1} \sinh j \frac{\pi k}{2}}{f_j} g(k). \end{aligned} \quad (3.62)$$

As usual, $\mathcal{F}_k [t_j(x)] := t_j(k)$. As can be seen by direct calculation, D_j from eq. (3.62) satisfies eq. (3.61) for $j = 1, \dots, m-2$. The function $g(k)$ has to be determined from the last equation $j = m-1$ and is found to be

$$g(k) = \left[2 \cos \frac{\pi}{m+2} \sinh(m+2) \frac{\pi k}{2} \right]^{-1}. \quad (3.63)$$

The first equation, $j = 0$, is already contained in eq. (3.62) by $t_0 \equiv 0$ and therefore $D_{j=0} \equiv 0$.

For $2S < m$, the impurity part of the free energy then reads

$$f_I(T, h \ll T_K) = -T \ln \frac{\sin \frac{\pi(2S+1)}{m+2}}{\sin \frac{\pi}{m+2}} - \frac{T}{2} \int_{-\infty}^{\infty} \frac{1}{\cosh \frac{\pi k}{2}} D_{2S}(k) e^{ik \ln T/T_K} dk.$$

Since $T < T_K$, only negative imaginary values for k are allowed.

Consider the analyticity properties of the integrand. It has a pole of second order in $k = 0$ ($D_m(x)$ is a steplike function and therefore its Fourier transform has a simple pole in $k = i0^+$. The zero in the denominator of $g(k = 0)$ gives the second singularity). This second order pole is circumvented by choosing an integration path slightly below the real axis. Then the leading order of the integral is given by the pole with imaginary part next to the real axis, corresponding to large values of x . There are simple poles at

$$\begin{aligned} k_n &= -(2n+1)i, \quad n = 0, \pm 1, \pm 2, \dots \\ k_p &= -2pi/(m+2), \quad p = \pm 1, \dots \end{aligned}$$

The residuum in $k_{p=1}$ vanishes. Depending on the value of m , there is a pole of first order (m uneven) or of second order (m even) in $k = -i$. However, its residuum vanishes, so that the value $m = 2$ is excluded here. It will be treated separately below. With $m > 2$, the leading behaviour therefore is given by the residuum in $k_{p=2}$:

$$\begin{aligned} f_I(T, h \ll T_K) &= -T \ln \frac{\sin \frac{\pi(2S+1)}{m+2}}{\sin \frac{\pi}{m+2}} - T \alpha_2 (h/T) \left(\frac{T}{T_K} \right)^{\frac{4n}{m+2}} \\ \alpha_p &= \frac{(-1)^p \left(\sin \frac{2\pi S p}{m+2} \sin \frac{2\pi(S+1)}{m+2} - \sin \frac{2\pi S}{m+2} \sin \frac{2\pi p(S+1)}{m+2} \right)}{(m+2) \cos \frac{\pi}{m+2} \cos \frac{\pi p}{m+2} \sin \frac{\pi(2S+1)}{m+2}} \int_{-\infty}^{\infty} e^{\frac{2\pi p x}{m+2}} \ln[\mathfrak{B}_m \overline{\mathfrak{B}}_m](x) dx \end{aligned} \quad (3.64)$$

The specific heat and susceptibility are derived:

$$C_I(T, h = 0) = \alpha_2|_{h=0} \frac{4(m+6)}{(m+2)^2} \left(\frac{T}{T_K} \right)^{\frac{4}{m+2}} \quad (3.65a)$$

$$\chi_I(T, h = 0) = \left(\frac{T}{T_K} \right)^{\frac{4}{m+2}-1} \frac{\partial^2}{\partial(\beta h)^2} \alpha_2 \Big|_{h=0} \quad (3.65b)$$

Note that for $h = 0$, $\ln \mathfrak{B}_m \overline{\mathfrak{B}}_m$ does not depend on T . The derivative in eq. (3.65b) only acts upon the integrand in eq. (3.64). Both C_I and χ_I show the same T -dependence, so that one may again calculate the low-temperature Wilson ratio, defined in eq. (3.11), once \mathfrak{B}_m , $\overline{\mathfrak{B}}_m$ and its derivatives with respect to βh are known:

$$R_w = \frac{\chi_I(T) C_h(T)}{C_I(T) \chi_h(T)} = \frac{4\pi^2}{3} \frac{(m+2)^2}{4(m+6)} \left. \frac{\frac{\partial^2 \alpha_2}{\partial (\beta h)^2}}{\alpha_2} \right|_{h=0} ; m = 3, 4, \dots \quad (3.66)$$

Despite the simple form of the integral eq. (3.64), we did not succeed in evaluating it analytically. Instead, $\ln \mathfrak{B}_m \overline{\mathfrak{B}}_m$ and its derivatives are calculated numerically, cf. chapter 4. The results are given below.

The case $m = 2$, $2S = 1$ is excluded from the above linearization scheme. The Wilson ratio is found analytically in this case. The relevant equations are:

$$\begin{aligned} \ln y_1(x) &= [s * \ln \mathfrak{B}_2 \overline{\mathfrak{B}}_2](x) \\ \ln \mathfrak{b}_2(x) &= -e^x + \frac{\beta h}{2} + [s * \ln Y_1](x) + [k * \ln \mathfrak{B}_2](x) - [k_- * \ln \overline{\mathfrak{B}}_2](x) \\ f_I(T, h) &= -\frac{T}{2\pi} \int_{-\infty}^{\infty} \frac{\ln Y_1(x)}{\cosh\left(x + \ln \frac{T}{T_K}\right)} dx . \end{aligned} \quad (3.67)$$

In section 3.1.1, we found (eq. (3.8) specialized to $m = 2$):

$$\lim_{x \gg 0} [s * \ln \mathfrak{B}_2 \overline{\mathfrak{B}}_2](x) = e^{-x} \left(\frac{\pi}{4} - \frac{(\beta h)^2}{2(\pi - 2\gamma)} \right) .$$

Consequently,

$$\lim_{x \gg 0} \ln Y_1(x) = \ln 2 + e^{-x} \left(\frac{\pi}{8} - \frac{(\beta h)^2}{4(\pi - 2\gamma)} \right) . \quad (3.68)$$

This is just the region of interest in the integral of the free energy, eq. (3.67). One approximates the kernel in the same scheme as in eq. (3.8),

$$\lim_{T \ll T_K} \frac{1}{2 \cosh(x + \ln T/T_K)} = \frac{T}{T_K} e^x + \mathcal{O}(T^2 e^{2x}) , x \leq \ln T/T_K . \quad (3.69)$$

The latter restriction is necessary for reasons of convergence: The integral eq. (3.67) exists. However the integrand after the approximation, eqs. (3.68), (3.69), is constant and therefore diverges when integrated over the whole real axis. The divergence is the same in both summands, so asymptotically,

$$\lim_{T, h \ll T_K} f_I(T, h) = -\frac{T}{4\pi} \ln 2 - \frac{T^2}{T_K} \left[\frac{1}{8} + \frac{(\beta h)^2}{4\pi(\pi - 2\gamma)} \right] \int_D^{\ln T/T_K} dx , D \ll 0$$

An auxiliary cutoff D has been introduced. The divergence connected with $D \ll 0$ is controlled since it occurs with a factor of T^2 or h^2 , and both of them are assumed to be small, we therefore neglect it in the following. The occurrence of the logarithm $\ln T/T_K$ is more interesting. It leads to

$$\lim_{T, h \ll T_K} C_I(T, h) = -\frac{1}{4} \frac{T \ln T/T_K}{T_K} \quad (3.70a)$$

$$\lim_{T, h \ll T_K} \chi_I(T, h) = -\frac{1}{2\pi(\pi - 2\gamma)} \frac{\ln T/T_K}{T_K} \quad (3.70b)$$

$$R_w|_{m=2, 2S=1} = R_w|_{m=2, 2S=2} = \frac{8}{3(1 - 3\gamma/\pi)} . \quad (3.70c)$$

Numerically, we find by methods described in appendix C for $\gamma = 0$ (note that $1/(2\pi^2) = 0.05066\dots$):

$$\begin{aligned}\lim_{T, h \ll T_K} C_I(T, h) &= - (0.25 \pm 10^{-2}) \frac{T \ln T/T_K}{T_K} \\ \lim_{T, h \ll T_K} \chi_I(T, h) &= - (0.05 \pm 10^{-2}) \frac{\ln T/T_K}{T_K}\end{aligned}\quad (3.71)$$

These results agree with numerical findings by Sacramento et. al. [75] ($\gamma = 0$), who treated the TBA equations within an approximative cutoff scheme. The Wilson ratio is in accordance with the prediction by Affleck [2], who performed an analytical investigation of the over-screened case (with $\gamma = 0$) using conformal field theory. He finds

$$\begin{aligned}C_I(T) &= \begin{cases} -\lambda^2 \pi^2 9T \ln(aT); & m = 2 \\ \lambda^2 \delta \frac{3\pi}{2} \left(\frac{4}{2+m}\right)^2 (m+4) T^{\frac{4}{2+m}}; & m = 3, 4, \dots \end{cases} \\ \chi_I(T) &= \begin{cases} -18\lambda^2 \ln(aT); & m = 2 \\ \lambda^2 \delta 2 \left(2 + \frac{m}{2}\right)^2 T^{\frac{4}{m+2}-1}; & m = 3, 4, \dots \end{cases} \\ \delta &= \frac{\Gamma\left(\frac{1}{2} - \frac{2}{2+m}\right) \Gamma\left(\frac{1}{2}\right)}{\Gamma\left(1 - \frac{2}{2+m}\right)} \\ R_w &= \frac{(2 + m/2)(2 + m)^2}{18}; \quad m = 2, 3, \dots\end{aligned}$$

a is some distance cutoff constant and λ^2 is the spin-exchange coupling constant. One observes that the T -dependence agrees with eqs. (3.65a), (3.65b), (3.70a), (3.70b). The amplitudes are difficult to compare, since the relation between the coupling constants, λ^2 and T_K , is unknown. However, whereas the coefficients found by Affleck are S -independent, those obtained from the asymptotic linearization depend on S . For illustrative reasons, define

$$C_I(T) = T^{\frac{4}{2+m}} \zeta_c; \quad m = 3, 4, \dots \quad (3.72)$$

$$\chi_I(T) = T^{\frac{4}{m+2}-1} \zeta_\chi; \quad m = 3, 4, \dots \quad (3.73)$$

In table 3.1, our findings are compared with those by Affleck. One observes a relative deviation of 4% for $m = 3, 4$ and of 10% for $m = 5$. This is due to numerical errors in predicting the low-temperature behaviour of the susceptibility, as shown in chapter 4. Finally, we give results for finite anisotropy in table 3.2. As expected, the coefficient of the specific heat is nearly not affected by γ , but only the susceptibility, which grows with growing γ , in analogy to the result in the exactly screened case, eq. (3.9). One expects a $1/(1 - m\gamma/\pi)$ dependence; however, the accuracy of the data does not suffice to confirm this expectation.

The results of this section shall be summarized together with those of the next section at the end of this chapter.

m	Affleck			Asymptotic linearization		
	ζ_c/λ^2	ζ_χ/λ^2	$3/(4\pi^2) R_w$	$\zeta_c/T_K^{4/(m+2)}$	$\zeta_\chi/T_K^{(2-m)/(2+m)}$	$3/(4\pi^2) R_w$
3	298.7	110.3	0.369	7.45	5.72	0.384
4	131	79.6	0.608	1.75	2.05	0.585
5	79	73.5	0.931	0.633	1.05	0.830

Table 3.1: Comparison of results for the low temperature Wilson ratio in the over-screened case $m > 2S$ between Affleck's CFT approach and the asymptotical linearization of the exact solution, applied here.

m	$\gamma(2m)/\pi$	$\zeta_c/T_K^{4/(m+2)}$	$\zeta_\chi/T_K^{(2-m)/(2+m)}$	$3/(4\pi^2) R_w$
3	0.2	7.455	6.371	0.4273
	0.5	7.454	7.718	0.517
	0.9	7.439	10.91	0.733
4	0.2	1.76	2.29	0.651
	0.5	1.76	2.76	0.786
	0.9	1.75	3.85	1.097
5	0.2	0.633	1.17	0.924
	0.5	0.633	1.41	1.113
	0.9	0.633	1.951	1.541

Table 3.2: Low temperature Wilson ratio in the over-screened case $m > 2S$ for finite anisotropy γ .

3.2 High Temperature Evaluation

In the limits of high (low) temperature, $T \gg T_K$ ($T \ll T_K$), the main contribution in the integral of the free energy stems from the regions $x \rightarrow -\infty$ ($x \rightarrow \infty$) of the auxiliary functions or of convolutions with these functions. By this we mean that the convolutions are carried out over the half axis $x \in]-\infty, \Delta]$ ($x \in [\Delta, \infty[$), with some cutoff Δ . Such an approximation only makes sense if the results are independent of Δ .

Our interest is on a systematic expansion of the auxiliary functions around the asymptotic values. It turns out that qualitatively, the $T \gg T_K$, $h = 0$ behaviour resembles the $h \gg T_h$, $T = 0$ results, as revealed in section 3.1.2 by rigorous linearization. In the under-screened case, this is also true for $T \ll T_K$, $h = 0$. On the other hand, in section 3.1.2 it has been shown that for $h \neq 0$, the over-screened models still fulfill the Fermi liquid relation $C \propto T\chi$, but $\lim_{T \ll T_K} \chi \sim (h \ln^{-2} h/T_K)$, eq. (3.53). The scenario of $h \rightarrow 0$ is not contained in this approach. This case is also treated in this section.

This section is divided into four parts. In the first part, the isotropic limit $\gamma = 0$ is considered, without magnetic field. A finite magnetic field is included in the second part. The third part treats the low-temperature limit of the under-screened case, which is conceptually very similar to the regime of high temperatures. The anisotropic case is treated in the last part.

The anisotropic case differs qualitatively from the isotropic one. The auxiliary functions show exponential corrections to their asymptotic values. However, we are not able to determine the coefficients of these corrections.

3.2.1 Isotropic case $\gamma = 0$, $h = 0$

In the high temperature regime, the first corrections to the asymptotic value of the free energy are merely given by the first asymptotic corrections of the concerned auxiliary function for $x \rightarrow -\infty$, and one can neglect the rest of the integration range. These corrections are of algebraic and logarithmic-algebraic nature and can be found within an asymptotic linearization scheme (contrary to the rigorous linearization $T \rightarrow 0$ with $h \neq 0$, cf. section 3.1.2). This is still true in the low-temperature limit, referring to the region $x \rightarrow \infty$. In this region, the set of l equations decouples into two sets of m and $l - m$ equations. For an under-compensated impurity spin, $l > m$, the high-temperature-linearization is directly transferable. In contrast to the case with magnetic field, the specific heat diverges as $\ln^{-4} T/T_K$. In the exactly screened and over-screened cases, the integral over the whole integration range is of importance, the asymptotic linearization scheme is more involved.

We begin with the asymptotic expansion of $\ln \mathfrak{B}_l$, $\ln \overline{\mathfrak{B}}_l$, $l \geq m$ in the region $x \rightarrow -\infty$. The case $m > l$ is obtained therefrom afterwards. Consider the equations for \mathfrak{B}_l , $\overline{\mathfrak{B}}_l$ in the $h = 0$ -case:

$$\ln \mathfrak{b}_l = s * \ln Y_{l-1} + k * \ln \mathfrak{B}_l - k_- * \ln \overline{\mathfrak{B}}_l \quad (3.74a)$$

$$\ln \overline{\mathfrak{b}}_l = s * \ln Y_{l-1} + k * \ln \overline{\mathfrak{B}}_l - k_+ * \ln \mathfrak{B}_l \quad (3.74b)$$

$$k_{\pm}(x) = k(x \pm i\pi)$$

We shall show that $\ln \mathfrak{B}_l(x)$, $\ln \overline{\mathfrak{B}}_l(x)$ approach their asymptotes $x \rightarrow -\infty$ as x^{-3} and calculate the corresponding coefficient $b_3^{(l)}$.

The first $l - 1$ integral equations determine the j -dependence of $\ln Y_j(x)$, $j = 1, \dots, l - 1$. To see

this, define

$$\begin{aligned}
\ln Y_j(x) &= 2 \ln(j+1) + 2\delta_j(x) & \ln \mathfrak{B}_l(x) &= \ln(l+1) + \delta_l(x) \\
\lim_{x \rightarrow -\infty} \delta_j(x) &= 0 \\
\lim_{x \ll 0} \ln y_j(x) &= \ln j(j+2) + 2 \frac{(j+1)^2}{j(j+2)} \delta_j(x) + \mathcal{O}(\delta_j^2) \\
\lim_{x \ll 0} \ln \mathfrak{b}_l(x) &= \ln l + \frac{l+2}{l} \delta_l(x) + \mathcal{O}(\delta_l^2) .
\end{aligned} \tag{3.75}$$

$\ln \overline{\mathfrak{B}}_l$ ($\ln \overline{\mathfrak{b}}_l$) is related to $\ln \mathfrak{B}_l$ ($\ln \mathfrak{b}_l$) by complex conjugation. The crucial approximation is

$$[s * \delta_j](x) \approx \delta_j(x)/2 + \mathcal{O}(\delta_j''(x)) . \tag{3.76}$$

s being an exponentially decaying kernel, this approximation is justified for algebraically decaying δ_j . Such an algebraic behaviour is indeed expected from the integration kernel $k(x)$, which itself decays algebraically for $\gamma = 0$. In the anisotropic case $\gamma \neq 0$, this is not true, since $\delta_j(x)$ also decays exponentially. The δ_j satisfy the recurrence relations

$$2 \frac{(j+1)^2}{j(j+2)} \delta_j(x) = \delta_{j+1}(x) + \delta_{j-1}(x) \tag{3.77a}$$

$$\delta_0(x) \equiv 0 \tag{3.77b}$$

$$\frac{l+1}{l} \delta_l(x) = \delta_{l-1}(x) + a \frac{f_l}{x^3} . \tag{3.77c}$$

These equations determine δ_j and f_l up to a constant factor. Note that from eqs. (3.77a), (3.77b)

$$\delta_j(x) = j(j+2)d(x) .$$

Summarizing,

$$\ln Y_j(x) = 2 \ln(j+1) + 2j(j+2)d(x) , \quad \ln \mathfrak{B}_l(x) = \ln(l+1) + l(l+1)d(x) . \tag{3.78}$$

According to eqs. (3.74a), (3.74b), \mathfrak{B}_l , $\overline{\mathfrak{B}}_l$ are related by complex conjugation, the Y_i are real-valued.

$$\ln \mathfrak{B}_l =: B_{1,l} + iB_{2,l} , \quad \ln \overline{\mathfrak{B}}_l =: B_{1,l} - iB_{2,l} . \tag{3.79}$$

Define the sum and the difference of the integration kernels,

$$\begin{aligned}
k^{(s)}(x) &= k\left(x + i\frac{\pi}{2}\right) + k\left(x - i\frac{\pi}{2}\right) = \mathcal{F}_k^{-1} \left[e^{-\frac{\pi}{2}|k|} \right] \\
k^{(d)}(x) &= k\left(x + i\frac{\pi}{2}\right) - k\left(x - i\frac{\pi}{2}\right) = \mathcal{F}_k^{-1} \left[e^{-\frac{\pi}{2}|k|} \frac{\sinh \frac{\pi}{2} k}{\cosh \frac{\pi}{2} k} \right] .
\end{aligned}$$

Asymptotically,

$$\begin{aligned}
k^{(s)}\left(x + i\frac{\pi}{2}\right) &\sim \frac{1}{2x^2} - \frac{i\pi}{2x^3} , & |x| \rightarrow \infty \\
k^{(d)}(x) &\sim -i\frac{\pi}{2x^3} , & |x| \rightarrow \infty .
\end{aligned} \tag{3.80}$$

The convolutions with the k -kernels are written in the following way:

$$\begin{aligned} k * \ln \mathfrak{B}_l - k_- * \ln \bar{\mathfrak{B}}_l &= k_-^{(d)} * B_{l,1} + i k_-^{(s)} * B_{l,2} \\ k_{\pm}^{(\nu)}(x) &= k^{(\nu)}\left(x \pm i\frac{\pi}{2}\right), \quad \nu = s, d. \end{aligned}$$

The first non-vanishing term in an asymptotic expansion of $B_{l,1}(x)$ around $|x| \rightarrow \infty$ is

$$B_{l,1}(x) \sim \ln(l - m + 1) + \ln \frac{l + 1}{l - m + 1} \theta(-x).$$

The θ -function has to be understood asymptotically for large x . This regime is equivalent to small k -values in Fourier-space, $\mathcal{F}_k[\theta(-x)] = -i/k + \pi\delta(k)$. In this region around the origin in Fourier space, $\pi k \mathcal{F}_k[k^{(s)}]/2 \sim \mathcal{F}_k[k^{(d)}]$. Thus it follows that

$$\left[k_-^{(d)} * B_{l,1} \right](x) \sim \ln \frac{l + 1}{l - m + 1} \left(\frac{\pi^2}{4x^3} - i \frac{\pi}{4x^2} \right) + \mathcal{O}(ix^{-3}). \quad (3.81)$$

It is useful to define correction terms to the asymptotic behaviour for $x \ll 0$:

$$\lim_{x \rightarrow -\infty} \ln \mathfrak{B}_l(x) = \ln(l + 1) + \frac{b_{1,3}^{(l)}}{x^3} + i \frac{b_{2,2}^{(l)}}{x^2}. \quad (3.82)$$

One then performs the asymptotic expansion

$$\begin{aligned} i \left[k_-^{(s)} * B_{l,2} \right](x) &\sim \frac{i}{x^2} \left(\frac{1}{2} \int_{-\infty}^{\infty} B_{l,2}(x) dx + b_{2,2}^{(l)} \int_{-\infty}^{\infty} k_s(x) dx \right) \\ &\quad - \frac{\pi}{x^3} \left(\frac{1}{2} \int_{-\infty}^{\infty} B_{l,2}(x) dx + b_{2,2}^{(l)} \int_{-\infty}^{\infty} k_s(x) dx \right) \\ \int_{-\infty}^{\infty} k^{(s)}(x) dx &= 1 \\ \int_{-\infty}^{\infty} B_{l,2}(x) dx &= \frac{\pi}{2} \left(-(m \pm 10^{-5}) + \ln \frac{l + 1}{l - m + 1} \right). \end{aligned} \quad (3.83)$$

The last integral is done numerically with the indicated precision, for technical details cf. appendix C. In the following, we set

$$\int_{-\infty}^{\infty} B_{l,2}(x) dx = \frac{\pi}{2} \left(-m + \ln \frac{l + 1}{l - m + 1} \right). \quad (3.84)$$

In order to relate it to $b_{1,3}^{(l)}$, $b_{2,2}^{(l)}$, we observe that eq. (3.79) implies

$$\begin{aligned} \ln \mathfrak{b}_l &= \ln \left(e^{\ln \mathfrak{B}_l} - 1 \right) \\ &= \ln l + \frac{l + 1}{l} \delta_l + \mathcal{O}(\delta_l^2). \end{aligned}$$

Insert eq. (3.82) and keep only the linear order in δ_l ,

$$\begin{aligned} \ln \mathfrak{b}_l(x) &\sim \ln l + \frac{l + 1}{l} \left(\frac{b_{1,3}^{(l)}}{x^3} + i \frac{b_{2,2}^{(l)}}{x^2} \right) \\ \ln \bar{\mathfrak{b}}_l(x) &\sim \ln l + \frac{l + 1}{l} \left(\frac{b_{1,3}^{(l)}}{x^3} - i \frac{b_{2,2}^{(l)}}{x^2} \right). \end{aligned} \quad (3.85)$$

Combining eq. (3.81), (3.83), (3.85) one expands eq. (3.74a) around $x \rightarrow -\infty$:

$$\begin{aligned} \ln l + \frac{l+1}{l} \frac{b_{1,3}^{(l)}}{x^3} &= \ln l + (l-1)(l+1)d(x) + \ln \frac{l+1}{l-m+1} \frac{\pi^2}{4x^3} - \frac{\pi}{x^3} \left(\frac{1}{2} \int_{-\infty}^{\infty} B_{2,l}(x) dx + b_{2,2}^{(l)} \right) \\ \frac{l+1}{l} \frac{b_{2,2}^{(l)}}{x^2} &= \frac{1}{x^2} \left(-\frac{\pi}{4} \ln \frac{l+1}{l-m+1} + \frac{1}{2} \int_{-\infty}^{\infty} B_{2,l}(x) dx + b_{2,2}^{(l)} \right). \end{aligned}$$

Using eq. (3.84), we find:

$$\begin{aligned} d(x) &= \frac{\pi^2}{12} \frac{m}{x^3} \\ b_{2,2}^{(l)} &= -\frac{l m \pi}{4} \\ b_{1,3}^{(l)} &= \frac{l(l+2)m}{3} \frac{\pi^2}{4} \\ \lim_{x \rightarrow -\infty} \ln Y_j(x) &= 2 \ln(j+1) + j(j+2) \frac{m \pi^2}{6x^3} \\ \lim_{x \rightarrow -\infty} \ln \mathfrak{B}_l(x) &= \ln(l+1) - i \frac{m l \pi}{4x^2} + \frac{m l(l+2)\pi^2}{12x^3} \\ \lim_{x \rightarrow -\infty} \ln \overline{\mathfrak{B}}_l(x) &= \ln(l+1) + i \frac{m l \pi}{4x^2} + \frac{m l(l+2)\pi^2}{12x^3}. \end{aligned}$$

Note that the x -dependence of the corrections is determined through the asymptotic behaviour of the kernel in the convolutions $k * \ln \mathfrak{B}_l$, $k * \ln \overline{\mathfrak{B}}_l$. The amplitudes follow from the Y -hierarchy.

We proceed with the asymptotic evaluation of $\partial_{\beta h} \ln Y_j(x)$, $\partial_{\beta h} \ln \mathfrak{B}_l(x)$ in the regime $x \ll 0$. The $\ln Y_j$ are symmetric with respect to βh : The system of NLIE remains the same upon replacing $\beta h \rightarrow -\beta h$ and substituting \mathfrak{B}_l by $\overline{\mathfrak{B}}_l$. So $\partial_{\beta h} \ln Y_j$ vanishes identically for $h = 0$. Define $B_l^{(m)} := \partial_{\beta h} \ln \mathfrak{B}_l$. Then the only equations which rest are

$$B_l^{(m)}(x) = \left(1 - e^{-\ln \mathfrak{B}_l(x)} \right) \left[\frac{1}{2} + [k * B_l^{(m)} - k_- * \overline{B}_l^{(m)}](x) \right] \quad (3.86a)$$

$$\overline{B}_l^{(m)}(x) = \left(1 - e^{-\ln \overline{\mathfrak{B}}_l(x)} \right) \left[-\frac{1}{2} + [k * \overline{B}_l^{(m)} - k_+ * B_l^{(m)}](x) \right]. \quad (3.86b)$$

$B_l^{(m)}$ and $\overline{B}_l^{(m)}$ are related by negation and complex conjugation,

$$B_l^{(m)} =: B_{l,1}^{(m)} + i B_{l,2}^{(m)} \quad \overline{B}_l^{(m)} = - [B_l^{(m)}]^* = -B_{l,1}^{(m)} + i B_{l,2}^{(m)}.$$

However, since $[s * (B_l^{(m)} + \overline{B}_l^{(m)})](\ln T/T_K)$ is a physical quantity (namely the magnetization), the imaginary part of $B_l^{(m)}$ vanishes for $h = 0$. Thus $B_l^{(m)} \equiv B_{l,1}^{(m)}$ is real valued. We shall determine asymptotic corrections to $B_l^{(m)}$ up to order $\mathcal{O}(x^{-2})$, so that corrections to $\ln \mathfrak{B}_l(\pm\infty)$ (of order $\mathcal{O}(x^{-3})$), can safely be neglected. In this approximation,

$$\lim_{x \rightarrow -\infty} \left(1 - e^{-\ln \mathfrak{B}_l(x)} \right) = \frac{l}{l+1} \left(1 + i \frac{\pi}{4x^2} \right) \quad \lim_{x \rightarrow \infty} \left(1 - e^{-\ln \mathfrak{B}_l(x)} \right) = \frac{l-m}{l-m+1} \left(1 + i \frac{\pi}{4x^2} \right) \quad (3.87)$$

and one finds the asymptotic equation for $B_l^{(m)}$,

$$\begin{aligned} \lim_{x \ll 0} B_l^{(m)}(x) &= \frac{l}{l+1} \left(1 + i \frac{\pi}{4x^2}\right) \left(\frac{1}{2} + k_-^{(s)} * B_l^{(m)}\right) \\ &= \frac{l}{l+1} \left(\frac{1}{2} + k^{(s)} * B_l^{(m)}\right). \end{aligned} \quad (3.88)$$

The imaginary contributions vanish as expected. The only unknown in eq. (3.88), namely $B_l^{(m)}$, enters linearly. Therefore eq. (3.88) is well suited for further analytical studies. Note that this possibility does not exist in the TBA-approach, where one deals with the infinitely many Y_j and their derivatives. As mentioned above, $Y_j^{(m)} \equiv 0 \forall j$.

The constant asymptotic behaviour of $B_l^{(m)}$ is

$$\lim_{x \rightarrow -\infty} B_l^{(m)}(x) = \frac{l}{2} \quad \lim_{x \rightarrow \infty} B_l^{(m)}(x) = \frac{l-m}{2}.$$

This behaviour is written in the compact form

$$\begin{aligned} B_l^{(m)}(x) &= \Delta_+ - \Delta_- \operatorname{sgn} x \\ \Delta_+ &= \frac{2l-m}{4} \quad \Delta_- = \frac{m}{4} \\ \Delta_+ + \Delta_- &= \frac{l}{2} \quad \Delta_+ - \Delta_- = \frac{l-m}{2}. \end{aligned} \quad (3.89)$$

Eq. (3.89) and similar equations in the following have to be understood asymptotically, for $|x| \rightarrow \infty$. As is shown in appendix B.2,

$$k^{(s)} * \operatorname{sgn} x = \operatorname{sgn} x - \frac{1}{x}, \quad k^{(s)} * \frac{\operatorname{sgn} x}{x} = \frac{\operatorname{sgn} x}{x} + \frac{\ln|x|}{x^2} - \frac{\Psi(2)}{x^2} \quad (3.90a)$$

$$k^{(s)} * \frac{1}{x} = \frac{1}{x}, \quad k^{(s)} * \frac{\ln|x|}{x^2} = \frac{\ln|x|}{x^2} \quad (3.90b)$$

$$k^{(s)} * \frac{1}{x^2} = \frac{1}{x^2} + \frac{1}{2x^2} \varepsilon. \quad (3.90c)$$

$\Psi(x)$ is the digamma function; $\Psi(2) = -C + 1$, $C = 0.577\dots$ is Euler's constant. The asymptotic evaluation of the convolutions has been done using distributions. Taken literally, these approximate $B_l^{(m)}$ by step-like functions with jumps at the origin. A test in how far one can rely on this asymptotic expansion is done by considering the integral

$$I_\Delta(x) := \int_{-\infty}^{\Delta} k(x-y) f_{corr}(y) dy, \quad (3.91)$$

where $f_{corr}(x) = x^{-1} + \ln|x|/x^2 + x^{-2}$ and Δ is some negative cutoff near to the origin, thus avoiding the singularities of f_{corr} in the integral. The use of distributions for describing the asymptotic behaviour only makes sense when the asymptotic expansion of the integral in eq. (3.91) does not depend on Δ . Indeed, this is the case in the orders $\mathcal{O}(x^{-1}, \ln|x|/x^2)$. In the order x^{-2} , however, the result does depend on Δ (in the form Δ/x^2). In other words, to determine accurately the x^{-2} -coefficient, the precise behaviour of the auxiliary functions around the origin must be known. The quantity ε in eq. (3.90c) accounts for the error made in the analytical evaluation, it is the integral over the whole

function which decays as $1/x^2$, see appendix B.1. We cannot determine ε analytically in this approach. It can be determined numerically as shown later on.

We make the following ansatz for $B_l^{(m)}$, which consists in extrapolating the asymptotic behaviour over the whole axis with the aid of distributions:

$$B_l^{(m)}(x) = \Delta_+ - \Delta_- \operatorname{sgn}x + \frac{1}{x}(\Delta_+^{(1)} - \Delta_-^{(1)} \operatorname{sgn}x) + \frac{\ln|x|}{x^2}(\Delta_+^{(1)} - \Delta_-^{(1)} \operatorname{sgn}x) + \frac{1}{x^2}(\Delta_+^{(2)} - \Delta_-^{(2)} \operatorname{sgn}x) \quad (3.92)$$

$$\begin{aligned} [k * B_l^{(m)}](x) &= \frac{\Delta_+ - \Delta_- \operatorname{sgn}x}{2} + \frac{1}{2x} \left(\Delta_- + \Delta_+^{(1)} - \Delta_-^{(1)} \operatorname{sgn}x \right) \\ &\quad - \left(\Delta_-^{(1)} - \Delta_+^{(l)} + \Delta_-^{(l)} \operatorname{sgn}x \right) \frac{\ln|x|}{2x^2} \\ &\quad + \left(\Delta_-^{(1)} \Psi(2) + \Delta_+^{(2)} - \Delta_-^{(2)} \operatorname{sgn}x + \frac{\varepsilon}{2} \right) \frac{1}{2x^2} . \end{aligned} \quad (3.93)$$

The convolutions are done with the help of eqs. (3.90a), (3.90b), (3.90c). One observes that only the terms $\operatorname{sgn}x$ and $\operatorname{sgn}x/x$ give the next higher order contribution when convoluted with the kernel. The asymptotic form of eq. (3.88) is found by inserting eqs. (3.92), (3.93).

By comparing coefficients, one finds

$$\begin{aligned} \Delta_+^{(1)} + \Delta_-^{(1)} &= l \Delta_- = \frac{m \cdot l}{4} & \Delta_+^{(1)} &= \frac{m(2l-m)}{8} \\ \Delta_+^{(1)} - \Delta_-^{(1)} &= (l-m) \Delta_- = \frac{m(l-m)}{4} & \Delta_-^{(1)} &= \frac{m^2}{8} \\ \Delta_+^{(l)} + \Delta_-^{(l)} &= -l \Delta_-^{(1)} = -\frac{m^2 \cdot l}{8} \\ \Delta_+^{(l)} - \Delta_-^{(l)} &= (l-m) \Delta_-^{(1)} = -\frac{m^2(l-m)}{8} \\ \Delta_+^{(2)} + \Delta_-^{(2)} &= l(\Delta_-^{(1)} \Psi(2) + \varepsilon/2) = \Psi(2) \frac{m^2 \cdot l}{8} + \frac{l\varepsilon}{2} \end{aligned} \quad (3.94)$$

$$\Delta_+^{(2)} - \Delta_-^{(2)} = (l-m)(\Delta_-^{(1)} \Psi(2) + \varepsilon/2) = \Psi(2) \frac{m^2 \cdot (l-m)}{8} + \frac{(l-m)\varepsilon}{2} \quad (3.95)$$

In the high-temperature regime, the $x \rightarrow -\ln T/T_K \ll 0$ behaviour is of importance,

$$\lim_{x \ll 0} B_l^{(m)}(x) = \frac{l}{2} + \frac{ml}{4x} - \frac{m^2 l}{8} \frac{\ln|x|}{x^2} + \frac{l}{x^2} \left(\frac{m^2 \Psi(2)}{8} + \frac{\varepsilon}{2} \right) . \quad (3.96)$$

Compare eq. (3.96) with the low temperature results eqs. (3.37), (3.38). Both are formally identical up to the order $\ln|x|/x^2$, $x = -\ln T/T_K$ in eq. (3.96), $x = -\ln h/\tilde{T}_h$ in eqs. (3.37), (3.38).

We shall focus on the $x \rightarrow +\infty$ asymptotes in the next paragraph.

Our analysis is continued by expanding $\partial_{\beta h}^2 \ln Y_j =: Y_j^{(\chi)}$, $\partial_{\beta h}^2 \ln \mathfrak{B}_l =: B_l^{(\chi)}$, $\partial_{\beta h}^2 \ln \bar{\mathfrak{B}}_l =: \bar{B}_l^{(\chi)}$.

These functions are given by the system

$$Y_j^{(\chi)} = \left(1 - e^{-\ln Y_j}\right) s * \left(Y_{j-1}^{(\chi)} + Y_{j+1}^{(\chi)}\right) \quad (3.97a)$$

$$Y_0^{(\chi)} \equiv 0 \quad (3.97b)$$

$$B_l^{(\chi)} = \frac{e^{-\ln \mathfrak{B}_l}}{1 - e^{-\ln \mathfrak{B}_l}} \left[B_l^{(m)}\right]^2 + \left(1 - e^{-\ln \mathfrak{B}_l}\right) s * Y_{l-1}^{(\chi)} + \left(1 - e^{-\ln \mathfrak{B}_l}\right) \left(k * B_l^{(\chi)} - k_- * \bar{B}_l^{(\chi)}\right) \quad (3.97c)$$

$$\bar{B}_l^{(\chi)} = \frac{e^{-\ln \bar{\mathfrak{B}}_l}}{1 - e^{-\ln \bar{\mathfrak{B}}_l}} \left[\bar{B}_l^{(m)}\right]^2 + \left(1 - e^{-\ln \bar{\mathfrak{B}}_l}\right) s * Y_{l-1}^{(\chi)} + \left(1 - e^{-\ln \bar{\mathfrak{B}}_l}\right) \left(k * \bar{B}_l^{(\chi)} - k_+ * B_l^{(\chi)}\right) \quad (3.97d)$$

$$B_l^{(\chi)} =: B_{l,1}^{(\chi)} + iB_{l,2}^{(\chi)}$$

$$\bar{B}_l^{(\chi)} = \left[B_l^{(\chi)}\right]^* .$$

The vanishing of $B_2^{(m)}$ helps to expand $B_1^{(\chi)}$:

$$B_{l,1}^{(\chi)} = \frac{1}{l} \left[B_{l,1}^{(m)}\right]^2 + \frac{l}{2(l+1)} Y_{l-1}^{(\chi)} + \frac{l}{l+1} \operatorname{Re} \left(k_-^{(d)} * B_{l,1}^{(\chi)} + ik_-^{(s)} * B_{l,2}^{(\chi)}\right) \quad (3.98a)$$

$$B_{l,2}^{(\chi)} = -\frac{\pi m}{4x^2} \left[B_{l,1}^{(m)}\right]^2 + \frac{lm}{l+1} \frac{\pi}{8x^2} Y_{l-1}^{(\chi)} + \frac{l}{l+1} \operatorname{Im} \left(k_-^{(d)} * B_{l,1}^{(\chi)} + ik_-^{(s)} * B_{l,2}^{(\chi)}\right) . \quad (3.98b)$$

From eq. (3.98b), $B_{l,2}^{(\chi)} = \mathcal{O}(x^{-2})$. Together with eq. (3.80), one concludes that the last term in brackets in eq. (3.98a) is $\mathcal{O}(x^{-3})$. This means that for our purposes, the convolutions in eq. (3.98a) can be entirely neglected. Thus in the asymptotic limit, eqs. (3.97a)-(3.97c) are simplified considerably:

$$Y_j^{(\chi)} = \frac{j(j+2)}{2(j+1)^2} \left(Y_{j-1}^{(\chi)} + Y_{j+1}^{(\chi)}\right)$$

$$Y_0^{(\chi)} \equiv 0$$

$$B_l^{(\chi)} = \frac{1}{l} \left[B_l^{(m)}\right]^2 + \frac{l}{2(l+1)} Y_{l-1}^{(\chi)}$$

This system bears similarity with eqs. (3.77a)-(3.77c). From the solution of those equations, we conclude

$$\lim_{x \rightarrow -\infty} Y_j^{(\chi)}(x) = \frac{j(j+2)}{6} \left(1 + \frac{m}{x} - \frac{m^2 \ln|x|}{2x^2} + \left(\frac{m^2}{2} \Psi(2) + \frac{m^2}{4} + 2\varepsilon\right) \frac{1}{x^2}\right)$$

$$\begin{aligned} \lim_{x \rightarrow -\infty} B_l^{(\chi)}(x) &= b_{l,0}^{(\chi)} + \frac{b_{l,1}^{(\chi)}}{x} + b_{l,2}^{(\chi)} \frac{\ln|x|}{x^2} + \frac{b_{l,2}^{(\chi)}}{x^2} \\ &= \frac{l(l+2)}{12} \left(1 + \frac{m}{x} - \frac{m^2 \ln|x|}{2x^2} + \left(\frac{m^2}{2} \Psi(2) + \frac{m^2}{4} + 2\varepsilon\right) \frac{1}{x^2}\right) \end{aligned}$$

ε is the error made in this analytical analysis. Concluding, a systematic asymptotic expansion of the auxiliary functions around their $x \rightarrow -\infty$ -asymptotes is possible. It can be done analytically up to the indicated orders.

We can go one step further with numerical efforts. In appendix C, a procedure for numerically determining the coefficient $\Delta_+^{(2)} - \Delta_-^{(2)} \operatorname{sgn} x$ of the x^{-2} -decay is described. It deviates slightly from the analytical estimate with $\varepsilon = 0$. We introduce an extra symbol ϕ ,

$$\phi(m) := \left(\Delta_+^{(2)} + \Delta_-^{(2)} \right) / (lm^3) = \frac{1}{m^3} \left(\frac{m^2}{8} \Psi(2) + \frac{\varepsilon}{2} \right) \quad (3.99)$$

Numerically, ϕ is found to be independent of l . However, our data do not suffice to exclude a dependence on m . These results are given in appendix C, table C.3. Let us cite the special case $m = 1$,

$$\phi(m = 1) = 0.04707 \pm 2 \cdot 10^{-7} \quad (3.100)$$

One makes use of the knowledge of the asymptotic behaviour of the auxiliary functions to extract the high-temperature behaviour of the free energy, the specific heat and magnetic susceptibility without magnetic field. Employing once again the approximation eq. (3.76), this time in the integral of the free energy, we find

$$\lim_{T \gg T_K} f(T, h = 0) = -T \ln(l + 1) + \frac{T}{\ln^3 \frac{T}{T_K}} \frac{ml(l + 2)\pi}{12} \quad (3.101a)$$

$$\lim_{T \gg T_K} C(T, h = 0) = \frac{T}{\ln^4 \frac{T}{T_K}} \frac{ml(l + 2)\pi^2}{4} \quad (3.101b)$$

$$\lim_{T \gg T_K} \chi(T, h = 0) = \frac{l(l + 2)}{12T} \left(1 - \frac{m}{\ln \frac{T}{T_K}} - \frac{m^2 \ln \ln T/T_K}{2 \ln \frac{T}{T_K}} + \frac{4m^3 \phi(m) + m^2/4}{\ln^2 \frac{T}{T_K}} \right) \quad (3.101c)$$

The leading orders of the specific heat and magnetic susceptibility are for the first time calculated for general m . Note that the $\ln^{-4} T/T_K$ divergence of $C(T \gg T_K, 0)$ in contrast to the $T/(h \ln^2 h/T_K)$ behaviour in the case with finite field and $T \ll T_K$, eq. (3.53). The single-channel case $m = 1$ agrees with known TBA-results, [90]. The same is true for the corrections to the magnetic susceptibility. Especially, note that we firstly determine the coefficient of the $(\ln T/T_K)^2$ -coefficient of the magnetic susceptibility in the framework of an exact solution. This allows for the calculation of Wilson's ratio, relating the high-temperature to the low-temperature scale, see below.

In section 2.2.2, the equivalence between the TBA equations and the NLIE has been established, based on the fusion hierarchy. In the framework of TBA equations, (2.164), it is possible to calculate the coefficient of the $1/\ln^3 T/T_K$ contribution to the free energy analytically for $m = 1$, [90]. The result agrees with eq. (3.101b). However, the TBA method fails for $m > 1$.

The over-screened case $m = l$ is obtained by setting $m = l$ and inserting $\ln Y_{j=l}$ and its derivatives into the definitions of the free energy, specific heat and susceptibility. The results are identical with eqs. (3.101a), (3.101b), (3.101c).

Wilson's ratio

In this section, we want to calculate Wilson's ratio, relating the low-temperature scale T_K to some high-temperature scale \tilde{T}_K , to be defined.

Let us first draw our attention to the exactly screened spin-1/2 case, $l = 1 = m$. In his numerical renormalization group approach, Wilson started from high temperatures and rescaled the temperature dependent coupling constant upon lowering the temperature. In this way, the low temperature regime of the impurity susceptibility was for the first time obtained non-perturbatively. His result [94] for

the zero-field spin-1/2 susceptibility is

$$\begin{aligned}\lim_{T \rightarrow 0} \chi(T) &= \frac{1}{2\pi T_K} = \frac{0.1032 \pm 0.0005}{\tilde{T}_K} \\ \frac{\tilde{T}_K}{T_K} &= 2\pi \cdot (0.1032 \pm 0.0005) =: 2\pi\xi.\end{aligned}\quad (3.102)$$

This ratio relates the low-temperature scale eq. (2.107) to the high-temperature scale \tilde{T}_K , defined by absorbing the term $\mathcal{O}(x^{-2})$ in the asymptotic expansion

$$\begin{aligned}\lim_{T \gg T_K} \chi(T) &= \frac{1}{2\pi T} \int_{-\infty}^{\infty} \frac{1}{\cosh(x + \ln T/T_K)} \partial_{\beta h}^2 [\ln \mathfrak{B}_1 \overline{\mathfrak{B}}_1](x) dx \\ &= \frac{1}{2T} \partial_{\beta h}^2 [\ln \mathfrak{B}_1 \overline{\mathfrak{B}}_1](x = -\ln T/T_K) + \mathcal{O}\left([\partial_{\beta h}^2 \ln \mathfrak{B}_1 \overline{\mathfrak{B}}_1]''(x)\right) \\ &= b_{1,0}^{(\chi)} + \frac{b_{1,1}^{(\chi)}}{x} + \frac{b_{1,1}^{(\chi)} \ln|x|}{x^2} + \frac{b_{1,2}^{(\chi)}}{x^2} \Bigg|_{x=-\ln T/T_K} \\ &= b_{1,0}^{(\chi)} + \frac{b_{1,1}^{(\chi)}}{x - \frac{b_{1,2}^{(\chi)}}{b_{1,1}^{(\chi)}}} + \frac{b_{1,1}^{(\chi)} \ln|x|}{x^2} \Bigg|_{x=-\ln T/T_K}.\end{aligned}\quad (3.103)$$

Wilson's ratio is identified to be

$$2\pi\xi = \exp\left(-\frac{b_{1,2}^{(\chi)}}{b_{1,1}^{(\chi)}}\right).\quad (3.104)$$

The reason for searching a scale \tilde{T}_K such that the term $\mathcal{O}(\ln^{-2} T/T_K)$ is absorbed in the asymptotic expansion of the zero-field high-temperature susceptibility is the aim to write physical quantities in a way that exhibits scaling behaviour. This means that it is possible to find an expansion

$$\lim_{T \gg T_K} \chi(T) = \frac{1}{4T} (1 + z + cz^2 + \mathcal{O}(z^3)),\quad (3.105)$$

where the *dynamical coupling constant*² z is scale-invariant: It is the product of two functions; the first depending on D, J (both changing upon rescaling), the second on the energy parameter ϵ , (T in this case), and invariant under scaling. Indeed, perturbation theory confirms eq. (3.105): By evaluating the relevant Green's functions, the result to order J^2 is [1, 94]:

$$\chi(T) = \frac{1}{4T} \left(1 - \frac{J}{2} + \frac{J^2}{4} \ln T/D + cJ^2 + \dots\right).$$

Upon defining

$$z = \frac{J/2}{1 + J \ln T/D}, \quad J > 0,$$

the susceptibility is written as in eq. (3.105).

²In [90], z is called the invariant charge.

z does not change as

$$D \rightarrow D', J \rightarrow J' = [J^{-1} - \ln D/D']^{-1}.$$

The cited form of z has been found in [1] by summing the leading \ln -contributions to the Green's functions. The phenomenological introduction of a dynamical or temperature dependent coupling constant in the framework of perturbation theory is justified in the renormalization group (RG) approach. A RG-transformation consists in changing the bandwidth D , resulting in a change of the initial coupling constant J , preserving the form of the initial Hamiltonian. Thus J gets the energy-dependent z and D is scaled until reaching the physical energy scale ϵ . Since z is assumed to show scaling behaviour,

$$\begin{aligned} \frac{dz}{d \ln \epsilon} &= \beta(z) \\ \int_D^\epsilon d(\ln \epsilon') &= \int_J^z \frac{1}{\beta(z')} dz'. \end{aligned} \quad (3.106)$$

where β is itself a function of z , which is determined perturbationally for $|z| \ll 1$. In [4, 42], it is shown that $\beta(z) = -z^2 + \frac{1}{2}z^3$. Then with the definition of the "high-temperature scale"

$$\tilde{T}_K := D e^{-1/J+1/2 \ln J + \mathcal{O}(J)} \quad (3.107)$$

one gets

$$\ln \frac{\epsilon}{\tilde{T}_K} = \frac{1}{z} - \frac{1}{2} \ln z. \quad (3.108)$$

One inverts eq. (3.108) asymptotically by defining $z = z_1 + z_2 + z_3 + \dots$, with $\lim_{\epsilon \gg \tilde{T}_K} z_{i+1}/z_i = 0$. The z_i are identified upon successively considering the i th leading order of magnitude. One finds:

$$\begin{aligned} z_1 &= \frac{1}{\ln \epsilon / \tilde{T}_K} \\ z_2 &= -\frac{z_1^2}{2} \ln z_1 = \frac{1}{2 \ln^2 \epsilon / \tilde{T}_K} \ln \ln \epsilon / \tilde{T}_K \\ z_3 &= \frac{z_2^2}{2(z_1 - z_2)} \approx \frac{z_2^2}{2z_1} + \mathcal{O}(z_2^3/z_1^2) = \frac{z_1^3}{8} \ln^2 z_1 + \mathcal{O}(z_2^3/z_1^2) \end{aligned} \quad (3.109)$$

Especially we see that there is no term $\mathcal{O}(\ln^{-2} \epsilon / \tilde{T}_K)$ occurring in eq. (3.109).³ This is the defining property of \tilde{T}_K . The scale ϵ may be either the magnetic field (when $T = 0$, then we rather write \tilde{T}_h) or the temperature. In the former case, at $T = 0$, one finds \tilde{T}_h analytically by linearizing the NLIE, section 3.1.2. With the help of the preceding paragraph, it is possible to give a numerical value for \tilde{T}_K . Note that our approach is somehow inverse to Wilson's: We defined T_K through the zero-temperature susceptibility, and rescaled it in the high-temperature regime.

The relation between T_K , \tilde{T}_K is given by eq. (3.102). This means that eq. (2.107) implies

$$T_K = \frac{D}{2\pi\xi} e^{-1/J+1/2 \ln J + \mathcal{O}(J)}.$$

When looking at T_K , defined from the effective model, eqs. (2.125), (2.153) in the isotropic limit for $|J| \ll 1$, agreement is found only in the leading order in J . This is due to the different cutoff-schemes denoted by the parameters D, \mathcal{D} . The latter is employed in the derivation of (2.153), justified heuristically.

³There would be such a term if on the rhs of eq. (3.108), a constant was added.

Andrei and Lowenstein [8] carried out a perturbative expansion of the $2S = m = 1$ free energy, both for $h/T \gg 0$ and $T/h \gg 0$. By requiring that in the first case, the result should depend on h/T_h , in the second case on T/\tilde{T}_K , they deduced the ratio T_h/\tilde{T}_K . Moreover, they determined the ratio T_h/T_K from the (conventional) BA. Arguing that the ratios of the energy scales are universal (unlike the scales themselves, which do depend on the cutoff-scheme used), they found by combining their two results (the analytical expression is due to Hewson, [42])

$$\xi = \frac{e^{C+3/4}}{4\pi^{3/2}} = 0.102676\dots \quad (3.110)$$

We generalize Wilson's definition (3.104) to the general spin- S case, in the presence of m channels. A scheme of numerically solving the integral equations is given in appendix C which allows for the calculation of the corresponding ratios. For general l, m , eq. (3.104) reads in the notation of section 3.2.1

$$2\pi\xi = \exp\left[-m^2\left(4\phi(m) + \frac{1}{4}\right)\right],$$

which does only depend on m , analogously to the ratio \tilde{T}_h/T_K for $T = 0$, eqs. (3.35), (3.36). This is in contradiction with [31]. There, the Wilson ratios for S arbitrary, $m = 1$ are calculated. The ratio T_K/T_h for $T = 0$ is found by BA techniques and agrees with ours, eq. (3.20) for $\gamma = 0$. T_h/\tilde{T}_K is found by conventional perturbation theory (unfortunately without the explicit calculations). The resulting T_K/\tilde{T}_K depends exponentially on $S(S+1)$. We leave this question to be clarified.

By inserting eq. (3.100), one gets for $m = 1$:

$$\xi = 0.102678 \pm 2 \cdot 10^{-6}.$$

This result agrees with eq. (3.102) and with eq. (3.110). Note that for $2S > m$, the susceptibility at low temperatures can be obtained from that at high temperatures by replacing $l \rightarrow (l - m)$. This does not change the value of ξ , which means that in the under-screened cases, only one scale (namely \tilde{T}_K) governs the low- and high-temperature behaviour.

3.2.2 High temperature expansion, $h \neq 0$

The strategy of asymptotically linearizing the equations is the same as above, the calculations are more involved. We want to include this case explicitly, since the first correction is needed for the numerical solution of the equations.

Therefore, define correction functions \mathfrak{D}_l, D_j ,

$$\begin{aligned} \ln \mathfrak{B}_l(x) &= \ln \mathfrak{B}_l^{(\infty)} + \mathfrak{D}_l(x), & \ln \overline{\mathfrak{B}}_l(x) &= \ln \overline{\mathfrak{B}}_l^{(\infty)} + \overline{\mathfrak{D}}_l(x) \\ \ln Y_j(x) &= \ln Y_j^{(\infty)} + D_j(x) \\ \mathfrak{D}_l + \overline{\mathfrak{D}}_l &= D_l. \end{aligned} \quad (3.111)$$

The last equation follows from the fusion hierarchy. $\mathfrak{D}_l, \overline{\mathfrak{D}}_l, D_j$ depend parametrically on

$$\zeta := \beta h/2,$$

especially $\mathfrak{D}_l|_\zeta = \overline{\mathfrak{D}}_l|_{-\zeta}$, since we expect $\mathfrak{D}(x), \overline{\mathfrak{D}}(x)$ to be real-valued. Furthermore, the x -dependence is the same as in the $h = 0$ -case, because merely the asymptotic values are altered. So one can again approximate $[s * \delta](x \ll 0) = \delta(x)/2$, with $\delta = \mathfrak{D}_l, \overline{\mathfrak{D}}_l, D_j$. We want to carry out the calculation

explicitly for the coefficients of the $1/x$ -correction, coefficients of higher orders follow along the same lines. Inserting values for the asymptotes, one gets

$$2 \frac{\sinh^2 \zeta(j+1)}{\sinh \zeta j \sinh \zeta(j+2)} D_j(x) = D_{j+1}(x) + D_{j-1}(x) \quad (3.112)$$

$$D_0 \equiv 0$$

$$2e^{-\zeta} \frac{\sinh \zeta(l+1)}{\sinh \zeta l} \mathfrak{D}_l(x) = D_{l-1}(x) + \left(\mathfrak{D}_l(x) - \overline{\mathfrak{D}}_l(x) + \frac{\alpha m}{x} \right) \quad (3.113)$$

$$2e^{\zeta} \frac{\sinh \zeta(l+1)}{\sinh \zeta l} \overline{\mathfrak{D}}_l(x) = D_{l-1}(x) - \left(\mathfrak{D}_l(x) - \overline{\mathfrak{D}}_l(x) + \frac{\alpha m}{x} \right). \quad (3.114)$$

The term in $1/x$ results from the $1/x$ contribution of the convolution $k * \left(\ln \mathfrak{B}_l^{(-\infty)} - \ln \mathfrak{B}_l^{(\infty)} \right)$, eq. (3.90a). Once again, we observe that the functional dependence on x of all correction functions is determined by the last equation. Thus one recognizes that for $h \neq 0$, already the auxiliary functions itself (and not only their derivatives with respect to h) acquire algebraical corrections of order $1/x$.

The solution of eqs. (3.112) can be extracted from eqs. (3.61), by replacing the asymptotes and carrying out the limit $k \rightarrow 0$ (since the convolution was replaced by a multiplication with $1/2$ in eqs. (3.112)):

$$D_j(x) = \left[\frac{\sinh \zeta j}{\sinh \zeta(j+1)}(j+2) - \frac{\sinh \zeta(j+2)}{\sinh \zeta(j+1)}j \right] \frac{d_l}{x}.$$

The factor d_l still depends on ζ , l , m , and has to be determined from the boundary condition eq. (3.113). Therefore, first observe that from eqs. (3.113), (3.114),

$$\mathfrak{D}_l - \overline{\mathfrak{D}}_l = \zeta m \frac{\cosh \zeta \sinh \zeta l}{\sinh \zeta \cosh \zeta l}.$$

d_l can now be calculated from equating eq. (3.111) with the actual value of $\mathfrak{D}_l + \overline{\mathfrak{D}}_l$ from eqs. (3.113), (3.114). We find

$$\begin{aligned} d_l &= -\frac{\zeta m}{2(l+1)} \frac{\sinh \zeta(l+1)}{\cosh \zeta l \sinh^2 \zeta} \\ \mathfrak{D}_l(x) &= \frac{\zeta m}{2(l+1)} \frac{1}{\sinh^2 \zeta \cosh \zeta l} \left(l e^{\zeta(l+1)} \sinh \zeta - \sinh \zeta l \right) \frac{1}{x} \\ \overline{\mathfrak{D}}_l &= \frac{\zeta m}{2(l+1)} \frac{1}{\sinh^2 \zeta \cosh \zeta l} \left(l e^{-\zeta(l+1)} \sinh \zeta - \sinh \zeta l \right) \frac{1}{x} \\ D_j &= \frac{\zeta m}{2(l+1)} \frac{\sinh \zeta(l+1)}{\cosh \zeta l \sinh^2 \zeta} \left(j \frac{\sinh \zeta(j+2)}{\sinh \zeta(j+1)} - (j+2) \frac{\sinh \zeta j}{\sinh \zeta(j+1)} \right) \frac{1}{x} \end{aligned}$$

A check of consistency with the results of section 3.2.1 is an expansion of \mathfrak{D}_l , $\overline{\mathfrak{D}}_l$, D_j in ζ up to $\mathcal{O}(\zeta^2)$ inclusively.

$$x \lim_{\zeta \rightarrow 0} \mathfrak{D}_l(x) = \frac{lm}{2} \zeta + \frac{ml(l+2)}{6} \zeta^2 + \mathcal{O}(\zeta^3) \quad (3.115a)$$

$$x \lim_{\zeta \rightarrow 0} \overline{\mathfrak{D}}_l(x) = -\frac{lm}{2} \zeta + \frac{ml(l+2)}{6} \zeta^2 + \mathcal{O}(\zeta^3) \quad (3.115b)$$

$$x \lim_{\zeta \rightarrow 0} D_j(x) = \frac{j(j+2)}{3} \zeta^2 + \mathcal{O}(\zeta^4) \quad (3.115c)$$

D_j is even in ζ as it must be. The first algebraic correction to $B_l^{(m)}$, $B_l^{(\chi)}$, $Y_j^{(\chi)}$ is obtained by partially deriving the coefficients of $\ln \mathfrak{B}_l$, $\ln \overline{\mathfrak{B}}_l$, $\ln Y_j$ with respect to h . As can be seen from eqs. (3.115a), (3.115b), (3.115c), the known results of the $h = 0$ -case are reproduced. Note that with finite magnetic field, there are also $1/x$ -corrections to the functions partially derived with respect to T , that is in the entropy and specific heat.

Higher order terms, namely those in $\ln|x|/x^2$, x^{-2} , can be calculated in the same way. However, we do not want to dwell on the coefficients of those orders, since they are of no practical use in the framework of this work and the calculations are cumbersome. Only the coefficient of the $1/x$ -decay is needed for the numerical solution, cf. chapter 4.

3.2.3 Low temperature evaluation in the under-screened case

We are interested in the behaviour of the auxiliary functions for large values $x \rightarrow \infty$ in the under-screened case $l > m$. In this limit, the set of NLIE decouples in two separate sets with exponential accuracy, as noted in the derivation of the asymptotes, eqs. (2.163). Consider first the field-free case $h = 0$. The last $l - m$ functions, namely $Y_{m+1}, \dots, \mathfrak{B}_l, \overline{\mathfrak{B}}_l$, satisfy a set of equations formally identical to eqs. (3.77a)-(3.77c), with j, l replaced by $j - m, l - m$. The whole analysis of paragraph 3.2.1 applies to this case; of special interest are now the corrections to the $x = \ln \frac{T_K}{T} \gg 0$ -behaviour of the auxiliary functions. The results are:

$$\begin{aligned} \lim_{x \rightarrow \infty} \mathfrak{B}_l(x) &= \ln(l - m + 1) - i \frac{m(l - m)\pi}{4x^2} + \frac{m(l - m)(l - m + 2)\pi^2}{12x^3} \\ \lim_{x \rightarrow \infty} \ln Y_{j > m}(x) &= \ln(l + 1 - j) + \frac{m(l - m)(l - m + 2)\pi^2}{6x^3} \\ \lim_{x \rightarrow \infty} B_l^{(m)}(x) &= \frac{l - m}{2} + \frac{m(l - m)}{4x} - \frac{m^2(l - m)}{8} \frac{\ln|x|}{x^2} + \frac{l - m}{x^2} \left(\frac{m^2 \Psi(2)}{8} + \frac{\varepsilon}{2} \right) \\ \lim_{x \rightarrow \infty} Y_j^{(\chi)}(x) &= \frac{(j - m)(j - m + 2)}{6} \left(1 + \frac{m}{x} - \frac{m^2 \ln|x|}{2x^2} + \left(\frac{m^2}{2} \Psi(2) + \frac{m^2}{4} + 2\varepsilon \right) \frac{1}{x^2} \right) \\ \lim_{x \rightarrow \infty} B_l^{(\chi)}(x) &= \frac{(l - m)(l - m + 2)}{12} \left(1 + \frac{m}{x} - \frac{m^2 \ln|x|}{2x^2} + \left(\frac{m^2}{2} \Psi(2) + \frac{m^2}{4} + 2\varepsilon \right) \frac{1}{x^2} \right) \end{aligned}$$

One deduces the low-temperature behaviour in the over-screened case of the following quantities:

$$\begin{aligned} \lim_{T \ll T_K} f(T, h = 0) &= -T \ln(l - m + 1) - \frac{T}{\ln^3 \frac{T_K}{T}} \frac{m(l - m)(l - m + 2)\pi}{12} \\ \lim_{T \ll T_K} C(T, h = 0) &= \frac{T}{\ln^4 \frac{T_K}{T}} \frac{m(l - m)(l - m + 2)\pi^2}{4} \\ \lim_{T \ll T_K} \chi(T, h = 0) &= \frac{(l - m)(l - m + 2)}{12T} \\ &\quad \times \left(1 + \frac{m}{\ln \frac{T_K}{T}} - \frac{m^2 \ln \ln T_K/T}{2 \ln \frac{T_K}{T}} + \frac{4m^3 \phi(m) + m^2/4}{\ln^2 \frac{T_K}{T}} \right) \end{aligned} \quad (3.116)$$

The low-temperature behaviour for exact screening is given in paragraph 3.1.1, where the expected Fermi liquid shows up. Similarly to $T = 0$, a change of sign in the leading corrections to the asymptotic values of the susceptibility is observed, cf. eqs. (3.101c), (3.116). Its physical interpretation has been given in the sequel of eq. (3.38). It applies analogously in this case.

More care is needed for the first m functions, i.e. the under-screened case. The asymptotes of $\ln Y_{j \leq m}$ do not depend on βh (eq. (2.160)), however, it is still possible to realize an asymptotic

linearization. The difficulty lies in the evaluation of the convolutions, since the correction functions do not decay algebraically with integer exponents. This case is treated in paragraph 3.1.3.

Low temperature evaluation in the under-screened case, $h \neq 0$

The arguments of the preceding paragraph apply also for finite magnetic field, so we directly give the results:

$$\begin{aligned} \lim_{x \rightarrow \infty} \ln Y_j(x) &= 2 \ln \left(\frac{\sinh \zeta(j-m+1)}{\sinh \zeta} \right) + \frac{\zeta m}{2(l-m+1)} \times \\ &\quad \frac{\sinh \zeta(l-m+1)}{\cosh \zeta(l-m) \sinh^2 \zeta} \left((j-m) \frac{\sinh \zeta(j-m+2)}{\sinh \zeta(j-m+1)} - \frac{(j-m+2) \sinh \zeta(j-m)}{\sinh \zeta(j-m+1)} \right) \frac{1}{x} \\ \lim_{x \rightarrow \infty} \ln \mathfrak{B}_l(x) &= \ln \left(e^{\zeta(l-m)} \frac{\sinh \zeta(l-m+1)}{\sinh \zeta} \right) \\ &\quad + \frac{\zeta m}{2(l-m+1)} \frac{1}{\sinh^2 \zeta \cosh \zeta(l-m)} \left(l e^{\zeta(l-m+1)} \sinh \zeta - \sinh \zeta(l-m) \right) \frac{1}{x} \\ \lim_{x \rightarrow \infty} \ln \overline{\mathfrak{B}}_l(x) &= \ln \left(e^{-\zeta(l-m)} \frac{\sinh \zeta(l-m+1)}{\sinh \zeta} \right) \\ &\quad + \frac{\zeta m}{2(l-m+1)} \frac{1}{\sinh^2 \zeta \cosh \zeta(l-m)} \left(l e^{-\zeta(l-m+1)} \sinh \zeta - \sinh \zeta(l-m) \right) \frac{1}{x} . \end{aligned}$$

3.2.4 Anisotropic case, $\gamma \neq 0$

As will be explained in appendix A.4, the crossing parameter is restricted to $0 \leq \gamma \leq \frac{\pi}{2l}$, where $l = \max(l, m)$. Since the kernel $k(x)$ decays exponentially in direct space, corrections to $\ln \mathfrak{B}_l^{(\infty)}$, $\ln Y_j^{(\infty)}$ are expected to be exponentially small. Thus it is no longer permitted to replace convolutions with $s(x)$ by algebraic multiplications. Instead, let us write eq. (3.74a) in direct space, with the same notations as eq. (3.75), however including a finite magnetic field from the beginning. First subtract the asymptotes ($\zeta := \beta h/2$),

$$\lim_{x \ll 0} 2e^{-\zeta} \frac{\sinh \zeta(l+1)}{\sinh \zeta l} \delta_l(x) = \lim_{x \ll 0} \left\{ -e^x + [s * \delta_{l-1} + k * \delta_l - k_- * \bar{\delta}_l](x) \right\} . \quad (3.117)$$

Contrary to the isotropic case, the driving term $-e^x$ must be kept since all quantities on the rhs of eq. (3.117) are exponentially small. We did not find a closed solution to eq. (3.117). All we can do is to determine the exponent of the exponential decay. Therefore first observe that the equation

$$\delta_-^{(0)}(x) = -e^x + \int_{-\infty}^0 k(x-y) \delta_-^{(0)}(y) dy$$

is directly solvable by Wiener-Hopf techniques. This solution relies on the fact that

$$1 - \mathcal{F}_k[k] = \frac{\sinh \frac{\pi k}{2} \frac{\pi}{\gamma}}{2 \cosh \frac{\pi k}{2} \sinh \frac{\pi k}{2} \left(\frac{\pi}{\gamma} - l \right)}$$

is factorizable in functions analytical in the upper and lower half planes. The leading decay is

$$\delta_-^{(0)}(x \ll 0) \sim e^{\frac{2\gamma}{\pi} x} .$$

Since

$$2e^{-\zeta} \frac{\sinh \zeta(l+1)}{\sinh \zeta l} = 1 + e^{-2\zeta} \coth \zeta l ,$$

we take the solution $\delta_-^{(0)}$ as an ansatz for δ_- . It is seen that there is no further restriction on the leading decay of δ_- , such that

$$\delta_-(x \ll 0) \sim e^{\frac{2\gamma}{\pi}x} .$$

However, we did not succeed in determining the coefficient. Of course it depends on ζ , especially,

$$\begin{aligned} \lim_{x \ll 0} [\delta_- + \bar{\delta}_-](x) &\sim (\tilde{a}_1 + (\beta h)^2 \tilde{a}_2) e^{\frac{2\gamma}{\pi}x} \\ \lim_{T \gg T_K} f(T, h=0) &= -T \ln(l+1) + (\tilde{a}_1 + (\beta h)^2 \tilde{a}_2) \left(\frac{T_K}{T}\right)^{\frac{2\gamma}{\pi}} \end{aligned} \quad (3.118)$$

$$C(T \gg T_K, h=0) \sim \left(\frac{T_K}{T}\right)^{\frac{2\gamma}{\pi}} \quad (3.119)$$

$$\chi(T \gg T_K, h=0) = \frac{l(l+2)}{12T} \left(1 - a_2 \left(\frac{T_K}{T}\right)^{\frac{2\gamma}{\pi}}\right) . \quad (3.120)$$

Note that both C and χ show similar decays, contrary to the isotropic case. A formally identical behaviour shows up at low temperatures for $h=0$ and $l > m$. If $h \neq 0$ and $l > m$, the rigorous linearization, section 3.1.2, is done. Then $\chi \sim h^{-1} \ln^{-2} h/T_K$, eq. (3.53): The T -dependent power-like divergence is replaced by a logarithmic, h -dependent divergence.

If $T \ll T_K$, one argues in close analogy to the isotropic case: The decoupling into two independent sets still holds. However, the asymptotic values of the auxiliary functions for $x \rightarrow \infty$ are related to their $x \rightarrow -\infty$ counterparts by substituting $l \rightarrow (l-m)$ and scaling $\beta h \rightarrow \alpha \beta h$, $\alpha = (1 - m\gamma/\pi)^{-1}$, eq. (2.163). This scaling affects the susceptibility:

$$\lim_{T \ll T_K} f(T, h=0) = -T \ln(l-m+1) + (\tilde{a}_1 + (\beta h \alpha)^2 \tilde{a}_2) \left(\frac{T}{T_K}\right)^{\frac{2\gamma}{\pi}} \quad (3.121)$$

$$\lim_{T \ll T_K} C(T, h=0) \sim \left(\frac{T}{T_K}\right)^{\frac{2\gamma}{\pi}} \quad (3.122)$$

$$\lim_{T \ll T_K} \chi(T, h=0) = \frac{(l-m)(l-m+2)\alpha^2}{12T} \left(1 - a_2 \left(\frac{T}{T_K}\right)^{\frac{2\gamma}{\pi}}\right) \quad (3.123)$$

The constants in eqs. (3.118)-(3.120) differ from those in eqs. (3.121)-(3.123). For ease of notation, the same symbols have been used.

3.3 Summary

At high temperatures, $T \gg T_K$, the impurity spin approaches asymptotically the behaviour of a free spin of magnitude $S = l/2$. Corrections to the asymptotic values depend in their amplitude on the channel number m . Especially, the Wilson ratio relating low- to high-temperature scales is determined, with the help of a numerical solution, cf. appendix C.

The low temperature case is characterized by Fermi liquid behaviour. In the exactly screened case $l = m$, it is investigated by the dilogarithm technique and by the dressed charge formalism, in the framework of a rigorous linearization.

The most striking feature of the not exactly screened models $l \neq m$ for $T \ll T_K$ is the non-commutativity of the limits $T \rightarrow 0, h \rightarrow 0$. Consider the under-screened case, $l > m$. A "formal" Fermi liquid behaviour occurs for $h \neq 0$, described by eq. (3.52), together with a rest spin, possibly non-integer, eq. (3.33). On the other hand, if $h = 0$, an asymptotic approach to free $(l - m)/2$ spin asymptotes is observed, formally analogous to the $T \gg T_K$ case, paragraph 3.2.3. These findings lead [79, 80] to speak of a quantum critical point (QCP) at $T = 0, h = 0$ for under-screening. The "formal" Fermi liquid behaviour is investigated in [20] by perturbational techniques; they come to the same results, differing from ours by trivial constant pre-factors. The behaviour of such field-induced Fermi liquids with divergent electron masses near a QCP is described in more detail in [21].

The over-screened models have been treated by asymptotic linearization for low temperatures. The limits mentioned above do not commute, compare eqs. (3.57), (3.58) and (3.65a), (3.65b). Furthermore, they also display a "formal" Fermi liquid behaviour, eqs. (3.66), (3.70c). The non-integer powers (or logarithms for $m = 2$) occurring in the specific heat and susceptibility are remarkable, equally well as the fractional rest entropy, implied by eq. (2.160). They give evidence of a many body state not fully understood yet. Especially at low temperatures the situation is not satisfactory: Thermodynamic quantities are derived from integrals over the auxiliary functions, eq. (3.64). The behaviour of the auxiliary functions themselves is unknown. This is a drawback for numerical solutions, as shown in the next chapter.

Whereas with analytical tools, the NLIE can be investigated in certain limiting regions of the parameters, the next chapter deals with a numerical treatment of the NLIE over the whole parameter ranges.

Chapter 4

Numerical Investigation

This chapter presents results for thermodynamic equilibrium response functions of the impurity calculated from a numerical solution of the NLIE over a wide range of temperature and magnetic field.

Previous numerical studies were based on the TBA equations. Their numerical solution requires, in the isotropic case, a cutoff scheme of the infinitely many equations. The first numerical solution of the isotropic S -spin single channel model with $h = 0$ is due to Mel'nikov, [68]. This approach has been generalized and carried out for finite fields in [75]. Further numerical work includes the $S = 1/2$, $m = 1$, $\gamma \neq 0$ case [22], and the isotropic m -channel problem [24, 76].

The cited works met two difficulties: Either the infinitely many TBA equations for $\gamma = 0$ are cut off or $\gamma \neq 0$ is restricted to values $\pi/(2n)$, the root of unity case, whence there rest a number of finite equations. The system of NLIE eq. (2.154) allows for exact numerical solutions. Neither sets it restrictions to γ , except eq. (2.142), which also has to be fulfilled in the TBA approach, [79, 80]. Our numerical data obtained from the system eq. (2.154) confirm and extend those in the cited references.

All cases show qualitatively equal high-temperature asymptotes $T \gg T_K$, independent of the anisotropy, namely that of a free spin of magnitude S in an external field h . The crucial differences between the above mentioned cases show up at smaller temperatures:

- The approach to the free field behaviour. This has been analyzed analytically in the foregoing chapter and the results will be confirmed numerically.
- The crossover region $T \sim \mathcal{O}(T_K)$, which is not accessible analytically.
- The limit of low temperatures, which has been studied by analytical methods in the preceding chapter.

In the absence of a magnetic field, the results are presented in two subsections, containing the exactly and under-screened first and then the over-screened cases, respectively. Each subsection starts with the isotropic case, being followed by a finite anisotropy.

Calculations for finite fields are not carried out as generally as for $h = 0$. We only want to point out that such calculations can principally be done, and therefore restrict ourselves to $S = 1/2, 1$, $m = 1, 2$, including a possible anisotropy. In these cases, the entropy and magnetization curves for a wide temperature range are given.

In the whole chapter, the integration range extends from $-L$ to L , N is the number of sampling points and N_{it} the number of iterations.

4.1 Thermodynamic quantities for $h = 0$

4.1.1 Under-screened and exactly screened cases

The impurity spin S exceeds half the channel number, $S = l/2 \geq m/2$. For exact screening, $l = m$, Fermi liquid behaviour is recovered at low temperatures, whereas in the under-screened case, $S > m/2$, Kondo-like behaviour occurs at high and low temperatures. Both cases are illustrated in the ongoing for $S = 5/2$.¹

The crossover from low to high temperatures is displayed by the entropy curves, fig. 4.1. The Fermi liquid behaviour is shown qualitatively in the case $2S = m = 5$, $\gamma = 0$, for the specific heat (fig. 4.2) and the susceptibility (fig. 4.3). Both can be combined to the low temperature Wilson ratio, which reaches a constant, eq. (3.9). Quantitative results are summarized in table 4.1. To get an idea how far the numerical solution reproduces the approach to the asymptotes, the first correction to the susceptibility in the high temperature regime (fig. 4.4) and low temperature regime (fig. 4.5) is plotted. Note that this Kondo-like behaviour at low temperatures only occurs for $m/2 < S$. Whereas these corrections are slightly overestimated at high temperatures, one remarks the underestimation at low temperatures. These deviations stem from the finite integration range in the numerical studies. In any case, further numerical studies, like the calculation of Wilson's ratio, do not rely on these numerical errors, but on integrals over the whole integration range, which can be determined much more accurately.

As a comparison with earlier numerical studies based on the TBA equations, the location and value of the maximum of the specific heat for some under-screened cases calculated by Mel'nikov [68] and in our approach are given in table 4.2. The deviations grow with increasing spin, which probably is due to the fact that in [68], the infinitely many TBA-equations had to be truncated. This procedure inevitably leads to numerical errors, which grow with growing spin.

$l = m$	$R_n/2$				$R_a/2$			
	$\gamma = 0$	$\frac{0.1\pi}{2l}$	$\frac{0.5\pi}{2l}$	$\frac{0.9\pi}{2l}$	0	$\frac{0.1\pi}{2l}$	$\frac{0.5\pi}{2l}$	$\frac{0.9\pi}{2l}$
1	0.999994	1.05263158*	1.33333333	1.81818182	1	1.05263157	$1.\bar{3}$	$1.\bar{81}$
2	1.3339	1.405*	1.78*	2.43*	$1.\bar{3}$	1.40350877	$1.\bar{7}$	$2.\bar{42}$
3	1.668	1.758*	2.227*	3.036*	$1.\bar{6}$	1.75438597	$2.\bar{2}$	$3.\bar{03}$
4	2.002	2.113*	2.68*	3.65*	2	2.10526316	$2.\bar{6}$	$3.\bar{63}$
5	2.336	2.1;2.468*	3.12	4.26	$2.\bar{3}$	2.45614035	$3.\bar{1}$	$4.\bar{24}$

Table 4.1: Numerical results R_n compared with analytical predictions R_a of the low-temperature Wilson ratio. The numerical calculation has been done with $N = 32768$, $L = 100$, $N_{it} = 100$. Results denoted by * are obtained by integration over an interval with $L = 700$.

Let us now permit an anisotropy $\gamma \neq 0$. The functions decay exponentially, which facilitates numerical calculations. However, numerical errors appear when γ tends to its limiting values, $\gamma \rightarrow 0$ or $\gamma \rightarrow \pi/(2l)$. In the former case, the exponential decay becomes too weak for finite integration ranges, we take $\gamma = 0.1\pi/(2l)$ as smallest value. On the other hand, the kernel shows a pole for $\gamma = \pi/(2l)$, causing not controlled divergences. $\gamma = 0.9\pi/(2l)$ will be the maximal value γ is allowed to adopt.

¹We solved the NLIE for $m, 2S \leq 5$. The value $5/2$ is arbitrary, but reflects both the confirmation of analytical results by the numerics as well as numerical limitations.

S	$\ln T_0/T_K$		$C(T_0)$	
	[68]	this work	[68]	this work
1/2	-0.7985	-0.7985	0.177	0.177
1	-0.6349	-0.6162	0.063	0.0634
3/2	-0.5798	-0.5109	0.033	0.0325

Table 4.2: Location $\ln T_0/T_K$ of the maximal value $C(T_0)$ of the specific heat, calculated by Mel'nikov [68] and in our approach in the presence of one channel, $m = 1$.

The specific heat is only slightly affected by the anisotropy: Table 4.3 gives the location and the value of the maximum for different values of γ and m , keeping the spin fixed. In all cases, the maximum of $C(T)$ grows with growing anisotropy - in agreement with the fact that we deal with an Ising-like anisotropy. As to the entropy, this means that the crossover from lower to higher temperatures gets steeper for increasing γ .

The low temperature behaviour of the magnetic susceptibility is neatly affected by $\gamma \neq 0$, as predicted by eq. (3.123). In table 4.4, the low-temperature values of the susceptibility are given, both from numerical and analytical studies. Furthermore, we are able to distinguish between the logarithmic corrections to the Curie-like behaviour for $\gamma = 0$ and algebraic corrections for $\gamma \neq 0$: In table 4.5, the exponent extracted from numerical data is compared with analytical predictions.²

To get an impression how the anisotropy generally influences the susceptibility, the $\gamma = 0$ case is compared with $\gamma = 0.5\pi/(4S)$, $S = 5/2$ and channels $m = 1, \dots, 5$ in fig. (4.6). In the anisotropic case, the crossover from low to high temperatures is more pronounced.

Numerical results for the low-temperature Wilson ratio are presented, table 4.1, and compared with analytical findings.

4.1.2 Over-screened cases

The channel number exceeds twice the impurity spin, $m > 2S$. Whereas at high temperature, the common spin- S Kondo-like behaviour occurs, the low temperature state is difficult to grasp: It shows fractional entropy, and non-integer powers of temperature and field for the specific heat and susceptibility.

Crossover from the low to the high temperature state in the entropy is shown in fig. 4.7. According to this crossover, the specific heat shows a maximum for $T \approx T_K$, which grows with increasing spin, fig. 4.8. As expected, the free spin behaviour is recovered at high temperatures, independently of the channel number, fig. 4.9. The amplitude of the first logarithmic correction to this high-temperature value is that of the channel number, fig. 4.10. The deviation of the numerical result from the analytical value is traced back to finite size errors.

The leading low temperature behaviour of both the specific heat and the susceptibility is given by

²The exponents were calculated numerically by differentiating $\ln(T\chi - \chi^{(0)})$ with respect to $\ln T$; $\chi^{(0)} = \lim_{T \rightarrow \pm\infty}$, depending on whether high or low temperatures are considered. In the low-temperature regime, the resulting function approaches its asymptotes unambiguously. In the high-temperature regime, this function shows a minimum at $\ln T/T_K \approx 50$. For $\gamma\pi/(4S) = 0.2, 0.5$, a turning point at higher temperature follows, above which the function approaches its asymptotic value. The minimal value for $\gamma\pi/(4S) = 0.2$ is about 0.08, and for $\gamma\pi/(4S) = 0.5$ about 0.11: The difference between the minimum and the asymptotic value as given in the table decreases with increasing γ . If γ gets too large, as in the case $\gamma\pi/(4S) = 0.9$, such a turning point does not occur, so that the function increases up to the boundary from the minimum. This effect is due to the finite system size and numerical errors (note that a pole in the kernel occurs for $\gamma\pi/(4S) = 1$). That's why for $\gamma\pi/(4S) = 0.9$, we take the minimum as asymptotic value for the exponent.

m	$\gamma \cdot \left(\frac{\pi}{4S}\right)^{-1}$	$\ln \frac{T_0}{T_K}$	$C(T_0)$
1	0	-0.3011	0.01327
	0.2	-0.3011	0.01327
	0.5	-0.3011	0.01328
	0.9	-0.3011	0.01341
2	0	-0.1393	0.03353
	0.2	-0.1393	0.03353
	0.5	-0.1393	0.03355
	0.9	-0.1278	0.03380
3	0	-0.21072	0.06816
	0.2	-0.21072	0.06816
	0.5	-0.21072	0.06818
	0.9	-0.21072	0.06852
4	0	-0.4620	0.1397
	0.2	-0.4620	0.1397
	0.5	-0.4620	0.1398
	0.9	-0.4620	0.1401
5	0	-0.8440	0.360
	0.2	-0.8440	0.360
	0.5	-0.8440	0.360
	0.9	-0.8440	0.3603

Table 4.3: Location $\ln T_0/T_K$ of the maximal value $C(T_0)$ of the specific heat for various anisotropies in the exactly and under-screened $S = 5/2$ cases.

non-integer exponents, eq. (3.72), (3.73). In order to gain insight into the deviation of our numerical findings for the low-temperature Wilson ration from the analytical prediction by Affleck, table 3.1, the exponential law of $C(T)$ and $T \cdot \chi(T)$, extracted by numerical studies, is compared with the exact result in table 4.6. Whereas numerical data for specific heat agree well with the exact result, the susceptibility shows significant deviations.³ These deviations cause the error made in calculating the low-temperature Wilson ratio in the over-screened case. They presumably originate from contributions to the auxiliary functions in the low-temperature regime which are difficult to control numerically. This region of low temperatures is not completely understood in the over-screened case: As pointed out in the preceding chapter, the behaviour of the auxiliary functions is unknown and thus cannot be accounted for in the numerics.

We now include a finite anisotropy into our considerations. As in the under-screened case, the maximum value of the specific heat increases slightly with γ , table 4.7. At high temperatures, the Curie-law of the susceptibility is approached in a power-like manner (eq. (3.120)), table 4.8 compares the numerical result with the exact value. Deviations between both are traced back to finite size effects. Fig. 4.11 compares qualitatively the crossover in the susceptibility between the isotropic and anisotropic cases. As expected, the crossover is more pronounced for $\gamma \neq 0$. As to the low temperature Wilson ratio, the behaviour of $C(T)$ and $\chi(T)$ is very similar to the isotropic case, table 4.6, with the

³The same behaviour as already observed in the high-temperature regime of finite anisotropy, footnote 2 in this chapter, occurs: The function $d\chi(T)/d\ln T$ does not approach its asymptotic value for $T \ll T_K$, but shows a maximum at $\ln T/T_K \approx -10$. This maximal value is taken as the numerically calculated exponent. On the other hand, the asymptotic value of the specific heat exponent can be read of without ambiguity.

m	$\gamma \cdot \left(\frac{\pi}{4S}\right)^{-1}$	$\chi_n^{(0)}$	$\chi_a^{(0)}$
1	0	2.08	2.0
	0.2	2.130	2.08247
	0.5	2.233	2.21607
	0.9	2.418	2.41517
2	0	1.347	1.25
	0.2	1.4142	1.35634
	0.5	1.5633	1.54321
	0.9	1.862	1.85901
3	0	0.742	0.66667
	0.2	0.80	0.75449
	0.5	0.938	0.92272
	0.9	1.253	1.25102
4	0	0.287	0.25
	0.2	0.318	0.29537
	0.5	0.398	0.39063
	0.9	0.6109	0.61035

Table 4.4: $\lim_{T \ll T_K} T \cdot \chi(T) =: \chi^{(0)}$, calculated numerically (index n) and analytically (index a), $\chi_a^{(0)} = \frac{(2S-m)(2S-m+1)}{12} \frac{1}{(1-m\gamma/\pi)^2}$ for $2S = 5$.

same difficulties concerning the susceptibility.

4.2 Thermodynamic quantities for $h \neq 0$

Numerical data for $h \neq 0$ are less accurate than those for $h = 0$. Problems occur if $\beta h \gg 1$, in the $\beta h \gg 1$ regime. Then $\ln Y_j(x)$, $\ln \mathfrak{B}_l(x)$, $\ln \overline{\mathfrak{B}}_l(x)$ show a crossover of order βh over a range of order $(\beta h)^{-1}$ around the origin. This sharp crossover is hard to resolve numerically with acceptable effort, lowest temperatures are $T/T_K = \mathcal{O}(10^{-10})$. Although smoothed functions are dealt with, appendix C.2.3, some trembling of the data at $\beta h \gg 1$, of the order $\mathcal{O}(10^{-3})$ is inevitable. It is a numerical artefact, with no physical meaning. Unintentionally, it is exaggerated in the corresponding plots. In the following, the exactly screened cases $S = 1 = m/2$, the under-screened case $S = 1 = m$ and the over-screened case $S = 1/2 = m/2$ are considered.

4.2.1 Under-screened and exactly screened cases

Fig. 4.12 shows the entropy in the exactly screened case $S = 1$, $m = 1$. The magnetic field shifts the onset of the crossover to higher temperatures. This confirms the intuitive idea of the magnetic field to induce "order" which competes with "disorder" caused by temperature. Consequently the peak in the specific heat shifts to higher temperatures, which is shown in fig. 4.13. There one also realizes that the anisotropy plays an increasingly important role with increasing magnetic field. This is in accordance with the intuitive expectation, since we are dealing with an Ising-like anisotropy. Note that the crossover in the susceptibility also is shifted to higher temperatures, the higher the magnetic field, fig. 4.14. The entropy of the under-screened case with and without magnetic field is shown in fig. 4.15. The non-commutativity of the limits $T \rightarrow 0$, $h \rightarrow 0$, known from analytical studies, is evident.

m	$\gamma \cdot \left(\frac{\pi}{4S}\right)^{-1}$	$\nu_n^{(l)}$	$\nu_n^{(h)}$	ν_a
1	0.2	0.068	0.040	0.04
	0.5	0.13	0.087	0.1
	0.9	0.20	0.179	0.18
2	0.2	0.069	0.040	0.04
	0.5	0.12	0.088	0.1
	0.9	0.22	0.179	0.18
3	0.2	0.068	0.041	0.04
	0.5	0.13	0.090	0.1
	0.9	0.25	0.179	0.18
4	0.2	0.069	0.040	0.04
	0.5	0.13	0.091	0.1
	0.9	0.28	0.178	0.18
5	0.2	n.d.	0.040	0.04
	0.5	n.d.	0.094	0.1
	0.9	n.d.	0.018	0.18

Table 4.5: The coefficient $\nu^{(l)}$ ($\nu^{(h)}$) of the low (high) temperature expansion of the susceptibility, $T \cdot \chi(T \ll T_K) = \chi^{(0)} + a(T/T_K)^{\nu^{(l)}}$ ($T \cdot \chi(T \gg T_K) = \chi^{(0)} + a(T_K/T)^{\nu^{(h)}}$) in the under-/exactly screened $m/2 \leq S = 5/2$ case. ν_n gives the numerical value, $\nu_a = 2\gamma/\pi$ the analytical result (n.d.: not defined)

Furthermore, the magnetic field has qualitatively a higher influence than in the exactly screened case. This is confirmed by the specific heat, fig. 4.16, and susceptibility curves, fig. 4.17.

The magnetization for $S = 1 = m/2$ is depicted in fig. 4.18. The magnetization of a free $S = 1$ spin is approached for high fields, where the coupling with the host becomes small in comparison with the field. An anisotropy is seen to enhance this effect. The magnetization for the under-screened case is depicted in fig. 4.19 and shows qualitatively the same behaviour.

4.2.2 Over-screened case

Let us now turn our attention to the over-screened case, $S = 1/2$, $m = 2$. The most striking feature is that a weak magnetic field induces a second crossover temperature $T_K^{(2)}$, fig. 4.20. The second scale coincides with T_K at higher fields. This is also reflected in the specific heat, fig. 4.21. This double peak structure has first been observed in [76] for the isotropic case. There it was argued that two energy scales are involved at low fields, $T_K(h/T_K)^{1+2/m}$ (in view of eq. (3.57)) and T_K . The physical picture behind is that Kondo screening gets less important for increasing m (l fixed) - in fact, the h dependent scale becomes h itself for $m \rightarrow \infty$. Numerical studies for $m > 2$ in [76] show that with increasing m at $h < T_K$, the impurity spin behaves more and more like a free spin in a magnetic field, the second peak at T_K vanishes. With increasing fields, the two peaks merge into one at $T \approx T_K$. This is the common Schottky anomaly.

The susceptibility behaves very similarly to the exactly screened case, so that we do not show it again here. The magnetization curve is depicted in fig. 4.22. As in the exactly screened case, the free spin function is approached for high fields, dominating the coupling with the host. This tendency is enforced by a finite anisotropy.

Summarizing, one observes that the numerical data shown in this chapter confirm analytical results

m	$2S$	$\kappa_n(C)$	$\kappa_n(\chi)$	$\kappa_a = \frac{4}{m+2}$
3	1	0.794	0.667	0.8
	2	0.883	0.75	
	3*	1.0	1.0	1.0
4	1	0.664	0.552	0.6667
	2	0.6662	0.591	
	3	0.67	0.693	
	4*	1.0	1.0	1.0
5	1	0.568	0.47	0.5714
	2	0.570	0.49	
	3	0.573	0.537	
	4	0.576	0.656	
	5*	1.0	1.0	1.0

Table 4.6: The exponents κ , defined by $C(T \ll T_K) \sim T^{\kappa(C)}$, $T \cdot \chi(T \ll T_K) \sim T^{\kappa(\chi)}$. Subscripts n denote numerical, a analytical results. In the exactly screened case, denoted by $*$, $\kappa = 1$.

for $h = 0$. Corrections to the asymptotic behaviour can be extracted; this extends numerical work based on the TBA approach, where such asymptotic investigations of numerical data have not been performed yet. At the same time, the analysis of these corrections reveals the limits of the numerical procedure. Only the Fermi liquid behaviour of the exactly screened cases is reproduced with arbitrary accuracy, in the not exactly screened cases, numerical errors seem to be unavoidable.

In the presence of a magnetic field, the NLIE are more difficult to be solved numerically with high accuracy, and asymptotic corrections cannot be extracted. The data give qualitative agreement with analytical predictions. On the other hand, the double peak structure in quantities of the overcompensated case for $h \neq 0$ has not been foreseen analytically, since it is located at $T = \mathcal{O}(T_K)$; this crossover region is not accessible by analytical tools yet.

$2S$	$\gamma \cdot \left(\frac{\pi}{4S}\right)^{-1}$	$\ln \frac{T_0}{T_K}$	$C(T_0)$
1	0	0.53063	0.00874
	0.2	0.53063	0.00874
	0.5	0.53063	0.00874
	0.9	0.53063	0.00878
2	0	0.2624	0.0263
	0.2	0.2624	0.0263
	0.5	0.2624	0.0263
	0.9	0.2624	0.0263
3	0	-0.0305	0.0601
	0.2	-0.0305	0.0601
	0.5	-0.0305	0.0601
	0.9	-0.0202	0.0602
4	0	-0.4155	0.1333
	0.2	-0.4155	0.1333
	0.5	-0.4155	0.1333
	0.9	-0.4005	0.1335

Table 4.7: Location $\ln T_0/T_K$ of the maximal value $C(T_0)$ of the specific heat for various anisotropies in the over-screened $S < m/2 = 5/2$ case.

$2S$	$\gamma \cdot \left(\frac{\pi}{4S}\right)^{-1}$	$\nu_n^{(h)}$	ν_a
1	0.2	0.038	0.04
	0.5	0.083	0.1
	0.9	0.179	0.18
2	0.2	0.038	0.04
	0.5	0.084	0.1
	0.9	0.177	0.18
3	0.2	0.038	0.04
	0.5	0.085	0.1
	0.9	0.179	0.18
4	0.2	0.038	0.04
	0.5	0.087	0.1
	0.9	0.179	0.18

Table 4.8: The coefficient $\nu^{(h)}$ of the high temperature expansion of the susceptibility, $T \cdot \chi(T \gg T_K) = \chi^{(0)} + a(T_K/T)^{\nu^{(h)}}$ in the over-screened $S < m/2 = 5/2$ case. $\nu_n^{(h)}$ gives the numerical value, $\nu_a = 2\gamma/\pi$ the analytical result. (cf. footnote 2 in section 4.2.1.)

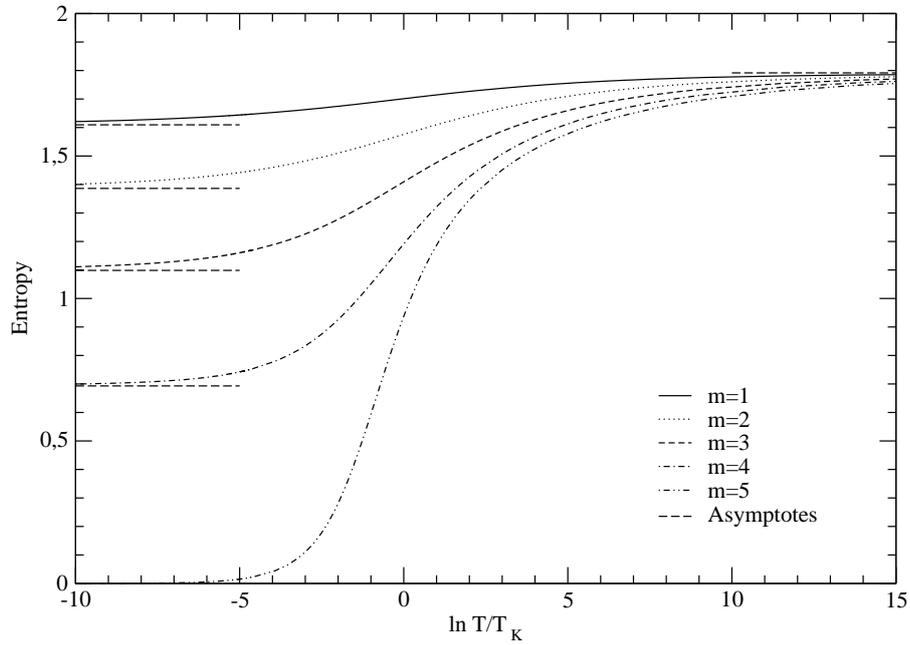


Figure 4.1: Entropy for impurity spin $S = 5/2$ and different channel numbers. Also shown are the asymptotes $\ln(2S + 1)$ at high temperatures and $\ln(2S - m)$ at low temperature.

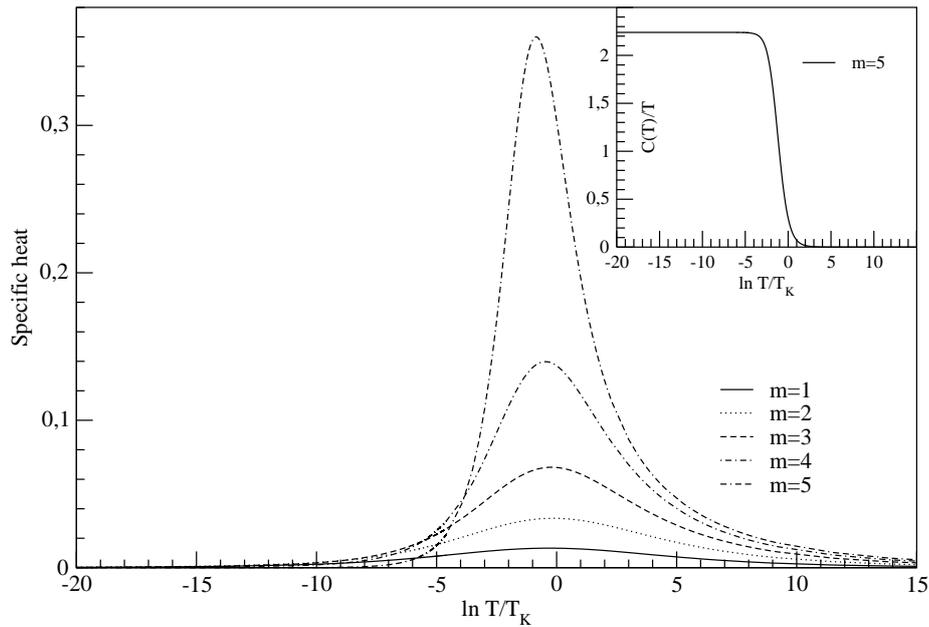


Figure 4.2: Specific heat for impurity spin $S = 5/2$ and different channel numbers. As an example for the exactly screened cases, the inset shows the Fermi liquid behaviour $\lim_{T \rightarrow 0} C(T)/T = \text{const.}$ for $2S = m = 5$. Curves for other values $2S = m$ look qualitatively the same.

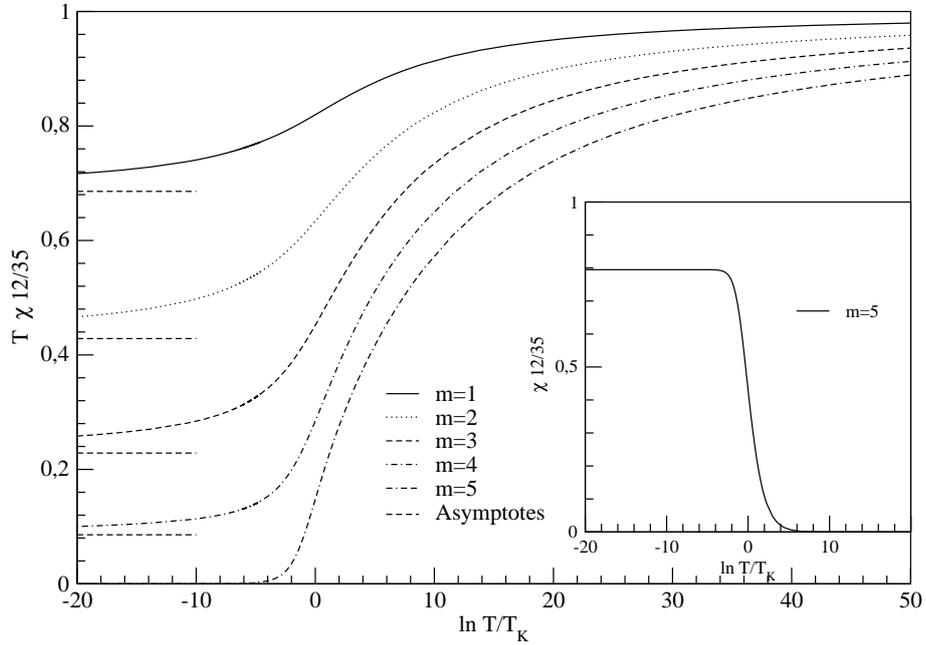


Figure 4.3: Susceptibility multiplied by temperature for impurity spin $S = 5/2$ and different channel numbers. For the sake of better comparison with known results, a scaling by $12/(2S(2S + 2))$ has been performed. The inset shows the Fermi liquid behaviour $\lim_{T \rightarrow 0} \chi(T) = \text{const.}$ for $2S = m = 5$. Curves for other values $2S = m$ look qualitatively the same.

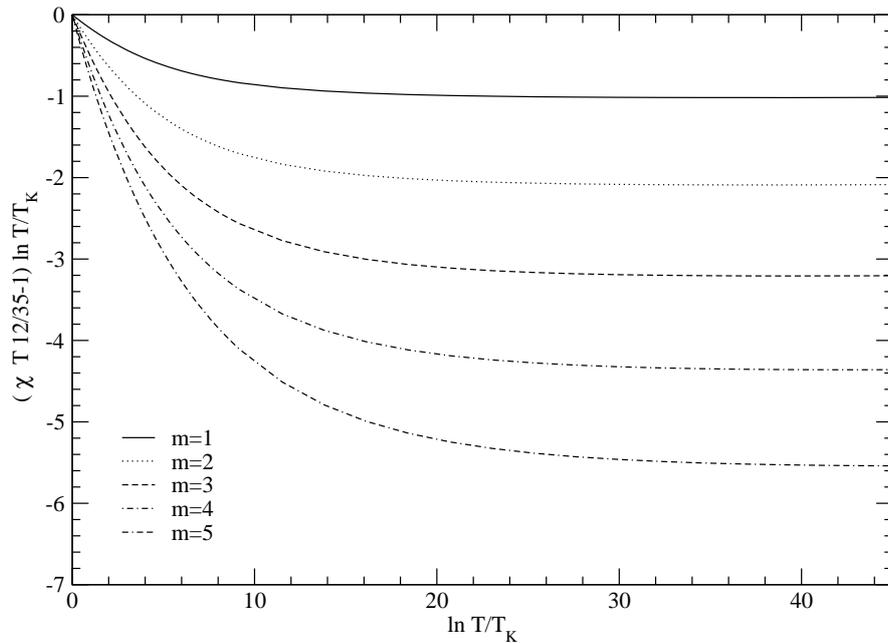


Figure 4.4: Convergence to the coefficient of the $(\ln T/T_K)^{-1}$ contribution to the susceptibility at high temperatures for $S = 5/2$. With increasing channel number m , the deviations from the analytical result, $-m$, become more pronounced.

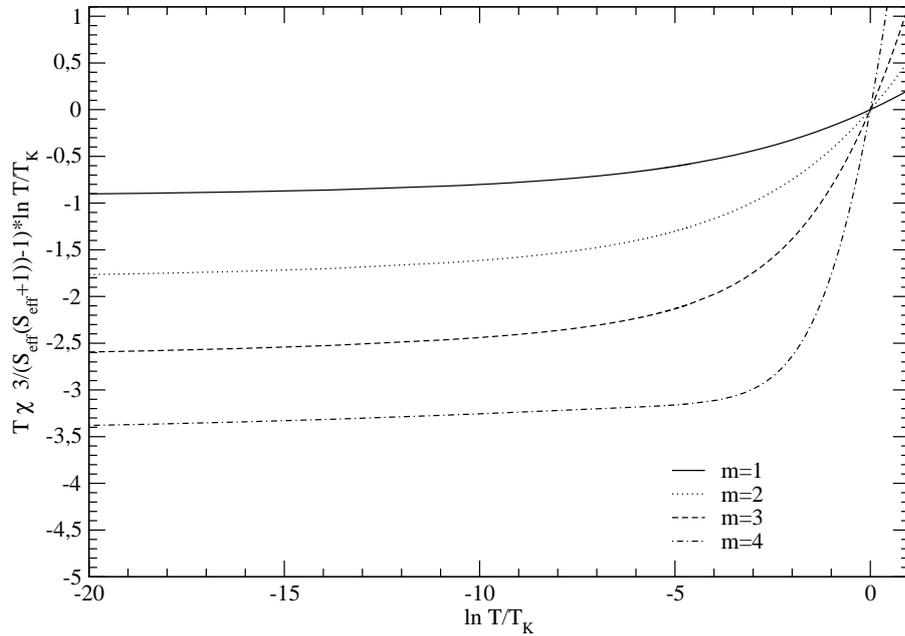


Figure 4.5: Convergence to the coefficient of the $(\ln T/T_K)^{-1}$ to the susceptibility at low temperatures for $S = 5/2$. $S_{eff} = S - m/2$. With increasing channel number m , the deviations from the analytical result, $-m$, become more pronounced.

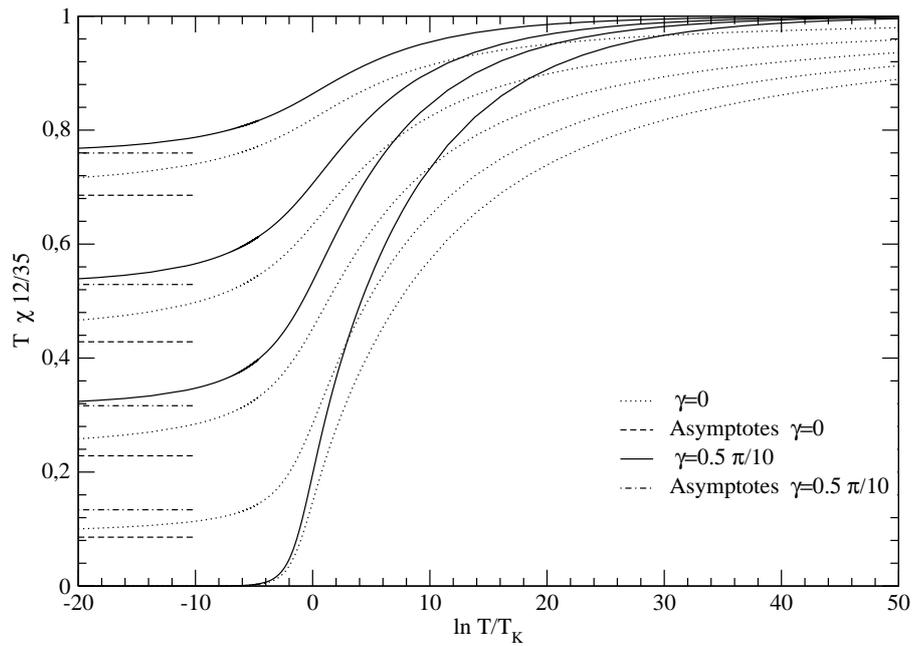


Figure 4.6: Susceptibility for $S = 5/2$ and channels $m = 1, \dots, 5$. Isotropic and anisotropic results are compared for $\gamma = 0.5\pi/(4S)$.

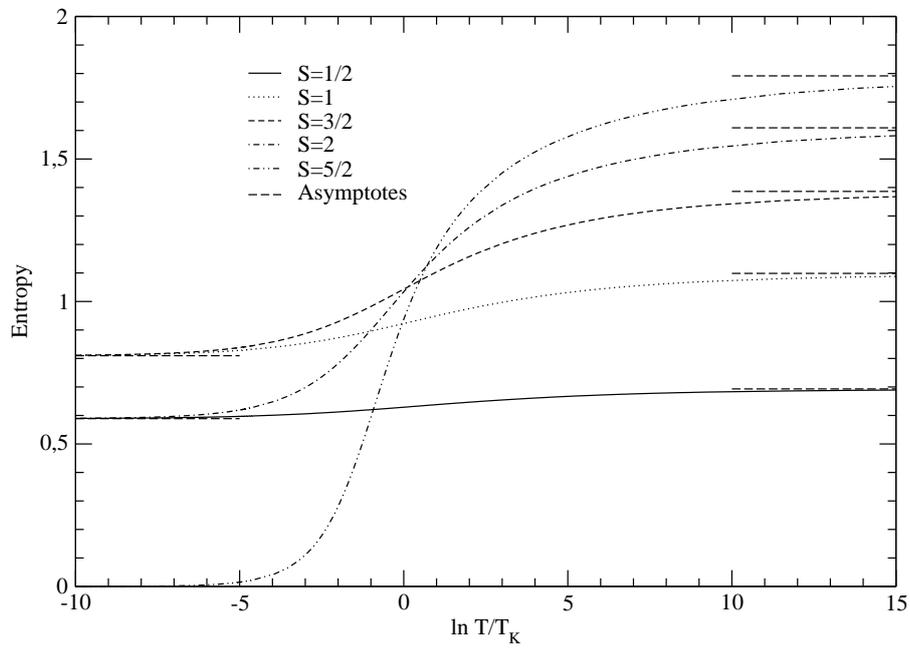


Figure 4.7: Entropy for $m = 5$ channels and spins $S = 1/2, \dots, 5/2$.

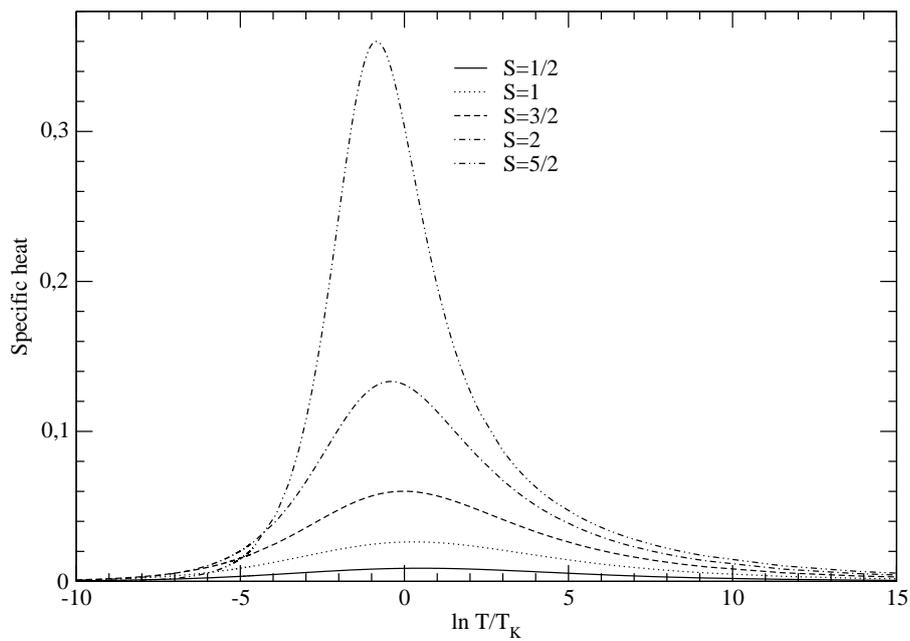


Figure 4.8: Specific heat for $m = 5$ channels and spins $S = 1/2, \dots, 5/2$.

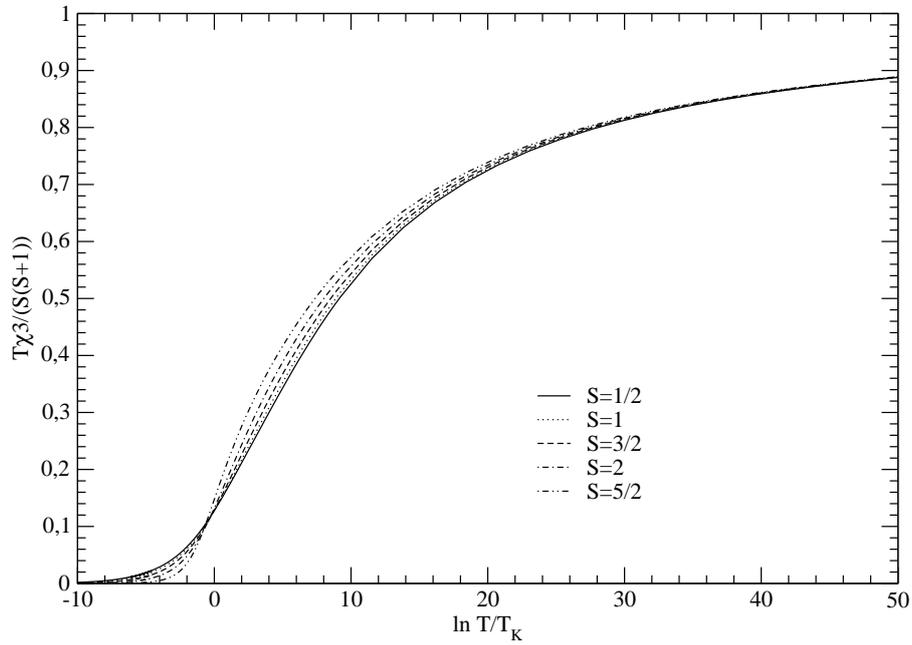


Figure 4.9: Susceptibility for $m = 5$ channels and spins $S = 1/2, \dots, 5/2$, normalized to the free spin values.

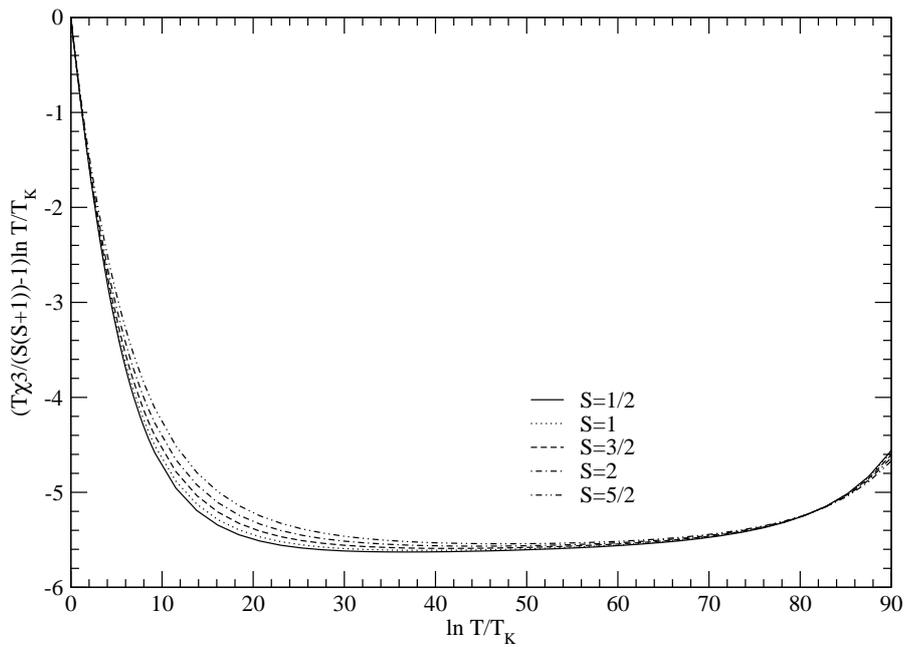


Figure 4.10: First correction to the high temperature susceptibility for $m = 5$ channels and spins $S = 1/2, \dots, 5/2$. Analytically, $(12/35 T \cdot \chi - 1) \ln T/T_K = -5$. Finite size effects are obvious.

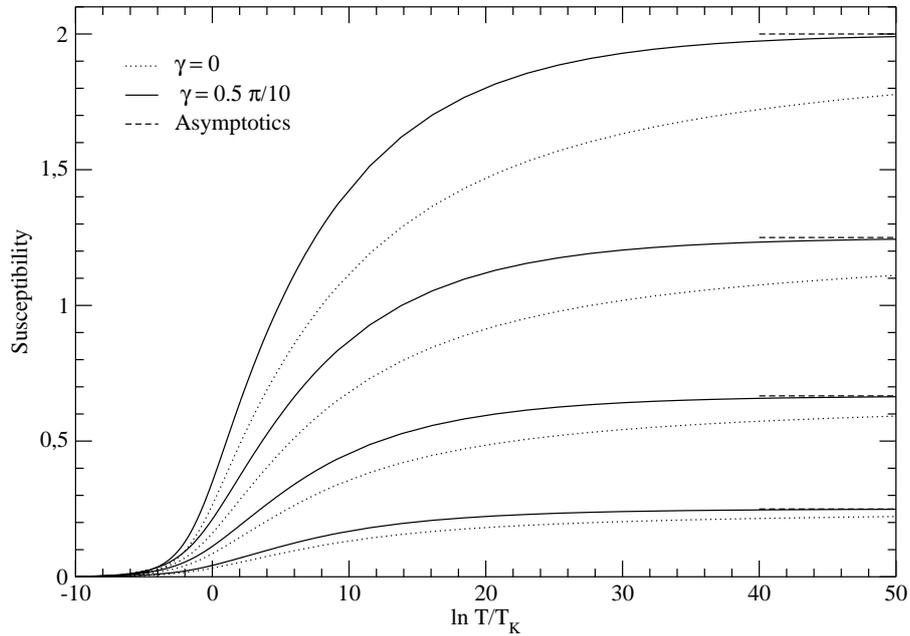


Figure 4.11: Susceptibility for $m = 5$ channels, spins $S = 1/2, \dots, 2$ and $\gamma = 0, 0.5\pi/(2m)$.

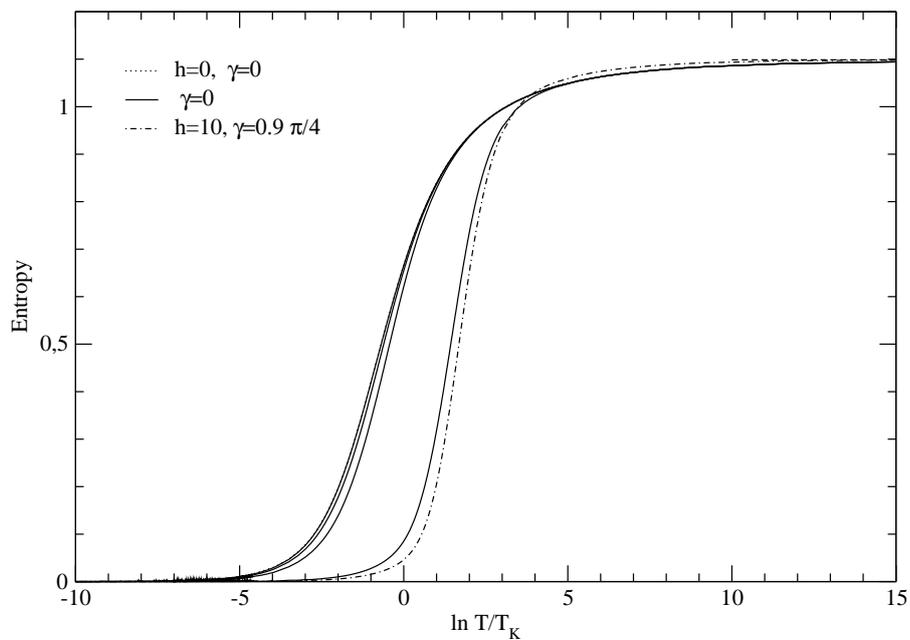


Figure 4.12: The entropy for exactly screened case $S = 1$, $m = 2$, with fields $h = 0, 0.1, 0.5, 1, 10$. For $h = 10$, the curve for finite anisotropy is shown. The field-free curve cannot be distinguished from the $h = 0.1$ curve in this resolution. Equally, the difference between the isotropic and anisotropic cases is weakly pronounced.

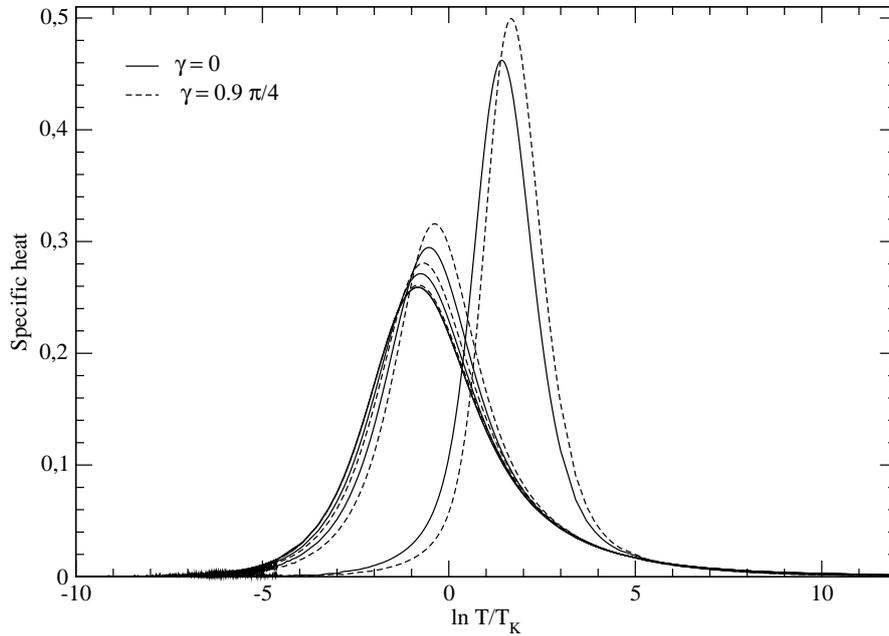


Figure 4.13: The specific heat for the exactly screened case $S = 1$, $m = 2$ with fields $h = 0, 0.5, 1, 10$ and anisotropies $\gamma = 0, \gamma = 0.9\pi/2$.

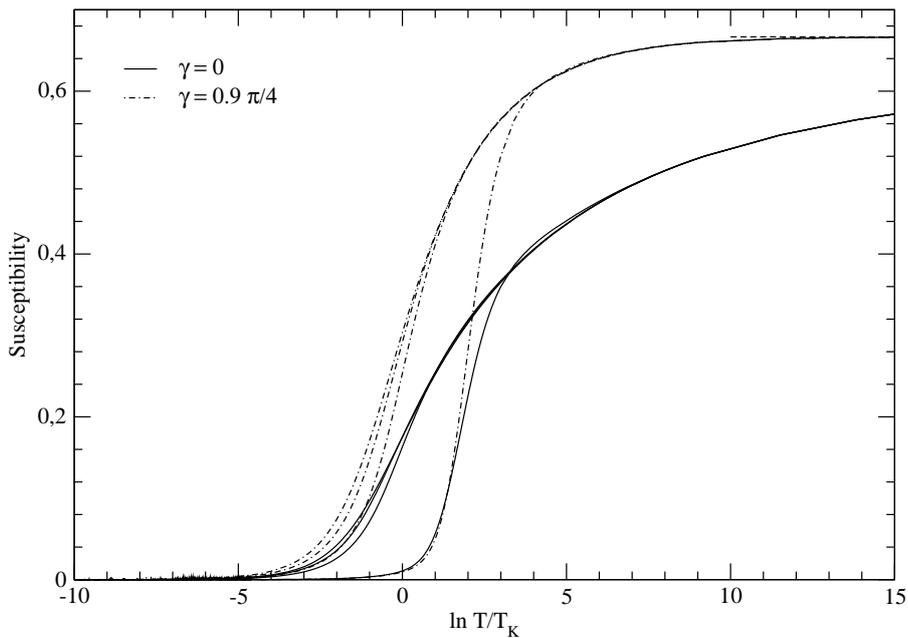


Figure 4.14: The susceptibility for the exactly screened case $S = 1$, $m = 2$ with fields $h = 0, 0.5, 1, 10$ for anisotropies $\gamma = 0, 0.9\pi/4$. The asymptotic values are given as horizontal bars.

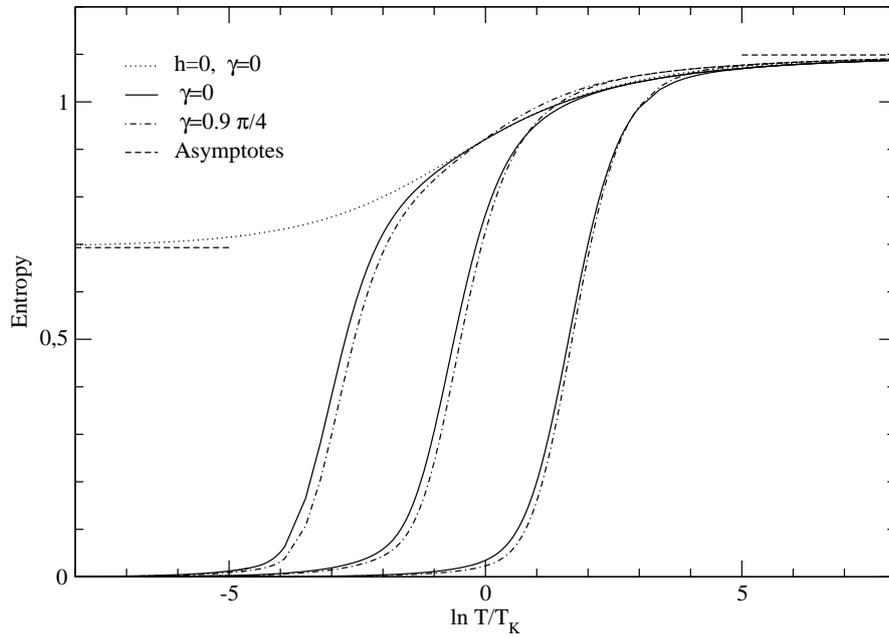


Figure 4.15: The entropy for the under-screened case $S = 1$, $m = 1$ with fields $h = 0, 0.1, 1, 10$ and anisotropies $\gamma = 0, \gamma = 0.9\pi/2$. The asymptotic values are given as horizontal bars.

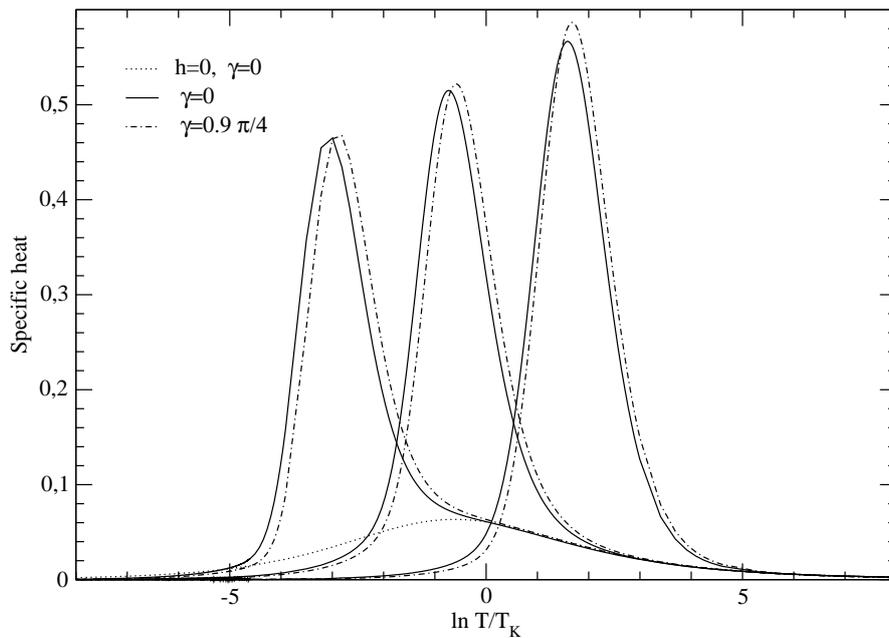


Figure 4.16: The specific heat for the under-screened case $S = 1$, $m = 1$ with fields $h = 0, 0.1, 1, 10$ for anisotropies $\gamma = 0, 0.9\pi/4$.

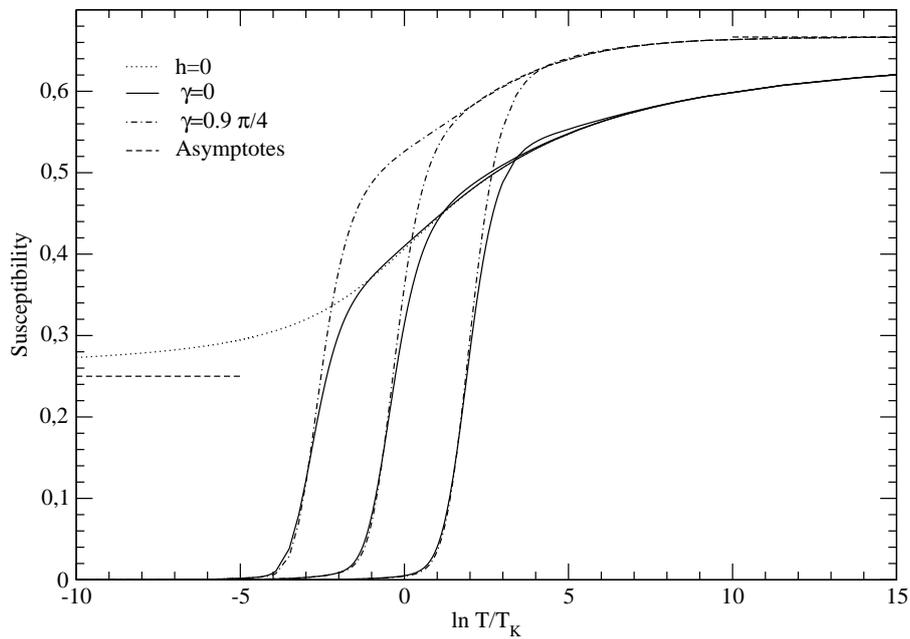


Figure 4.17: The susceptibility for the under-screened case $S = 1$, $m = 1$ with fields $h = 0, 0.1, 1, 10$ and anisotropies $\gamma = 0, \gamma = 0.9\pi/2$. The asymptotic values are given as horizontal bars on the right.

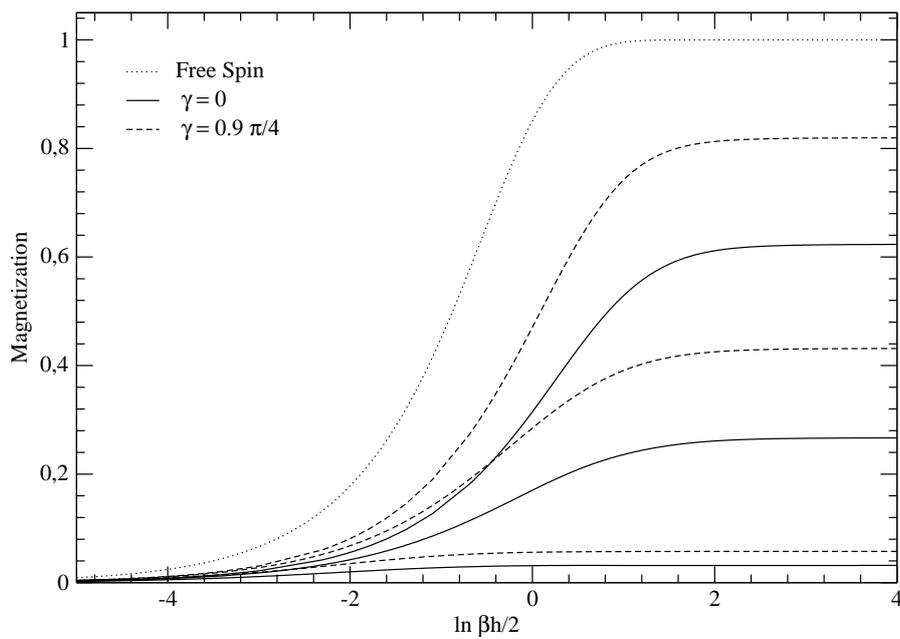


Figure 4.18: The magnetization in the exactly screened case $S = 1$, $m = 2$ with fields $h = 0.1, 1, 10$ and anisotropies $\gamma = 0, \gamma = 0.9\pi/4$.

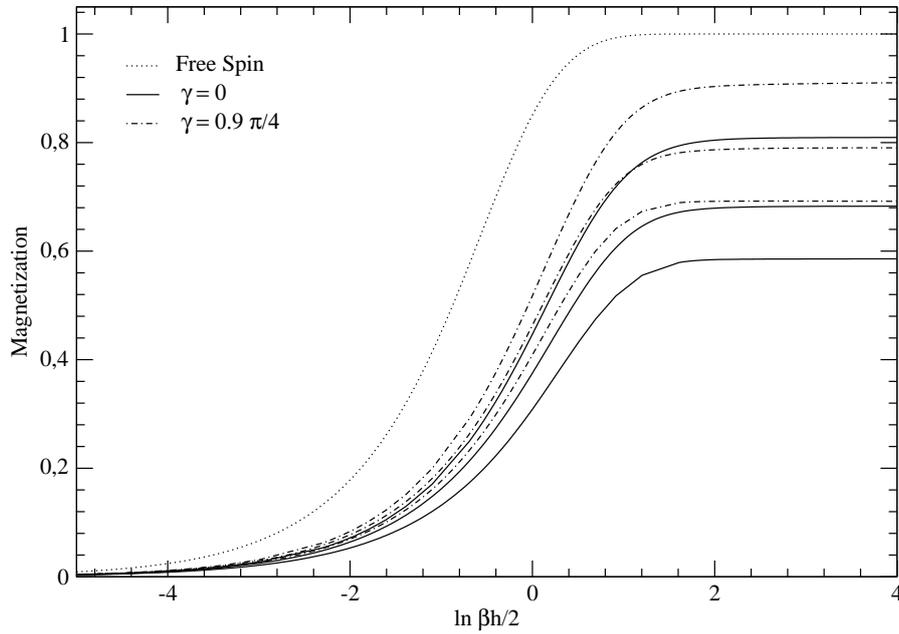


Figure 4.19: The magnetization in the under-screened case $S = 1$, $m = 1$ with fields $h = 0.1, 1, 10$ and anisotropies $\gamma = 0$, $\gamma = 0.9\pi/4$.

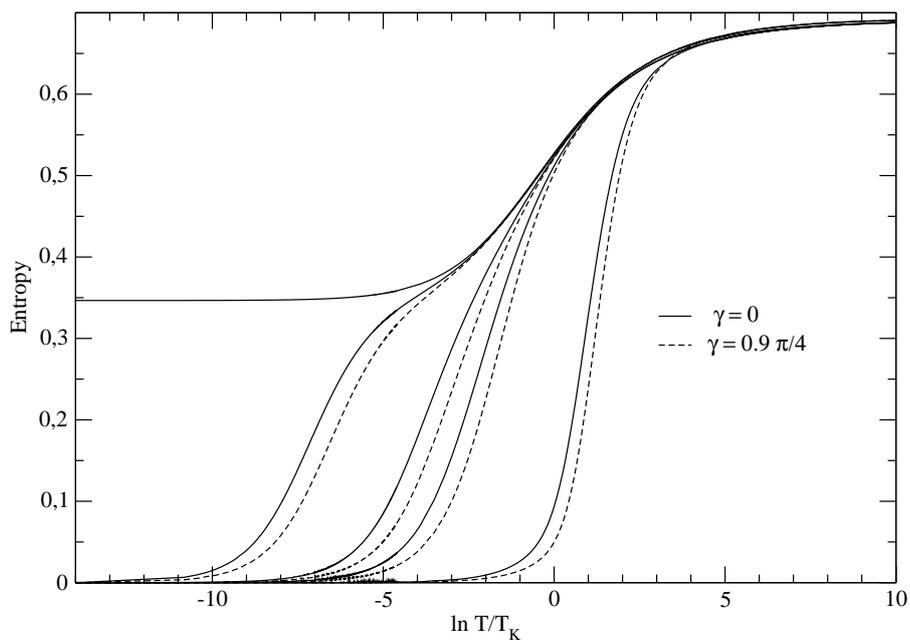


Figure 4.20: The entropy in the over-screened case $S = 1/2$, $m = 2$ with fields $h = 0, 0.1, 0.5, 1, 10$ and anisotropies $\gamma = 0$, $\gamma = 0.9\pi/4$.

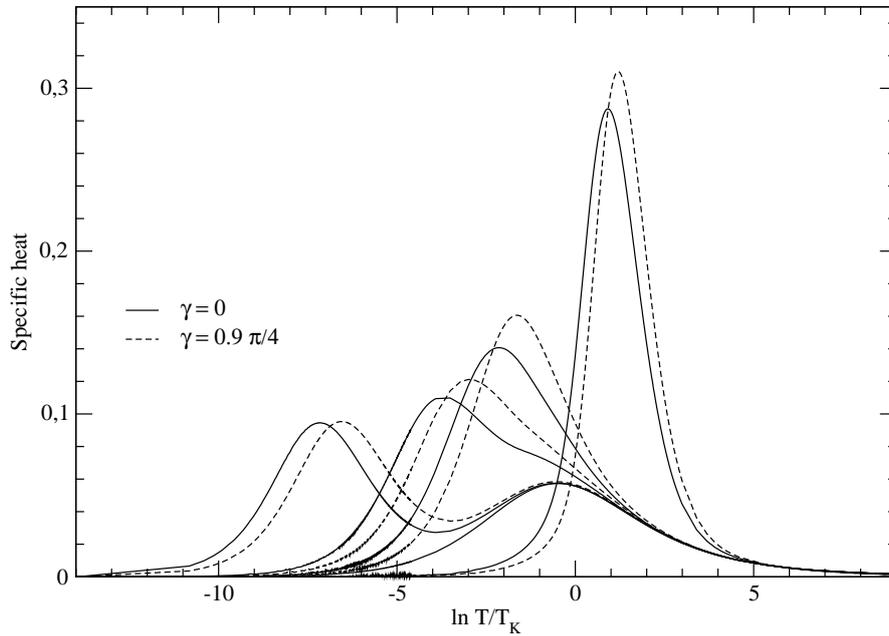


Figure 4.21: The specific heat in the overcreened case $S = 1/2$, $m = 2$ with fields $h = 0, 0.1, 0.5, 1, 10$ and anisotropies $\gamma = 0, \gamma = 0.9\pi/4$.

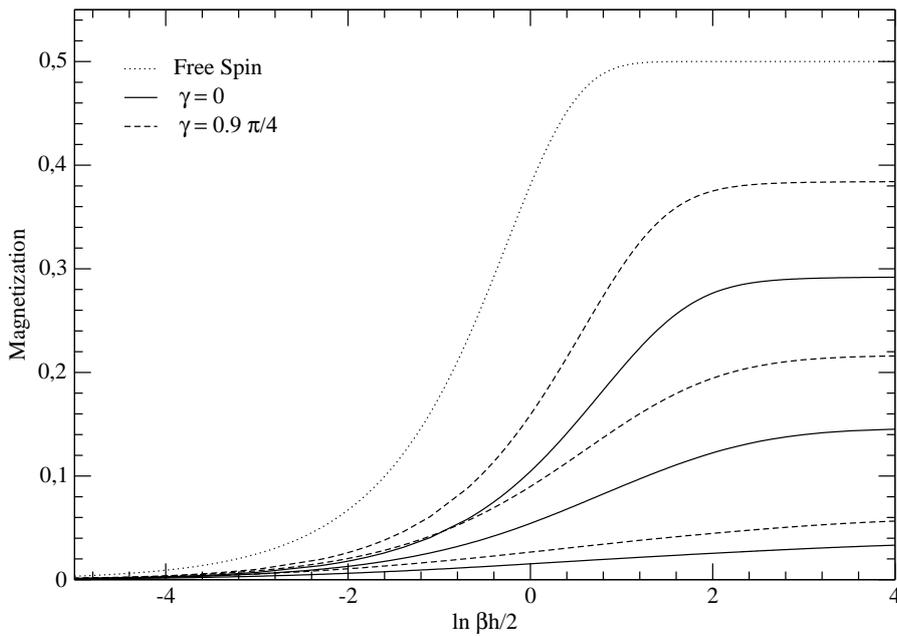


Figure 4.22: The magnetization in the overcreened case $S = 1/2$, $m = 2$ with fields $h = 0.1, 1, 10$ and anisotropies $\gamma = 0, \gamma = 0.9\pi/4$.

Chapter 5

Conclusion and Outlook

A lattice regularization of the continuous Kondo model has been presented. The Hamiltonian, host and impurity, is obtained as the logarithmic derivative of a $\mathfrak{gl}(2|1)$ symmetric transfer matrix, allowing for the calculation of the free energy of the host and impurity in the same approach. The procedure is purely algebraic, and does not need the explicit construction of wave functions as in the coordinate BA in previous works. The QTM-formalism has been applied to the model, resulting in NLIE which simultaneously determine the free energy of the host and of the impurity.

The impurity contribution has been studied in the limit of single occupation, described by the common Kondo model. This limit reduces the underlying Lie super-algebra $\mathfrak{gl}(2|1)$ to one of its even Lie sub-algebras, $\mathfrak{su}(2)$. The resulting transfer matrix is generalized to symmetry with respect to higher dimensional irreps of $U_q(\mathfrak{su}(2))$. These effective matrices contain all information about the impurity contribution to thermodynamic equilibrium response functions of the anisotropic m -channel S -spin Kondo model. The thermodynamic functions are given by a system of $[\max(2S, m) + 1]$ NLIE.

In certain limiting ranges of temperature and magnetic field, the NLIE are solved analytically, numerical studies are carried out over the whole range of parameters. Most importantly, both Wilson ratios are calculated in the framework of one approach. Furthermore, results known from other exact solutions are confirmed. However, while agreeing qualitatively with Schlottmann [79, 80] in the anisotropic under-screened case, quantitative disagreement is found.

This work exclusively concentrates on the Kondo limit of the impurity model, realized by $\mu, D, \alpha \gg 1$. The model presented in section 2.1.2 with these parameters left finite is of interest itself: It describes a correlated host interacting with an impurity on which double occupation is forbidden. The study of such a model is expected to be in reach: The NLIE leading to the impurity contribution of the free energy are the same as those for the host, which have been investigated extensively in [47, 77]. One still has to take account of the different functional dependence of the free energy on the auxiliary functions. Such investigations are motivated by CFT-results by [29, 30], where the low-temperature properties of an impurity embedded in an interacting one-dimensional host are calculated.

At the end of section 2.1.3 it has been stated that in the $\mathfrak{gl}(2|1)$ -symmetric model, the host-host interaction is determined by the same parameter which yields the host-impurity coupling, namely α . On the other hand, the final equations for host and impurity are independent of α , and the limits $D, \alpha \rightarrow \infty$ can be taken rigorously, only T_K must remain constant. One may speculate whether an additional degree of freedom exists which allows for a further parameter, say α_h , which tunes the correlations in the host, so that $\alpha_h \rightarrow \infty$ results in free fermions, but a finite spin-exchange coupling between host and impurity remains.

Actually, $R^{(4,4)}$ -matrices exist which intertwine two four-dimensional representations of $\mathfrak{gl}(2|1)$, but these representations may differ in the parameters α, α' [40, 71]. An impurity model may thus be

constructed by a transfermatrix $T^{(4,4)}$, where in the language of fig. 2.2, α lives on the "horizontal" bonds, and α' on the "vertical" bonds. It remains to be explored in how far such a model leads to a decoupling of host-host and host-impurity interaction amplitudes.

Another approach to this challenge is a closer study of $\mathfrak{gl}(2|1)$. One is tempted to perform the limit which reduces $\mathfrak{gl}(2|1)$ to $\mathfrak{su}(2)$ on the impurity site already on an algebraic level, rather than on the Hamiltonian level by the canonical transformation or in the NLIE framework by eliminating one auxiliary function. This addresses the question whether it is possible to embed a $\mathfrak{u}(1) \otimes \mathfrak{su}(2)$ -symmetric R -matrix for the impurity from the beginning in a $\mathfrak{gl}(2|1)$ dimensional host.

Whereas in section 2.1.2 the host (impurity) is realized by a four- (three-) dimensional representation of $\mathfrak{gl}(2|1)$, in [14] the "inverse" model is developed: The host (impurity) relies on the three- (four-) dimensional representation of $\mathfrak{gl}(2|1)$. This corresponds to an impurity permitting charge fluctuation, which is embedded in a $t - J$ -like host. Thermodynamic quantities are studied for $T = 0$ and low temperatures, as well as for high temperatures by TBA-techniques and compared with findings by CFT, [29, 30]. The formalism presented in this work is suited to contribute further insight into the exact solution of that model.

The following questions could not be clarified in this work:

- i) Our "hybrid" method, which combines analytical with numerical results to calculate the high-temperature Wilson ratio, motivates further analytical studies of the NLIE. It is an intriguing question how to obtain this number analytically (and to solve the contradiction between our results for $S > 1/2 = m/2$ and those of [31]). This question may be intimately related to the calculation of the integral over the imaginary part of $\ln \mathfrak{B}_l$, eq. (3.84).
- ii) The multichannel models still remain somehow mysterious: Neither the fusion of electronic degrees of freedom in the Hamiltonian, nor the low-temperature behaviour of the over-screened models is fully understood.

Regularizations of the anisotropic and the isotropic $m, 2S > 1$ models, similar to that proposed in this work for $\gamma = 0, 2S = m = 1$, are left as a future challenge. Such a regularization is particularly desired for the multichannel $m > 1$ case, see item ii). The strategy to find the $m = 1 = 2S$ Kondo model with anisotropic exchange is to employ the q -deformed algebra $U_q(\mathfrak{gl}(2|1))$, [40, 67, 37]. As to the realization of higher impurity spins, remember that $\mathfrak{su}(2)$ is an even sub-algebra of $\mathfrak{gl}(2|1)$. Thus one is tempted to find representations of $\mathfrak{gl}(2|1)$ which embed higher dimensional representations of $\mathfrak{su}(2)$. A starting point might be [78].

Once a lattice path integral approach to the simplest case, $\gamma = 0, S = 1/2 = m/2$, is found, the next question addresses dynamical response functions. Since the spectrum with the corresponding eigenstates of the model are known, those quantities can be calculated in principle. The difficulties are twofold: Matrix elements between local operators and next-leading eigenvalues must be calculated.

For example, consider the spin-spin correlation function between the $S = 1/2$ impurity and the $m = 1$ host without external fields. Let σ_I^ν (σ_r^ν) be the ν -th component of the spin operator at the impurity (at the r -th lattice site in the host). $|\Phi^{(Q)}\rangle \equiv |k\rangle$, eq. (A.29), is a common eigenstate of $\tau_I^{(Q)}, \tau_h^{(Q)}$, with parity $p[k]$. $|\Phi_{\max}^{(Q)}\rangle$ is the eigenstate leading to the largest eigenvalues of $\tau_I^{(Q)}, \tau_h^{(Q)}$.

$$\mathcal{Z} = \text{tr} e^{-\beta H} = \lim_{N \rightarrow \infty} \text{str} \left\{ \tau_I^{(Q)} \left[\tau_h^{(Q)} \right]^L \right\}$$

$$\begin{aligned}
c(r, T) &:= \langle \sigma_I^\nu \sigma_r^\mu \rangle = \frac{1}{\mathcal{Z}} \text{tr} \left[e^{-\beta H} \sigma_I^\nu \sigma_r^\mu \right] \\
&= \lim_{N \rightarrow \infty} \frac{1}{\mathcal{Z}} \sum_k (-1)^{p[k]} \langle k | \tau_I^{(Q)} \sigma_I^\nu \left[\tau_h^{(Q)} \right]^r \sigma_r^\mu \left[\tau_h^{(Q)} \right]^{L-r} |k \rangle \\
&= \lim_{N \rightarrow \infty} \frac{\sum_{k,q} (-1)^{p[k]} \langle k | \sigma_I^\nu |q \rangle \langle q | \sigma_r^\mu |k \rangle \Lambda_I^{(k)} \left[\Lambda_h^{(q)} \right]^r \left[\Lambda_h^{(k)} \right]^{L-r}}{\sum_p (-1)^{p[p]} \Lambda_I^{(p)} \left[\Lambda_h^{(p)} \right]^L} \tag{5.1}
\end{aligned}$$

$$\begin{aligned}
&= \langle \Phi_{\max}^{(Q)} | \sigma_I^\nu | \Phi_{\max}^{(Q)} \rangle \langle \Phi_{\max}^{(Q)} | \sigma_r^\mu | \Phi_{\max}^{(Q)} \rangle \\
&\quad + \lim_{N \rightarrow \infty} \sum_{q \neq \max} (-1)^{p[q]} \langle \Phi_{\max}^{(Q)} | \sigma_I^\nu | q \rangle \langle q | \sigma_r^\mu | \Phi_{\max}^{(Q)} \rangle \left(\frac{\Lambda_h^{(q)}}{\Lambda_h^{\max}} \right)^r \\
&=: \text{const.} + \sum_{q \neq \max} (-1)^{p[q]} a_q e^{-r/\xi_q}, \tag{5.2}
\end{aligned}$$

with

$$\begin{aligned}
a_q &:= \langle \Phi_{\max}^{(Q)} | \sigma_I^\nu | q \rangle \langle q | \sigma_r^\mu | \Phi_{\max}^{(Q)} \rangle \\
\xi_q^{-1} &= - \lim_{N \rightarrow \infty} \ln \frac{\Lambda_h^{(q)}}{\Lambda_h^{\max}}.
\end{aligned}$$

A finite gap between the largest and next-leading eigenvalues persists in the limit $N \rightarrow \infty$, such that (eq. (5.1) in the denominator only the leading term rests and k in the nominator is restricted to $k = \max$. The first term in eq. (5.2) is constant. The second summand contains an r -dependence through the ratios of next-leading to leading eigenvalues of the host matrix. The ξ_q are correlation lengths of the host. In the limit of large distances,

$$\lim_{r \gg 1} \langle \sigma_I^\nu \sigma_j^\mu \rangle = \text{const.} + (-1)^{p[2]} a_2 e^{-r/\xi_2}. \tag{5.3}$$

$|2\rangle$ is the eigenstate pertaining to the next-leading eigenvalue of the host QTM. Eq. (5.3) states that for large distances, the impurity enters the correlation function only through a constant pre-factor, the exponential decay is determined by the host. Such a behaviour is expected.

For smaller distances, near the impurity site, the restriction to the next-leading eigenvalue of eq. (5.3) does not suffice. Rather, sufficiently many terms of the series in eq. (5.2) must be added. In that case, the impurity-dependent pre-factors a_q are important. The result is expected to deviate from the corresponding correlation function with host operators only.

So two tasks are to accomplish: The evaluation of next-leading eigenvalues of the host and the calculation of the matrix elements a_q .

Next-leading eigenvalues are defined by the deviation of their BAN-distribution in the complex plane from the BAN-distribution of the leading eigenvalue. This leads to additional terms in the NLIE, as has been demonstrated for the host QTM in [77].

Improvements in evaluating matrix elements for $T = 0$ have recently been made by Müller, [16, 17], relying on methods by Kitanine, [53, 43]. These techniques require the numerical determination of BAN in the complex plane.

Whether the two techniques for calculating $\Lambda_q^{(h)}$ and a_q help to evaluate eq. (5.2) remains a challenge for future research.

In view of debates about the characteristics of a possible screening cloud around the impurity, such progress is highly desirable. The question whether such a screening cloud exists in the low-temperature limit is not answered unambiguously. $c(r, T \ll T_K)$ has been calculated perturbationally by Keiter [49]. Besides a diverging contribution $\sim \ln T/D$, he found non-oscillating J^2/r^3 and $J^3(\ln k_f r)/r^3$ -contributions. These terms predict an extremely long-range behaviour at zero temperature, which would require, in eq. (5.2), the summation of infinitely many terms. Affleck et al. [11, 12, 83] interpolate between high and low temperatures by scaling arguments. They also describe the Kondo screening as a long-range many-particle phenomenon. This statement contradicts results by Gan [32], who, after performing a $1/m$ development, concludes the non-existence of a long-range screening cloud.

Finally, progress in the evaluation of correlation functions in the framework of the BA is of theoretical significance itself: The models are exactly solvable since they display infinitely many conservation laws. The question is, how to exploit them with least effort.

Appendix A

Appendix to Chapter 2

Some details in the diagonalization of $\tau_I^{(Q)}$, $\tau_h^{(Q)}$, $\tau_{eff}^{(l,m)}$ are provided.

A.1 Eigenvalue of $\tau_I^{(Q)}$

In the following, details in the calculation of the eigenvalue of the impurity quantum transfer matrix are given.

Let

$$T^{(d,d')}(v) := R_{a,N}^{(d,d')}(v + v_N) R_{a,N-1}^{(d,d')}(v + v_{N-1}) \cdots R_{a,1}^{(d,d')}(v + v_1) \quad (\text{A.1})$$

be a monodromy matrix, with d -dimensional auxiliary space, and N quantum spaces, each of dimension d' . At each site j , the spectral parameter may be shifted by a site dependent constant v_j . The definition eq. (A.1) thus includes both $T_h^{(Q)}$ and $T_I^{(Q)}$, eqs. (2.63), (2.64).

$T^{(d,d')}$ is regarded as a $d \times d$ matrix in auxiliary space, with operator valued entries acting in the quantum spaces. From the YBE (2.2), the direct product of two monodromy matrices is intertwined by a R -matrix,

$$\begin{aligned} & (-1)^{p[\beta'](p[\alpha]+p[\alpha'])} \left[\bar{T}^{(d,d')} \otimes T^{(d'',d')} \right]_{\beta',\alpha'}^{\beta,\alpha} \left[R^{(d'',d)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} \\ &= \left[R^{(d'',d)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[T^{(d'',d')} \otimes \bar{T}^{(d,d')} \right]_{\alpha'',\beta''}^{\alpha',\beta'} (-1)^{p[\beta'](p[\alpha']+p[\alpha''])} \end{aligned} \quad (\text{A.2})$$

$$\begin{aligned} & \left[R^{(d'',d)}(v-u) \right]_{\alpha',\beta'}^{\alpha,\beta} \left[T^{(d'',d')} \otimes_s \bar{T}^{(d,d')} \right]_{\alpha'',\beta''}^{\alpha',\beta'} = \left[\bar{T}^{(d,d')} \tilde{\otimes}_s T^{(d'',d')} \right]_{\alpha',\beta'}^{\alpha,\beta} \left[R^{(d'',d)}(v-u) \right]_{\alpha'',\beta''}^{\alpha',\beta'} \\ & T =: T(v), \quad \bar{T} = T(u). \end{aligned} \quad (\text{A.3})$$

The symbol $\tilde{\otimes}_s$ is defined as

$$[A \tilde{\otimes}_s B]_{\gamma,\delta}^{\alpha,\beta} = [A \otimes B]_{\delta,\gamma}^{\beta,\alpha} (-1)^{p[\delta](p[\alpha]+p[\gamma])}.$$

It is introduced in eq. (A.3) in order to arrange the matrices such that both sides can be written as a conventional matrix multiplication. Note that usually in literature, the entries of the R -matrix in eq.

(A.2) are permuted to achieve a matrix multiplication like structure. This works well for $d'' = d$. In this work, however, the cases

$$d'' = d = 3; d' = 4 \quad (\text{A.4})$$

$$d'' = 3; d = d' = 4 \quad (\text{A.5})$$

are treated, so that we work with the slightly modified formalism.

$R^{(d'',d)}$ is a regular matrix (indeed, it is unitary: $R(u)R(-u) = 1$), so that eq. (A.2) can be multiplied by $[R^{(d'',d)}]^{-1}$. Then take the trace and employ invariance of cyclic permutations under the trace operation to end up with

$$\begin{aligned} [\tau^{(d,d')}(u), \tau^{(d'',d')}(v)] &= 0 \\ \tau^{(d,d')}(u) &:= \text{tr} T^{(d'',d')} . \end{aligned} \quad (\text{A.6})$$

So in spite of differing in the dimensions of their auxiliary spaces and in the spectral parameters, both $\tau^{(d,d')}(u)$ and $\tau^{(d'',d')}(v)$ share a common system of eigenstates. It is essential that the quantum spaces of both have the same dimension.

One may include twisted boundary conditions of the transfer matrices. Define matrices

$$\begin{aligned} \mathcal{E}^{(3,3)} &= \hat{\varepsilon}^{(3)} \otimes_s \hat{\varepsilon}^{(3)} \\ \mathcal{E}^{(3,4)} &= \hat{\varepsilon}^{(3)} \otimes_s \hat{\varepsilon}^{(4)} \\ \hat{\varepsilon}^{(3)} &= \begin{pmatrix} \varepsilon_1 \varepsilon_2 & & \\ & \varepsilon_1 \varepsilon_2^{-1} & \\ & & 1 \end{pmatrix} \\ \hat{\varepsilon}^{(4)} &= \begin{pmatrix} \varepsilon_1^2 & & & \\ & \varepsilon_1 \varepsilon_2 & & \\ & & \varepsilon_1 \varepsilon_2^{-1} & \\ & & & 1 \end{pmatrix} \end{aligned}$$

$\hat{\varepsilon}^{(3)}$ acts in three-dimensional, $\hat{\varepsilon}^{(4)}$ in four-dimensional auxiliary space; the entries are numbers, i.e. the unity operator with respect to the quantum spaces. One verifies that

$$[R^{(d,d')}, \mathcal{E}^{(d,d')}] = 0 . \quad (\text{A.7})$$

Furthermore,

$$\hat{\varepsilon}^{(d)} \otimes_s \hat{\varepsilon}^{(d')} = \hat{\varepsilon}^{(d')} \tilde{\otimes}_s \hat{\varepsilon}^{(d)} . \quad (\text{A.8})$$

Multiply eq. (A.3) from left with $\mathcal{E}^{(d'',d)}$:

$$\begin{aligned} \mathcal{E}^{(d'',d)} R^{(d'',d)}(v-u) [T^{(d'',d')} \otimes_s \bar{T}^{(d,d')}] &= \mathcal{E}^{(d'',d)} [\bar{T}^{(d,d')} \tilde{\otimes}_s T^{(d'',d')}] R^{(d'',d)}(v-u) \\ \Leftrightarrow R^{(d'',d)}(v-u) \mathcal{E}^{(d'',d)} [T^{(d'',d')} \otimes_s \bar{T}^{(d,d')}] &= \mathcal{E}^{(d'',d)} [\bar{T}^{(d,d')} \tilde{\otimes}_s T^{(d'',d')}] R^{(d'',d)}(v-u) \\ \Leftrightarrow R^{(d'',d)}(v-u) \left[\left(\hat{\varepsilon}^{(d'')} T^{(d'',d')} \right) \otimes_s \left(\hat{\varepsilon}^{(d)} \bar{T}^{(d,d')} \right) \right] &= \left[\left(\hat{\varepsilon}^{(d)} \bar{T}^{(d,d')} \right) \tilde{\otimes}_s \left(\hat{\varepsilon}^{(d'')} T^{(d'',d')} \right) \right] \\ &\quad \times R^{(d'',d)}(v-u) \end{aligned}$$

$|4\rangle^{\otimes N}$ - this is the essential, but not the whole story, so we postpone the explicit construction of $|\Phi\rangle$ to some later moment. As a verification, one has to commute A, D through C .

The intertwining $R^{(3,3)}$ is defined by eq. (2.3),

$$R^{(3,3)}(u) = u + \begin{pmatrix} e_1^1 & e_2^1 & e_3^1 \\ e_1^2 & e_2^2 & e_3^2 \\ e_1^3 & e_2^3 & -e_3^3 \end{pmatrix}.$$

Before comparing matrix entries on both sides of eq. (A.3), it proves ingenious to apply a similarity transformation to eq. (A.3) (this idea is borrowed from [33], where it helped to diagonalize $\tau^{(3,3)}$). Define

$$Z := \begin{pmatrix} \mathbb{1}_2 & & & \\ & 1 & & \\ & & 1 & \\ & & & \mathbb{1}_4 \end{pmatrix}.$$

Z induces a similarity transformation:

$$\begin{aligned} ZR^{(3,3)}Z^T Z [T \otimes_s \bar{T}] Z^T &= Z [\bar{T} \tilde{\otimes}_s T] Z^T ZR^{(3,3)}Z^T \\ R &\equiv R(v-u). \end{aligned}$$

This transformation arranges the elements in the fermionic sector in eq. (A.3) in a "natural" order. It is written explicitly

$$\begin{aligned} &\left(\begin{array}{c|c} r_4 & \\ \hline g\mathbb{1}_2 & \mathbb{1}_2 \\ \hline \mathbb{1}_2 & g\mathbb{1}_2 \\ & z \end{array} \right) \left(\begin{array}{cc|cc} A \otimes_s \bar{A} & A \otimes_s \bar{B} & B \otimes_s \bar{A} & B \otimes_s \bar{B} \\ A \otimes_s \bar{C} & A \otimes_s \bar{D} & B \otimes_s \bar{C} & B \otimes_s \bar{D} \\ \hline C \otimes_s \bar{A} & C \otimes_s \bar{B} & D \otimes_s \bar{A} & D \otimes_s \bar{B} \\ C \otimes_s \bar{C} & C \otimes_s \bar{D} & D \otimes_s \bar{C} & D \otimes_s \bar{D} \end{array} \right) \\ &= \left(\begin{array}{cc|cc} \bar{A} \tilde{\otimes}_s A & \bar{B} \tilde{\otimes}_s A & \bar{A} \tilde{\otimes}_s B & \bar{B} \tilde{\otimes}_s B \\ \bar{C} \tilde{\otimes}_s A & \bar{D} \tilde{\otimes}_s A & \bar{C} \tilde{\otimes}_s B & \bar{D} \tilde{\otimes}_s B \\ \hline \bar{A} \tilde{\otimes}_s C & \bar{B} \tilde{\otimes}_s C & \bar{A} \tilde{\otimes}_s D & \bar{B} \tilde{\otimes}_s D \\ \bar{C} \tilde{\otimes}_s C & \bar{D} \tilde{\otimes}_s C & \bar{C} \tilde{\otimes}_s D & \bar{D} \tilde{\otimes}_s D \end{array} \right) \left(\begin{array}{c|c} r_4 & \\ \hline g\mathbb{1}_2 & \mathbb{1}_2 \\ \hline \mathbb{1}_2 & g\mathbb{1}_2 \\ & z \end{array} \right). \end{aligned} \quad (\text{A.11})$$

The entries of the R -matrix are

$$\begin{aligned} g(v-u) &= v-u, & z(v-u) &= v-u-1 \\ r_4(v-u) &= \begin{pmatrix} h(v-u) & & & \\ & g(v-u) & 1 & \\ & 1 & g(v-u) & \\ & & & h(v-u) \end{pmatrix} \\ h(v-u) &= v-u+1. \end{aligned} \quad (\text{A.12})$$

Horizontal and vertical lined in eq. (A.11) separate fermionic from bosonic sectors. The searched commutators of A and D with C are now read off:

$$A \otimes_s \bar{C} = \bar{C} \tilde{\otimes}_s A \frac{r_4}{g} - \frac{1}{g} C \otimes_s \bar{A} \quad (\text{A.13})$$

$$\bar{D} \tilde{\otimes}_s C = \frac{z}{g} C \otimes_s \bar{D} - \frac{1}{g} \bar{C} \tilde{\otimes}_s D. \quad (\text{A.14})$$

The graded tensor products can be written without grading,

$$D \tilde{\otimes}_s C = -D \otimes C, \quad A \otimes_s C = A \otimes C \quad (\text{A.15})$$

$$C \tilde{\otimes}_s D = -C \otimes D, \quad C \tilde{\otimes}_s A = C \tilde{\otimes} A \quad (\text{A.16})$$

$$A \otimes \bar{C} = \bar{C} \tilde{\otimes} A \frac{r_4}{g} - \frac{1}{g} C \otimes \bar{A} \quad (\text{A.17})$$

$$\bar{D} \otimes C = \frac{z}{g} C \otimes \bar{D} + \frac{1}{g} \bar{C} \otimes D. \quad (\text{A.18})$$

Eqs. (A.18) results from eq. (A.14) by inserting eqs. (A.15), (A.16). For later use, note that

$$C \otimes \bar{C} = \bar{C} \tilde{\otimes} C \frac{r_4}{z} \quad (\text{A.19})$$

$$gB \otimes_s \bar{C} + D \otimes_s \bar{A} = \bar{D} \tilde{\otimes}_s A + g\bar{C} \tilde{\otimes}_s B$$

$$A \otimes_s \bar{D} + gC \otimes_s \bar{B} = g\bar{B} \tilde{\otimes}_s C + \bar{A} \tilde{\otimes}_s D.$$

In the last two preceding equations, graded tensor products are again replaced by the non-graded versions. Exchanging arguments in the latter ($\tilde{g}(v-u) = g(u-v)$), one adds both and finds:

$$-(g+\tilde{g})\bar{C} \otimes B = (g+\tilde{g})B \otimes \bar{C} + A \otimes \bar{D} + D \otimes \bar{A} - \bar{A} \otimes D - \bar{D} \otimes A. \quad (\text{A.20})$$

In the common language of BA, the first terms on the rhs in eqs. (A.17) are "wanted", the second terms "unwanted". The latter must cancel when acting with τ on $|\Phi\rangle$. Furthermore, $|\Phi\rangle$ must diagonalize Ar_4 . Since A is already diagonal with respect to $|4\rangle^{\otimes N}$, this is achieved by finding a "subeigenstate", on which

$$\begin{aligned} \tilde{T} &:= T^{(2,2)} := [r_4]_{a,m} \cdots [r_4]_{a,1} \\ &=: \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} \end{aligned} \quad (\text{A.21})$$

acts. \tilde{T} is intertwined by r_4 :

$$\begin{aligned} &\begin{pmatrix} h & & & \\ & g & 1 & \\ & 1 & g & \\ & & & h \end{pmatrix} \begin{pmatrix} A \otimes \bar{\tilde{A}} & A \otimes \bar{\tilde{B}} & B \otimes \bar{\tilde{A}} & B \otimes \bar{\tilde{B}} \\ A \otimes \bar{\tilde{C}} & A \otimes \bar{\tilde{D}} & B \otimes \bar{\tilde{C}} & B \otimes \bar{\tilde{D}} \\ \hline C \otimes \bar{\tilde{A}} & C \otimes \bar{\tilde{B}} & D \otimes \bar{\tilde{A}} & D \otimes \bar{\tilde{B}} \\ C \otimes \bar{\tilde{C}} & C \otimes \bar{\tilde{D}} & D \otimes \bar{\tilde{C}} & D \otimes \bar{\tilde{D}} \end{pmatrix} \\ &= \begin{pmatrix} \bar{\tilde{A}} \otimes A & \bar{\tilde{B}} \otimes A & \bar{\tilde{A}} \otimes B & \bar{\tilde{B}} \otimes B \\ \bar{\tilde{C}} \otimes A & \bar{\tilde{D}} \otimes A & \bar{\tilde{C}} \otimes B & \bar{\tilde{D}} \otimes B \\ \hline \bar{\tilde{A}} \otimes C & \bar{\tilde{B}} \otimes C & \bar{\tilde{A}} \otimes D & \bar{\tilde{B}} \otimes D \\ \bar{\tilde{C}} \otimes C & \bar{\tilde{D}} \otimes C & \bar{\tilde{C}} \otimes D & \bar{\tilde{D}} \otimes D \end{pmatrix} \begin{pmatrix} h & & & \\ & g & 1 & \\ & 1 & g & \\ & & & h \end{pmatrix} \end{aligned} \quad (\text{A.22})$$

The operator valued entries of \tilde{T} act on m two-dimensional quantum spaces. Call the basis system of each quantum state $\{|\tilde{1}\rangle, |\tilde{2}\rangle\}$. \tilde{T} acquires a lower triangular structure by acting on $|\tilde{2}\rangle^{\otimes m}$. So one needs commutators of \tilde{A} , \tilde{D} with \tilde{C} ,

$$\tilde{A}\tilde{C} = \frac{h}{g}\tilde{C}\tilde{A} - \frac{1}{g}\tilde{C}\tilde{A} \quad (\text{A.23})$$

$$\tilde{D}\tilde{C} = \frac{h}{g}\tilde{C}\tilde{D} - \frac{1}{g}\tilde{C}\tilde{D}. \quad (\text{A.24})$$

The second terms on the rhs, "unwanted", again have to vanish if the eigenstate property is to be fulfilled.

$$|\Phi\rangle = \left[C(v_1^{(1)}) \otimes \cdots \otimes C(v_m^{(1)}) \right] \tilde{C}(v_1^{(2)}) \cdots \tilde{C}(v_{\tilde{m}}^{(2)}) \left(|\tilde{2}\rangle^{\otimes m} \otimes |4\rangle^{\otimes N} \right) \quad (\text{A.25})$$

is an eigenvector of $\tau(v)$. The proof uses the same strategy as [33], where the $\mathfrak{gl}(2|1)$ symmetric transfer matrix with threedimensional auxiliary and quantum spaces is diagonalized. This proof is rigorous for arbitrary N . We have verified that all arguments needed are given in [33] and are directly transferable to and valid for our problem. We thus only give the result here:

$$\begin{aligned} \tau(v)|\Phi\rangle &= \Lambda(v)|\Phi\rangle \\ \Lambda(v) &= \omega_1(u) \left[\frac{q_2(v+1)}{q_2(v)} + \frac{q_2(v-1)}{q_2(v)} \frac{q_1(v+1)}{q_1(v)} \right] + \omega_2(u) \frac{q_1(v+1)}{q_1(v)} \end{aligned} \quad (\text{A.26})$$

$$\begin{aligned} q_1(v) &= \prod_{k=1}^m (v - v_k^{(1)}), \quad q_2(v) = \prod_{l=1}^{\tilde{m}} (v - v_l^{(2)}) \\ -1 &= \frac{q_2(v_k^{(2)} - 1) q_1(v_k^{(2)} + 1)}{q_2(v_k^{(2)} + 1) q_1(v_k^{(2)})} \end{aligned} \quad (\text{A.27})$$

$$-\frac{q_2(v_l^{(1)})}{q_2(v_l^{(1)} - 1)} = \frac{\omega_1(v_l^{(1)})}{\omega_2(v_l^{(1)})}. \quad (\text{A.28})$$

In eq. (A.25), the 2^m row vector $\left[C(v_1^{(1)}) \otimes_s \cdots \otimes_s C(v_m^{(1)}) \right]$ is multiplied with the 2^m column vector $\tilde{C}(v_1^{(2)}) \cdots \tilde{C}(v_{\tilde{m}}^{(2)}) \left(|\tilde{2}\rangle^{\otimes m} \otimes |4\rangle^{\otimes N} \right)$.

The eigenstate depends on $m + \tilde{m}$ many quantum numbers, which are arranged in two sets, each one being the zeroes of q_1, q_2 . They are determined by the vanishing of the "unwanted" terms: q_2 stems from the "inner" BA, which diagonalizes r_4 , and eq. (A.27) reflects the cancellation of unwanted terms produced by eqs. (A.23), (A.24). q_1 originates in the "outer" BA, and eq. (A.28) ensures the cancellation of unwanted terms stemming from eqs. (A.17), (A.18). Both sets of eqs. (A.27), (A.28) are seen to equivalent to the analyticity of Λ .

The eigenvalue $\Lambda_I^{(Q)}$ differs from Λ only by the vacuum expectation values, eq. (2.64) and the external fields h, μ . As mentioned in the main part, $v \rightarrow -iv$ and $v_k^{(1,2)} \rightarrow -iv_k^{(1,2)}$. Furthermore, shift $v_k^{(1)} \rightarrow v_k^{(1)} + i/2 \forall k$ (this shift has only "cosmetic" reasons). For the moment, let Λ_{++-} be the eigenvalue of $\tau_I^{(Q)}(v)$, where the indices $++-$ denote the grading in auxiliary space. The fields are

Note that the spaces 2, 3 in auxiliary space have been permuted in comparison to eq. (A.9). Now the fermionic reference state $|2\rangle^{\otimes N} (|[3] \otimes |2\rangle)^{\otimes N/2}$ serves as a starting point to construct the eigenstate of τ ($\tau^{(Q)}$), and T ($T^{(Q)}$) (which is not the same as above!) becomes upper diagonal. With this modification one finds along exactly the same lines as above:

$$\begin{aligned}\Lambda_{+-+}(v) &= \lambda_-(v) + \lambda_+(v) + \lambda_0(v) \\ &:= \phi_+ \left(v + i\frac{\alpha}{2} \right) \phi_- \left(v - i\frac{\alpha}{2} - i \right) \frac{q_-(v+i)}{q_-(v)} e^{\beta(\mu+h/2)} \\ &\quad + \phi_- \left(v - i\frac{\alpha}{2} \right) \phi_+ \left(v + i\frac{\alpha}{2} + i \right) \frac{q_+(v-i/2)}{q_+(v+i/2)} e^{\beta(\mu-h/2)} \\ &\quad + \phi_+ \left(v - i\frac{\alpha}{2} \right) \phi_- \left(v + i\frac{\alpha}{2} \right) \frac{q_-(v+i)}{q_-(v)} \frac{q_+(v-i/2)}{q_+(v+i/2)}\end{aligned}\tag{A.35}$$

$$q_-(v) = \prod_{j=1}^{\widetilde{M}} (v - v_j), \quad q_+(v) = \prod_{k=1}^M (v - v_k)$$

$$-\frac{q_-(v_k + i/2)}{q_-(v_k - i/2)} e^{-\beta(\mu-h/2)} = \frac{\phi_-(v_k - i\alpha/2 - i/2) \phi_+(v_k + i\alpha/2 + i/2)}{\phi_+(v_k - i\alpha/2 - i/2) \phi_-(v_k + i\alpha/2 - i/2)}\tag{A.36}$$

$$-\frac{q_+(\widetilde{v}_j - i/2)}{q_+(\widetilde{v}_j + i/2)} e^{-\beta(\mu+h/2)} = \frac{\phi_+(\widetilde{v}_j + i\alpha/2) \phi_-(\widetilde{v}_j - i\alpha/2 - i)}{\phi_+(\widetilde{v}_j - i\alpha/2) \phi_-(\widetilde{v}_j + i\alpha/2)}.\tag{A.37}$$

Using a technique proposed in [82], we want to show that

$$\Lambda_{++-}(v) = \Lambda_{+-+}(v)$$

$$q_2(v) = q_-(v), \quad \widetilde{m} = \widetilde{M}\tag{A.38a}$$

$$q_1^{(h)}(v) = q_+^{(h)}(v), \quad N + \widetilde{m} - m = N + M - \widetilde{M}\tag{A.38b}$$

$$q_1(v) = q_-^{(h)}(v), \quad m = N + \widetilde{M} - M\tag{A.38c}$$

$$q_2^{(h)}(v) = q_+(v), \quad 2N - m = M.\tag{A.38d}$$

To start with, one observes that eq. (A.32) is equivalent to eq. (A.36), immediately allowing for eq. (A.38a).

As already mentioned in the main part, eq. (A.37) also permits $N + M - \widetilde{M}$ many hole solutions $\widetilde{v}_k^{(h)}$, the zeroes of $q_+^{(h)}$. In analogy to eq. (A.38a), one is lead to eq. (A.38b).

Motivated by eq. (A.36), define a polynomial P ,

$$\begin{aligned}P(v) &= q_- \left(v + \frac{i}{2} \right) \phi_+ \left(v - i\frac{\alpha}{2} - \frac{i}{2} \right) \phi_- \left(v + i\frac{\alpha}{2} - \frac{i}{2} \right) e^{-\beta(\mu-h/2)} \\ &\quad + q_- \left(v - \frac{i}{2} \right) \phi_- \left(v - i\frac{\alpha}{2} - \frac{i}{2} \right) \phi_+ \left(v + i\frac{\alpha}{2} + \frac{i}{2} \right)\end{aligned}\tag{A.39}$$

$$\equiv q_+(v) q_-^{(h)}(v)\tag{A.40}$$

P is of degree $\widetilde{M} + N$, and by construction (eq. (A.36)) has M zeroes $\{v_k\}$. The remaining $N + \widetilde{M} - M$ zeroes are contained in $q_-^{(h)}$, which has already been defined in eq. (2.71).

Consider the quotient

$$\frac{P(\widetilde{v}_k + i/2)}{P(\widetilde{v}_k - i/2)},$$

which gives an expression for $q_+(\tilde{v}_k - i/2)/q_+(\tilde{v}_k + i/2)$. It is inserted into eq. (A.37), resulting in

$$\frac{q_-(\tilde{v}_k - i) q_-^{(h)}(\tilde{v}_k + i/2)}{q_-(\tilde{v}_k + i) q_-^{(h)}(\tilde{v}_k - i/2)} e^{-\beta h} = -1 .$$

The equivalence with eq. (A.31) is evident and gives eq. (A.38c).

Eq. (A.38d) completes eqs. (A.38a), (A.38b), (A.38c).

The equivalence of the BAE has been shown. The eigenvalues are equal and can be mapped onto each other. One directly sees

$$\lambda_- \equiv \lambda_1 .$$

As to the remaining terms, consider

$$\frac{P(v + i/2)}{P(v - i/2)} .$$

This quotient can be expressed in two ways, using eqs. (A.39), (A.40). One is lead to

$$\begin{aligned} \frac{q_-(v + i)}{q_-(v)} \frac{q_+(v - i/2)}{q_+(v + i/2)} \phi_+ \left(v - i \frac{\alpha}{2} \right) \phi_- \left(v + i \frac{\alpha}{2} \right) e^{-\beta(\mu - h/2)} + \frac{q_+(v - i/2)}{q_+(v + i/2)} \phi_- \left(v - i \frac{\alpha}{2} \right) \phi_+ \left(v + i \frac{\alpha}{2} + i \right) \\ = \frac{q_-(v - i)}{q_-(v)} \frac{q_-^{(h)}(v + i/2)}{q_-^{(h)}(v - i/2)} \phi_+ \left(v + i \frac{\alpha}{2} \right) \phi_- \left(v - i \frac{\alpha}{2} - i \right) \\ + \frac{q_-^{(h)}(v + i/2)}{q_-^{(h)}(v - i/2)} \phi_- \left(v - i \frac{\alpha}{2} - i \right) \phi_- \left(v + i \frac{\alpha}{2} - i \right) e^{-\beta(\mu - h/2)} \\ \Leftrightarrow \lambda_+ + \lambda_0 = \lambda_2 + \lambda_3 \end{aligned}$$

This completes the proof of equivalence between the $+ - +$ and $+ + -$ sets.

NB: One may find a third equivalent set, $- + +$. Since it is of no importance in this work, we omit to give it explicitly.

Shifting the roots $v_k \rightarrow v_k - i/2$ in eq. (A.35), one gets eq. (2.69). Note that the largest eigenvalue is given by $M = \widetilde{M} = N/2$ particle solutions and, following eqs. (A.38b), (A.38c), by N hole solutions. This means that in fig. (2.4), only half the number of possible hole solutions are depicted. They are, however, expected not to deviate substantially from those shown.

A.2 Host Hamiltonian

Let us list some properties of $R^{(4,4)}(u)$, useful in calculating the corresponding Hamiltonian afterwards.

From the definition eq. (2.5) and by using the projection property eq. (2.13),

$$\begin{aligned} R^{(4,4)}(0) &= -(\mathbf{1} - 2\check{P}_1 - 2\check{P}_3) \neq \mathbf{1} \\ \left[R^{(4,4)}(0) \right]^2 &= \mathbf{1} \end{aligned} \tag{A.41}$$

So $R^{(4,4)}(0)$ is a permutation operator. Indeed, inserting explicit expressions from eqs. (2.7), (2.8),

$$\begin{aligned} \left[R^{(4,4)}(0) \right]_{c,d}^{a,b} &= (-1)^{p[a]p[b]} \delta_d^a \delta_c^b \\ &=: [\mathcal{P}]_{c,d}^{a,b} . \end{aligned}$$

\mathcal{P} is the graded permutation operator in four-dimensional space. Now $\mathcal{P} = \mathcal{P}_\downarrow \mathcal{P}_\uparrow$, where $\mathcal{P}_{\downarrow, \uparrow}$ are permutation operators in two distinct two-dimensional spaces with grading $p[1] = 0, p[2] = 1$. So from eq. (A.41)

$$\check{P}_1 + \check{P}_3 = \frac{1}{2} \mathbf{1} + \frac{1}{2} \mathcal{P}_\downarrow \mathcal{P}_\uparrow = \frac{1}{4} (\mathcal{P}_\downarrow + \mathcal{P}_\uparrow)^2$$

Since on the other hand $(-\check{P}_1 + \check{P}_3)^2 = \check{P}_1 + \check{P}_3$, it follows that

$$-\check{P}_1 + \check{P}_3 = \frac{1}{2} (\mathcal{P}_\downarrow + \mathcal{P}_\uparrow) = \frac{1}{2} h^{(ff)} \quad (\text{A.42})$$

Eq. (A.42) directly permits the identification with the free fermion Hamiltonian between two lattice sites, defined in eq. (2.25).

Consider

$$\left[\frac{d}{du} R^{(4,4)}(u) \right]_{u=0} = \frac{2}{\alpha} \check{P}_1 - \frac{2}{\alpha+1} \check{P}_3.$$

Using eq. (A.41),

$$\left[\frac{d}{du} \ln R^{(4,4)}(u) \right]_{u=0} = \frac{2}{\alpha} \check{P}_1 - \frac{2}{\alpha+1} \check{P}_3. \quad (\text{A.43})$$

With

$$\lim_{\alpha \rightarrow \infty} \left[(\alpha+1) \left(\frac{2}{\alpha} \check{P}_1 - \frac{2}{\alpha+1} \check{P}_3 \right) \right] = 2\check{P}_1 - 2\check{P}_3$$

eq. (2.25) follows.

Let us now calculate the host contribution to the Hamiltonian. In the main part, it has been shown that it is the sum of local contributions, (2.23). These are identified with the logarithmic derivative of $R^{(4,4)}(u)$, eq. (A.43). All one has to do is inserting the explicit expressions eqs. (2.7), (2.8), and making the identification eq. (2.17). For the ease of notation, operators acting in j -th space are not labeled, those acting in $j+1$ -th space are over-lined.

$$\begin{aligned} & -(\alpha+1) \left[\frac{2}{\alpha} [\check{P}_1]_{j,j+1} - \frac{2}{\alpha+1} [\check{P}_3]_{j,j+1} \right] \\ &= [-e_1^1 (\bar{e}_1^1 + \bar{e}_2^2 + \bar{e}_3^3) - (e_1^1 + e_2^2 + e_3^3) \bar{e}_1^1 + e_4^4 (\bar{e}_2^2 + \bar{e}_3^3 + \bar{e}_4^4) + (e_2^2 + e_3^3 + e_4^4) \bar{e}_4^4] \\ & \quad - \frac{1}{\alpha} [e_1^1 (\bar{e}_1^1 + \bar{e}_2^2 + \bar{e}_3^3) + (e_1^1 + e_2^2 + e_3^3) \bar{e}_1^1] \\ & \quad (e_1^2 + e_3^4) (\bar{e}_2^1 + \bar{e}_4^3) + (e_1^3 - e_2^4) (\bar{e}_3^1 - \bar{e}_4^2) - (e_2^1 + e_4^3) (\bar{e}_1^2 + \bar{e}_3^4) - (e_3^1 - e_4^2) (\bar{e}_1^3 - \bar{e}_2^4) \\ & \quad + \frac{1}{\alpha} (e_1^2 \bar{e}_2^1 - e_2^1 \bar{e}_1^2 + e_1^3 \bar{e}_3^1 - e_3^1 \bar{e}_1^3 - e_4^4 \bar{e}_4^1 - e_1^1 \bar{e}_4^4 - e_4^1 \bar{e}_1^4 - e_1^4 \bar{e}_4^1) \\ & \quad + \left(\sqrt{\frac{\alpha+1}{\alpha}} - 1 \right) (e_3^4 \bar{e}_2^1 + e_1^2 \bar{e}_4^3 - e_4^3 \bar{e}_1^2 - e_2^1 \bar{e}_3^4 - e_2^2 \bar{e}_3^3 - e_1^3 \bar{e}_4^2 + e_4^2 \bar{e}_1^3 + e_3^1 \bar{e}_2^4). \end{aligned}$$

The Hamiltonian is obtained by identifications implied by eq. (2.17).

A.2.1 $\mathfrak{gl}(2|1)$ invariance

The invariance of $\tau(u)$ with respect to $\mathfrak{gl}(2|1)$ is shown by expanding eq. (A.2) in the limit $v \rightarrow \infty$, including only terms $\mathcal{O}(1)$, $\mathcal{O}(1/v)$.

$$R^{(3,4)}(v) \sim 1 + \frac{1}{v} \left(\frac{\alpha}{2} + 1 + (-1)^b e_a^b E_b^a \right) + \mathcal{O} \left(\frac{1}{v^2} \right) \quad (\text{A.44})$$

$$\begin{aligned} T^{(3,4)}(v) &=: R_{a,L}^{(3,4)}(v) R_{a,L-1}^{(3,4)}(v) \dots R_{a,0}^{(3,3)}(v + iu_0) \\ &\sim 1 + \frac{1}{v} \left\{ \sum_{j=1}^L \left[\frac{\alpha}{2} + 1 + (-1)^b [e_a]_a^b [E_j]_b^a \right] + (-1)^b [e_a]_a^b [e_0]_b^a \right\} + \mathcal{O} \left(\frac{1}{v^2} \right) \\ &=: 1 + \frac{W}{v} + \mathcal{O} \left(\frac{1}{v^2} \right). \end{aligned} \quad (\text{A.45})$$

$T^{(4,4)} \equiv T$ is defined in eq. (2.19).

Eqs. (A.44), (A.45) are inserted into eq. (A.2) with $d'' = 3; d = d' = 4$, while keeping the full $T^{(4,4)}(u)$. The constant terms on both sides are identically equal. In order $\mathcal{O}(1/v)$, one gets

$$\begin{aligned} &(-1)^{p[\beta'']p[\alpha]+p[\alpha'']} \overline{T_{\beta''}^\beta} W_{\alpha''}^\alpha + \overline{T_{\beta''}^\beta} \left[(-1)^{p[a]p[b]} e_a^b E_b^a \right]_{\alpha'',\beta''}^{\alpha,\beta'} \\ &= (-1)^{p[\beta](p[\alpha]+p[\alpha''])} W_{\alpha''}^\alpha \overline{T_{\beta''}^\beta} + \left[(-1)^{p[a]p[b]} e_a^b E_b^a \right]_{\alpha'',\beta'}^{\alpha,\beta} \overline{T_{\beta''}^{\beta'}}. \end{aligned}$$

Set $\beta = \beta''$, multiply with $(-1)^\beta$ and sum over β . The second terms on each side are identically equal. The first terms give the commutator of the transfer matrix $\bar{\tau}$ with W :

$$\begin{aligned} \bar{\tau} &:= \sum_{\beta} (-1)^\beta \overline{T_{\beta}^\beta} \\ [\bar{\tau}, W_{\alpha''}^\alpha] &= 0. \end{aligned} \quad (\text{A.46})$$

Dropping constants in W , eq. (A.46) states that:

$$\left[\tau(u), \sum_{j=1}^L [E_j]_b^a + [e_0]_b^a \right] = 0.$$

Thus τ commutes with all global $\mathfrak{gl}(2|1)$ symmetry operators. In a very similar way, one starts with eq. (2.11) to show

$$\left[\bar{\tau}(u), \sum_{j=1}^L [E_j]_b^a + [e_0]_b^a \right] = 0,$$

where $\bar{\tau}(u)$ is defined in eq. (2.20). Consequently, the Hamiltonian, defined by eq. (2.21), is $\mathfrak{gl}(2|1)$ -symmetric.

A.3 Eigenvalue of $\tau_h^{(Q)}$

The eigenvalue Λ_h of $\tau_h^{(Q)}$ is calculated in two steps: The first part is dedicated to the formal diagonalization. The result for the largest eigenvalue is used in the second part to set up NLIE.

Given the settings of eq. (A.5), one can directly compare matrix entries on both sides of eq. (A.3). Before, apply a similarity transformation to eq. (A.3), very similar to the procedure in section A.1. Let

$$X_1 = \begin{pmatrix} 1 & & & & \\ & s & & & \\ & & s^T & & \\ & & & 1 & \\ & & & & \mathbb{1}_4 \end{pmatrix}$$

$$s = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

X_1 arranges the elements in the fermionic sector on both sides of eq. (A.3) in their "natural" order. The structure gets even nicer by acting with

$$X_2 = \begin{pmatrix} 1 & & & & \\ & & & 1 & \\ & & \mathbb{1}_4 & & \\ & 1 & & & \\ & & & & 1 \\ & & & & & \mathbb{1}_4 \end{pmatrix}.$$

Using $X := X_2 \cdot X_1$, eq. (A.3) is transformed as

$$X [\underline{T} \tilde{\otimes}_s T] X^T X R^{(3,4)} X^T = X R^{(3,4)} X^T X [T \otimes_s \overline{T}] X^T. \quad (\text{A.47})$$

The shorthand notations are

$$\overline{T} := T(u), \quad R \equiv R(v - u). \quad (\text{A.48})$$

We assign different symbols to the entries of \underline{T} :

$$\underline{T} =: \begin{pmatrix} \underline{D}_1^1 & \underline{C}_1 & \underline{D}_1^2 \\ \underline{B}_1 & \underline{A} & \underline{B}_2^1 \\ \underline{D}_2^1 & \underline{C}_2 & \underline{D}_2^2 \end{pmatrix}$$

$$\underline{B}_1 =: (\underline{T}_2^1, \underline{T}_3^1)^T, \quad \underline{B}_2 =: (\underline{T}_2^4, \underline{T}_3^4)^T, \quad \underline{C}_1 =: (\underline{T}_1^2, \underline{T}_1^3), \quad \underline{C}_2 =: (\underline{T}_4^2, \underline{T}_4^3)$$

$$\underline{A} =: \begin{pmatrix} \underline{A}_1^1 & \underline{A}_1^2 \\ \underline{A}_2^1 & \underline{A}_2^2 \end{pmatrix} := \begin{pmatrix} \underline{T}_2^1 & \underline{T}_2^3 \\ \underline{T}_3^2 & \underline{T}_3^3 \end{pmatrix}$$

Elements \underline{A}_j^k belong the fermionic sector, \underline{D}_j^k to the bosonic sector. $\underline{C}_j, \underline{B}_j$ are the transition elements.

This notation is formally equal to eq. (A.10). Now eq. (A.47) reads

$$\begin{aligned}
& \left(\begin{array}{ccc|ccc} d\mathbf{1}_2 & & & \xi & & \\ & r_4 & & & & \\ & & f\mathbf{1}_2 & & \phi\mathbf{1}_2 & \\ \hline & & \xi^T & & a & \\ & & & & & b\mathbf{1}_2 \\ & & & & & c \end{array} \right) \left(\begin{array}{ccc|ccc} A \otimes_s \overline{D_1^1} & A \otimes_s \overline{C_1} & A \otimes_s \overline{D_2^2} & B \otimes_s \overline{D_1^1} & B \otimes_s \overline{C_1} & B \otimes_s \overline{D_2^2} \\ A \otimes_s \overline{B_1} & A \otimes_s \overline{A} & A \otimes_s \overline{B_2} & B \otimes_s \overline{B_1} & B \otimes_s \overline{A} & B \otimes_s \overline{B_2} \\ A \otimes_s \overline{D_2^1} & A \otimes_s \overline{C_2} & A \otimes_s \overline{D_2^2} & B \otimes_s \overline{D_2^1} & B \otimes_s \overline{C_2} & B \otimes_s \overline{D_2^2} \\ \hline C \otimes_s \overline{D_1^1} & C \otimes_s \overline{C_1} & C \otimes_s \overline{D_2^2} & D \otimes_s \overline{D_1^1} & D \otimes_s \overline{C_1} & D \otimes_s \overline{D_2^2} \\ C \otimes_s \overline{B_1} & C \otimes_s \overline{A} & C \otimes_s \overline{B_2} & D \otimes_s \overline{B_1} & D \otimes_s \overline{A} & D \otimes_s \overline{B_2} \\ C \otimes_s \overline{D_2^1} & C \otimes_s \overline{C_2} & C \otimes_s \overline{D_2^2} & D \otimes_s \overline{D_2^1} & D \otimes_s \overline{C_2} & D \otimes_s \overline{D_2^2} \end{array} \right) \\
& = \left(\begin{array}{ccc|ccc} \overline{D_1^1} \otimes_s A & \overline{C_1} \otimes_s A & \overline{D_2^2} \otimes_s A & \overline{D_1^1} \otimes_s B & \overline{C_1} \otimes_s B & \overline{D_2^2} \otimes_s B \\ \overline{B_1} \otimes_s A & \overline{A} \otimes_s A & \overline{B_2} \otimes_s A & \overline{B_1} \otimes_s B & \overline{A} \otimes_s B & \overline{B_2} \otimes_s B \\ \overline{D_2^1} \otimes_s A & \overline{C_2} \otimes_s A & \overline{D_2^2} \otimes_s A & \overline{D_2^1} \otimes_s B & \overline{C_2} \otimes_s B & \overline{D_2^2} \otimes_s B \\ \hline \overline{D_1^1} \otimes_s C & \overline{C_1} \otimes_s C & \overline{D_2^2} \otimes_s C & \overline{D_1^1} \otimes_s D & \overline{C_1} \otimes_s D & \overline{D_2^2} \otimes_s D \\ \overline{B_1} \otimes_s C & \overline{A} \otimes_s C & \overline{B_2} \otimes_s C & \overline{B_1} \otimes_s D & \overline{A} \otimes_s D & \overline{B_2} \otimes_s D \\ \overline{D_2^1} \otimes_s C & \overline{C_2} \otimes_s C & \overline{D_2^2} \otimes_s C & \overline{D_2^1} \otimes_s D & \overline{C_2} \otimes_s D & \overline{D_2^2} \otimes_s D \end{array} \right) \left(\begin{array}{ccc|ccc} d\mathbf{1}_2 & & & \xi & & \\ & r_4 & & & & \\ & & f\mathbf{1}_2 & & \phi\mathbf{1}_2 & \\ \hline & & \xi^T & & a & \\ & & & & & b\mathbf{1}_2 \\ & & & & & c \end{array} \right) \tag{A.49}
\end{aligned}$$

The entries of the R -matrix are

$$\begin{aligned}
a(v-u) &= v-u+1-\frac{\alpha}{2}; \quad b(v-u) = v-u-\frac{\alpha}{2}; \quad c(v-u) = v-u-\frac{\alpha}{2}-1 \\
d(v-u) &= v-u+1+\frac{\alpha}{2}; \quad f(v-u) = v-u+\frac{\alpha}{2}; \quad \phi = \sqrt{\alpha+1} \\
\xi^T &= (0, \sqrt{\alpha}, -\sqrt{\alpha}, 0) \\
r_4(v-u) &= \begin{pmatrix} d(v-u) & & & & & \\ & f(v-u) & & 1 & & \\ & & 1 & & f(v-u) & \\ & & & & & d(v-u) \end{pmatrix}
\end{aligned}$$

Horizontal and vertical lines in eq. (A.49) separate fermionic from bosonic sectors in the auxiliary space of T .

In eq. (A.49), fermionic (bosonic) operators have been summarized in the matrix \underline{A} (\underline{D}). This structure is made explicit by transforming eq. (A.49) again with the matrix \tilde{X} :

$$\tilde{X} = \left(\begin{array}{ccc|ccc} 0 & 1 & 0 & & & \\ 1 & 0 & 0 & & & \\ 0 & 0 & 1 & & & \\ \hline & & & 0 & 1 & 0 \\ & & & 1 & 0 & 0 \\ & & & 0 & 0 & 1 \end{array} \right).$$

The notation is symbolical, the dimensions of the unity operators are chosen such that the matrix multiplication is properly defined. \tilde{X} permutes the first and second rows/columns and the fourth and

fifth rows/columns. By transforming eq. (A.49), one gets

$$\begin{aligned} & \left(\begin{array}{c|c} r_4 & \zeta \\ \hline p_4 & \phi \mathbf{1}_2 \\ \phi^T \mathbf{1}_2 & b \mathbf{1}_2 \\ \hline \zeta^T & p_2 \end{array} \right) \left(\begin{array}{cc|cc} A \otimes_s \overline{A} & A \otimes_s \overline{B} & B \otimes_s \overline{A} & B \otimes_s \overline{B} \\ A \otimes_s \overline{C} & A \otimes_s \overline{D} & B \otimes_s \overline{C} & B \otimes_s \overline{D} \\ \hline C \otimes_s \overline{A} & C \otimes_s \overline{B} & D \otimes_s \overline{A} & D \otimes_s \overline{B} \\ C \otimes_s \overline{C} & C \otimes_s \overline{D} & D \otimes_s \overline{C} & D \otimes_s \overline{D} \end{array} \right) \\ &= \left(\begin{array}{cc|cc} \overline{A} \tilde{\otimes}_s A & \overline{B} \tilde{\otimes}_s A & \overline{A} \tilde{\otimes}_s B & \overline{B} \tilde{\otimes}_s B \\ \overline{C} \tilde{\otimes}_s A & \overline{D} \tilde{\otimes}_s A & \overline{C} \tilde{\otimes}_s B & \overline{D} \tilde{\otimes}_s B \\ \hline \overline{A} \tilde{\otimes}_s C & \overline{B} \tilde{\otimes}_s C & \overline{A} \tilde{\otimes}_s D & \overline{B} \tilde{\otimes}_s D \\ \overline{C} \tilde{\otimes}_s C & \overline{D} \tilde{\otimes}_s C & \overline{C} \tilde{\otimes}_s D & \overline{D} \tilde{\otimes}_s D \end{array} \right) \left(\begin{array}{c|c} r_4 & \zeta \\ \hline p_4 & \phi \mathbf{1}_2 \\ \phi^T \mathbf{1}_2 & b \mathbf{1}_2 \\ \hline \zeta^T & p_2 \end{array} \right). \end{aligned} \quad (\text{A.50})$$

The entries of the R -matrix are

$$\begin{aligned} \phi^T &= (0_{2 \times 2}, \phi \mathbf{1}_2), & \zeta &= (\xi, 0_{4 \times 1}) \\ p_4 &= \begin{pmatrix} d \mathbf{1}_2 & 0 \\ 0 & f \mathbf{1}_2 \end{pmatrix}, & p_2 &= \begin{pmatrix} a & 0 \\ 0 & c \end{pmatrix}. \end{aligned}$$

$0_{j \times k}$ is a $j \times k$ matrix with 0 entries. Eq. (A.50) is of 8 vertex model structure. This is very similar to corresponding equations of the Hubbard model, [34]. The main difference to analogous equations with $R^{(3,3)}$ as inter-twiner is the existence of four off-diagonal entries instead of two. This makes the calculation of the eigenvalue little more involved. The price to pay for the compactness of eq. (A.50) is that it has to be deciphered, once the proper commutation relations are found.

The eigenstates of T (and thereby of \underline{T}) are constructed by acting with C on $(|4\rangle)^{\otimes N}$. So let us dive into the commutation relations between the diagonal elements of \underline{T} with C , given by eq. (A.49):

$$\xi^T A \otimes_s \overline{B}_1 + a C \otimes_s \overline{D}_1^1 = \overline{D}_1^1 \tilde{\otimes}_s C d \quad (\text{A.51a})$$

$$\phi A \otimes_s \overline{C}_2 + b C \otimes_s \overline{A} = \overline{A} \tilde{\otimes}_s C r_4 + \overline{C}_2 \tilde{\otimes}_s D \xi^T \quad (\text{A.51b})$$

$$c C \otimes_s \overline{D}_2^2 = \overline{D}_2^2 \tilde{\otimes}_s C f + \overline{C}_2 \tilde{\otimes}_s D \phi. \quad (\text{A.51c})$$

On the rhs, terms wished to be calculated and "unwanted" terms (in eqs. (A.51b), (A.51c)) occur. On the lhs, there appear wanted terms and, in eqs. (A.51a), (A.51b), terms which are "annoying": They are of the same structure as the "wanted" terms, but are neither "wanted" nor "unwanted". To get rid of them, the only possibility is to make use of

$$r_4 A \otimes_s \overline{B}_1 + \xi C \otimes_s \overline{D}_1^1 = \overline{B}_1 \tilde{\otimes}_s A d \quad (\text{A.52})$$

$$f A \otimes_s \overline{C}_2 + \phi C \otimes_s \overline{A} = \overline{C}_2 \tilde{\otimes}_s A r_4 + \overline{D}_2^1 \tilde{\otimes}_s B \xi^T. \quad (\text{A.53})$$

Eliminating $A \otimes_s \overline{B}_1$ from eq. (A.51a) by eq. (A.52) and $A \otimes_s \overline{C}_2$ from eq. (A.51b) by eq. (A.53) gives

$$\overline{D}_1^1 \tilde{\otimes}_s C = \frac{a - \xi^T r_4^{-1} \xi}{d} C \otimes_s \overline{D}_1^1 + \xi^T r_4^{-1} \overline{B}_1 \tilde{\otimes}_s A \quad (\text{A.54})$$

$$\overline{A} \tilde{\otimes}_s C = C \otimes_s \overline{A} \left(b - \frac{\phi^2}{f} \right) r_4^{-1} + \overline{C}_2 \tilde{\otimes}_s A \frac{\phi}{f} - \overline{B}_1 \tilde{\otimes}_s D \xi^T r_4^{-1} + \overline{D}_2^1 \tilde{\otimes}_s B \frac{\xi^T \phi r_4^{-1}}{f} \quad (\text{A.55})$$

$$\left(b - \frac{\phi^2}{f} \right) r_4^{-1} = \frac{d(u-v)}{b(u-v)} \frac{1}{a(u-v)} \begin{pmatrix} a(u-v) & & & \\ & b(u-v) & 1 & \\ & 1 & b(u-v) & \\ & & & a(u-v) \end{pmatrix} \quad (\text{A.56})$$

$$\overline{D}_2^2 \tilde{\otimes}_s C = \frac{c}{f} C \otimes_s \overline{D}_2^2 - \frac{\phi}{f} \overline{C}_2 \tilde{\otimes}_s D \quad (\text{A.57})$$

In the last line, eq. (A.51c) has been rewritten. Note that r_4 defined in eq. (A.56) differs from eq. (A.12) only by a normalizing pre-factor and a constant shift by $-\alpha/2$. The first terms on the rhs of eqs. (A.54), (A.55), (A.57) are "wanted", the others "unwanted". Let us write eqs. (A.54), (A.55), (A.57) with non-graded tensor products:

$$\overline{D_1^1} \tilde{\otimes} C = \frac{a - \xi^T r_4^{-1} \xi}{d} C \otimes \overline{D_1^1} + \xi^T r_4^{-1} \overline{B_1} \tilde{\otimes} A \quad (\text{A.58a})$$

$$\overline{A} \tilde{\otimes} C = C \otimes \overline{A} \left(b - \frac{\phi^2}{f} \right) r_4^{-1} - \overline{C_2} \tilde{\otimes} A \frac{\phi}{f} + \overline{B_1} \tilde{\otimes} D \xi^T r_4^{-1} - \overline{D_2^1} \tilde{\otimes} B \frac{\xi^T \phi r_4^{-1}}{f} \quad (\text{A.58b})$$

$$\overline{D_2^2} \tilde{\otimes} C = \frac{c}{f} C \otimes \overline{D_2^2} - \frac{\phi}{f} \overline{C_2} \tilde{\otimes} D \quad . \quad (\text{A.58c})$$

Eqs. (A.58a), (A.58b), (A.58c) are contained in analogous relations, derived from eq. (A.50) by a similar procedure:

$$\overline{A} \tilde{\otimes}_s C = (b - \phi^T p_4^{-1} \phi) C \otimes_s \overline{A} r_4^{-1} + \phi^T p_4^{-1} \overline{C} \tilde{\otimes}_s A + \phi^T p_4^{-1} \overline{D} \tilde{\otimes}_s B \zeta^T r_4^{-1} - \overline{B} \tilde{\otimes}_s D \zeta^T r_4^{-1} \quad (\text{A.59a})$$

$$\overline{D} \tilde{\otimes}_s C = \frac{p_2 - \zeta^T r_4^{-1} \zeta}{p_4} C \otimes_s D + \zeta^T r_4^{-1} \overline{B} \tilde{\otimes}_s A + \zeta^T r_4^{-1} \overline{A} \tilde{\otimes}_s B \phi^T p_4^{-1} - \overline{C} \tilde{\otimes}_s D \phi^T p_4^{-1} \quad (\text{A.59b})$$

The basic difference between the "wanted" terms is that in the fermionic case, eq. (A.59a), the matrix r_4^{-1} appears. It requires the nested BA with a "sub-vacuum", corresponding to the model discussed in section A.1. On the other hand, the pre-factor of the "wanted" term in eq. (A.59b) is already diagonal. Since eqs. (A.59a), (A.59b) do not contain further information for the problem we wish to solve, we continue with eqs. (A.58a), (A.58b), (A.58c).

An eigenvalue can only be obtained by acting with the "wanted" terms on the eigenstate, the "unwanted" terms must vanish. Let us sketch the main ideas:

- Consider the unwanted terms which substitute C -particles by $\overline{C_2}$ -particles (eqs. (A.58b), (A.58c)). The pre-factors of both terms are the same, so $D(v_i^{(1)}) + \text{tr} A(v_i^{(1)})$ must be carried through the remaining C -operators of $|\Phi\rangle$, eq. (A.25). Eqs. (A.17), (A.18) tell how to do this, the procedure is equal to the derivation of τ in section A.1. Again there are "wanted" and "unwanted" terms. The "wanted" terms are essentially given by (cf. eq. (A.26)):

$$q \left(v_i^{(1)} \right) \Lambda \left(v_i^{(1)} \right) .$$

They cancel if eq. (A.28) is obeyed. Together with eq. (A.27) this is also the condition that the "unwanted" terms in the diagonalization of $D(v_i^{(1)}) + \text{tr} A(v_i^{(1)})$ vanish.

- In eqs. (A.58a), (A.58b), two "unwanted" terms which create a $\overline{B_1}$ -excitation appear. Up to a common constant factor, these are

$$\xi^T \propto (01) \tilde{\otimes} (10) - (10) \tilde{\otimes} (01)$$

$$\xi^T \overline{B_1} \tilde{\otimes} A \propto \overline{T_3^1} \tilde{\otimes} (A_1^1, A_1^1) - \overline{T_2^1} \tilde{\otimes} (A_2^1, A_2^1) \quad (\text{A.60})$$

$$\text{tr} \overline{B_1} \tilde{\otimes} D \xi^T = \overline{T_3^1} \tilde{\otimes} D - \overline{T_2^1} \tilde{\otimes} D \quad (\text{A.61})$$

$$A_2^1 |4\rangle^{\otimes N} = 0 = A_1^2 |4\rangle^{\otimes N} . \quad (\text{A.62})$$

If there is still a sequence of C -operators to the right on the lhs of eqs. (A.60), (A.61), the A, D -operators are first carried through them, before multiplying with ξ^T . Then in eq. (A.60), only the diagonal elements of A remain (cf. eq. (A.62)), together with those in eq. (A.61). Eq. (A.28) again leads to the cancellation of these terms.

- In eq. (A.58b), a term with $\overline{D}_2^1 \widetilde{\otimes} B \xi^T$ is left. If it directly meets the vacuum, it is annihilated by $B|4\rangle^{\otimes N} = 0$. Other ways, $B(v)$ must be commuted through remaining $C(v_l^{(1)})$ by eq. (A.20). The "wanted" terms in this procedure are $C(v_l^{(1)})B(v)$, which ultimately annihilate. The "unwanted" terms are

$$\propto \overline{A} \otimes D - D \otimes A + \overline{D} \otimes A - A \otimes \overline{D}.$$

The direct product with \overline{D}_2^1 and the multiplication with ξ^T of this expression still have to be done. Then diagonal terms (because of the tr operation in eq. (A.58b)) of this term meet the vacuum. They vanish, since $|4\rangle^{\otimes N}$ is simultaneous eigenstate of A_1^1, A_2^2, D .

Finally, r_4 has to be diagonal, which is achieved by vanishing of unwanted terms in the frame of the "subeigenstate":

$$-1 = \frac{q_2(v_k^{(2)} - i) q_1(v_k^{(2)} + i/2)}{q_2(v_k^{(2)} + i) q_1(v_k^{(2)} - i/2)} e^{-\beta h}. \quad (\text{A.63})$$

It is very nice (and consistent) to observe that "unwanted" terms vanish if eqs. (A.32), (A.31) are obeyed.

The arguments presented for the vanishing of the "unwanted" terms do constitute a mathematical rigorous proof only for $m = 1$. For arbitrary m , we expect that the rigorous proof can be realized with the arguments given above together with the diagonalization procedure of the impurity matrix.

The eigenvalue is analytic. Analyticity of this eigenvalue is equivalent to its very property of being an eigenvalue, i.e. to the cancellation of the unwanted terms. Then the eigenstates that diagonalize \overline{T} are those that diagonalize T , which is conceptually clear from eq. (A.6). This statement is now verified explicitly, since these eigenstates are known from eq. (A.25). Compare the wanted terms of eqs. (A.58a), (A.58b), (A.58c) with those of eqs. (A.17), (A.18). They do not only set in evidence that eq. (A.25) is the eigenstate we need also here, but also permit to read off the eigenvalue (good accounts on the nested ABA procedure are [33, 82]):

$$\begin{aligned} \overline{\Lambda} &= \underline{\omega}_1(u) \frac{q_1(u+1+\alpha/2)}{q_1(u+1-\alpha/2)} \\ &+ \underline{\omega}_2(u) \left[\frac{q_1(u+1+\alpha/2)}{q_1(u-\alpha/2)} \frac{q_2(u-1)}{q_2(u)} + \frac{q_1(u+\alpha/2+1)}{q_1(u-\alpha/2+1)} \frac{q_2(u+1)}{q_2(u)} \right] \\ &+ \underline{\omega}_3(u) \frac{q_1(u+\alpha/2+1)}{q_1(u-\alpha/2)} \\ q_1(v) &= \prod_{k=1}^m (v - v_k^{(1)}), \quad q_2 = \prod_{l=1}^{\tilde{m}} (v - v_l^{(2)}). \end{aligned}$$

$\underline{\omega}_1, \underline{\omega}_2, \underline{\omega}_3$ are the eigenvalues of $\underline{A}, \underline{D}, \underline{F}$ with respect to $(|4\rangle)^{\otimes N}$. Constant shifts of $v_l^{(2)}$ by $\alpha/2$ are absorbed in a redefinition.

Ultimately, we are interested in the eigenvalues of $\tau_h^{(Q)}(v)$, the staggered quantum transfer matrix of a lattice site in the host. It differs from $\overline{\Lambda}$ merely by modified vacuum expectation values, eq. (2.63) and external fields μ and h , realized by twisted boundary conditions (they are included as described at the beginning of this appendix). As mentioned in the main part, $v \rightarrow -iv$ and $v_k^{(1,2)} \rightarrow -iv_k^{(1,2)}$.

Shifting $v_k^{(1)} \rightarrow v_k^{(1)} - i/2 + i\alpha/2 \forall k$ leads us to the final result

$$\begin{aligned}
\Lambda_h(v) &= \underline{\lambda}_1(v) + \underline{\lambda}_2(v) + \underline{\lambda}_3(v) + \underline{\lambda}_4(v) \\
&=: \phi_1(v) \frac{q_1(v + i/2 + i\alpha)}{q_1(v + i/2)} e^{2\beta\mu} \\
&\quad + \phi_2(v) e^{\beta\mu} \left[e^{\beta h/2} \frac{q_1(v + i\alpha + i/2)}{q_1(v + i/2)} \frac{q_2(v + i)}{q_2(v)} + e^{-\beta h/2} \frac{q_1(v + i\alpha + i/2)}{q_1(v - i/2)} \frac{q_2(v - i)}{q_2(v)} \right] \\
&\quad + \phi_3(v) \frac{q_1(v + i\alpha + i/2)}{q_1(v - i/2)} \\
\phi_1(v) &= \frac{\phi_+(v) \phi_+(v + i) \phi_-(v - i\alpha)}{\phi_+(v - i\alpha) \phi_+(v + i\alpha + i) \phi_-(v + i\alpha)} \\
\phi_2(v) &= \frac{\phi_+(v) \phi_-(v)}{\phi_+(v + i(\alpha + 1)) \phi_-(v + i\alpha)} \\
\phi_3(v) &= \phi_1(-v)|_{\alpha \rightarrow -\alpha - 1} .
\end{aligned}$$

Requiring analyticity determines the sets $\{v_k^{(1)}\}$, $\{v_l^{(2)}\}$:

$$-1 = \frac{q_2(v_k^{(2)} - i) q_1(v_k^{(2)} + i/2)}{q_2(v_k^{(2)} + i) q_1(v_k^{(2)} - i/2)} e^{-\beta h} \quad (\text{A.64})$$

$$\frac{q_2(v_l^{(1)} + i/2)}{q_2(v_l^{(1)} - i/2)} e^{-\beta(\mu - h/2)} = \frac{\phi_1(v_l^{(1)} - i/2)}{\phi_2(v_l^{(1)} - i/2)} . \quad (\text{A.65})$$

Eqs. (A.64), (A.65) are identical to eqs. (A.31), (A.32) upon shifting $v_l^{(1,2)} \rightarrow v_l^{(1,2)} - i\alpha/2$ in eqs. (A.64), (A.65). This means that both the host and the impurity share the same pattern of BAN, only the functional dependence of the eigenvalue on these BAN is different. It reflects the fact that both possess the same symmetry, namely $\text{gl}(2|1)$.

A.3.2 Solution (NLIE)

When one thinks of setting up NLIE for $\Lambda_h^{(\max)}$, the largest eigenvalue of $\tau_h^{(Q)}$, one may infer without any further calculation that auxiliary functions which determine $\Lambda_h^{(\max)}$ are the same as those of the impurity - only the functional dependence of the eigenvalue on these functions is different, in complete analogy to the pattern of BA roots (this is true for all eigenvalues; however, we derive NLIE only for the largest one). This statement is proved in the following.

The host is derived from a four-dimensional representation of $\text{gl}(2|1)$. The corresponding q -deformed model has been treated in the QTM-approach in [47, 77]. We adopt the ansatz from [77] for auxiliary functions (and, by using the same symbols, anticipate the result that the auxiliary functions are identical to those defined in section 2.1.3):

$$\begin{aligned}
\mathfrak{b} &= \frac{\underline{\lambda}_2}{\underline{\lambda}_3 + \underline{\lambda}_4}, & \mathfrak{B} &= \frac{\underline{\lambda}_2 + \underline{\lambda}_3 + \underline{\lambda}_4}{\underline{\lambda}_3 + \underline{\lambda}_4} \\
\bar{\mathfrak{b}} &= \frac{\underline{\lambda}_1(\underline{\lambda}_3 + \underline{\lambda}_4)}{\underline{\lambda}_2 \underline{\Lambda}}, & \bar{\mathfrak{B}} &= \frac{(\underline{\lambda}_1 + \underline{\lambda}_2)(\underline{\lambda}_2 + \underline{\lambda}_3 + \underline{\lambda}_4)}{\underline{\lambda}_2 \underline{\Lambda}} \\
\mathfrak{c} &= \frac{\underline{\lambda}_1}{\underline{\lambda}_2 + \underline{\lambda}_3 + \underline{\lambda}_4}, & \mathfrak{c} &= \frac{\underline{\Lambda}}{\underline{\lambda}_2 + \underline{\lambda}_3 + \underline{\lambda}_4} .
\end{aligned}$$

With arguments of analyticity very similar to eqs. (2.71), (A.40), a hole-distribution is introduced:

$$\begin{aligned}\underline{\lambda}_1(v) + \underline{\lambda}_2(v) &= \frac{q_1(v + i/2 + i\alpha)}{q_2(v)} q_1^{(h)}(v) \phi_2(v) \frac{e^{2\beta\mu}}{\phi_+(v - i\alpha) \phi_-(v - i\alpha - i)} \\ \underline{\lambda}_3(v) + \underline{\lambda}_4(v) &= \frac{q_1(v + i/2 + i\alpha)}{q_2(v)} q_1^{(h)}(v - i) \phi_2(v) \frac{e^{2\beta\mu}}{\phi_+(v) \phi_-(v - i\alpha - i)} \\ q_1^{(h)}(v) &= \prod_{k=1}^{N+\tilde{m}-m} (v - v_k^{(1,h)})\end{aligned}$$

In order to determine the functional dependence of the eigenvalue on the auxiliary functions, write it in a factorized form: Without the q -functions, the ϕ -terms in the denominator would cause poles. The product of these gives a polynomial of degree $2N$. In the nominator, a factor $q_1(v + i/2 + i\alpha)$ can be isolated, of degree m . The nominator is balanced by $q_2^{(h)}$, of degree $2N - m$:

$$\begin{aligned}\underline{\Lambda}(v) &\propto \frac{q_1(v + i/2 + i\alpha) q_2^{(h)}(v)}{\phi_+(v - i\alpha) \phi_+(v + i(\alpha + 1)) \phi_-(v + i\alpha) \phi_-(v - i(\alpha + 1))} \\ q_2^{(h)}(v) &= \prod_{j=1}^{2N-m} (v - v_j^{(2,h)}) .\end{aligned}\tag{A.66}$$

Shift $v \rightarrow v + i\alpha/2$ to render the vacuum eigenvalues symmetric in $\alpha/2$ -shifts. Then

$$\begin{aligned}\mathfrak{b}(v) &\propto \phi_+(v + i\alpha/2) \phi_-(v - i\alpha/2 - i) \frac{q_2(v + i + i\alpha/2)}{q_1(v + i/2 + i\alpha/2) q_1^{(h)}(v + i\alpha/2 - i)} \\ \bar{\mathfrak{b}}(v) &\propto \phi_+(v + i\alpha/2 + i) \phi_-(v - i\alpha/2) \frac{q_1^{(h)}(v + i\alpha/2 - i)}{q_2(v + i\alpha/2 + i) q_2^{(h)}(v + i\alpha/2)} \\ \frac{\mathfrak{c}(v)}{\mathfrak{c}(v)} &\propto \frac{q_1(v + i\alpha/2 + i/2) q_2^{(h)}(v + i\alpha/2)}{\phi_+(v + i\alpha/2) \phi_-(v - i\alpha/2) \phi_+(v + i + i\alpha/2) \phi_-(v - i\alpha/2 - i)} \\ \bar{\mathfrak{B}}(v) \mathfrak{C}(v) &\propto \frac{1}{\phi_+(v - i\alpha/2) \phi_-(v + i\alpha/2)} \frac{q_1^{(h)}(v + i\alpha/2) q_1(v + i\alpha/2 + i/2)}{q_2(v + i + i\alpha/2)} \\ \mathfrak{B}(v) \mathfrak{C}(v) &\propto \frac{1}{\phi_-(v + i\alpha/2) \phi_+(v - i\alpha/2)} \frac{q_2(v + i\alpha/2) q_2^{(h)}(v + i\alpha/2)}{q_1^{(h)}(v + i\alpha/2 - i)}\end{aligned}$$

Constant exponentials as pre-factors, stemming von external fields, were not mentioned explicitly. They merely determine the asymptotic behaviour of the auxiliary functions, eqs. (2.80), (2.81). The further procedure is principally clear: Carry out the Fourier transform eq. (2.73). The logarithmic derivative makes disappear the constant exponential pre-factors. It is essential to know the domains of analyticity of the unknown q -functions. However, this task has already been solved: Eqs. (A.38a), (A.38b), (A.38c), (A.38d) identify the four q -functions with those from another set, whose analyticity properties have been investigated numerically (figs. 2.3, 2.4) and analytically (eq. (2.84)) in an approximate manner for the largest eigenvalue case. So one states

$$\begin{aligned}q_{1,2}(v + i(\alpha + 1)/2) &: \text{ ANZ in } \mathbb{C}^+ \\ q_1^{(h)}(v + i\alpha/2 - i), q_2^{(h)}(v + i\alpha/2) &: \text{ ANZ in } \mathbb{C}^- .\end{aligned}$$

As in section 2.1.3, the Fourier transforms are carried out for $k < 0$, $k > 0$ separately. For simplicity, the k -dependence of the functions is not mentioned explicitly.

$$\hat{\mathbf{b}} = \begin{cases} e^{-\alpha/2k} \hat{\phi}_+ + e^{-(\alpha/2+1)k} \hat{q}_2 - e^{-(\alpha/2+1/2)k} \hat{q}_1 & , k > 0 \\ \hat{q}_2 - \hat{q}_1 & , k = 0 \\ e^{(\alpha/2+1)k} \hat{\phi}_- - e^{-(\alpha/2+1)k} \hat{q}_1^{(h)} & , k < 0 \end{cases} \quad (\text{A.67a})$$

$$\hat{\bar{\mathbf{b}}} = \begin{cases} e^{-(\alpha/2+1)k} \hat{\phi}_+ - e^{-(\alpha/2+1)k} \hat{q}_2 & , k > 0 \\ -\hat{q}_2 & , k = 0 \\ e^{\alpha/2k} \hat{\phi}_- + e^{-(\alpha/2+1)k} \hat{q}_1^{(h)} - e^{-\alpha/2k} \hat{q}_2^{(h)} & , k < 0 \end{cases} \quad (\text{A.67b})$$

$$\hat{\mathbf{c}} - \hat{\mathbf{c}} = \begin{cases} e^{-(\alpha/2+1/2)k} \hat{q}_1 - e^{-\alpha/2k} \hat{\phi}_+ - e^{-(\alpha/2+1)k} \hat{\phi}_+ & , k > 0 \\ \hat{q}_1 & , k = 0 \\ e^{-\alpha/2k} \hat{q}_2^{(h)} - e^{\alpha/2k} \hat{\phi}_- - e^{(\alpha/2+1)k} \hat{\phi}_- & , k < 0 \end{cases} \quad (\text{A.67c})$$

$$\hat{\mathbf{c}} + \hat{\bar{\mathbf{B}}} = \begin{cases} -e^{-\alpha/2k} \hat{\phi}_- + e^{-(\alpha/2+1/2)k} \hat{q}_1 - e^{-(\alpha/2+1)k} \hat{q}_2 & , k > 0 \\ \hat{q}_1 - \hat{q}_2 & , k = 0 \\ -e^{\alpha/2k} \hat{\phi}_+ + e^{-\alpha/2k} \hat{q}_1^{(h)} & , k < 0 \end{cases} \quad (\text{A.67d})$$

$$\hat{\mathbf{c}} + \hat{\mathfrak{B}} = \begin{cases} -e^{-\alpha/2k} \hat{\phi}_- + e^{-\alpha/2k} \hat{q}_2 & , k > 0 \\ \hat{q}_2 & , k = 0 \\ -e^{\alpha/2k} \hat{\phi}_+ + e^{-\alpha/2k} \hat{q}_2^{(h)} - e^{-(\alpha/2+1)k} \hat{q}_1^{(h)} & , k < 0 \end{cases} \quad (\text{A.67e})$$

From eqs. (A.67d), (A.67e), the four unknowns are expressed in terms of auxiliary functions and inserted into eqs. (A.67a), (A.67b), (A.67c). One then obtains eqs. (2.77a), (2.77b), (2.77c).

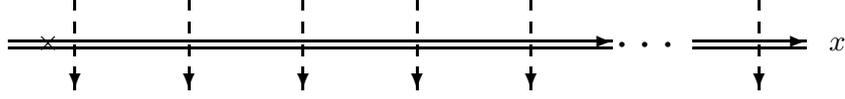
In a very similar fashion, eq. (A.66) is converted to

$$\hat{\Lambda} = \begin{cases} e^{-(\alpha+1)k} (\hat{\phi}_- - \hat{\phi}_+) + e^{-\alpha/2k} \hat{\bar{\mathbf{B}}} + e^{-(\alpha/2+1)k} \hat{\mathfrak{B}} + (e^{-\alpha/2k} + e^{-(\alpha/2+1)k}) \hat{\mathbf{c}} & , k > 0 \\ e^{(\alpha+1)k} (\hat{\phi}_+ - \hat{\phi}_-) + e^{(\alpha/2+1)k} \hat{\bar{\mathbf{B}}} + e^{\alpha/2k} \hat{\mathfrak{B}} + (e^{\alpha/2k} + e^{(\alpha/2+1)k}) \hat{\mathbf{c}} & , k < 0 \end{cases}$$

The inverse Fourier transform yields eq. (2.115).

A.4 Eigenvalue of $\tau_{eff}^{(l,m)}$

Let $T^{(l,m)}(x)$ be the monodromy matrix acting in the direct product of the $l + 1$ -dimensional auxiliary space and the $[m + 1]^{\otimes N}$ dimensional quantum space, eq. (2.137); the index $_{eff}$ is omitted. Graphically, it is translated as



The orientation of arrows is analogous to section 2.1.2. The N dashed vertical lines depict the quantum space, the horizontal double line represents the auxiliary space. The cross stands for twisted boundary conditions, with an imaginary twist angle depending on the spin in auxiliary space (it is included in the same manner as described at the beginning of this appendix for the $\mathfrak{gl}(2|1)$ symmetric matrices). $[T^{(l,m)}]$ is composed of N local R -matrices $\hat{R}^{(l,m)}(x)$, each one acting in the direct product of a $l + 1$ -dimensional auxiliary space and a $m + 1$ -dimensional quantum space. According to tensor notation, the elements of \hat{R} are denoted by $[\hat{R}^{(l,m)}(x)]_{j,k}^{i,p}$, where i, j (p, k) refer to in- and out-coming auxiliary (quantum) states:

$$[\hat{R}^{(l,m)}(x)]_{j,k}^{i,p} = i \begin{array}{c} p \\ | \\ | \\ | \\ x \\ | \\ | \\ | \\ j \\ \downarrow \\ k \end{array}$$

This notation is the same as in section 2.1.1. The $\hat{R}^{(l,m)}$ obey a non-graded YBE:

$$\begin{aligned} & [\hat{R}_{2,3}^{(l,m)}(u)]_{i',p'}^{i,p} [\hat{R}_{1,2}^{(l',m)}(v)]_{k',p''}^{k,p'} [\hat{R}_{1,3}^{(l',l)}(v-u)]_{k'',i''}^{k',i'} \\ &= [\hat{R}_{1,3}^{(l',l)}(v-u)]_{k',i'}^{k,i} [\hat{R}_{1,2}^{(l',m)}(v)]_{k'',p'}^{k',p} [\hat{R}_{2,3}^{(l,m)}(u)]_{i'',p''}^{i',p'} \end{aligned} \quad (\text{A.68})$$

$T^{(l,m)}(x)$ is constructed such that the commutator

$$[\text{tr}_a T^{(l,m)}(x), \text{tr}_a T^{(l',m)}(y)] = 0, \quad \forall l, l' \quad (\text{A.69})$$

vanishes because of eq. (A.68), see eq. (A.6). So the eigensystem of $\text{tr}_a T^{(l,m)}(x)$ does not depend on the dimension of the auxiliary space l . The explicit form of $\hat{R}^{(1,m)}(x)$ is easily found and will be given below. Then our strategy to find the eigenvalues of $\text{tr}_a T^{(1,m)}(x)$ is to calculate its action on the eigenvector $|\Phi\rangle$ of $\text{tr}_a T^{(1,m)}(x)$: It is simultaneously an eigenvector of $\text{tr}_a T^{(l,m)}(x)$. This procedure is analogous to that employed to diagonalize the host QTM in appendix A.3.

$T^{(1,m)}$ is a 2×2 matrix in quantum space, eq. (2.133); set

$$T^{(1,m)} = \begin{pmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{pmatrix}.$$

Then $T^{(1,m)}(x)$, $T^{(1,m')}(y)$ are intertwined by the R -matrix eq. (A.12), with entries

$$\begin{aligned} \hat{R}^{(1,1)}(x) &= \begin{pmatrix} \sinh(x+i\gamma) & & & \\ & \sinh x & \sinh i\gamma & \\ & \sinh i\gamma & \sinh x & \\ & & & \sinh(x+i\gamma) \end{pmatrix} \\ &=: \sinh i\gamma \begin{pmatrix} h_\gamma(x) & & & \\ & g_\gamma(x) & 1 & \\ & 1 & g_\gamma(x) & \\ & & & h_\gamma(x) \end{pmatrix} \end{aligned} \quad (\text{A.70})$$

This matrix is formally identical to the isotropic version, eq. (A.12), up to normalization. From eq. (A.22), the following commutators are identified:

$$\hat{A}(x)\hat{B}(y) = \frac{h_\gamma(y-x)}{g_\gamma(y-x)}\hat{B}(y)\hat{A}(x) - \frac{1}{g_\gamma(y-x)}\hat{B}(x)\hat{A}(y) \quad (\text{A.71a})$$

$$\hat{D}(x)\hat{B}(y) = \frac{h_\gamma(x-y)}{g_\gamma(x-y)}\hat{B}(y)\hat{D}(x) - \frac{1}{g_\gamma(x-y)}\hat{B}(x)\hat{D}(y) \quad (\text{A.71b})$$

$$\hat{B}(x)\hat{B}(y) = \hat{B}(y)\hat{B}(x) \quad (\text{A.71c})$$

$$\begin{aligned} \hat{A}(x)\hat{D}(y) + g_\gamma(x-y)\hat{C}(x)\hat{B}(y) &= g_\gamma(x-y)\hat{B}(y)\hat{C}(x) + \hat{A}(y)\hat{D}(x) \\ \hat{D}(x)\hat{A}(y) + g_\gamma(x-y)\hat{B}(x)\hat{C}(y) &= g_\gamma(x-y)\hat{C}(y)\hat{B}(x) + \hat{D}(y)\hat{A}(x). \end{aligned}$$

The last two equations are combined to

$$\begin{aligned} (g_\gamma(x-y) + g_\gamma(y-x))\hat{B}(y)\hat{C}(x) + \hat{D}(y)\hat{A}(x) + \hat{A}(y)\hat{D}(x) = \\ (g_\gamma(x-y) + g_\gamma(y-x))\hat{C}(x)\hat{B}(y) + \hat{D}(x)\hat{A}(y) + \hat{A}(x)\hat{D}(y). \end{aligned} \quad (\text{A.72})$$

Let us choose the maximal weight state $|1\rangle$ as reference state. It is defined by

$$\sum_{k=1}^N \sigma_k^z |1\rangle = N m |1\rangle. \quad (\text{A.73})$$

The choice $|m+1\rangle$ with

$$\sum_{k=1}^N \sigma_k^z |m+1\rangle = -N m |1\rangle.$$

leads to the same results. Then $T^{(1,m)}$ is upper diagonal with respect to $|1\rangle$, and eigenvectors are created by acting with \hat{B} on $|1\rangle$:

$$\begin{aligned} |\Phi\rangle &:= \prod_{\nu=1}^{\mathcal{N}} \hat{B}(x_\nu) |1\rangle \\ \hat{A}(x) |1\rangle &=: \Lambda_A(x) |1\rangle = \sinh^N \left(x + \frac{i\gamma}{2} (1+m) \right) |1\rangle \\ \hat{D}(x) |1\rangle &=: \Lambda_D(x) |1\rangle = \sinh^N \left(x + \frac{i\gamma}{2} (1-m) \right) |1\rangle \\ \text{tr}_a T^{(l,m)}(x) |\Phi\rangle &= \Lambda^{(l)}(x) |\Phi\rangle. \end{aligned} \quad (\text{A.74})$$

Substitution of eq. (A.76) into eq. (A.75) results in

$$\begin{aligned}
\left[T^{(l,m)}(x) \right]_j^j \hat{B}(y) = & \frac{\left[\hat{R}^{(1,l)} \right]_{1,j}^{1,j} \left[\hat{R}^{(1,l)} \right]_{2,j-1}^{2,j-1} - \left[\hat{R}^{(1,l)} \right]_{2,j-1}^{1,j} \left[\hat{R}^{(1,l)} \right]_{1,j}^{2,j-1}}{\left[\hat{R}^{(1,l)} \right]_{2,j}^{2,j} \left[\hat{R}^{(1,l)} \right]_{2,j-1}^{2,j-1}} \Bigg|_{y-x} \hat{B}(y) \left[T^{(l,m)}(x) \right]_j^j \\
& - \frac{\left[\hat{R}^{(1,l)} \right]_{1,j+1}^{2,j}}{\left[\hat{R}^{(1,l)} \right]_{2,j}^{2,j}} \Bigg|_{y-x} \left[T^{(l,m)}(x) \right]_j^{j+1} \hat{A}(y) + \frac{\left[\hat{R}^{(1,l)} \right]_{1,j}^{2,j-1}}{\left[\hat{R}^{(1,l)} \right]_{2,j-1}^{2,j-1}} \Bigg|_{y-x} \left[T^{(l,m)}(x) \right]_{j-1}^j \hat{D}(y) \\
& + \frac{\left[\hat{R}^{(1,l)} \right]_{1,j+1}^{2,j} \left[\hat{R}^{(1,l)} \right]_{1,j}^{2,j-1}}{\left[\hat{R}^{(1,l)} \right]_{2,j}^{2,j} \left[\hat{R}^{(1,l)} \right]_{1,j}^{2,j-1}} \Bigg|_{y-x} \left[T^{(l,m)}(x) \right]_{j-1}^{j+1} \hat{C}(y) \tag{A.77}
\end{aligned}$$

Finally, the sum over $j = 1, \dots, l+1$ has to be taken. Let us first discuss the "unwanted" terms, these are the last three summands in eq. (A.77).

- The pre-factors of \hat{A} (\hat{D}) in the second (third) term result from each other by shifting $j \rightarrow j-1$. Thus in the sum, two consecutive pre-factors are oppositely equal. \hat{A} and \hat{D} still have to be commuted through the remaining $\hat{B}(x_\nu)$ of $|\Phi\rangle$. This is done with eqs. (A.71a)-(A.71c), again producing "wanted" and "unwanted" terms. Eventually, in both terms \hat{A} and \hat{D} act on the bare vacuum $|1\rangle$. Both vanish if the $\{x_\nu\}$ fulfill the BAE

$$\frac{\Lambda_A(x_\nu)}{\Lambda_D(x_\nu)} = \prod_{\mu \neq \nu}^N \frac{\sinh(x_\nu - x_\mu + i\gamma)}{\sinh(x_\nu - x_\mu - i\gamma)}.$$

In [84], the distribution of the $\{x_\nu\}$ in the complex x -plane was examined for the isotropic case $\gamma = 0$, $l = m$. In the thermodynamic limit $N \rightarrow \infty$, the BAN were found to be aligned parallel to the real axis, with imaginary parts

$$(l+1-2j)/2, \quad j = 1, \dots, l. \tag{A.78}$$

We infer that this statement holds principally true for eqs. (2.140) with $\gamma \neq 0$. So we expect the BAN in our case to have imaginary parts $\gamma(l+1-2j)/2$; $j = 1, \dots, l$. This means that there are effectively l sets of BAE, each one characterized by the imaginary part of its elements.

- In the fourth term, \hat{C} acts on the remaining $\hat{B}(x_\nu)$. If there are no $\hat{B}(x_\nu)$, \hat{C} annihilates $|1\rangle$. Otherwise, it is commuted through them by eq. (A.72). This produces a "wanted" term $\propto \hat{B}(x_\nu)\hat{C}(y)$, which ultimately meets $|1\rangle$ and vanishes. The "unwanted" terms are essentially given by

$$\propto \hat{D}(x_\nu)\hat{A}(x) + \hat{A}(x_\nu)\hat{D}(x) - \hat{D}(x)\hat{A}(x_\nu) - \hat{A}(x)\hat{D}(x_\nu).$$

These are again carried through the $\hat{B}(x_\nu)$, until they act upon $|1\rangle$. Since $|1\rangle$ is a simultaneous eigenstate of \hat{A}, \hat{D} , these terms also cancel.

The cancellation of unwanted terms has been shown. The "wanted" term contributes to the eigenvalue by collecting the BAN of the $\hat{B}(x_\nu)$:

$$\Lambda^{(l)}(x) = \sum_{j=1}^{l+1} \left[\hat{T}^{(l,m)}(x) \right]_{j,1}^{j,1} \frac{q\left(x + \frac{i\gamma}{2}(l+1)\right) q\left(x - \frac{i\gamma}{2}(l+1)\right)}{q\left(x + \frac{i\gamma}{2}(l-2j+1)\right) q\left(x + \frac{i\gamma}{2}(3+l-2j)\right)} \quad (\text{A.79})$$

$$q(x) = \prod_{\nu=1}^{\mathcal{N}} \sinh(x - x_\nu).$$

To tackle the calculation of $\left[\hat{R}^{(l,m)}(x) \right]_{j,1}^{j,1}$, one specializes eq. (A.75) to \hat{R} -operators:

$$\begin{array}{c} \begin{array}{ccccccc} 1 & j & x & k & j & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ j & 1 & y & k-1 & 2 & & \end{array} & + & \begin{array}{ccccccc} 1 & j-1 & x & k & j & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ j & 2 & y & k-1 & 2 & & \end{array} & = & \begin{array}{ccccccc} 1 & k & y & 2 & j & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ j & k-1 & x & j & 2 & & \end{array} & + & \begin{array}{ccccccc} 1 & k & y & 1 & j & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ j & k-1 & x & j+1 & 2 & & \end{array} \end{array} \quad (\text{A.80})$$

We are interested in the terms containing diagonal elements of $\left[\hat{R}^{(l,m)} \right]_j^j$. The second term on the rhs certainly does not belong to those, it vanishes by choosing

$$y = y_1 := -i\frac{\gamma}{2}(5 + m - 2k).$$

The second term on the lhs still disturbs, but let us consider eq. (A.80), with j shifted to $j-1$:

$$\begin{array}{c} \begin{array}{ccccccc} j-1 & x & k-1 & j-1 & 1 & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ 2 & y & k & 1 & j-1 & & \end{array} & + & \begin{array}{ccccccc} j-1 & x & k-1 & j-2 & 1 & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ 2 & y & k & 2 & j-1 & & \end{array} & = & \begin{array}{ccccccc} j-1 & 2 & k-1 & y & 2 & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ 2 & j-1 & k & x & j-1 & & \end{array} & + & \begin{array}{ccccccc} j-1 & 1 & k-1 & y & 1 & & \\ \diagdown & \diagup & \diagdown & \diagup & \diagdown & \diagup & \\ \diagup & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\ 2 & j & k & x & j-1 & & \end{array} \end{array}$$

Now the second term on the lhs disappears while choosing

$$y = y_2 := i\frac{\gamma}{2}(1 + m - 2k).$$

On the rhs, the second term contains the disturbing factor of the second term on the lhs of eq. (A.80). Correspondingly, one equates:

$$\begin{aligned} & \left[\hat{R}^{(l,m)}(x) \right]_{j-1,k}^{j,k-1} \frac{\left[\hat{R}^{(1,l)} \right]_{1,j}^{2,j-1}}{\left[\hat{R}^{(1,m)} \right]_{1,k}^{2,k-1}} \\ &= \left[\hat{R}^{(l,m)}(x) \right]_{j,k}^{j,k} \left[\hat{R}^{(1,l)}(y_1 - x) \right]_{2,j}^{2,j} - \left[\hat{R}^{(l,m)}(x) \right]_{j,k-1}^{j,k-1} \left[\hat{R}^{(1,l)}(y_1 - x) \right]_{1,j}^{1,j} \\ &= \left[\hat{R}^{(l,m)}(x) \right]_{j-1,k-1}^{j-1,k-1} \left[\hat{R}^{(1,l)}(y_2 - x) \right]_{1,j-1}^{1,j-1} - \left[\hat{R}^{(l,m)}(x) \right]_{j-1,k}^{j-1,k} \left[\hat{R}^{(1,l)}(y_2 - x) \right]_{2,j-1}^{2,j-1}. \quad (\text{A.81}) \end{aligned}$$

Arguments on the lhs of the first line have been partially omitted, since the concerned elements do not depend on the spectral parameter. Eq. (A.81) is a recursion relation, in which the recursion is

defined by a shift of both indices, j and k . However, one only needs the eigenvalue of \hat{R}_j^j with respect to the highest weight state, that is the matrix element $\hat{R}_{j,1}^{j,1}$. According to eq. (A.81),

$$\frac{\left[\hat{R}^{(l,m)}(x)\right]_{j,1}^{j,1}}{\left[\hat{R}^{(l,m)}(x)\right]_{j-1,1}^{j-1,1}} \propto \frac{\sinh\left(x + \frac{i\gamma}{2}(4+l-2j-m)\right)}{\sinh\left(x + \frac{i\gamma}{2}(4+l-2j+m)\right)} \quad (\text{A.82})$$

Eq. (A.82) defines $\hat{R}_{j,1}^{j,1}$ except a multiplicative constant. It is chosen to be

$$-\frac{\prod_{p=1}^{l+1} \sinh\left(x + i\frac{\gamma}{2}(4+l-2p+m)\right)}{\sinh\left(x + i\frac{\gamma}{2}(2+l-m)\right)}.$$

Then the special cases $\left[\hat{R}^{(1,m)}\right]_{1,1}^{1,1} = \sinh(x + i\gamma/2(1+m))$ and $\left[\hat{R}^{(1,m)}\right]_{2,1}^{2,1} = \sinh(x + i\gamma/2(1-m))$ are reproduced:

$$\left[\hat{R}^{(l,m)}(x)\right]_{j,1}^{j,1} = \prod_{p=1}^{j-1} \sinh\left(x + \frac{i\gamma}{2}(2-2p+l-m)\right) \prod_{p=1}^{l-j+1} \sinh\left(x + \frac{i\gamma}{2}(4-2p-2j+l+m)\right).$$

Taking account of the twist angle,

$$\begin{aligned} \left[T^{(l,m)}\right]_{j,1}^{j,1}(x) &= e^{-\frac{\beta h}{2}(l-2j+2)} \\ &\times \prod_{p=1}^{j-1} \sinh^N\left(x + \frac{i\gamma}{2}(2-2p+l-m)\right) \prod_{p=1}^{l-j+1} \sinh^N\left(x + \frac{i\gamma}{2}(4-2p+l+m-2j)\right) \end{aligned}$$

We are now ready to combine our two results, that is the commutator of $\text{tr}_a T^{(l,m)}(x)$ with $\left[T^{(1,m)}(x)\right]_{1,2}^{1,2}$ and the eigenvalue of $\left[T^{(l,m)}\right]_j^j$ with respect to $|1\rangle$. Then we find the eigenvalue of $\text{tr}_a T^{(l,m)}(x)$ with respect to $|\Phi\rangle$, eq. (2.139). It agrees with the analogous expression given in [84] for the staggered $l = m$ QTM with $\gamma = 0$.

Appendix B

Appendix to Chapter 3

B.1 Calculation of $\hat{A}(k)$

The calculation of \hat{A} , eq. (3.23), is done by using the Z transform.

The $l \times l$ matrix \hat{A}^{-1} is known, eq. (3.13). It permits to set up a recursion relation for d_n , the determinant of the $n \times n$ sub-matrix with corner elements $\left[\hat{A}^{-1}\right]_{l-n+1, l-n+1}$, $\left[\hat{A}^{-1}\right]_{l-n+1, l}$, $\left[\hat{A}^{-1}\right]_{l, l-n+1}$, $\left[\hat{A}^{-1}\right]_{l, l}$. Set $k := \mathcal{F}_k[k]$, $s := \mathcal{F}_k[s]$, the Fourier transform of the integration kernels.

$$\begin{aligned} d_1 &= 1 - k \\ d_2 &= (1 - k) - s^2 \\ d_l &= d_{l-1} - s^2 d_{l-2} \end{aligned} \tag{B.1}$$

The shift operator T is defined as

$$d_{l+1} =: T d_l .$$

The Z -transform converts the action of T into multiplication with a complex number z :

$$\begin{aligned} T d_l &= z d_l - d_1 z \\ T^2 d_l &= z^2 d_l - d_2 z - d_1 z^2 \end{aligned}$$

Then, from eq. (B.1),

$$d_l (z^2 - z + s^2) = (1 - k) z^2 - z s^2 .$$

Factorize

$$\begin{aligned} z^2 - z + s^2 &=: (z - z_1)(z - z_2) \\ \Rightarrow d_l &= \left(\frac{z z_1}{z - z_1} - \frac{z z_2}{z - z_2} \right) \frac{1 - k}{z_1 - z_2} - \left(\frac{z_1}{z - z_1} - \frac{z_2}{z - z_2} \right) \frac{s^2}{z_1 - z_2} \\ &= \left(z_1^l - z_2^l \right) \frac{1 - \hat{k}}{z_1 - z_2} - \left(z_1^{l-1} - z_2^{l-1} \right) \frac{s^2}{z_1 - z_2} . \end{aligned}$$

The last equation was obtained upon applying the inverse transform. The rest is pure algebra. Insert $z_{1,2} = \exp(\pm \pi k / 2) / (2 \cosh \pi k / 2)$ to get d_l , eq. (3.24).

Consider \hat{A}^{-1} with the kernel $k \equiv 0$. Let the determinants of the corresponding sub-matrices be D_j . Analogously as above, one finds

$$D_j = \frac{\sinh(j+1)\frac{\pi k}{2}}{(2 \cosh \frac{\pi k}{2})^j \sinh \frac{\pi k}{2}}.$$

From the definition eq. (3.23), one derives the following matrix elements:

$$\begin{aligned}\hat{A}_{l,l} &= \frac{D_{l-1}}{d_l} \\ \hat{A}_{j,l} &= \frac{s^{j-l} D_{j-1}}{d_l} \\ \hat{A}_{j,j} &= \frac{D_{j-1} d_{l-j}}{d_l}.\end{aligned}$$

These are employed in the main part, following eq. (3.23).

B.2 Convolutions

Techniques for asymptotically evaluating convolutions of auxiliary functions with integration kernels are provided. Two classes are distinguished: Kernels with algebraic and with exponential decay in direct space. To the first class belong those occurring in the NLIE for $\gamma = 0$ in convolutions with $\ln \mathfrak{B}_l$, $\ln \overline{\mathfrak{B}}_l$ and its derivatives. The second class includes the integral of the free energy, convolutions with $\ln Y_j$ and, for $\gamma > 0$, with $\ln \mathfrak{B}_l$, $\ln \overline{\mathfrak{B}}_l$.

The convolutions are conveniently done in Fourier space. An algebraic decay $\mathcal{O}(x^{-n})$ is traced back to discontinuities in the $(n - 1)$ st derivative of the Fourier transformed kernel. Exponential decay with an exponent ν corresponds to a pole with imaginary part $|\nu|$ in the Fourier transformed kernel.

B.2.1 Convolutions with algebraically decaying kernels

In [66], methods how to Fourier transform distributions are given. The relations needed for our purposes are:

$$\begin{aligned} \theta(-x) &= \int_{-\infty}^{\infty} \frac{1}{2\pi} \left(\pi\delta(k) - \frac{i}{k} \right) e^{-ikx} dk \\ \theta(-x) \frac{1}{x} &= \int_{-\infty}^{\infty} \frac{1}{4\pi} (i\pi \operatorname{sgn} k + 2 \ln |k| + a_1) e^{-ikx} dk \\ \theta(-x) \frac{1}{x^2} &= \int_{-\infty}^{\infty} \frac{-k}{4\pi} (\pi \operatorname{sgn} k - 2i(\ln |k| + a_2)) e^{-ikx} dk \\ \theta(-x) \frac{\ln |x|}{x^2} &= \int_{-\infty}^{\infty} \frac{1}{4\pi} (\pi |k| (\ln |k| - \Psi(2)) - ik ((\ln |k| - \Psi(2))^2 + a_l)) e^{-ikx} dk \\ \int_{-\infty}^{\infty} \frac{1}{|x|} e^{ikx} dx &= -2 \ln |k| \\ \int_{-\infty}^{\infty} \frac{\operatorname{sgn} x}{x^2} e^{ikx} dx &= -2ik \ln |k| \end{aligned}$$

$\Psi(x)$ is the digamma function; $\Psi(2) = -C + 1$, $C = 0.577 \dots$ is Euler's constant. Note that $\theta(-x) = (1 - \operatorname{sgn} x)/2$, so that each transform $\theta(-x)f(x)$ (f even or odd) is the sum of an even and an odd term, depending on the parity of f . The constants $a_{1,2,l}$ are not determined. Only upon regularizing the above relations, that is finding functions which are asymptotically equal to the asymptotic behaviour of the distributions, the constants acquire precise values. These then depend on the regularizing functions.

In order to derive eqs. (3.90a), (3.90b), note that

$$\begin{aligned} k(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-\frac{\pi}{2}|k|}}{2 \cosh \frac{\pi k}{2}} dk \sim \frac{1}{4x^2}, \quad |x| \gg 0 \\ \mathcal{F}_k[k^{(s)}(x)] &= e^{-\frac{\pi}{2}|k|} \stackrel{|k| \ll 1}{\approx} 1 - \frac{\pi}{2}|k| + \mathcal{O}(k^2). \end{aligned} \tag{B.2}$$

By inserting the asymptotic behaviour of the kernel, eq. (B.2), and of the auxiliary functions into the convolution of both, eqs. (3.90a), (3.90b) follow.

Let f be an auxiliary function. The crucial point in the application of the above technique is that the kernel decays faster (namely as x^{-2}) than the first three orders of f ($\theta(-x)$, $\theta(-x)/x$, $\theta(-x) \ln |x|/x^2$). However, the x^{-2} decay of f is of the same order as the decay of the kernel, so that one is no longer justified to replace f by its asymptotic behaviour in terms of a distribution: The knowledge of f over the whole real axis is necessary to evaluate the x^{-2} order of $k * f$.

For simplicity, assume $f(x) \sim (\Delta_+ - \Delta_- \text{sgn}x)/x^2$, and $k^{(s)}(x) \sim 1/(2x^2)$. Then

$$[f * k^{(s)}](x) \sim \frac{\Delta_+ - \Delta_- \text{sgn}x}{x^2} \int_{-\infty}^{\infty} k^{(s)}(x) dx + \frac{1}{2x^2} \int_{-\infty}^{\infty} f(x) dx . \quad (\text{B.3})$$

The appearance of the second term in eq. (B.3) prohibits - up to now - an analytical determination of the x^{-2} decay of $B^{(m)}$, as it was initialized in section 3.2.1. Fortunately, the result depends on the integral $\int_{-\infty}^{\infty} f$, which can be done numerically with high accuracy. Details are given in appendix C.

B.2.2 Convolutions with exponentially decaying kernels

Let $f(x)$ be an algebraically decaying function, and $s(x)$ be an exponentially decaying kernel. Then

$$\begin{aligned} [f * s](x) &= \int_{-\infty}^{\infty} f(x-y)s(y) dy \\ &= f(x) \int_{-\infty}^{\infty} s(y) dy + f'(x) \int_{-\infty}^{\infty} (-y)s(y) dy + f''(x) \int_{-\infty}^{\infty} y^2 s(y)/2 dy + \mathcal{O}\left(f^{(3)}(x)\right) . \end{aligned}$$

Especially, for $s(x) = 1/\cosh x$:

$$[f * s](x) = \pi f(x) + \frac{\pi^3}{8} f''(x) + \mathcal{O}\left(f^{(4)}(x)\right)$$

For all cases of interest in this work, it suffices to include only the leading order.

Now let an exponentially decaying function $f(x) \sim e^{\nu_f x}$ meet an exponentially decaying kernel $s(x) \sim e^{\nu_s x}$. Their convolution

$$[f * s](x) \sim e^{\sigma \min\{|\nu_f|, |\nu_s|\}x} .$$

σ is the sign of the exponent whose minimal absolute value is taken. The leading order is given by the pole next to the real axis in Fourier space.

Appendix C

Appendix to Chapter 4

Details of the numerical investigation are presented in three sections. First, schemes of numerically performing the convolutions are described. Special attention has to be paid to the fact that some of the auxiliary functions are not Fourier-transformable. These contributions must be subtracted before applying a Fast Fourier Transform (FFT) routine to the convolutions. The second section presents variations of the general iterative approach to solve the NLIE. Finally, results of applying these methods to calculate the integral over the imaginary part of $\ln \mathfrak{B}_l$, the x^{-2} decay of $B_l^{(m)}$ and the Wilson ratio are presented.

C.1 Regularization schemes

In this section, the $h = 0$ case is treated. $h \neq 0$ is set in paragraph C.2.3. For reasons of computational efficiency, we wish to treat the convolutions by FFT. From the analytical analysis of the NLIE, non-Fourier-transformable terms were found, namely those $\mathcal{O}(1)$, $\mathcal{O}(x^{-1})$ in the limit $|x| \rightarrow \infty$.¹ In Fourier space, these appear as simple poles and discontinuities in the origin, see appendix B.1. They are therefore subtracted from the auxiliary functions *before* performing the FFT, the corresponding singularities in Fourier space can be treated "by hand". After having applied the inverse FFT, the analytically convoluted terms are re-added. Two forms of this regularization have been implemented:

$$k * \ln Y = \underbrace{k * (\ln Y - f) + (k * f - f_{komp})}_{\text{N}} + \underbrace{f_{komp}}_{\text{A}} \quad (\text{C.1})$$

$$k * \ln Y = \underbrace{k * (\ln Y - f)}_{\text{N}} + \underbrace{k * f}_{\text{A}} \quad (\text{C.2})$$

$$\lim_{|x| \rightarrow \infty} \ln Y(x) \sim f(x), \quad \lim_{|k| \rightarrow 0} \mathcal{F}_k[k * f] \sim \mathcal{F}_k[f_{komp}]. \quad (\text{C.3})$$

k is a kernel, $\ln Y$ an auxiliary function. f is asymptotically equal to $\ln Y$, eq. (C.3) and contains the non-transformable contributions. The difference $\ln Y - f$ is therefore numerically transformable. The terms denoted by N are treated numerically, those labeled by A analytically. The Fourier-transforms of f , f_{komp} and k are known.

In the first case, the divergences in Fourier space due to $k * f$ are subtracted by f_{komp} , which is chosen to be asymptotically equal to $\mathcal{F}_k[k * f]$ around $k = 0$, eq. (C.3). Afterwards, f_{komp} is added analytically. This method is applied to the anisotropic case. We call this procedure "scheme I".

¹Algebraic corrections to the asymptotes do only occur in the isotropic case.

In the second case, the convolution $k * f$ is solved completely by hand, such that no further manipulations in Fourier space are necessary. This is only possible for $\gamma = 0$. The advantage of this "scheme II" is its compactness and the restriction of "manual" manipulations to the direct space, the price to pay are computational costs higher compared to scheme I, since $k * f$ involves transcendental functions, see below.

Parameters are built in f , such that the first of eqs. (C.3) is still valid, but $f(x \approx 0)$ depends on the parameters. The final results should be independent of these parameters. This is indeed the case as will be illustrated below.

C.1.1 Scheme I

Only the case $\gamma \neq 0$ is treated within this scheme. Because of the exponential approach to the asymptotic values, only the constant asymptotic behaviour must be regularized. Suppose

$$\begin{aligned} \lim_{|x| \rightarrow \infty} Y(x) &\sim (y_+ \theta(-x) - y_- \theta(x)) \\ f(x) &= y_- + (y_+ - y_-) f_0(x) \\ \lim_{|x| \rightarrow \infty} f_0(x) &\sim \theta(-x). \end{aligned}$$

We choose

$$f_0(x) = \frac{1}{1 + e^{\pi x}}.$$

The Fourier-transform is found to be

$$\mathcal{F}_k[f_0(x)] = \frac{-i}{2\pi \sinh k}.$$

f_{komp} is required to compensate the divergences of $k * f$:

$$\begin{aligned} f_{komp} &:= (y_+ - y_-) f_{komp,0} \\ \mathcal{F}_k[f_{komp,0}] &= \frac{i}{k} \frac{\sinh \frac{bk}{2}}{\sinh ck}, \quad b = \pi \left(\frac{\pi}{\gamma} - (l+1) \right), \quad c = \pi \left(\frac{\pi}{\gamma} - l \right) \\ f_{komp,0}(x) &= \frac{1}{\pi} \operatorname{Im} \ln \left(1 + e^{-\frac{\pi}{c}(x-ib/2)} \right) \stackrel{|x| \rightarrow \infty}{\sim} \frac{b}{2c} \theta(-x). \end{aligned} \quad (\text{C.4})$$

The compensating function f_{komp} has been determined such that

$$\lim_{|k| \rightarrow \infty} \mathcal{F}_k[f^{(komp)}] \sim \mathcal{O} \left(e^{-(\pi+\alpha)|k|} \right), \quad \alpha \in \mathbb{R}^{>0}. \quad (\text{C.5})$$

Since the regularization is applied to convolutions with arguments shifted by $\pm i\pi$ in direct space, it is essential to choose $\alpha > 0$ in eq. (C.5). With eq. (C.4),

$$\lim_{|k| \rightarrow \infty} \mathcal{F}_k[f^{(komp)}] \sim \mathcal{O} \left(\exp \left[-\frac{\pi}{2} \left(\frac{\pi}{\gamma} - l + 1 \right) \right] \right)$$

and eq. (C.5) is fulfilled because of $\pi/\gamma > 2l$.

The convolution with s is manipulated along the same lines:

$$\begin{aligned} f_0(x) &= \frac{1}{1 + e^{\pi x}} \\ \mathcal{F}_k[f_{komp,0}] &= \frac{i}{4\pi k \cosh \frac{\pi k}{2}} \\ f_{komp,0}(x) &= \frac{1}{2\pi i} [\ln(e^x + i) - \ln(e^x - i)]. \end{aligned}$$

C.1.2 Scheme II

Only the isotropic case can be treated in the following manner. Extend the asymptotic expansion of paragraph C.1.1,

$$\begin{aligned}
\lim_{|x| \rightarrow \infty} Y(x) &\sim (y_+ - y_- \operatorname{sgn} x) + \frac{1}{x} (y_+^{(1)} - y_-^{(1)} \operatorname{sgn} x) + \frac{\ln |x|}{x^2} (y_+^{(l)} - y_-^{(l)} \operatorname{sgn} x) \\
f(x) &= y_- + (y_+ - y_-) f_0(x) + (y_+^{(1)} + y_-^{(1)}) f_1^+(x) + (y_+^{(1)} - y_-^{(1)}) f_1^-(x) \\
&\quad + (y_+^{(l)} + y_-^{(l)}) f_l^+(x) + (y_+^{(l)} - y_-^{(l)}) f_l^-(x) \\
\lim_{|x| \rightarrow \infty} f_0(x) &\sim \theta(-x) \\
f_1^-(x) &= -f_1^+(-x) \stackrel{|x| \rightarrow \infty}{\sim} \theta(x)/x \\
f_l^-(x) &= f_1^+(-x) \stackrel{|x| \rightarrow \infty}{\sim} \theta(x) \ln |x|/x^2 .
\end{aligned}$$

In the ongoing, Fourier transforms are calculated, we just give the results. They can be derived by standard techniques. One integral is calculated explicitly in paragraph C.1.3, since its expression given in several integral tables is wrong.

We choose the following functions:

$$\begin{aligned}
f_0(x) &= \frac{1}{1 + e^{\pi x/a_0}}, 0 < a_0 \\
&\stackrel{|x| \rightarrow \infty}{\sim} \frac{1}{2}(1 - \operatorname{sgn} x) \\
\mathcal{F}_k[f_0] &= -\frac{1}{2\pi i} \frac{a_0}{\sinh(a_0 k - i\epsilon)} = -\text{P} \frac{a_0}{2\pi i \sinh a_0 k} + \frac{1}{2\pi} \pi \delta(k) \\
f_1^+(x) &= \operatorname{Re} \left[\frac{1}{(x + i\delta)(1 + e^{\pi(x+i\delta)/a_1})} \right] \\
&\stackrel{|x| \rightarrow \infty}{\sim} \frac{1}{2x}(1 - \operatorname{sgn} x) \\
\mathcal{F}_k[f_1^+] &= \frac{1}{2\pi} \frac{1}{2} \left[(e^{\delta k} + e^{-\delta k}) \ln \tanh \frac{a_1 |k|}{2} - i\pi \operatorname{sgn} k e^{-\delta |k|} \right], 0 < \delta < a_1
\end{aligned}$$

$$\begin{aligned}
f_l^+(x) &= \frac{1}{2} \left\{ -\operatorname{Re} \left[\frac{\ln(a_l^{(1)} + ix)}{(a_l + ix)^2} \right] + \operatorname{Im} \left[\frac{\ln^2(a_l + ix)}{\pi(a_l + ix)^2} \right] \right\}, 0 < a_l \\
&\stackrel{|x| \rightarrow \infty}{\sim} \frac{\ln |x|}{2x^2}(1 - \operatorname{sgn} x) \\
\mathcal{F}_k[f_l^+] &= e^{-a_l |k|} \frac{|k|}{2} (\ln |k| - \Psi(2)) - \frac{ik}{2\pi} e^{-a_l |k|} \left[(\Psi(2) - \ln |k|)^2 + 1 - \frac{\pi^2}{6} \right].
\end{aligned}$$

First, consider the numerical procedure to determine $\ln \mathfrak{B}_l$, $\ln \overline{\mathfrak{B}}_l$. The asymptotes have to be subtracted. That's all, since the next leading term is $\mathcal{O}(x^{-3})$. The convolutions are rewritten in the

form

$$\begin{aligned}
[k * \ln \mathfrak{B}_l](x) - [k * \ln \overline{\mathfrak{B}}_l](x - i\pi) &= [k * (\ln \mathfrak{B}_l - (\ln \mathfrak{B}_l^{(-\infty)} - \ln \mathfrak{B}_l^{(\infty)}) f_0 - \ln \mathfrak{B}_l^{(\infty)})](x) \\
&\quad - [k * (\ln \overline{\mathfrak{B}}_l - (\ln \mathfrak{B}_l^{(-\infty)} - \ln \mathfrak{B}_l^{(\infty)}) f_0 - \ln \mathfrak{B}_l^{(\infty)})](x - i\pi) \\
&\quad + (\ln \mathfrak{B}_l^{(-\infty)} - \ln \mathfrak{B}_l^{(\infty)}) ([k * f_0](x) - [k * f_0](x - i\pi)) .
\end{aligned}$$

We exploited $\mathfrak{B}_l^{(\pm\infty)} = \overline{\mathfrak{B}}_l^{(\pm\infty)}$ and $k * \ln \mathfrak{B}_l^{(\pm\infty)} = \mathfrak{B}_l^{(\pm\infty)}/2$. The asymptotic behaviour is included in the last term, where it cancels because of the difference. Therefore, it is evaluated in Fourier-space, which constitutes numerically a more precise procedure than Fourier-transforming the asymptotic terms back separately and subtracting them in direct space.

Next, tackle the calculation of $B_l^{(m)}, \bar{B}_l^{(m)}$. This situation is slightly more involved: The real parts differing in their sign, the asymptotic parts of the convolutions do not cancel each other, but are added. In this case, numerical results are expected to be more precise by evaluating the relevant convolutions analytically. These are

$$[k * f_\nu^\pm](x) + [k * f_\nu^\pm](x - i\pi), \quad \nu = 1, l .$$

A glance into the Fourier space reveals that the two summands can be pulled together:

$$\begin{aligned}
[k * f_\nu^+](x) + [k * f_\nu^+](x - i\pi) &= [k^{(s)} * f_\nu^+](x - i\frac{\pi}{2}) & (C.6) \\
\mathcal{F}_k [k^{(s)}] &= \frac{1}{2\pi} e^{-\frac{\pi}{2}|k|} \\
[k * f_\nu^-](x) + [k * f_\nu^-](x - i\pi) &\stackrel{\nu=1}{=} -[k^{(s)} * f_1^+](x - i\frac{\pi}{2}) \\
&\stackrel{\nu=l}{=} [k^{(s)} * f_1^+](x - i\frac{\pi}{2}) .
\end{aligned}$$

In the following, the relevant integrals for the analytic transformations are listed.

$$\begin{aligned}
[k^{(s)} * f_0](x) &= -\frac{1}{2\pi i} \left[\Psi \left(\frac{\pi}{4a_0} + \frac{1}{2} + \frac{ix}{2a_0} \right) - \Psi \left(\frac{\pi}{4a_0} + \frac{1}{2} - \frac{ix}{2a_0} \right) \right] + \frac{1}{2} \\
|x| \xrightarrow{\sim} \infty &\frac{1}{2}(1 - \operatorname{sgn}x) + \frac{1}{2x} + \mathcal{O}(x^{-3}) \\
[k^{(s)} * f_1^+](x) &= \frac{1}{4\pi} \left[\frac{1}{\pi/2 - \delta - ix} \left(C - 2 \ln 2 - \Psi \left(\frac{\pi/2 - \delta + a_1 - ix}{2a_1} \right) \right) \right. \\
&\quad \left. + \frac{1}{\pi/2 + \delta - ix} \left(C - 2 \ln 2 - \Psi \left(\frac{\pi/2 + \delta + a_1 - ix}{2a_1} \right) \right) \right] + cc \\
|x| \xrightarrow{\sim} \infty &\frac{1}{2x}(1 - \operatorname{sgn}x) - \frac{\ln|x|}{2x^2} + \frac{\Psi(2) + \ln a_1/2}{2x^2} \\
[k^{(s)} * f_l^+](x) &= \frac{1}{4} \left[-\frac{\ln(a_l + \frac{\pi}{2} + ix)}{(a_l + \frac{\pi}{2} + ix)^2} - i \frac{\ln(a_l + \frac{\pi}{2} + ix)}{\pi(a_l + \frac{\pi}{2} + ix)^2} + cc \right] \\
|x| \xrightarrow{\sim} \infty &\frac{1}{2}(1 - \operatorname{sgn}x) \frac{\ln|x|}{x^2} + \mathcal{O}(x^{-3})
\end{aligned}$$

The asymptotic expansions have been done with the help of

$$\Psi(z) \stackrel{z \rightarrow \infty}{\sim} \ln z - \frac{1}{2z}$$

On the same footing, one calculates

$$\begin{aligned} [s * f_0](x) &= \frac{1}{2(1+e^x)}, \quad a_0 = \frac{\pi}{2} \\ [s * f_1^+](x) &= -\frac{1}{4x} \left(\tanh \frac{\pi x}{2a_1} + \left(1 - \frac{x}{\sinh x}\right) \right), \quad \delta = \frac{\pi}{2}. \end{aligned}$$

As was emphasized in section 3.2, the calculation of the x^{-2} -decay requires the integral over the regular function B_{reg} , where $B_{reg} := B_l^{(m)} - B_{as}$.

$$B_{as} = \frac{l-m}{2} + \frac{m}{2}f_0 + \frac{ml}{4}f_1^+ + \frac{m(l-m)}{4}f_1^- - \frac{m^2l}{8}f_l^+ - \frac{m^2(l-m)}{8}f_l^-$$

contains the asymptotic behaviour of $B_l^{(m)}$ up to $\mathcal{O}(x^{-2})$ exclusively. Thus the leading decay of B_{reg} is $B_{reg} \sim b_2^+ \theta(-x) + b_2^- \theta(x)$, with

$$\begin{aligned} b_2^+ &= \Delta_+^{(2)} + \Delta_-^{(2)} = \Psi(2) \frac{m^2 \cdot l}{8} + \frac{l\varepsilon}{2} \\ b_2^- &= \Delta_+^{(2)} - \Delta_-^{(2)} = \Psi(2) \frac{m^2 \cdot (l-m)}{8} + \frac{(l-m)\varepsilon}{2}. \end{aligned}$$

These identifications are made in section 3.2, eqs. (3.94), (3.95). Whereas ε is unknown analytically, it is calculated numerically. The convolution $k_s * B_l^{(m)}$ is split into two parts:

$$\left[k_s * B_l^{(m)} \right] (x - i\pi) = \underbrace{\left[k_s * B_{reg} \right] \left(x \pm i \frac{\pi}{2} \right)}_{\text{I)}} + \underbrace{\left[k_s * B_{as} \right] \left(x \pm i \frac{\pi}{2} \right)}_{\text{II)}}$$

I) The first non-vanishing order of the product in the integrand is for both factors $\sim x^{-2}$:

$$\text{I)} \sim \frac{1}{2x^2} \int_{-\infty}^{\infty} B_{reg}(x) dx + \frac{1}{x^2} (b_2^+ \theta(-x) + b_2^- \theta(x)) \underbrace{\int_{-\infty}^{\infty} k_s(x) dx}_1$$

II) Known exactly up to $\mathcal{O}(x^{-2})$ inclusively,

$$\begin{aligned} \left[k_s * B_{as} \right] \left(x - i \frac{\pi}{2} \right) \quad |x| \rightarrow \infty & \sim \frac{l}{2} \theta(-x) + \frac{l-m}{2} \theta(x) + \frac{1}{x} \left(\frac{m}{4} + \frac{lm}{4} \theta(-x) + \frac{(l-m)m}{4} \theta(x) \right) \\ & + \frac{\ln|x|}{x^2} \left(-\frac{m}{8} + \frac{m^2l}{8} \theta(-x) + \frac{m^2(l-m)}{8} \theta(x) \right) \\ & + \frac{1}{x^2} \left(\frac{m^2}{8} \frac{\Psi(2) + \ln \frac{a_1}{2}}{2} + b_2^+ \theta(-x) + b_2^- \theta(x) \right) \\ & + i \frac{\pi}{2x^2} \left(\frac{m}{4} + \frac{lm}{4} \theta(-x) + \frac{(l-m)m}{4} \theta(x) \right) \end{aligned} \quad (\text{C.7})$$

Note the agreement with eq. (3.93), where now an explicit value has been assigned to the unknown quantity ε . Instead of solving numerically for $B_l^{(m)}$, $\bar{B}_l^{(m)}$, we treat the regularized function $B_{reg} =$

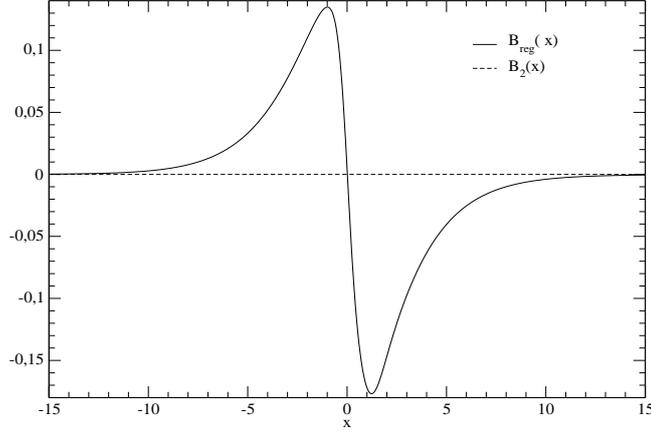


Figure C.1: The functions $B_{reg}(x)$ and $\text{Im } B_2^{(m)}(x)$ around the origin for $a_1 = \pi$, $\delta = \pi/2$, $l = 1 = m$.

$B_l^{(m)} - B_{as}$. As an illustration, $B_{reg}(x)$ is plotted for $m = 1 = 2S$ in fig. C.1. The task then consists in numerically treating the following equation:

$$B_{reg}(x) = \left(1 - e^{-\ln \mathfrak{B}_l(x)}\right) \left(\frac{1}{2} + [k_s * B_{reg}] \left(x - i\frac{\pi}{2}\right) + [k_s * B_{as}] \left(x - i\frac{\pi}{2}\right)\right) - B_{as}. \quad (\text{C.8})$$

Bearing in mind eqs. (2.161c), (C.7), one confirms explicitly that B_2 vanishes up to order $\mathcal{O}(x^{-2})$ inclusively. The coefficients b_2^\pm are found to be

$$b_2^+ = l(b_2^{(a)} + b_2^{(n)}) = lm^3\phi(m) \quad (\text{C.9})$$

$$b_2^- = (l - m)(b_2^{(a)} + b_2^{(n)}) = (l - m)m^3\phi(m)$$

$$b_2^{(a)} = \frac{m^2}{8} \left(\Psi(2) + \ln \frac{a_1}{2}\right) \quad (\text{C.10})$$

$$b_2^{(n)} = \frac{1}{2x^2} \int_{-\infty}^{\infty} B_{reg}(x) dx. \quad (\text{C.11})$$

In eq. (C.9), b_2^+ is identified with the scaled quantity ϕ , introduced in eq. (3.99). Variation of the parameters δ, a_0, a_l does not influence the numerical values for $b_2^{(n)}$. There is a slight dependence of a_1 , where $a_1 \in [\pi, 10\pi]$.² This dependence can be fitted well by linear regression, results are given in table C.2. This variation of $b_2^{(n)}$ is found to be smaller than the error induced by the finite integration range. We thus state that $b_2^{(n)}$ is independent of all variation parameters. Results for $\phi(m)$, are given in table C.2 below.

Finally, concentrate on an appropriate treatment of $B_l^{(\chi)}(x)$. The constant asymptotes are treated as for $\ln \mathfrak{B}_l$, $\ln \overline{\mathfrak{B}}_l$. The next leading order is $\mathcal{O}(1/x)$, not Fourier transformable. Instead of summing

² a_1 is, roughly speaking, the width of the crossover region of f_1 . a_1 must be chosen "reasonably", that is neither extremely small (then the crossover could not be resolved numerically) neither too large (such that the crossover would hinder the functions from attaining their asymptotic behaviour). So the slight a_1 -dependence is a finite size effect.

the kernels as in eq. (C.6), now the difference of both enters the game:

$$\begin{aligned}
 [k * f_1^+](x) - [k * f_1^+](x - i\pi) &= [k^{(d)} * f_1^+]\left(x - i\frac{\pi}{2}\right) & (C.12) \\
 \mathcal{F}_k [k^{(d)}] &= \frac{1}{2\pi} e^{-\frac{\pi}{2}|k|} \frac{\sinh \frac{\pi}{2}k}{\cosh \frac{\pi}{2}k} \\
 [k^{(d)} * f_1^+] &\stackrel{\delta=\pi/2}{=} \frac{1}{4\pi} \left[\frac{i}{x} \left(2C - 4 \ln 2 - \Psi \left(\frac{1}{2} - \frac{ix}{2a_1} \right) - \Psi \left(\frac{1}{2} + \frac{ix}{2a_1} \right) \right) \right. \\
 &\quad - \frac{1}{\pi - ix} \left(C - 2 \ln 2 - \Psi \left(\frac{1}{2} + \frac{\pi}{2a_1} - \frac{ix}{2a_1} \right) \right) \\
 &\quad - \frac{1}{\pi + ix} \left(C - 2 \ln 2 - \Psi \left(\frac{1}{2} + \frac{\pi}{2a_1} + \frac{ix}{2a_1} \right) \right) \\
 &\quad - 2i \left(\frac{\pi}{2ix - 2\pi} + \frac{1}{2} \left[\Psi \left(1 - \frac{ix}{2\pi} \right) - \Psi \left(\frac{1}{2} - \frac{ix}{2\pi} \right) \right] \right) \\
 &\quad \left. - \frac{\pi}{2\pi + 2ix} + \frac{1}{2} \left[\Psi \left(1 + \frac{ix}{2\pi} \right) - \Psi \left(\frac{1}{2} + \frac{ix}{2\pi} \right) \right] \right]
 \end{aligned}$$

C.1.3 Integrals

In common integral tables [39, 72], there is a mistake in the expression for the integral eq. (C.13) and therefore in eq. (C.14). The purpose of this paragraph is to give expressions for the integrals eqs. (C.14) and (C.15), these are needed in the context of exact regularization. The integrations were carried out with the help of [50].

One employs the integral representation of the digamma function,

$$\Psi(z) + C = \int_0^\infty \frac{e^{-x} - e^{-zx}}{1 - e^{-x}} dx .$$

Then

$$\begin{aligned}
 \int_0^\infty e^{-\mu x} \ln \cosh x dx &= \int_0^\infty e^{-\mu x} [\ln(e^x + e^{-x}) - \ln 2] dx \\
 &= -\frac{1}{\mu} e^{-\mu x} [\ln(e^x + e^{-x}) - \ln 2] \Big|_0^\infty + \frac{1}{\mu} \int_0^\infty e^{-\mu x} \frac{e^x - e^{-x}}{e^x + e^{-x}} dx \\
 &= \frac{1}{\mu} \int_0^\infty \frac{e^{-(\mu-1)x}}{2 \cosh x} - \frac{e^{-(\mu+1)x}}{2 \cosh x} dx, \quad \text{Re} \mu > 0 \\
 &= \frac{1}{4\mu} \left[\Psi \left(\frac{\mu-1}{4} + \frac{3}{4} \right) - \Psi \left(\frac{\mu-1}{4} + \frac{1}{4} \right) - \Psi \left(\frac{\mu-1}{4} + \frac{3}{4} \right) + \Psi \left(\frac{\mu+1}{4} + \frac{1}{4} \right) \right] \\
 &= \frac{1}{\mu} \left[\frac{1}{2} \Psi \left(\frac{\mu}{4} + \frac{1}{2} \right) - \frac{1}{2} \Psi \left(\frac{\mu}{4} \right) - \frac{1}{\mu} \right]
 \end{aligned}$$

$$\begin{aligned}
\int_0^\infty e^{-\mu x} (\ln \sinh x - \ln x) dx &= \int_0^\infty e^{-\mu x} [\ln(e^x - e^{-x}) - \ln 2x] dx \\
&= -\frac{1}{\mu} e^{-\mu x} [\ln(e^x - e^{-x}) - \ln 2x] \Big|_0^\infty + \frac{1}{\mu} \int_0^\infty e^{-\mu x} \left(\frac{e^x + e^{-x}}{e^x - e^{-x}} - \frac{1}{x} \right) dx \\
&= \frac{1}{\mu} \int_0^\infty \left[-\frac{e^{-\mu x}}{x} + \frac{e^{-\mu x}}{1 - e^{-2x}} + \frac{e^{-(\mu+2)x}}{1 - e^{-2x}} \right] dx, \operatorname{Re} \mu > 0 \\
&= \frac{1}{2\mu} \int_0^\infty \left[-\frac{e^{-x}}{x} + \frac{e^{-\frac{\mu}{2}x}}{1 - e^{-x}} - \frac{e^{-x}}{x} + \frac{e^{-(\frac{\mu}{2}+1)x}}{1 - e^{-x}} - 2\frac{e^{-\frac{\mu}{2}x} - e^{-x}}{x} \right] dx \\
&= \frac{1}{2\mu} \left[-\Psi\left(\frac{\mu}{2}\right) - \Psi\left(\frac{\mu}{2} + 1\right) - \ln \frac{2}{\mu} \right] \\
&= \frac{1}{\mu} \left[-\Psi\left(\frac{\mu}{2}\right) - \frac{1}{\mu} + \ln \frac{\mu}{2} \right] \tag{C.13}
\end{aligned}$$

$$\begin{aligned}
\int_0^\infty \frac{e^{-\mu x} - e^{-\nu x}}{x} dx &= \ln \frac{\nu}{\mu}, \quad \operatorname{Re} \mu > 0, \operatorname{Re} \nu > 0 \\
\int_0^\infty e^{-\mu x} \ln x dx &= -\frac{1}{\mu} [C + \ln \mu], \quad \operatorname{Re} \mu > 0
\end{aligned}$$

$$\begin{aligned}
\int_0^\infty e^{-\mu x} \ln \sinh x dx &= -\frac{1}{\mu} \left[C + \ln 2 + \frac{1}{\mu} + \Psi\left(\frac{\mu}{2}\right) \right], \operatorname{Re} \mu > 0 \\
&= -\frac{1}{\mu} \left[C + \ln 2 + \frac{1}{\mu} + \frac{1}{2} \Psi\left(\frac{\mu}{4}\right) + \frac{1}{2} \Psi\left(\frac{\mu}{4} + \frac{1}{2}\right) + \ln 2 \right]
\end{aligned}$$

Use has been made of

$$\Psi(2z) = \frac{1}{2} \Psi(z) + \frac{1}{2} \Psi\left(z + \frac{1}{2}\right) + \ln 2.$$

$$\int_0^\infty e^{-\mu x} \ln \tanh x dx = \frac{1}{\mu} \left[-C - 2 \ln 2 - \Psi\left(\frac{\mu}{4} + \frac{1}{2}\right) \right], \operatorname{Re} \mu > -2 \tag{C.14}$$

$$\begin{aligned}
\frac{1}{\mu} \left[-C - 2 \ln 2 - \Psi\left(\frac{\mu}{4} + \frac{1}{2}\right) \right] &|\mu| \xrightarrow{\sim} \infty \quad \frac{1}{\mu} \left[-C - 2 \ln 2 - \ln\left(\frac{\mu}{4} + \frac{1}{2}\right) + \frac{2}{\mu + 2} \right] \\
&\sim \frac{1}{\mu} (-C - \ln \mu) \\
\int_0^\infty \frac{e^{-\mu x}}{\cosh \nu x} dx &= \frac{1}{2\nu} \left[\Psi\left(\frac{\mu}{4\nu} + \frac{3}{4}\right) - \Psi\left(\frac{\mu}{4\nu} + \frac{1}{4}\right) \right] \\
\int_0^\infty e^{-\mu x} \tanh x dx &= \frac{1}{2} \left[\Psi\left(\frac{1}{2} + \frac{\mu}{4}\right) - \Psi\left(\frac{\mu}{4}\right) \right] - \frac{1}{\mu}. \tag{C.15}
\end{aligned}$$

C.2 Algorithms

The most simple and straightforward algorithm consists in iterating the $l + 1$ many equations simultaneously,

$$\begin{aligned} \ln y_j^{(i+1)} &= F \left[\left\{ \ln Y_j^{(i)} \right\} \right] \\ \ln Y_j^{(i+1)} &= \ln \left(1 + e^{\ln y_j^{(i+1)}} \right), \quad i = 1, \dots, N_{it}, \end{aligned}$$

where the functional F on the rhs denotes the rhs of the NLIE (2.154). Equivalently, one proceeds with eqs, (2.165), (2.166). In some cases however the numerical accuracy can be improved by slightly modifying the iteration procedure. Especially, this is the case concerning the integral over the imaginary part $\int_{-\infty}^{\infty} \text{Im} \ln \mathfrak{B}_l(x) dx$ and the integral over the regular part of $B_l^{(m)}$. These quantities play a crucial role in the evaluation of the asymptotic behaviour of the specific heat and the magnetic susceptibility, cf. section 3.2. In order to demonstrate the principal possibility to determine these quantities with high precision for arbitrary l, m , algorithms numerically more involved than the straightforward iteration have been implemented for special cases.

C.2.1 Recursive calculation of $\ln \mathfrak{B}_l$

As stated in eq. (2.148),

$$\ln Y_n = \ln \mathfrak{B}_n \overline{\mathfrak{B}}_n, \quad n \geq m.$$

m is the channel number. This means that one can build up the Y -hierarchy recursively in the over-screened case $2S > m$: In a first step, $\ln \mathfrak{B}_m, \ln \overline{\mathfrak{B}}_m$ are calculated together with the $\ln Y_{j < m}$. These are $m + 1$ unknown functions. Then the system of $m + 2$ NLIE, including $\ln Y_{1, \dots, m}, \ln \mathfrak{B}_{n=m+1}, \ln \overline{\mathfrak{B}}_{n=m+1}$ is solved by setting $\ln Y_m = \ln \mathfrak{B}_m \overline{\mathfrak{B}}_m$. Thus only two new functions have to be calculated, namely $\ln \mathfrak{B}_{n=m+1}, \ln \overline{\mathfrak{B}}_{n=m+1}$. This procedure is continued until $n = 2S$. The advantage of this strategy is that once the first $m + 1$ unknown functions have been determined, at each step only two new unknown functions have to be included. The alternative would be to calculate simultaneously the system of $2S + 1$ unknowns. In table C.1, results for the integral over the imaginary part are compared, calculated by recursively building up the Y -hierarchy and by conventional solution of the NLIE.

C.2.2 Extended integration range

The most important error in all calculations is caused by the finite integration range of length $2L$. So one is tempted to enlarge the considered interval. It is interesting to note that the results get not better upon enlarging the interval asymmetrically. However, improvements are possible by a symmetrical enlargement (with higher computational costs). Probably this is due to the fact that FFT is optimized to symmetric integration ranges. Concerning the integral over the imaginary part of the NLIE, we show that such an enlargement leads to results with arbitrary high accuracy, table C.1.

C.2.3 Smoothed functions for $h \neq 0$

The numerical iteration procedure gets more complex for $h \neq 0$: Then the auxiliary functions are T -dependent because of the βh -dependent driving terms. Thus the NLIE have to be solved for each temperature. Since the auxiliary functions themselves show sharp crossovers for $\beta h \gg 1$, we shall

deal with "smoothed" functions. This technique has been proposed by [22], who carried out similar calculations in the TBA approach. Write the NLIE in the following form:

$$\begin{aligned}
\ln Y_0 &= 0 \\
s * \ln Y_j &= s * \ln [1 + \exp(-\delta_{m,j}e^x + s * \ln Y_{j-1} + s * \ln Y_{j+1})] \\
s * \ln Y_{l-1} &= s * \ln [1 + \exp(-\delta_{m,l-1}e^x + s * \ln Y_{l-2} + k * \ln \ln \mathfrak{B}_l \overline{\mathfrak{B}}_l)] \\
k_{(+)} * \ln \mathfrak{B}_l &= k_{(+)} * \ln [1 + \exp(-\delta_{m,l}e^x + c\beta h + s * \ln Y_{l-1} + k * \ln \mathfrak{B}_l - k_- * \ln \overline{\mathfrak{B}}_l)] \\
k_{(-)} * \ln \overline{\mathfrak{B}}_l &= k_{(-)} * \ln [1 + \exp(-\delta_{m,l}e^x - c\beta h + s * \ln Y_{l-1} + k * \ln \overline{\mathfrak{B}}_l - k_+ * \ln \mathfrak{B}_l)] .
\end{aligned}$$

$k_{\pm}(x) = k(x \pm i\pi)$. Consider the convoluted functions on the lhs as unknowns; because of the convolutions, they are smoothed in comparison with the auxiliary functions themselves. These are equations for $l+3$ unknowns, which are solved iteratively for $h \neq 0$. The asymptotes are subtracted in a manner similar as for $h = 0$. In spite of these efforts, the data for $h \neq 0$ in the low-temperature regime are less accurate than for $h = 0$. For example, we are not able to confirm numerically the low-temperature Wilson ratios for $h \neq 0$, especially in the over-screened case eq. (3.52). However, without this modified iteration scheme, numerical low T errors would be even worse. The high-temperature regime causes no problems, the free spin behaviour is recovered. Illustrating curves are shown in chapter 4.

C.3 Results

Numerical results for the integral over the imaginary part $\int_{-\infty}^{\infty} B_2^{(l)}$ and the high-temperature Wilson ratio are presented. Since $B_2^{(l)}(x) \sim x^{-2}$ for large x , the error in $\int_{-\infty}^{\infty} B_2^{(l)}(x)dx$ is of order $1/L$, that is $1.4 \cdot 10^{-3}$ for $L = 700$. The accuracy gets slightly worse with increasing l , but is improved by building up the Y -hierarchy recursively by two orders of magnitude. This is only possible for $l > m$ and has been demonstrated for $m = 1$. The extension of the integration range with simultaneous increase of N in the case $l = m = 1$ leads to

$$\frac{2}{\pi} \int_{-\infty}^{\infty} B_2^{(1)}(x)dx - \ln 2 = -1 \pm 10^{-9} .$$

The data in table C.1 suggest that the value

$$\frac{1}{m} \left(\frac{2}{\pi} \int_{-\infty}^{\infty} B_2^{(l)}(x)dx - \ln \frac{l+1}{l-m+1} \right) = -1$$

may be confirmed numerically with arbitrary precision. It is interesting to observe that an asymmetric integration range does not improve the accuracy.

To calculate the x^{-2} -decay of $B_l^{(m)}$, the regularization procedure described in section C.1.2 is employed. During all calculations, $\delta = \frac{\pi}{4}$, $a_l = a_1$ has been set. It has been checked that the results do not depend on δ , neither on a_l . However, a slight dependence on a_1 is observed, which is well described by a linear fit. The errors given in table C.2 follow from the linear regression of $b_2(a_1)$. However, the numerical contribution to b_2 is an integral over a function decaying as $1/x^2$ (for $m = l$ as $\theta(-x)/x^2$) for large x . Thus the leading error is of order $1/L$, that is $1.4 \cdot 10^{-3}$ for $L = 700$ and $2 \cdot 10^{-5}$ for $L = 50000$. For $l = m = 1$, these exceed the error induced by the a_1 -dependence. For $l = m = 2$, the result could not be improved by extending the integration range; it is chosen to be $L = 700$ in all other cases. Then the a_1 dependence is dominated by the finite-size error. One may thus consider b_2 independent of a_1 . Up to an accuracy of 10^{-3} , the results in table C.2 are seen to coincide for equal m , independently of l such that we infer that b_2 is independent of l . The data do

l	m	$\frac{1}{m} \left(\frac{2}{\pi} \int_{-\infty}^{\infty} B_2^{(l)}(x) dx - \ln \frac{l+1}{l-m+1} \right)$
1	1	-0.999985
**1	1	-0.999999995
***1	1	-1.0007
2	1	-0.999119
2	2	-0.999173
**2	2	-0.99999
*2	1	-0.999985
3	1	-0.99896
3	2	-0.998963
3	3	-0.998913
*3	1	-0.999985
4	1	-0.99887
4	2	-0.998857
4	3	-0.998806
4	4	-0.998677
*4	1	-0.999985
5	1	-0.998766
5	2	-0.998756
5	3	-0.998707
5	4	-0.99861
5	5	-0.99842
*5	1	-0.999984

Table C.1: Numerical results for the integral over the imaginary part of $\ln \mathfrak{B}_l$, calculated in scheme II with $L = 700$, $N = 2^{15}$, $N_{it} = 70$. The results denoted by a star * are done by building up the Y -hierarchy recursively. The ** result has been obtained with the following choice of parameters: $L = 50000$, $N = 2^{19}$, $N_{it} = 100$. The *** calculation has been done with identical parameters as **, but over an asymmetric integration range $[-(2L - 700), 700]$.

not suffice to extract the m -dependence (if there is one at all). We expect those values derived from least equations as possible to be the most accurate. These are given, together with the corresponding Wilson ratios, in table C.3.

l	m	$b_2(a_1)/m^3$	
1	1	$0.04678 \pm 4 \cdot 10^{-5}$	$-(10^{-6} \pm 2 \cdot 10^{-6}) \cdot a_1$
**1	1	$0.04707 \pm 2 \cdot 10^{-7}$	$-(2 \cdot 10^{-8} \pm 10^{-9}) \cdot a_1$
2	1	$0.04721 \pm 1.5 \cdot 10^{-5}$	$-(1.03 \cdot 10^{-5} \pm 8 \cdot 10^{-7}) \cdot a_1$
2	2	$0.0501 \pm 4 \cdot 10^{-4}$	$+(1.1 \cdot 10^{-5} \pm 5 \cdot 10^{-6}) \cdot a_1$
**2	2	$0.0502 \pm 1 \cdot 10^{-4}$	$+(2 \cdot 10^{-5} \pm 6 \cdot 10^{-6}) \cdot a_1$
*2	1	$0.04652 \pm 5 \cdot 10^{-5}$	$+(10^{-3} \pm 2 \cdot 10^{-4}) \cdot a_1$
3	1	$0.04733 \pm 1 \cdot 10^{-5}$	$-(2.10 \cdot 10^{-5} \pm 7 \cdot 10^{-7}) \cdot a_1$
3	2	$0.05033 \pm 5 \cdot 10^{-5}$	$+(2 \cdot 10^{-6} \pm 2 \cdot 10^{-6}) \cdot a_1$
3	3	$0.0436 \pm 1.4 \cdot 10^{-4}$	$+(2.1 \cdot 10^{-5} \pm 7.3 \cdot 10^{-6}) \cdot a_1$
*3	1	$0.04139 \pm 9.6 \cdot 10^{-5}$	$+(4 \cdot 10^{-3} \pm 10^{-4}) \cdot a_1$
4	1	$0.04716 \pm 5 \cdot 10^{-5}$	$-(3.4 \cdot 10^{-5} \pm 3 \cdot 10^{-6}) \cdot a_1$
4	2	0.050369 ± 10^{-6}	$-(5 \cdot 10^{-6} \pm 10^{-6}) \cdot a_1$
4	3	$0.04380 \pm 7 \cdot 10^{-5}$	$+(9 \cdot 10^{-6} \pm 3 \cdot 10^{-6}) \cdot a_1$
4	4	$0.0382 \pm 2 \cdot 10^{-4}$	$+(2.8 \cdot 10^{-5} \pm 9 \cdot 10^{-6}) \cdot a_1$
*4	1	$0.0408 \pm 2 \cdot 10^{-4}$	$+(3.8 \cdot 10^{-3} \pm 2 \cdot 10^{-4}) \cdot a_1$
5	1	$0.01638 \pm 8 \cdot 10^{-5}$	$-(4.7 \cdot 10^{-5} \pm 4 \cdot 10^{-6}) \cdot a_1$
5	2	$0.046661 \pm 6 \cdot 10^{-6}$	$-(1.3 \cdot 10^{-5} \pm 3 \cdot 10^{-7}) \cdot a_1$
5	3	$0.04280 \pm 3 \cdot 10^{-5}$	$+(2 \cdot 10^{-6} \pm 2 \cdot 10^{-6}) \cdot a_1$
5	4	$0.03803 \pm 8 \cdot 10^{-5}$	$+(1.3 \cdot 10^{-5} \pm 4 \cdot 10^{-6}) \cdot a_1$
5	5	$0.0338 \pm 2 \cdot 10^{-4}$	$+(3 \cdot 10^{-5} \pm 10^{-5}) \cdot a_1$
*5	1	$0.04353 \pm 6.3 \cdot 10^{-5}$	$-(3.8 \cdot 10^{-5} \pm 3 \cdot 10^{-6}) \cdot a_1$

Table C.2: Numerical results for the coefficient of the x^{-2} -decay of $B_l^{(m)}$ in the under-compensated and exact compensated case, $m \leq l$, done with scheme II ($N = 2^{15}$, $L = 700$, $N_{it} = 100$). The values are obtained by linear regression of the dependence $b_2(a_1)$, the errors given are those due to the regression. The results denoted by * are done by building up the Y-hierarchy recursively. Note the improvement of the $l = 5$, $m = 1$ result due to this procedure. The ** result is obtained from an integration with the following choice of parameters: $L = 50000$, $N = 524288$, $N_{it} = 100$.

m	$\phi(m)$	ξ
1	$0.04707 \pm 2 \cdot 10^{-5}$	$0.102678 \pm 2 \cdot 10^{-6}$
2	$0.0502 \pm 1 \cdot 10^{-4}$	$6.4604 \cdot 10^{-2} \pm 6 \cdot 10^{-6}$
3	$0.0436 \pm 1.4 \cdot 10^{-3}$	$4.455 \cdot 10^{-2} \pm 8 \cdot 10^{-5}$
4	$0.0382 \pm 1.4 \cdot 10^{-3}$	$3.178 \cdot 10^{-2} \pm 7 \cdot 10^{-5}$
5	$0.0338 \pm 1.4 \cdot 10^{-3}$	$2.124 \cdot 10^{-2} \pm 6 \cdot 10^{-5}$

Table C.3: Combined analytical and numerical results for $\phi(m)$, defined in eqs. (3.99), (C.9). They are taken from table C.2, assuming no l dependence for equal m . Since the value calculated with least equations is expected to be the most accurate, the $l = m$ data from table C.2 are considered. Except for $m = 2$, the errors are those given by the finite integration ranges.

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