

Persistent currents

– Exact Bethe Ansatz results

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Abstract

We solve a class of 1-dimensional many-electron impurity models exactly on a ring with the Bethe Ansatz technique. The finite-size correction to the ground state energy is then computed within the Bethe Ansatz framework. In particular we obtain the additional contribution to the ground state energy from the impurity. We conclude with a discussion on the effect of persistent currents in small normal-metal rings. We focus on the impact of single scatterers and the interaction between electrons on the persistent current.

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Chapter 1

Introduction

There are few many-particle problems in physics that are exactly solvable. In most cases one has to use different approximations in order to obtain a problem that is solvable or even to be able to use numerical methods. However, there is a class of *integrable* systems that can be solved analytically. These are usually low-dimensional and have some special kind of symmetry that allows one to find infinitely many constants of motion. With the exact solution at hand it is possible to compare the exact answer with the results obtained by approximative methods. This is an important opportunity and has in many cases revealed approximations that don't work and give even qualitatively wrong results.

One exact method that works in some 1-Dimensional (1D) systems is the *Bethe Ansatz*. The origin of the method can be traced back to the early days of quantum mechanics when Hans Bethe found a wave-function that diagonalized the 1D isotropic Heisenberg spin-chain [1]. After that the method was not used extensively for some time. In the 60's the method experienced a revival and was extended to yield solutions to other problems. One important step forward was the solution of the repulsive δ -function interacting fermion gas by Yang [2]. In the 70's and the 80's the method continued to yield new results. Models that were solved include among others the 1D Hubbard model, the Kondo-model, the multi-channel Kondo model and the chiral Gross-Neveu model.

The Bethe Ansatz works only for systems in one dimension.¹ The one-dimensionality allows one to order the objects (e.g. particles or spins) on the line. With the help of the Hamiltonian it is possible to construct scattering matrices that connects the wave-functions in the different regions describing different orderings of the objects. One crucial property that the system must have is that it must be possible to factor many-particle scatterings into a product of two-particle scatterings. If the two-particle scattering matrices fulfill the so called Yang-Baxter Equations (YBE) it is possible to construct a consistent wave-function of the Bethe Ansatz form. To derive the energy spectrum one im-

¹The usual Kondo problem is formulated in 3 dimensions. Using the fact that the scattering is dominated by the spherically symmetric part it is a very good approximation to keep only this part. Then it is possible to map the problem onto one that is effectively 1D.

poses periodic boundary conditions on the system; this results in a matrix eigenvalue problem. This “spin” problem can be solved by a “second Bethe Ansatz” (this was the method that Yang used). This procedure is nowadays often replaced by the Quantum Inverse Scattering Method. This method originated from the work of Baxter [3] and was further extended by the St. Petersburg school [4].

One effect that is extremely sensitive to approximations is that of persistent currents in small normal-metal rings. The magnitude of the current is of the order of what a single electron at the Fermi energy carries; thus it is easy to wash away the effect by using wrong averaging procedures or too crude approximations. In some simple models it is possible to obtain a closed expression for the current; e.g. free electrons [5, 6, 7] and a one-band model where the (spin-less) electrons interact with a fixed scattering potential [8].

The exact Bethe Ansatz solution can be used to get exact results for the persistent currents in interacting spin-full systems. Examples of models studied with this method include the 1D Hubbard model [9, 10], and its limiting case, the δ -function interacting fermion gas [11].

There has been some controversy about what will happen with the persistent current when one couples a quantum dot in the Kondo regime to a mesoscopic ring [12]. In this regime the system can be described by a localized magnetic impurity interacting with the electrons in the ring. The Bethe Ansatz solution works for chiral electrons and a magnetic impurity [13]. In more typical cases the linear spectrum results in some problems [12]. This is why we in this thesis primarily study models with quadratic dispersion.

The usual way of getting the physics out of the Bethe Ansatz solution is to take the thermodynamic limit and let the size of the system go to infinity. The solution is then obtained in the form of coupled integral equations. This averaging procedure is not accurate enough to obtain the persistent current in a mesoscopic system. The magnitude of the persistent current is $\propto 1/L$ and hence taking the limit $L \rightarrow \infty$ kills the current. Thus one has to study finite-size corrections to the quantities obtained in the thermodynamic limit. The procedure for calculating the finite-size contribution to the ground state energy from the Bethe Ansatz solution that we outline in this thesis follows the one of Woynarovich [14]. Apart from the application to persistent currents the finite-size corrections to the ground state energy also has very important connections with conformal field theory, this is beyond the scope of this thesis however.

In this thesis we will apply the Bethe Ansatz to a class of model problems where we have a special kind of impurity (non-magnetic or ferro-magnetic) embedded in a repulsive δ -function interacting fermion gas with a quadratic dispersion. For some special values of the coupling constants the model is exactly solvable with the Bethe Ansatz. The construction of the Bethe Ansatz solution will be the topic of Chapter 2. In Chapter 3 we will go through the derivation of the finite-size correction to the ground state energy from the Bethe Ansatz solution. In particular we obtain the contribution from the impurity. Finally, in Chapter 4 we discuss the effect of persistent currents in small normal-metal rings.

Chapter 2

Bethe Ansatz solution

In the solution of the Kondo model with the Bethe Ansatz a linear energy dispersion is usually employed. This is motivated by the fact that the most important physics goes on around the Fermi point(s) and that the dispersion relation can be linearized in this active region. Thus the procedure is sound and can be motivated by the physics. This practice has a couple of advantages and a couple of drawbacks.

The main advantage of this procedure with this thesis in mind is that it makes the wave-function of the Schrödinger equation highly degenerate. The reason for this is that its dependence on the difference of any two of the electron coordinates, say $x_2 - x_1$, is not specified by the eigenvalue problem. This means that we can choose this dependence to our liking. This nice feature is no longer present when one uses a non-linear dispersion.

A drawback with the linear spectrum is that the energy spectrum is unbounded from below. This is not so severe, however, and a remedy is to implement an energy cut-off somehow. This can be subtle but is not a big problem if one is only interested in “universal” quantities, i.e. such quantities that are independent of the particular form of the cut-off.

A feature that can be a drawback but for the most part is an advantage is that the charge and spin sectors in the model with a linear dispersion are entirely decoupled. This makes the analysis of the excitations easier and computations and derivations less complicated. It is also interesting on mere physical grounds. The fact that it is possible to have independent charge- and spin-excitations is indeed very remarkable and leads to that we must change our view on the electron as the fundamental particle in this case.

We will see that the pure Heisenberg exchange term is not enough to get an integrable model in the case of a non-linear spectrum. One needs to add “counter-terms” into the Hamiltonian to get the Bethe Ansatz solution to be consistent. Yet another subtlety appears when one uses a non-linear spectrum. This is connected with the derivatives of the non-continuous wave-function at the impurity and will be discussed in more detail later.

There are a couple of instances in the literature where a non-linear spectrum

is used in the Bethe Ansatz solution of models that are similar to the Kondo model. The first is the one of Rudin [15], where a small third-order term is added to the linear spectrum in the backscattering model.

Another appearance is in the solution of the multi-channel Kondo model where a small second-order term is added to the linear spectrum to provide a built-in cut-off. The result of adding this term is to single out the actual form of the rapidities from the many possibilities. This results in the so-called “fusion” in the Bethe Ansatz equations. In the early paper [16] the details of the construction is not presented. However, in a much later paper [17] most of the details of how the “fusion” comes about are presented. The construction in this thesis is quite similar to the one presented in the latter paper.

A few Kondo models with a purely quadratic dispersion has also been solved exactly. These involve a special form of the impurity and an explicit electron-electron interaction. The first treatment is by Schulz [18, 19]. Similar models are treated by Wang and Voit [20] and Li and Bares [21]. We will come back to these cases later on.

The construction of the Bethe Ansatz solution is fairly straightforward as there exists a recipe to follow. Let us now start with this task.

2.1 Electron-impurity scattering matrix

We start here with the simple problem consisting of just one electron interacting with one localized magnetic impurity. Let us assume that we have a dispersion of the form $\epsilon(k) = a_1k + a_2k^2 + a_3k^3 + \dots$, where the zero of the energy is taken to be at zero wave-vector. In the case where the linear term dominates everything is measured relative to the Fermi surface. Let us also define the quantity $g = \epsilon(k)/k$ that will appear in the equations below. The one-particle case means that we want to solve the Schrödinger equation

$$\{\epsilon(-i\partial_1) + \delta(x_1)(2J\vec{\sigma}_1 \cdot \vec{S} + J')\}\psi = E\psi, \quad (2.1)$$

where x_1 is the coordinate of the electron. J and J' are coupling constants. $\vec{\sigma}_1$ are the usual Pauli matrices corresponding to the spin of the electron, \vec{S} is the spin operator of the impurity.

Away from the impurity the electron is free and we therefore take the wave-function to be a plane wave. To encode the information of the spin we introduce a quantization direction (\hat{z}) and a coefficient matrix in the wave function. We then make the Ansatz that we can write the wave-function as

$$\psi = A_{a_0 a_1} e^{ik_1 x_1} \theta(-x_1) + B_{a_0 a_1} e^{ik_1 x_1} \theta(x_1), \quad (2.2)$$

where a_1 label the spin coordinate of the electron (taking the values ± 1) and a_0 is the spin coordinate of the impurity. $\theta(x)$ is the Heaviside step function.

We are interested in the relation between the matrices A and B . To encode this we introduce the electron-impurity scattering matrix S defined by $B = S^{10}A$, or written more properly with the indices displayed

$$B_{a_0 a_1} = S_{a_1 a_0}^{a'_1 a'_0} A_{a'_0 a'_1}. \quad (2.3)$$

The simplest way to get S is to integrate the eigenvalue equation (2.1) over the origin, i.e. we multiply by $\int_{0^-}^{0^+} dx_1$. As long as our wave-function is continuous at the origin this poses no problem and we can easily get an expression for the scattering matrix. The wave-function is not generally continuous however (this would imply a trivial scattering matrix). Since the δ -function is usually defined when it multiplies a continuous function this gives us a problem. If we make the plausible prescription

$$\int_{0^-}^{0^+} dx \delta(x) \psi(x) = \frac{\psi(0^-) + \psi(0^+)}{2},$$

we get the following expression for the scattering matrix:

$$S^{j0} = \frac{g - i(2J\vec{\sigma}_j \cdot \vec{S} + J')/2}{g + i(2J\vec{\sigma}_j \cdot \vec{S} + J')/2}. \quad (2.4)$$

If we specialize to the case of spin -1/2 this can be simplified to

$$S^{j0} = \frac{g^2 + J''^2 - J^2 - i2gJ\mathcal{P}^{j0}}{g^2 - J''^2 + J^2 + i2gJ''}, \quad (2.5)$$

where we have defined $J'' = (J' - J)/2$. \mathcal{P} denotes the operator that permutes the indices of the matrix it acts on: $A_{s_1 s_0} = \mathcal{P}^{01} A_{s_0 s_1}$. This follows because we can write the permutation operator with the help of the usual Pauli matrices as $\mathcal{P}^{ij} = (\vec{\sigma}_i \cdot \vec{\sigma}_j + 1)/2$.

Note that the usual solution with a purely linear dispersion corresponds to $g = 1$ and that in this case our expression in (2.4) is the same as equation (57) in [22].

2.2 The need for counter-terms

We used the integral property of the δ -function to derive the electron-impurity scattering matrix in (2.5). Does the wave-function we constructed in this way really fulfill the Schrödinger equation we started out with? In particular, what happens when a higher order derivative acts on our discontinuous solution? Here we shall see that the linear dispersion makes life a lot easier.

Let us for simplicity work with the dispersion $\epsilon(k) = a_1 k + a_2 k^2$. Let it act in the coordinate basis as a differential operator on our trial wave-function in (2.2), the result is

$$\begin{aligned} \epsilon(-i\partial)\psi &= \epsilon(k)\psi - i\delta(x)(-A(a_1 + a_2k) + B(a_1 + a_2k))e^{ikx} \\ &\quad - a_2(-A + B)\delta'(x)e^{ikx}. \end{aligned} \quad (2.6)$$

If we use the prescription (see e.g. [22]) $\theta(x)\delta(x) = \theta(-x)\delta(x) = \delta(x)/2$ the δ -function in the second term on the right hand side of (2.6) and that in the Hamiltonian (2.1) matches up to get us the scattering matrix in (2.4). There is

also the the third term $\propto \delta'(x)$, which is not accounted for in the Schrödinger equation. In the previously mentioned papers [15, 17], this is taken care of by a local counter-term of the form

$$V_{cc}(x) = a_2 \frac{x}{|x|} (\delta'(x^+) + \delta'(x^-)), \quad (2.7)$$

that is added to the Hamiltonian to ensure that the eigenvalue equation is fulfilled at the origin. In these solutions this counter-term disappears when the non-linear terms are removed (i.e. taking the limit $a_2 \rightarrow 0$).

Another aspect of the linear dispersion is an ambiguity in the form of the first-quantized Hamiltonian given the scattering matrix. A solution to this problem is proposed by Schulz in the appendix of [23].

2.3 Electron-electron scattering matrix

Now when we have got the electron-impurity scattering matrix we also need an electron-electron scattering matrix to be able to proceed with the Bethe Ansatz solution. This scattering matrix must be such that the Yang-Baxter Equations are fulfilled, otherwise the Bethe-Ansatz solution is not consistent. We will comment more on this feature later in this chapter. The physical content of this relation is that it does not matter in which order the scattering takes place.¹ In symbols the equations can be written

$$\begin{aligned} S^{ij} S^{ik} S^{jk} &= S^{jk} S^{ik} S^{ij} \\ S^{ij} S^{i0} S^{j0} &= S^{j0} S^{i0} S^{ij}. \end{aligned} \quad (2.8)$$

The second of these equations including the impurity is the one we start with to construct the electron-electron scattering matrix. Now let us assume that the the electron-impurity scattering matrix is of the form $S^{i0} = \alpha_i + ic\mathcal{P}^{i0}$ and that the electron-electron scattering matrix is of the form $S^{ij} = \alpha_{ij} + ic\mathcal{P}^{ij}$. This assumption is quite general since the overall constant of proportionality is not important for the YBE. Simple algebra then gives that we must have $\alpha_{ij} = \alpha_i - \alpha_j$ for the YBE to be fulfilled. Writing out the result explicitly we get

$$S^{ij} = \frac{\alpha_i - \alpha_j + ic\mathcal{P}^{ij}}{\alpha_i - \alpha_j + ic}, \quad (2.9)$$

where we use that the matrix should be unitary to get the correct normalization. An arbitrary phase is also possible but we don't keep it here.

What physical interpretation can we make of an electron-electron scattering matrix of this form if we put in our values of the α_i 's? Is there a Hamiltonian that would give this kind of relation? We could ignore this question and just suppose that there is one but we don't know exactly what it is. This way of dealing with the problem is not very satisfactory for a physicist, we would like

¹In fact there is a lot more to it than this. It is deeply connected with the property of integrability, and that the solution works well only in one dimension.

to know what is going on and interpret it physically. There are a number of special cases where the electron-electron-interaction Hamiltonian can be specified however. Let us now take a closer look at some of these cases.

2.4 Special cases

The easiest case is probably the case of a non-magnetic impurity corresponding to the choice of $J = 0$ in our Hamiltonian (2.1). With this choice the electron-impurity scattering matrix is just a phase. We will not study this case in detail in this thesis. There are two more special cases corresponding to the case where $J'' = \pm J$ in (2.5), and in these cases the scattering matrix simplifies considerably to

$$S^{j0} = \frac{g - i2J\mathcal{P}^{j0}}{g + i2gJ''}. \quad (2.10)$$

These two cases turn up in a couple of papers where a solution to a Kondo-problem with a quadratic dispersion is presented. It seems that the first treatment is the one by Schulz [18, 19]. Wang and Voit treat a similar model in [20]; yet another model is the one presented by Li and Bares [21]. These two cases corresponds to a Hamiltonian proportional to the symmetric and antisymmetric spin projector respectively. In symbols this reads

$$(2J\vec{\sigma}_j \cdot \vec{S} + J') \propto (1 \pm \mathcal{P}^{j0})/2.$$

The third case is the one used in the solution of the multi-channel Kondo model [16, 17]. One supposes that the bending of the spectrum is very small. In the case of a small quadratic deviation from a linear dispersion we take $g = 1 + a_2k \equiv 1 + \epsilon$. The smallness is guaranteed if $\epsilon \ll 1$ for all relevant values of k . If we work only to first order in ϵ we are allowed to write $g^{-1} = 1 - \epsilon$ and the expression for the scattering matrix becomes

$$Y = \frac{1 + \epsilon + (J''^2 - J^2)(1 - \epsilon) - i2J\mathcal{P}}{1 + \epsilon - (J''^2 - J^2)(1 - \epsilon) + i2J''}. \quad (2.11)$$

In all these cases (if we don't go beyond third order in the dispersion - see below) we can find a simple Hamiltonian that provides us with the desired electron-electron scattering matrix. A comparison with the scattering matrix in a Fermi gas with δ -function interaction and quadratic dispersion [2] suggests that we could use this form of the interaction also in our case. The simplest potential to use is a δ -function potential ($\propto \delta(x_2 - x_1)$) and it works also in the case of a third-order term.² This means that in all these cases the Hamiltonian in the first quantization form can be taken to be

$$H = \sum_i \{\epsilon(k_i) + (J\vec{\sigma}_i \cdot \vec{\sigma}_0 + J')\delta(x_i)\} + \sum_i V_{cc}(x_i) + \sum_{i < j} K \delta(x_j - x_i), \quad (2.12)$$

²It is also possible to include permutation operators ($\propto \mathcal{P}^{12}\delta(x_2 - x_1)$) in the interaction term, but this gives no qualitatively new behavior.

where the explicit value of K depends on J and J' and whether we have a quadratic or a cubic term in the spectrum and which special case that we are dealing with. Note that in the case of $J'' = \pm J$ we are not free to choose J and J' independently (remember $J'' = (J' - J)/2$). In all cases however, K and J have opposite signs. This implies that for a ferromagnetic (antiferromagnetic) coupling we need to have a repulsive (attractive) interaction between the electrons in order for the Bethe Ansatz method to work.

One might ask whether a local counter-term is needed for the electron-electron interaction as well. The answer is that it is not needed. To see this we look at the case of two particles. Let us change to center-of-mass coordinates $y = x_2 - x_1$ and $X = (x_1 + x_2)/2$. Our Bethe Ansatz wave-function can then be written as

$$\psi = e^{iKX} \{ \theta(-y)(Ae^{iky} + Be^{-iky}) + \theta(y)(Ce^{iky} + De^{-iky}) \}, \quad (2.13)$$

where $K = k_1 + k_2$ and $k = (k_2 - k_1)/2$.

Here we get one equation from integrating the eigenvalue equation from $y = 0^-$ to $y = 0^+$, one from continuity and one from the requirement of antisymmetry. The three equations together result in a unique scattering matrix. Letting two derivatives act on the step functions gives us zero contribution since the wave function is continuous ($A + B = C + D$). Moreover, with these notations the kinetic energy terms of the first few orders are given by

$$k_1 + k_2 = \partial_1 + \partial_2 = \partial_X \quad (2.14a)$$

$$k_1^2 + k_2^2 = \partial_1^2 + \partial_2^2 = \frac{1}{2}\partial_X^2 + 2\partial_y^2 \quad (2.14b)$$

$$k_1^3 + k_2^3 = \partial_1^3 + \partial_2^3 = \frac{1}{4}\partial_X^3 + 3\partial_X\partial_y^2 \quad (2.14c)$$

$$k_1^4 + k_2^4 = \partial_1^4 + \partial_2^4 = \frac{1}{8}\partial_X^3 + 3\partial_X^2\partial_y^2 + 2\partial_y^4. \quad (2.14d)$$

If we don't go beyond third order we have just one quadratic ∂_y^2 -dependent term and hence no counter-term is needed. Note also that the first order term is independent of y , so in the case of a linear dispersion any y -dependence of the wave-function is allowed.

2.5 Bethe Ansatz solution

When we have constructed scattering matrices from the one- and two-particle cases that fulfill the YBE we can solve the N -particle problem with the help of the Bethe Ansatz. What we do is that we “guess” the form of the wave-function, i.e. we make an Ansatz. Then we prove that our guess is indeed a consistent solution. In fact this is not necessary since consistency is guaranteed by the YBE as we will see.

To derive the spectrum we put our problem in a box with periodic boundary conditions (or twisted ones, see Chapter 4 on persistent currents). We then move one particle around the system and arrive at a matrix eigenvalue problem.

The matrix eigenvalue problem can be solved by another “generalized” Bethe Ansatz (this was the way it was first done by Yang [2]) or by using the Quantum Inverse Scattering Method. Here we will use the latter method. The solution is then given as a set of algebraic equations for the momenta $\{k_j\}$ and the so-called spin rapidities $\{\Lambda_\gamma\}$. There are M spin rapidities corresponding to the total (conserved) number of “down” spins in the system.

The beauty of the method is that once you know the technique and have got the scattering matrices you can immediately write down the solution to the eigenvalue problem. The derivation can be done once and for all and is quite general. It is possible to extend the procedure to treat particles with more degrees of freedom (like for example in the multi-channel Kondo problem). There are a number of good references explaining the method [22, 24, 25]. The outline of the method here is to a large extent based on Andrei’s treatment [22].

We write the Bethe Ansatz wave-function as

$$\psi(x_1, \dots, x_N, a_0, a_1, \dots, a_N) = \mathcal{A} e^{i \sum_j k_j x_j} \sum_Q A_{a_0, a_1, \dots, a_N} \theta(Q), \quad (2.15)$$

where x_n are the position coordinates, a_n the spin indices of the electrons and a_0 is the spin index of the impurity. \mathcal{A} denotes the antisymmetrization operator. The sum over Q goes over all permutations of the $N+1$ integers $\{Q_0, Q_1, \dots, Q_N\}$ and

$$\theta(Q) = \begin{cases} 1 & \text{if } x_{Q_0} < x_{Q_1} < \dots < x_{Q_N} \\ 0 & \text{otherwise.} \end{cases}$$

Thus we have a (properly antisymmetrized) solution that in each region defined by the Q ’s is a linear superposition of plane waves. The Schrödinger equation in (2.12) is thus trivially fulfilled inside the regions. The coefficient matrices in different regions are connected via the scattering matrices or by the requirement of antisymmetry. If the regions Q and Q' are adjacent, i.e. they differ only by a transposition, then they are connected by the scattering matrix we constructed previously in this section. More explicitly, let $Q = \{\dots, Q_i, Q_{i+1}, \dots\}$ and $Q' = \{\dots, Q_{i+1}, Q_i, \dots\}$. Then according to our construction (suppressing the indices) $A(Q') = S^{Q_i Q_{i+1}} A(Q)$.

If the regions are not adjacent they can be connected by a number of transpositions, and hence the corresponding coefficient matrices can be connected by a product of S -matrices. However, the path of connection is usually not unique. Consider for instance the case of three particles. Then we can go from region $x_1 < x_2 < x_3$ to region $x_3 < x_2 < x_1$ either by the path via $x_2 < x_1 < x_3 \rightarrow x_2 < x_3 < x_1$ or via $x_1 < x_3 < x_2 \rightarrow x_3 < x_1 < x_2$. In order for our solution to be consistent it must not depend on which way we go between the regions. In terms of the scattering matrices the requirement in the three-particle example reads $S^{12} S^{13} S^{23} = S^{23} S^{13} S^{12}$, but this is nothing other than the aforementioned Yang-Baxter Equations (2.8). We explicitly constructed our scattering matrices to fulfill these relations without stating the reason, now we know why it was a good idea. It turns out that we do not need

to impose any further restrictions on the scattering matrices in order to have a consistent solution. Even when the number of particles and paths are extended, the YBE are enough to insure integrability [22]. Thus we can write our Bethe Ansatz wave-function as

$$\psi(x_1, \dots, x_N, a_0, a_1, \dots, a_N) = \mathcal{A} e^{ik_j x_j} \sum_Q S(Q) A(I) \theta(Q), \quad (2.16)$$

where $A(I)$ is the matrix in some reference region I , and $S(Q)$ is the appropriate product of scattering matrices. We can take the reference region to be $I = \{0, 1, 2, \dots, N\}$ for simplicity.

We then have a solution to our eigenvalue problem (2.12). To get the energy spectrum we impose periodic boundary conditions (PBC) $\phi(\dots, x_j + L, \dots) = \phi(\dots, x_j, \dots)$. If we start with region I and move particle j to the far left or to the far right the difference in the result according to the PBC would be a phase of $e^{ik_j L}$. Thus we have transformed our original problem to the following one:

$$S^{0j} \dots S^{j-2j} S^{j-1j} A(I) = S^{jN} \dots S^{jj+2} S^{jj+1} e^{k_j L} A(I). \quad (2.17)$$

When we move all the scattering matrices to one side we get the matrix eigenvalue problem

$$T_j A(I) \equiv S^{j+1j} S^{j+2j} \dots S^{Nj} S^{0j} \dots S^{j-2j} S^{j-1j} A(I) = e^{k_j L} A(I). \quad (2.18)$$

Now we note that in all the special cases above the scattering matrix can be written on the form

$$S^{ij} = \frac{\alpha_i - \alpha_j + ic \mathcal{P}^{ij}}{\alpha_i - \alpha_j + ic}.$$

The diagonalization of the matrix problem with this form of the scattering matrix can be accomplished by a ‘‘second’’ Bethe Ansatz or by the Quantum Inverse Scattering Method. The solution is then obtained as a set of algebraic equations. There are a number of nice derivations in the literature of this method [22, 24, 25] so we will consider it quite briefly in this thesis. The idea is to start from the state where all spins are up and construct and apply M lowering operators to get a state with M down spins. It is easy to construct operators that almost are lowering operators. To get at a pure lowering operator one introduces ‘‘spin rapidities’’ to insure that no unwanted terms are generated. The result is that the solution to the general problem is given by the following equations

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{\Lambda_\gamma - \alpha_j - ic/2}{\Lambda_\gamma - \alpha_j + ic/2} \quad (2.19a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \prod_{j=1}^N \frac{\Lambda_\gamma - \alpha_j - ic/2}{\Lambda_\gamma - \alpha_j + ic/2}, \quad (2.19b)$$

where the $\{\Lambda_\gamma\}$ are the spin rapidities. There are M of these corresponding to the (conserved) number of down spins in the system. If we put in the explicit form of our α_j 's we get our solution.

So now we have the solution to the problem, i.e. we have algebraic equations determining the spectrum of the model. There is some work left to do however. One has to extract the physics from the equations. For example, we might want to identify the ground state, compute the magnetization, treat non-zero temperatures etc. In this thesis we will study the problem of persistent currents at zero temperature. To study this effect we must first find an expression for the ground state energy. The way it is usually done is to take the thermodynamic limit (where $L \rightarrow \infty$). The solution is then obtained in the form of coupled integral equations. It turns out that this procedure is not accurate enough for our purposes. This means that we have to study finite-size effects, this will be the topic of the next chapter.

2.6 Explicit solutions in some special cases

Before concluding this chapter we will write down the Bethe Ansatz equations (BAE) for the Kondo model with a linear spectrum, the Kondo model with a small quadratic deviation and the attractive delta-function interacting fermion gas. This can give some insight into the similarities of these models.

The usual Kondo model solution with linear dispersion gives [22]

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{\Lambda_\gamma - 1 + ic/2}{\Lambda_\gamma - 1 - ic/2} \quad (2.20a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \left(\frac{\Lambda_\gamma - 1 - ic/2}{\Lambda_\gamma - 1 + ic/2} \right)^N \left(\frac{\Lambda_\gamma - ic/2}{\Lambda_\gamma + ic/2} \right). \quad (2.20b)$$

For the Kondo model with a small quadratic term ($\epsilon(k) = 1 + a_2 k$) and an attractive δ -function electron-electron interaction we get

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{\Lambda_\gamma - 1 - \lambda_j + ic/2}{\Lambda_\gamma - 1 - \lambda_j - ic/2} e^{i\theta(k_j)} \quad (2.21a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \prod_{j=1}^N \frac{\Lambda_\gamma - 1 - \lambda_j - ic/2}{\Lambda_\gamma - 1 - \lambda_j + ic/2} \left(\frac{\Lambda_\gamma - ic/2}{\Lambda_\gamma + ic/2} \right), \quad (2.21b)$$

where $\lambda_j = \text{const} \cdot a_2 k_j$ and $e^{i\theta(k_j)}$ is a phase. The case of an attractive δ -function interacting Fermi gas with a purely quadratic dispersion gives [2]

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{\Lambda_\gamma - k_j + ic/2}{\Lambda_\gamma - k_j - ic/2} \quad (2.22a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \prod_{j=1}^N \frac{\Lambda_\gamma - k_j - ic/2}{\Lambda_\gamma - k_j + ic/2}. \quad (2.22b)$$

Comparing these three equations it is apparent that the solutions to all three problems are quite similar and that an attractive potential between the electrons is somehow built into the usual Kondo problem, without being written out explicitly.³ When we add a non-linear term (quadratic or cubic) we need to write out an attractive interaction potential explicitly. Also when a linear spectrum is employed it is not possible to form pairs corresponding to complex values of k .

Another interesting fact is that a δ -function-interaction potential between the electrons in the linear Kondo problem has no effect because the wave-function is chosen so that it is zero at these points. To prove this, look at the wave-function in the two-particle case (2.13): The requirement of antisymmetry gives $D = -\mathcal{P}A$ and $B = -\mathcal{P}C$. Choosing the scattering operator to be just \mathcal{P} (i.e. $C = \mathcal{P}A$) immediately gives $\lim_{x_2 \rightarrow x_1^\pm} \psi(x_1, x_2) = 0$.

Finally, we will write down the class of impurity models and their solutions in the two special cases discussed above. We choose to focus on the ferromagnetic case since it is more natural to have a repulsive interaction between the electrons. The Hamiltonian is then given by

$$H = \sum_i \{-k_i^2 + (J\vec{\sigma}_i \cdot \vec{\sigma}_0 + J')\delta(x_i)\} + \sum_i V_{cc}(x_i) + \sum_{i < j} 2c \delta(x_j - x_i), \quad (2.23)$$

where $2J = -c < 0$. The two special cases above corresponding to the two solvable cases $J'' = J$ ($-J$) gives $J' = 3J$ ($-J$). The BAE in these two cases are given by

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{k_j - \Lambda_\gamma + ic/2}{k_j - \Lambda_\gamma - ic/2} \left(\frac{k_j - ic}{k_j + ic} \right)^\eta \quad (2.24a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \prod_{j=1}^N \frac{\Lambda_\gamma - k_j - ic/2}{\Lambda_\gamma - k_j + ic/2} \left(\frac{\Lambda_\gamma - ic/2}{\Lambda_\gamma + ic/2} \right), \quad (2.24b)$$

where $\eta = 1$ (0) for $J' = 3J$ ($-J$) respectively. Note that except for the impurity factors (the last factors on the right-hand side of (2.24)) these are just the BAE for the repulsive δ -function interacting fermion gas due to Yang [2]. The equations (2.24) are similar to the ones in [18, 20, 21] although the authors of [21, 18] have no local counter-term of the form V_{cc} . These BAE will be the starting point in our analysis of the finite-size corrections in the next chapter.

³This reflects the fact that a Kondo impurity *induces* correlations among otherwise non-interacting electrons.

Chapter 3

Finite-size corrections

Finite-size corrections to various quantities obtained in the thermodynamic limit are interesting in many ways. They are important for the calculation of certain types of excitation energies. There are also very interesting connections to conformal field theory that we will not consider here.

In this section we will derive an expression for the finite-size correction to the energy of the ground state from the Bethe Ansatz solution. The way how to do this was originally proposed in [26]. The original construction in the case of the 1D Hubbard model is due to Woynarovich [14]. Here we will stick to his treatment but generalize it slightly. The generalization includes keeping the α 's in (2.19) unspecified throughout (we will make some assumptions about them though). This allows us to extend the result to the δ -function interacting Fermi gas. Finally we obtain the contribution from certain types of impurities to the the ground state energy. In particular, the two special cases introduced in the previous chapter can be treated in the formalism.

The pure δ -function interacting Fermi gas case is treated extensively by Schlottmann [11, 27], while impurity contributions to the ground state energy have been studied by Fujimoto and Kawakami *et al.* for some similar models [28, 29, 30]. In the next chapter we will use the expression for the finite-size correction to the ground state energy to study the interesting effect of persistent currents in small normal-metal rings. This chapter will be quite technical. At the end, however, the result is simple and a nice interpretation in “dressed” physical quantities is possible. Let us now start the derivation.

3.1 Density corrections

In the last section we found the solution to our problem as the BAE in (2.24). At this point we remove the impurity contributions (the last factors on the right hand side of the BAE in (2.24)) to simplify the treatment. Taking the logarithm

of the remaining factors we arrive at the following equations

$$Lk_j = 2\pi I_j + \sum_{\gamma} \theta_{1/2}(\alpha_j - \lambda_{\gamma}) \quad (3.1a)$$

$$\sum_j \theta_{1/2}(\lambda_{\gamma} - \alpha_j) = -2\pi J_{\gamma} + \sum_{\delta} \theta_1(\lambda_{\gamma} - \lambda_{\delta}), \quad (3.1b)$$

where we have defined $\theta_n(x) = -2 \tan^{-1}(x/nc)$ and write α_j for $\alpha(k_j)$.¹ The I_j 's (J_{γ} 's) are integers or half-integers depending on whether M ($N - M - 1$) is even or odd. This follows from the fact that when we take the logarithm we get an extra π for each θ . Also observe that (3.1b) gives restrictions on the allowed values of the J_{γ} since $|\theta_n| \leq \pi$. In the case of $2M = N$ for instance there is no freedom at all in the choice of the J_{γ} 's.

Rewriting (3.1) slightly we define the quantities z_c and z_s via

$$z_c(k) = \frac{k}{2\pi} - \frac{1}{2\pi L} \sum_{\gamma} \theta_{1/2}(\alpha(k) - \lambda_{\gamma}) \quad (3.2a)$$

$$z_s(\lambda) = -\frac{1}{2\pi L} \sum_j \theta_{1/2}(\lambda - \alpha_j) + \frac{1}{2\pi L} \sum_{\delta} \theta_1(\lambda - \lambda_{\delta}). \quad (3.2b)$$

These will be useful because of the relations

$$z_c(k_j) = \frac{I_j}{L} \quad z_s(\lambda_{\gamma}) = \frac{J_{\gamma}}{L}. \quad (3.3)$$

Now let us also define

$$\rho_c(k) = \frac{\partial z_c(k)}{\partial k} \quad \rho_s(\lambda) = \frac{\partial z_s(\lambda)}{\partial \lambda}, \quad (3.4)$$

which will denote the density of the solutions in the charge and spin sector respectively. Taking the derivatives of the functions in (3.2) we arrive at the following equations for $\vec{\rho} \equiv (\rho_c, \rho_s)$:²

$$\rho_c(k) = \frac{1}{2\pi} + \frac{1}{L} \sum_{\gamma} \alpha'(k) K_{1/2}(\alpha(k) - \lambda_{\gamma}) \quad (3.5a)$$

$$\rho_s(\lambda) = \frac{1}{L} \sum_j K_{1/2}(\lambda - \alpha_j) - \frac{1}{L} \sum_{\delta} K_1(\lambda - \lambda_{\delta}). \quad (3.5b)$$

We have here defined $K_n(x) \equiv nc/\pi(x^2 + (nc)^2)$. In the ground state of the system the I 's and the J 's are supposed to be consecutive integers (holes in the sequence introduce excitations in the system). We denote the upper and lower

¹In our case $\alpha(k) = k$ and in the 1D Hubbard model $\alpha(k) = \sin k$. We will keep $\alpha(k)$ unspecified throughout so that we can use the result for both models. The only assumption that we will make is that α is an odd function of k .

²We will often use this kind of vector notation for various quantities from now on.

limit of these consecutive integers I^\pm and J^\pm respectively. In this case we can define the following parameters:

$$N_c = I^+ - I^- + 1 \quad N_s = J^+ - J^- + 1 \quad (3.6a)$$

$$D_c = \frac{I^+ + I^-}{2} \quad D_s = \frac{J^+ + J^-}{2}. \quad (3.6b)$$

Now we are ready to use the second Euler-Maclaurin formula to convert the sums into integrals (for details, see Appendix A). In our case we use the formula in the forms

$$\frac{1}{L} \sum_j f(k_j) = \int_{k^-}^{k^+} \rho_c(k) f(k) dk + \frac{1}{24L^2} \left\{ \frac{f'(k^-)}{\rho_c(k^-)} - \frac{f'(k^+)}{\rho_c(k^+)} \right\} \quad (3.7a)$$

$$\frac{1}{L} \sum_\gamma f(\Lambda_\gamma) = \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda) f(\lambda) d\lambda + \frac{1}{24L^2} \left\{ \frac{f'(\lambda^-)}{\rho_s(\lambda^-)} - \frac{f'(\lambda^+)}{\rho_s(\lambda^+)} \right\}, \quad (3.7b)$$

which are correct to order $O(1/L^2)$. The parameters k^\pm and λ^\pm are defined via the relations

$$z_c(k^\pm) = \frac{I^\pm \pm \frac{1}{2}}{L} \quad z_s(\lambda^\pm) = \frac{J^\pm \pm \frac{1}{2}}{L}. \quad (3.8)$$

Note that k^\pm and λ^\pm will play the role of Fermi-points in our system. With the help of these formulas we can rewrite (3.5) as

$$\begin{aligned} \rho_c(k) &= \frac{1}{2\pi} + \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda') \alpha'(k) K_{1/2}(\alpha(k) - \lambda') d\lambda' \\ &+ \frac{1}{24L^2} \left\{ \alpha'(k) \frac{K'_{1/2}(\alpha(k) - \lambda^+)}{\rho_s(\lambda^+)} - \alpha'(k) \frac{K'_{1/2}(\alpha(k) - \lambda^-)}{\rho_s(\lambda^-)} \right\} \end{aligned} \quad (3.9a)$$

$$\begin{aligned} \rho_s(\lambda) &= \int_{k^-}^{k^+} \rho_c(k') K_{1/2}(\lambda - \alpha(k')) dk' - \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda') K_1(\lambda - \lambda') d\lambda' \\ &+ \frac{1}{24L^2} \left\{ \frac{\alpha'(k^+) K'_{1/2}(\lambda - \alpha(k^+))}{\rho_c(k^+)} - \frac{\alpha'(k^-) K'_{1/2}(\lambda - \alpha(k^-))}{\rho_c(k^-)} \right. \\ &\quad \left. + \frac{K'_1(\lambda - \lambda^-)}{\rho_s(\lambda^-)} - \frac{K'_1(\lambda - \lambda^+)}{\rho_s(\lambda^+)} \right\}. \end{aligned} \quad (3.9b)$$

To clean up some of the notation we note that the following type of coupled integral equations will often appear

$$x_c(k|k^\pm, \lambda^\pm) = x_{c0}(k) + \int_{\lambda^-}^{\lambda^+} d\lambda' \alpha'(k) K_{1/2}(\alpha(k) - \lambda') x_s(\lambda'|k^\pm, \lambda^\pm) \quad (3.10a)$$

$$x_s(\lambda|k^\pm, \lambda^\pm) = x_{s0}(\lambda) + \int_{k^-}^{k^+} dk' K_{1/2}(\lambda - \alpha(k')) x_c(k'|k^\pm, \lambda^\pm) - \int_{\lambda^-}^{\lambda^+} d\lambda' K_1(\lambda - \lambda') x_s(\lambda'|k^\pm, \lambda^\pm), \quad (3.10b)$$

which we will write in a compact matrix form as

$$\vec{x} = \vec{x}_0 + \hat{K} \otimes \vec{x}. \quad (3.11)$$

Another important equation is the same type of integral equation with the kernel matrix transposed

$$\vec{y} = \vec{y}_0 + \hat{K}^T \otimes \vec{y}. \quad (3.12)$$

Given two solutions \vec{x} and \vec{y} (one of each type) to these we get the following useful property for inner products:

$$\vec{x}^T \otimes \vec{y}_0 \equiv \int_{k^-}^{k^+} x_c(k) y_{0c}(k) dk + \int_{\lambda^-}^{\lambda^+} x_s(\lambda) y_{0s}(\lambda) d\lambda = \vec{x}_0^T \otimes \vec{y}. \quad (3.13)$$

Since the integral equations are linear we can write the solution of (3.9) in a quite compact form as

$$\vec{\rho}(k, \lambda) = \vec{\rho}_\infty + \frac{1}{24L^2} \left\{ \frac{\vec{\rho}_1(k, \lambda|k^\pm, \lambda^\pm)}{\rho_c(k^+)} + \frac{\vec{\rho}_1(-k, -\lambda| -k^\mp, -\lambda^\mp)}{\rho_c(k^-)} + \frac{\vec{\rho}_2(k, \lambda|k^\pm, \lambda^\pm)}{\rho_s(\lambda^+)} + \frac{\vec{\rho}_2(-k, -\lambda| -k^\mp, -\lambda^\mp)}{\rho_s(\lambda^-)} \right\}, \quad (3.14)$$

where we used that $\alpha(k)$ is an odd function. This is the most important result of this section. The functions $\vec{\rho}_\infty$, $\vec{\rho}_1$ and $\vec{\rho}_2$ are solutions of (3.11) with the inhomogeneous part given by

$$\vec{\rho}_{\infty 0} = \begin{bmatrix} 1/2\pi \\ 0 \end{bmatrix} \quad \vec{\rho}_{10} = \begin{bmatrix} 0 \\ \alpha'(k^+) K'_{1/2}(\lambda - \alpha(k^+)) \end{bmatrix} \quad (3.15) \\ \vec{\rho}_{20} = \begin{bmatrix} \alpha'(k) K'_{1/2}(\alpha(k) - \lambda^+) \\ -K'_1(\lambda - \lambda^+) \end{bmatrix}.$$

3.2 Energy corrections

After these preliminaries it is now time to start looking at the energy of our system. The general form of the energy is given by

$$E = \sum_j \epsilon_{c0}(k_j) + \sum_\gamma \epsilon_{s0}(\lambda_\gamma). \quad (3.16)$$

The second term allows for a spin-dependent energy, a Zeeman term for instance. If we would like to study the system's response to a magnetic field we would

have to include such a term. Now we use the Euler-Maclaurin formula for the energy expression and arrive at

$$E = L \left[\int_{k^-}^{k^+} \rho_c(k') \epsilon_{c0}(k') dk' + \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda') \epsilon_{s0}(\lambda') d\lambda' \right] + \frac{1}{24L} \left\{ \frac{\epsilon'_{c0}(k^-)}{\rho_c(k^-)} - \frac{\epsilon'_{c0}(k^+)}{\rho_c(k^+)} + \frac{\epsilon'_{s0}(\lambda^-)}{\rho_s(\lambda^-)} - \frac{\epsilon'_{s0}(\lambda^+)}{\rho_s(\lambda^+)} \right\}. \quad (3.17)$$

With the help of our solution for $\vec{\rho}$ in (3.14) we can rewrite the energy expression (3.17) in a very compact form

$$E = L \epsilon_\infty(k^\pm, \lambda^\pm) + \frac{1}{24L} \{ \epsilon_1(k^\pm, \lambda^\pm) + \epsilon_1(-k^\mp, -\lambda^\mp) + \epsilon_2(k^\pm, \lambda^\pm) + \epsilon_2(-k^\mp, -\lambda^\mp) \}. \quad (3.18)$$

We will not specify the explicit form of the $O(1/L)$ term here (for details see Woynarovich's paper [14]); it is also easy to obtain the explicit form from (3.14) and (3.17). As these corrections are already $O(1/L)$ they are not affected to this order by the applied flux that we shall be interested in in the next chapter.

The important part of the energy for our purposes is that of the infinite system. It can be rewritten with the help of the inner-product relation in (3.13) as

$$\epsilon_\infty = \vec{\rho}_\infty^T \otimes \vec{\epsilon}_0 = \vec{\rho}_{\infty 0}^T \otimes \vec{\epsilon} = \frac{1}{2\pi} \int_{k^-}^{k^+} \epsilon_c(k) dk, \quad (3.19)$$

where we used the explicit form of $\vec{\rho}_{\infty 0}$ given in (3.15). Note that $\epsilon_c(k)$ is also a function of the endpoints and should more properly be written as $\epsilon_c(k|k^\pm, \lambda^\pm)$.

The quantity $\vec{\epsilon}$ is usually called the ‘‘dressed energy’’ and is given by the solution of (3.12) with the appropriate inhomogeneous $\vec{\epsilon}_0$ (e.g. $[k^2, 0]^T$ in the Fermi gas). The ground state energy of the infinite system is minimal with respect to k^\pm and λ^\pm . Taking the derivative of (3.19) with respect to these variables we find the condition we need to guarantee that the energy is minimal. For example it is possible to derive expressions like $\partial_{k^+} \epsilon_\infty = \epsilon_c(k^+) \rho_{\infty c}(k^+)$. The conditions that we need is to take the dressed energy to be zero at the four Fermi points, i.e.

$$\begin{aligned} \epsilon_c(k^+) &= 0 & \epsilon_c(k^-) &= 0 \\ \epsilon_s(\lambda^+) &= 0 & \epsilon_s(\lambda^-) &= 0. \end{aligned} \quad (3.20)$$

In the ground state of the infinite system we expect k^\pm and λ^\pm to be distributed symmetrically around the origin. Let us denote these points $\pm k_0$ and $\pm \lambda_0$. Then we can do a Taylor expansion of ϵ_∞ in $\Delta k^\pm \equiv (k^\pm \mp k_0)$ and $\Delta \lambda^\pm \equiv (\lambda^\pm \mp \lambda_0)$. There are no cross-terms because of (3.20). The result is

$$\begin{aligned} \epsilon_\infty &= \frac{1}{2\pi} \int_{-k_0}^{k_0} \epsilon_c(k|\pm k_0, \pm \lambda_0) dk + \frac{\epsilon'_c(k_0)}{2\rho_{\infty c}(k_0)} \rho_{\infty c}(k_0)^2 [\Delta k^{+2} + \Delta k^{-2}] \\ &\quad + \frac{\epsilon'_s(\lambda_0)}{2\rho_{\infty s}(\lambda_0)} \rho_{\infty s}(\lambda_0)^2 [\Delta \lambda^{+2} + \Delta \lambda^{-2}]. \end{aligned} \quad (3.21)$$

We want to express our result in some quantities that are easy to obtain from the Bethe Ansatz solution. The following quantities are the ones that we will use for this purpose:

$$\nu_c \equiv \frac{N_c}{L} = \int_{k^-}^{k^+} \rho_c(k') dk' \quad (3.22a)$$

$$\nu_s \equiv \frac{N_s}{L} = \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda') d\lambda' \quad (3.22b)$$

$$\delta_c \equiv \frac{D_c}{L} = \frac{1}{2} \left\{ z_c(k_\infty^+) + z_c(k_\infty^-) + \int_{k_\infty^-}^{k^-} \rho_c(k') dk' + \int_{k_\infty^+}^{k^+} \rho_c(k') dk' \right\} \quad (3.22c)$$

$$\delta_s \equiv \frac{D_s}{L} = \frac{1}{2} \left\{ z_s(\lambda_\infty^+) + z_s(\lambda_\infty^-) + \int_{\lambda_\infty^-}^{\lambda^-} \rho_s(\lambda') d\lambda' + \int_{\lambda_\infty^+}^{\lambda^+} \rho_s(\lambda') d\lambda' \right\}. \quad (3.22d)$$

We are free to choose the quantities k_∞^\pm and λ_∞^\pm to get as simple an expression as possible. For the Hubbard model we can choose them to lie at the band edges ($k_\infty^\pm = \pm\pi \equiv \pm D$) and at infinity ($\lambda_\infty^\pm = \pm\infty$) as in [14]. When we are interested in the δ -function interacting Fermi gas we use $k_\infty^\pm = \lambda_\infty^\pm = 0$ instead as it is slightly more general.³ It is also a convenient choice when we want to consider the impurity contribution to the finite-size correction later on in this chapter. From (3.2) we get the following relations:

$$z_c(0) = \frac{1}{2\pi} \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda) \theta_{1/2}(\lambda) d\lambda \quad (3.23a)$$

$$z_s(0) = \frac{1}{2\pi} \int_{k^-}^{k^+} \rho_c(k) \theta_{1/2}(\alpha(k)) dk - \frac{1}{2\pi} \int_{\lambda^-}^{\lambda^+} \rho_s(\lambda) \theta_1(\lambda) d\lambda, \quad (3.23b)$$

which are correct to $O(1/L)$ (this is all we need).

Now our construction is almost complete. What is left to do is to express Δk^\pm and $\Delta \lambda^\pm$ in terms of $\Delta \delta_c$, $\Delta \delta_s$, $\Delta \nu_c$ and $\Delta \nu_s$ (where the Δ 's denote the deviations in these quantities from their values in the infinite system). To this end we differentiate the quantities in (3.22). It is enough to compute these quantities with an accuracy of order $O(1/L)$ as they will multiply quantities that are $O(1/L)$. This means that we are allowed to compute them in the infinite system limit, i.e. we employ $\vec{\rho}_\infty$ and use $k^\pm = \pm k_0$ and $\lambda^\pm = \pm \lambda_0$. The derivation that follows is rather straightforward but tedious. To simplify the notation we begin by defining two functions $\vec{\sigma}_1$ and $\vec{\sigma}_2$ which are the solutions of (3.11) with the inhomogeneous parts given by

$$\vec{\sigma}_{10} = \begin{bmatrix} 0 \\ K_{1/2}(\alpha(k_0) - \lambda) \end{bmatrix} \quad \vec{\sigma}_{20} = \begin{bmatrix} \alpha'(k) K_{1/2}(\alpha(k) - \lambda_0) \\ -K_1(\lambda - \lambda_0) \end{bmatrix}. \quad (3.24)$$

³In fact, this choice works also in the Hubbard case. It is possible to carry through the derivation with any symmetrically spaced k_∞^\pm (inside the band) and λ_∞^\pm . The easiest choice might be $k_\infty^\pm = 0$ and $\lambda_\infty^\pm = \pm\infty$.

Note that these are just the columns of the \hat{K} -matrix in (3.11) evaluated at $k' = k_0$ and $\lambda' = \lambda_0$. In addition, we introduce two matrices $\hat{\xi}$ and \hat{Z} with matrix elements satisfying

$$\frac{\partial \nu_c}{\partial k^+} = -\frac{\partial \nu_c}{\partial k^-} = \rho_{\infty c}(k_0) \left(1 + \int_{-k_0}^{k_0} \sigma_{1c}\right) \equiv \rho_{\infty c}(k_0) \xi_{11} \quad (3.25a)$$

$$\frac{\partial \nu_s}{\partial k^+} = -\frac{\partial \nu_s}{\partial k^-} = \rho_{\infty c}(k_0) \int_{-\lambda_0}^{\lambda_0} \sigma_{1s} \equiv \rho_{\infty c}(k_0) \xi_{12} \quad (3.25b)$$

$$\frac{\partial \nu_c}{\partial \lambda^+} = -\frac{\partial \nu_c}{\partial \lambda^-} = \rho_{\infty s}(\lambda_0) \int_{-k_0}^{k_0} \sigma_{2c} \equiv \rho_{\infty s}(\lambda_0) \xi_{21} \quad (3.25c)$$

$$\frac{\partial \nu_s}{\partial \lambda^+} = -\frac{\partial \nu_s}{\partial \lambda^-} = \rho_{\infty s}(\lambda_0) \left(1 + \int_{-\lambda_0}^{\lambda_0} \sigma_{2s}\right) \equiv \rho_{\infty s}(\lambda_0) \xi_{22} \quad (3.25d)$$

$$\begin{aligned} \frac{\partial \delta_c}{\partial k^+} = \frac{\partial \delta_c}{\partial k^-} &= \rho_{\infty c}(k_0) \frac{1}{2} \left(1 + \frac{2}{\rho_{\infty c}(k_0)} \frac{\partial z_c(0)}{\partial k^+}\right) + \int_0^{-k_0} \sigma_{1c} + \int_0^{k_0} \sigma_{1c} \\ &\equiv \rho_{\infty c}(k_0) Z_{11} \end{aligned} \quad (3.26a)$$

$$\begin{aligned} \frac{\partial \delta_s}{\partial k^+} = \frac{\partial \delta_s}{\partial k^-} &= \rho_{\infty c}(k_0) \frac{1}{2} \left(\frac{2}{\rho_{\infty c}(k_0)} \frac{\partial z_s(0)}{\partial k^+}\right) + \int_0^{-\lambda_0} \sigma_{1s} + \int_0^{\lambda_0} \sigma_{1s} \\ &\equiv \rho_{\infty c}(k_0) Z_{12} \end{aligned} \quad (3.26b)$$

$$\begin{aligned} \frac{\partial \delta_c}{\partial \lambda^+} = \frac{\partial \delta_c}{\partial \lambda^-} &= \rho_{\infty s}(\lambda_0) \frac{1}{2} \left(\frac{2}{\rho_{\infty s}(\lambda_0)} \frac{\partial z_c(0)}{\partial \lambda^+}\right) + \int_0^{-k_0} \sigma_{2c} + \int_0^{k_0} \sigma_{2c} \\ &\equiv \rho_{\infty s}(\lambda_0) Z_{21} \end{aligned} \quad (3.26c)$$

$$\begin{aligned} \frac{\partial \delta_s}{\partial \lambda^+} = \frac{\partial \delta_s}{\partial \lambda^-} &= \rho_{\infty s}(\lambda_0) \frac{1}{2} \left(1 + \frac{2}{\rho_{\infty s}(\lambda_0)} \frac{\partial z_s(0)}{\partial \lambda^+}\right) + \int_0^{-\lambda_0} \sigma_{2s} + \int_0^{\lambda_0} \sigma_{2s} \\ &\equiv \rho_{\infty s}(\lambda_0) Z_{22}. \end{aligned} \quad (3.26d)$$

The matrix $\hat{\xi}$ is generally referred to as the “dressed charge” matrix. It is given by the solution to the following matrix integral equation evaluated at $k = k_0, \lambda = \lambda_0$ (or at $k = -k_0, \lambda = -\lambda_0$ due to symmetry):

$$\begin{bmatrix} \xi_{11}(k) & \xi_{12}(k) \\ \xi_{21}(\lambda) & \xi_{22}(\lambda) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \hat{K}^T \otimes \begin{bmatrix} \xi_{11}(k') & \xi_{12}(k') \\ \xi_{21}(\lambda') & \xi_{22}(\lambda') \end{bmatrix}. \quad (3.27)$$

There is a simple relation between the matrices $\hat{\xi}$ and \hat{Z} although it is not obvious at the moment. The derivation of this is not explained very well in [14]

so we will do it more careful here. Start by taking the derivative with respect to k of (3.27) which gives

$$\begin{bmatrix} \xi'_{11}(k) & \xi'_{12}(k) \\ 0 & 0 \end{bmatrix} = \partial_k(\hat{K}^T) \otimes \begin{bmatrix} \xi_{11}(k') & \xi_{12}(k') \\ \xi_{21}(\lambda') & \xi_{22}(\lambda') \end{bmatrix}. \quad (3.28)$$

Using the explicit form of the kernel we can do a partial integration and move the derivative to $\hat{\xi}(k', \lambda')$. Doing the same thing starting with taking a derivative with respect to λ we get the result

$$\begin{aligned} \begin{bmatrix} \xi'_{11}(k) & \xi'_{12}(k) \\ \xi'_{21}(\lambda) & \xi'_{22}(\lambda) \end{bmatrix} &= \hat{K} \otimes \begin{bmatrix} \xi'_{11}(k') & \xi'_{12}(k') \\ \xi'_{21}(\lambda') & \xi'_{22}(\lambda') \end{bmatrix} \\ + \begin{bmatrix} 0 & \alpha'(k)K_{1/2}(\alpha(k) - \lambda') \\ K_{1/2}(\lambda - \alpha(k')) & -K_1(\lambda - \lambda') \end{bmatrix} &\hat{\xi}(k', \lambda') \Big|_{k', \lambda' = -k_0, -\lambda_0}^{k', \lambda' = k_0, \lambda_0}. \end{aligned} \quad (3.29)$$

Note that the partial integration takes \hat{K}^T into \hat{K} . Linearity and the definition of $\bar{\sigma}_{10}$ and $\bar{\sigma}_{20}$ in (3.24) give

$$\begin{aligned} \begin{bmatrix} \xi'_{11}(k) & \xi'_{12}(k) \\ \xi'_{21}(\lambda) & \xi'_{22}(\lambda) \end{bmatrix} &= \\ - ([\bar{\sigma}_1(k, \lambda) & \bar{\sigma}_2(k, \lambda)] - [\bar{\sigma}_1(-k, -\lambda) & \bar{\sigma}_2(-k, -\lambda)]) &\hat{\xi}. \end{aligned} \quad (3.30)$$

Now we can re-integrate the first row from 0 to k_0 and the second from 0 to λ_0 and arrive at

$$\begin{aligned} \hat{\xi}(k_0, \lambda_0) - \hat{\xi}(0, 0) &= -2Z^T \cdot \hat{\xi}(k_0, \lambda_0) \\ + \begin{bmatrix} 1 + \frac{2}{\rho_{\infty c}(k_0)} \frac{\partial z_c(0)}{\partial k^+} & \frac{2}{\rho_{\infty c}(k_0)} \frac{\partial z_s(0)}{\partial k^+} \\ \frac{2}{\rho_{\infty s}(\lambda_0)} \frac{\partial z_c(0)}{\partial \lambda^+} & 1 + \frac{2}{\rho_{\infty s}(\lambda_0)} \frac{\partial z_s(0)}{\partial \lambda^+} \end{bmatrix} &\hat{\xi}(k_0, \lambda_0). \end{aligned} \quad (3.31)$$

Using the fact that $\hat{\xi}(0, 0) = I + \hat{K}^T(0, 0, k', \lambda') \otimes \hat{\xi}$ we find that $\hat{\xi} - \hat{K}^T(0, 0, k', \lambda') \otimes \hat{\xi}$ exactly cancel the second term on the right hand side of (3.31).⁴ Cancelling these terms we arrive at the simple relation

$$\hat{Z}^T \hat{\xi} = 1/2. \quad (3.32)$$

This imply that we get the following rather simple expression for the matrix connecting $[\rho_{\infty c}(k_0)\Delta k^+ \quad \rho_{\infty s}(\lambda_0)\Delta \lambda^+ \quad \rho_{\infty c}(k_0)\Delta k^- \quad \rho_{\infty s}(\lambda_0)\Delta \lambda^-]^T$ and $[\Delta \nu_c \quad \Delta \nu_s \quad \Delta \delta_c \quad \Delta \delta_s]^T$

$$\begin{bmatrix} \hat{\xi} & -\hat{\xi} \\ \hat{Z}^T & \hat{Z}^T \end{bmatrix}^{-1} = \begin{bmatrix} \hat{Z}^T & \hat{\xi} \\ -\hat{Z}^T & \hat{\xi} \end{bmatrix}. \quad (3.33)$$

⁴This statement hides some work. The idea is to make a partial integration in $\hat{K}^T(0, 0, k', \lambda') \otimes \hat{\xi}$ and utilizing the fact that the functions are even. Then one compares this expression with the derivatives of the z 's in (3.23) and find that they are equal.

Using the explicit form of ϵ_1 , ϵ_2 and ϵ' we find that to order $O(1/L)$ we can define Fermi velocities by [14]

$$\begin{aligned} v_c &\equiv \frac{\epsilon'_c(k_0)}{\rho_{\infty c}(k_0)} = -\epsilon_1 \\ v_s &\equiv \frac{\epsilon'_s(\lambda_0)}{\rho_{\infty s}(\lambda_0)} = -\epsilon_2. \end{aligned} \quad (3.34)$$

Putting it all together (using (3.18), (3.21), (3.32), (3.33) and (3.34)) we get our final result

$$\begin{aligned} E &= L\epsilon_{\infty}(\pm k_0, \pm \lambda_0) \\ &+ \frac{v_c}{L} \left[\frac{[\xi_{22}(N_c - \nu_c N) - \xi_{21}(N_s - \nu_s N)]^2}{4(\det\xi)^2} + [\xi_{11}D_c + \xi_{12}D_s]^2 - \frac{1}{12} \right] \\ &+ \frac{v_s}{L} \left[\frac{[\xi_{11}(N_c - \nu_c N) - \xi_{12}(N_s - \nu_s N)]^2}{4(\det\xi)^2} + [\xi_{21}D_c + \xi_{22}D_s]^2 - \frac{1}{12} \right]. \end{aligned} \quad (3.35)$$

3.3 Impurity effects

So far the treatment in this chapter works for the pure δ -function interacting Fermi gas. It is now time to put the impurity back into the system. When we add an impurity of the special kind that we discussed in Chapter 2 this results in the last factors on the right hand side of the BAE in (2.24). We will now show how an extra factor in the BAE contributes to the finite-size correction to the ground state energy. Our treatment here is similar to the one by Fujimoto and Kawakami *et al.* for a class of similar models [28, 29, 30].

Taking the logarithm of the BAE, the impurity contributes to terms in the equation for \vec{z} in (3.1). These end up in the equations for $\vec{\rho}$, i.e. (3.9) will contain additional terms encoding the presence of the impurity. As a result there is an additional term $\vec{\rho}_i/L$ in our solution for $\vec{\rho}$ in (3.14). $\vec{\rho}_i$ is given by the solution to (3.11) with the appropriate inhomogeneous part $\vec{\rho}_{i0}$. Note that in the limit of an infinite system ($L \rightarrow \infty$) this term gives no contribution to the total density $\vec{\rho}$ as it is multiplied by $1/L$.

The part of the density due to the impurity, i.e. $\vec{\rho}_i$, adds an additional term in the expression for the energy in (3.18) of the form

$$\epsilon_i = \vec{\rho}_i^T \otimes \vec{c}_0.$$

This can be rewritten with the the help of the inner-product relation (3.13) as

$$\epsilon_i = \vec{\rho}_{i0}^T \otimes \vec{c}.$$

Expanding this term in Δk^{\pm} and $\Delta \lambda^{\pm}$ we get

$$\epsilon_i = \int_{-k_0}^{k_0} \rho_{ic0}(k') \epsilon_c(k') dk' + \int_{-\lambda_0}^{\lambda_0} \rho_{is0}(\lambda') \epsilon_s(\lambda') d\lambda' + O\left(\frac{1}{L^2}\right), \quad (3.36)$$

where we used the fact that Δk^\pm and $\Delta \lambda^\pm$ is of order $(1/L)$. The $O(1/L)$ contribution vanishes because the dressed energy is zero at the Fermi points (3.20). Hence we can write

$$\epsilon_i = \epsilon_i(\pm k_0, \pm \lambda_0) + O\left(\frac{1}{L^2}\right) \equiv \epsilon_{i\infty} + O\left(\frac{1}{L^2}\right). \quad (3.37)$$

The impurity also gives a contribution to the quantities $(N_c, N_s, D_c$ and $D_s)$ that we use in the finite-size correction formula above (3.35). It is easy to see that the changes in these induced by the impurity are given by

$$\Delta N_{ic} = \int_{-k_0}^{k_0} \rho_{ic}(k') dk' \quad (3.38a)$$

$$\Delta N_{is} = \int_{-\lambda_0}^{\lambda_0} \rho_{is}(\lambda') d\lambda' \quad (3.38b)$$

$$D_{ic} = z_{ic}(0) + \frac{1}{2} \left(\int_0^{k_0} \rho_{ic}(k') dk' + \int_0^{-k_0} \rho_{ic}(k') dk' \right) \quad (3.38c)$$

$$D_{is} = z_{is}(0) + \frac{1}{2} \left(\int_0^{\lambda_0} \rho_{is}(\lambda') d\lambda' + \int_0^{-\lambda_0} \rho_{is}(\lambda') d\lambda' \right). \quad (3.38d)$$

Thus we can conclude that the contribution of the impurity to the energy of the system to order $O(1/L)$ consists of two parts. First an additional term in (3.35) given by $\epsilon_{i\infty}$. Second the impurity induces a change in the parameters in the $1/L$ -term of (3.35) that is given by (3.38).

3.4 The dressed charge

In some limits it is possible to get a more explicit form of the dressed charge matrix. For example, in the important special case of no macroscopic magnetization we get $\lambda_0 = \infty$ and we can use a Fourier transform to solve the integral equation. The evaluation of ξ_{21} and ξ_{22} requires Wiener-Hopf techniques [31]. The form of the matrix is then [14]

$$\begin{bmatrix} \xi_{11} & \xi_{12} \\ \xi_{21} & \xi_{22} \end{bmatrix} = \begin{bmatrix} \xi & \xi/2 \\ 0 & 1/\sqrt{2} \end{bmatrix}. \quad (3.39)$$

Here $\xi \equiv \xi(\alpha(k_0))$, where $\xi(l)$ is the solution to the integral equation

$$\xi(l) = 1 + \int_{\alpha(-k_0)}^{\alpha(k_0)} dk' \tilde{K}(l-k') \xi(k'), \quad (3.40)$$

where the kernel is given by

$$\tilde{K}(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-c|\omega|}}{1 + e^{-c|\omega|}} e^{i\omega x}.$$

This gives the final form of the finite-size spectrum of the δ -function interacting Fermi gas with an impurity of the form discussed above:

$$E = L\epsilon_\infty + \epsilon_{i_\infty} + \frac{1}{L} \left[v_c \left(\frac{\Delta N_c^2}{4\xi^2} + \xi^2 [D_c + D_s]^2 - \frac{1}{12} \right) + v_s \left(\frac{(\Delta N_c - 2\Delta N_s)^2}{4} + \frac{1}{2} D_s^2 - \frac{1}{12} \right) \right]. \quad (3.41)$$

The leading impurity contribution is the ϵ_{i_∞} -term. The impurity also affects the parameters in the $1/L$ -term as discussed below equation (3.38).

This expression (or more generally, the one in (3.35) plus ϵ_{i_∞}) for the finite-size spectrum is the one that we will use in the next chapter. The explicit form of v_c and v_s can also be obtained as the solution of similar integral equations as the one in (3.40). In some limits it is also possible to evaluate ξ explicitly with the help of Wiener-Hopf techniques [14].

Chapter 4

Persistent currents

The effect of persistent currents in superconducting samples is well known. You have probably heard the story of the superconducting ring in the cellar that has been there for years, upholding a current that is not attenuated.

Less well known is probably the possibility to have a persistent current in a normal metal ring. In this case you have to pierce it with a magnetic flux¹ to induce a steady current in the ring. It is also necessary to work at sufficiently low temperature and with a small enough ring. The effect is possible if the phase information can be transported around the ring. This means that the phase coherence length of the electronic wave-function must be larger than the size of the ring. For this to be possible a small sample is needed and the temperature has to be low enough, otherwise thermal fluctuations remove the effect.

The effect was predicted theoretically in the early eighties although the earlier treatment of the superconducting case also mentioned the possibility of having a persistent current in a normal metal. The first experimental verification of the reality of the effect was accomplished in the early nineties [32]. An excellent review on the subject is the one by Zvyagin and Krive [7]. Another good reference for the interested reader is Chapter 8 in the book by Efetov [6]. These references include references to the original papers and experiments. After this general introduction let us go on and study the origin of the effect.

4.1 Free electrons

The easiest case to start with is the one with spin-less, non-interacting fermions. As we are interested in an isolated ring we let the number of fermions in the

¹It is also possible to drive the current with a “spin flux” describing the effect of piercing the ring with a charged wire. This case is referred to as the Aharonov-Casher effect [33] and gives a spin-dependent current. This effect has not yet been shown to exist experimentally.

ring be fixed. The Hamiltonian is then given by

$$H = \sum_{j=1}^N \epsilon_j = \frac{1}{2} \sum_{j=1}^N k_j^2, \quad (4.1)$$

in units where $\hbar = 1$ and $m = 1$. The energy spectrum is usually determined by imposing periodic boundary conditions on the system as $\psi(x_j + L) = \psi(x_j)$. This is also the natural thing to do in a 1D ring. When the ring encloses a magnetic flux, the effect of this (i.e. the Aharonov-Bohm effect [34]) can be encoded as twisted boundary conditions via a gauge transformation as [35]

$$\psi(x_j + L) = \psi(x_j)e^{i\varphi}, \quad (4.2)$$

where $\varphi = 2\pi \frac{\Phi}{\Phi_0} \equiv 2\pi\varphi_e$. Φ denotes the magnetic flux that is piercing the ring, while Φ_0 is the quantum flux unit given by $hc/|e|$. It is apparent from this that everything is periodic in the flux with period Φ_0 .

The eigenfunctions of the Hamiltonian are just plane waves. The twisted boundary conditions imply that the momenta are given by $k_j L = 2\pi(n_j + \varphi_e)$. Hence the total energy of our system is given by

$$E = \sum_j \epsilon_j = \frac{2\pi^2}{L^2} \sum_j (n_j + \varphi_e)^2. \quad (4.3)$$

To find the ground state of our system we should simply find the set of integers $\{n_j\}$ that minimize the energy. This is rather straightforward but gives different formulas whether there are an odd or an even number of particles. For odd N , the correct choice is $\{n_j\} = \{-(N-1)/2, \dots, (N-1)/2\}$ for $-1/2 < \varphi_e < 1/2$. For even N the correct choice is to take $\{n_j\} = \{-N/2, \dots, N/2-1\}$ for $0 < \varphi_e < 1$. We use different intervals (for φ_e) in the two cases because this gives a unique set of integers for the full interval. If we take the interval $-1/2 < \varphi_e < 1/2$ for the even case the choice of the integers change whether φ_e is greater than or smaller than zero. With the help of the periodicity we can easily extend the result to arbitrary φ_e so the choice of the interval does not matter.

To see that the flux results in a current we note that equation (4.2) is analogous to a Bloch state with crystal (quasi-) momentum φ/L where the elementary cell is the whole ring. The velocity of the j th electron is given by its group velocity $v_{gj} = L\partial_\varphi \epsilon_j$. Since each electron carries the charge density $-e/L$, we can sum up the contribution from all electrons and hence arrive at the general formula for the persistent current

$$I = -e \frac{\partial E}{\partial \varphi}. \quad (4.4)$$

It is possible to put back the standard SI units; this gives the formula $I = -c \frac{\partial E}{\partial \Phi}$, where c is the speed of light. Note that we only used equation (4.2) and the group-velocity argument to arrive at the formula (4.4), hence we expect it to

hold for an arbitrary dispersion relation. Using this formula and the explicit values of the integers $\{n_j\}$ above we get the following characteristic sawtooth pattern for the persistent current

$$I_{even} = -I_0(\varphi_e - 1/2) \quad 0 < \varphi_e < 1 \quad (4.5a)$$

$$I_{odd} = -I_0\varphi_e \quad -1/2 < \varphi_e < 1/2, \quad (4.5b)$$

where $I_0 \equiv e(2\pi N/L^2)$. Note also that I_0 can be written as $2ev_f/L$ to order $O(1/N)$, where $v_f = \pi N/L$ is the Fermi velocity. The result is plotted in Figure 4.1. The difference between the persistent currents for an even and an odd number of fermions is usually referred to as the *parity effect*.

Figure 4.1: Persistent current for spin-less free fermions.

It is now straightforward to treat spin-full electrons in our simple model. The effect of the spin is just to make every state doubly degenerate. Then we get four different cases depending on the number of particles. For $N_e = 4M$ we use twice (each level holds two electrons) the even case above with $N = N_e/2$. The case $N_e = 4M + 2$ corresponds to twice the odd case above with $N = N_e/2$. The cases $N_e = 4M + 1$ and $N_e = 4M + 3$ are also straightforward to evaluate but now we get a period halving. The reason for this is that the best choice for the last odd integer (e.g. n_{N_e}) to minimize the energy changes with the flux. The result is that the persistent current in this case is just the sum of the even and odd spin-less cases.² Summarizing the case of free spin-full electrons we get

²Consider the interval $0 < \varphi_e < 1/2$. The best choice for the integers for $N_e = 4M$ is then $\{n_j\} = 2 \times \{-2M, \dots, 2M-1\}$, while for $N_e = 4M+2$ it is $\{n_j\} = 2 \times \{-2M, \dots, 2M\}$. Thus it is natural that the best choice for $N_e = 4M+1$ is $\{n_j\} = 2 \times \{-2M, \dots, 2M-1\} \cup \{2M\}$. This is just the sum of the even and odd spin-less cases. The treatments of the interval $-1/2 < \varphi_e < 0$ and the case $N_e = 4M+3$ are similar.

the persistent currents

$$I_{4M} = -I_0(\varphi_e - \frac{1}{2}) \quad 0 < \varphi_e < 1 \quad (4.6a)$$

$$I_{4M+2} = -I_0\varphi_e \quad -1/2 < \varphi_e < 1/2 \quad (4.6b)$$

$$I_{4M+3} = I_{4M+1} = -I_0(\varphi_e \mp 1/4) \quad 0 < \pm\varphi_e < 1/2, \quad (4.6c)$$

which are correct to $O(I_0/M)$. Note that $I_0 = 4\epsilon v_f/L$ to order $O(1/N_e)$ and hence varies with N . The results are shown in Figure 4.2 where we ignore the small difference in I_0 for the different cases (i.e. we put $v_f(4M) = v_f(4M+1)$ etc.).

Figure 4.2: Persistent current for spin-full free fermions.

4.2 Impurity effects

The case of a quadratic spectrum and a localized non-magnetic impurity can be solved exactly by the use of the transfer matrix method. The original treatment is by Gogolin and Prokof'ev [8]. We point out that the result is more general than the one presented here and is claimed to hold for an arbitrary dispersion relation.

The Hamiltonian of the problem is taken to be a modification of the non-interacting case above in (4.1)

$$H = \frac{1}{2} \sum_j k_j^2 + V(x_j), \quad (4.7)$$

where $V(x)$ is an impurity potential. We assume that the impurity is localized within $|x| < a < L$. For simplicity we assume that $a \ll L$ so that the phase shift induced by the impurity is small (this is actually unimportant as discussed in [8]).

If we have spin-less fermions we can start by solving the one-particle problem. The general form of energy eigenfunction is given by

$$\Psi = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ Ce^{ikx} + De^{-ikx} & x > a, \end{cases} \quad (4.8)$$

where $k \geq 0$. We have explicitly included the back-scattering terms allowed by energy conservation. The coefficients are related by the transfer matrix $\hat{T}(k)$ which is defined by

$$\begin{bmatrix} C \\ D \end{bmatrix} = \hat{T} \begin{bmatrix} A \\ B \end{bmatrix}.$$

Here we will use the scattering matrix $\hat{S}(k)$ instead because it is easier to apply symmetry arguments to it. It is defined by

$$\begin{bmatrix} B \\ C \end{bmatrix} = \hat{S} \begin{bmatrix} A \\ D \end{bmatrix}. \quad (4.9)$$

This matrix is unitary because of probability conservation and symmetric because of time reversal symmetry. These statements are easy to prove (see e.g. [36]). It follows that we can write

$$\hat{S}(k) = \begin{bmatrix} \sqrt{1-T(k)}e^{i\alpha(k)} & \sqrt{T(k)}e^{i\delta(k)} \\ \sqrt{T(k)}e^{i\delta(k)} & \sqrt{1-T(k)}e^{i\beta(k)} \end{bmatrix}, \quad (4.10)$$

where in addition $e^{i(\alpha+\beta)} = -e^{2i\delta}$. The forward scattering solution is defined by C when $D = 0$, i.e. $C = \sqrt{T}e^{i\delta}A$.

Imposing twisted boundary conditions on our wave-function we get the eigenvalue equation

$$\begin{bmatrix} 0 & e^{ikL}e^{i\varphi} \\ e^{ikL}e^{-i\varphi} & 0 \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} = \hat{S}(k) \begin{bmatrix} A \\ D \end{bmatrix}. \quad (4.11)$$

Solving the quadratic secular equation for e^{ikL} we get

$$kL = 2\pi n + \delta(k) \pm \cos^{-1}(\sqrt{T(k)} \cos \varphi) \equiv 2\pi n + \Phi_{\pm}(k, \varphi). \quad (4.12)$$

Note that the case $n = 0$ only gives the Φ_+ -solution since we assumed $k > 0$.³ Expanding k in $1/L$ yields

$$k = x + \frac{1}{L}\Phi_{\pm}(x, \varphi) + \frac{1}{L^2}\Phi_{\pm}(x, \varphi) \frac{\partial \Phi_{\pm}(x, \varphi)}{\partial x} + O\left(\frac{1}{L^3}\right), \quad (4.13)$$

³Another way to look at it is that there is only one state that evolves from $n = 0$ as the flux is applied. For $n \neq 0$ the state we start out with contains two degenerate states, one left-going and one right-going. The applied flux splits these into two with unequal momenta. The analog in the free case is that for the right-going state $k_r \rightarrow k_r + \varphi$, while for the left-going state $-k_l \rightarrow -k_l + \varphi$. Thus when $k_r = k_l = k$ we start with two degenerate energy states which splits into two, with absolute values of the momenta $k + \varphi$ and $k - \varphi$ after the flux is applied.

where $x = 2\pi n/L$. Assuming that the number of electrons on the ring is odd (i.e. N_e is odd) we can easily sum up the contributions to get the total energy

$$E(\varphi) = \frac{1}{2} \sum_j k_j^2 = \sum_x \left[x^2 + \frac{2x}{L} \delta(x) + \frac{1}{2L^2} \frac{\partial}{\partial x} \left(x \sum_{\pm} \Phi_{\pm}(x, \varphi)^2 \right) \right] - \frac{1}{2L^2} \Phi_-(0, \varphi)^2 + \sum_x O(1/L^3). \quad (4.14)$$

The flux contribution to the energy is then

$$\Delta E(\varphi) = E(\varphi) - E(0) = \sum_{x=2\pi n/L} \left[\frac{1}{2L^2} \frac{\partial}{\partial x} \left(x \sum_{\pm} \Phi_{\pm}(x, \varphi)^2 - \Phi_{\pm}(x, 0)^2 \right) \right] + \frac{1}{2L^2} (\Phi_-(0, 0)^2 - \Phi_-(0, \varphi)^2) + \sum_{x=2\pi n/L} O(1/L^3). \quad (4.15)$$

Converting the sum into an integral gives the integral of a perfect derivative plus some small corrections. Using the explicit form of Φ_{\pm} we get

$$\Delta E(\varphi) = \frac{v_f}{2\pi L} \left[(\cos^{-1}[\sqrt{T_f} \cos \varphi])^2 - (\cos^{-1}[\sqrt{T_f}])^2 \right] + O\left(\frac{1}{L^2}\right), \quad (4.16)$$

where $T_f = T(k_f)$ is the transmission amplitude at the Fermi energy. Turning to the formula (4.4) for the persistent current we get

$$I_{odd} = -e \frac{v_f}{\pi L} \frac{\sqrt{T_f} \sin \varphi}{\sqrt{1 - T_f \cos^2 \varphi}} \cos^{-1}[\sqrt{T_f} \cos \varphi], \quad (4.17)$$

which is correct to $O(1/L)$. It is reassuring to see that taking the limit $T \rightarrow 1$ results in the free-fermion case above in (4.5b). The even particle case gives an additional unpaired particle on top of the spectrum. This results in an additional contribution to the current:

$$I_{even} = I_{odd} + e \frac{v_f}{L} \frac{\sqrt{T_f} \sin \varphi}{\sqrt{1 - T(k_f) \cos^2 \varphi}}. \quad (4.18)$$

Taking the limit $T \rightarrow 1$ again gives us back the free-fermion case in (4.5a).

In the case of a pure δ -function scatterer we have that $T_f = k_f^2 / (k_f^2 + J'^2)$. Thus $T_f \rightarrow 0$ as the strength of the scatterer goes to infinity. This results in a vanishing persistent current. One might worry that this is not the case in the Bethe Ansatz solution of the similar problem we mentioned in the first section, i.e. a non-magnetic impurity corresponding to $J = 0$ in (2.23). The reason for this is the counter-term at the origin. This term allows for the Bethe Ansatz wave-function where each particle has a definite momentum and hence no back-scattering is present. Thus in this case $T_f = 1$ and the persistent current is not affected by the scatterer, even in the case of a very strong scatterer. This means that the counter-term V_{cc} is indeed important.

4.3 Interacting particles and the BAE

The simple picture of non-interacting particles is often not satisfactory to describe real phenomena, especially in 1D. For instance we know that electrons interact through the Coulomb force. It is then natural to ask how the interaction between the particles changes the nature of the persistent current. We can find some indications of what the interaction effect can be by studying the δ -function interacting (repulsive) Fermi gas. In this crude model of a real electron system we can answer the question of the interaction effect via the exact Bethe Ansatz solution. We follow here the equivalent discussion for the Hubbard model originally due to Yu and Fowler [10]. In [37] Schlottmann treats the δ -function interacting Fermi gas extensively.

Since persistent currents is a small effect ($\propto 1/L$), it is not accurate enough to take the thermodynamic limit $L \rightarrow \infty$. Luckily, the finite-size corrections to the ground-state energy that we worked out in the previous chapter is just what we need to proceed. Note that adding the Aharonov-Bohm flux is equivalent to shift all the charge quantum numbers by the same amount φ_e . This just affects D_c in the formula (3.35) (or (3.41)) where we let $D_c \rightarrow D_c + \varphi_e$. The finite-size correction to the ground state energy that is flux dependent is thus given by

$$\Delta E(\varphi) = \frac{1}{L} v_c [\xi_{11} D_c + \xi_{11} \varphi_e + \xi_{12} D_s]^2 + \frac{1}{L} v_s [\xi_{21} D_c + \xi_{21} \varphi_e + \xi_{22} D_s]^2. \quad (4.19)$$

Using our expression (4.4) for the persistent current we get

$$I(\varphi) = -\frac{e}{\pi L} (\xi_{11} v_c [\xi_{11} D_c + \xi_{11} \varphi_e + \xi_{12} D_s] + \xi_{21} v_s [\xi_{21} D_c + \xi_{21} \varphi_e + \xi_{22} D_s]). \quad (4.20)$$

The parity effect is readily incorporated by the choices of D 's in the ground state; for a discussion of this procedure in the case of the Hubbard model, see [10]. The possibility to adjust the D 's to minimize the energy when the flux is applied gives rise to level crossings. Similarly to the case of non-interacting particles, this results in a saw-tooth pattern for the persistent current with period Φ_0 or $\Phi_0/2$.

It is possible to get a more explicit expression for the ξ -matrix in the limit of strong and weak coupling [14]. It turns out that the limit of strong coupling is a bit tricky and must be treated with care. We remind the reader that in the derivation of the finite-size correction, the distribution of the k 's and the λ 's are treated as dense when $L \rightarrow \infty$. When L is large but not infinite this is still a viable assumption for the distribution of the k 's. In the limit of large coupling (c) the spacing between the λ 's are of the order of c . Thus for the solutions to be dense the relation $c/L \ll 1$ must be fulfilled. Thus keeping L fixed and letting $c \rightarrow \infty$ is not allowed in the derivation. In this case, however, all the k 's are small compared to all the λ 's (except for maybe one single λ that can lie between $-k_0$ and k_0). This means that we can do a Taylor expansion directly in the logarithm of the BAE in (3.1), treating $\alpha(k)/\lambda = k/\lambda$ as small.

The crudest approximation is to neglect all α 's. This leads to

$$k_j L = 2\pi \left(n_j + \varphi_e + \frac{1}{N_e} \sum_{\gamma} J_{\gamma} \right).$$

The ground state of this system is highly degenerate because there are many ways to choose the J 's to arrive at the same value for their sum. This allows for the spin system (i.e. the J 's) to compensate for the flux in order to minimize the energy of the system. This induces “microscopic oscillations” in the persistent current. The period of the oscillations is Φ_0/N_e . The nature of the case of very large but finite repulsion is treated in [10]. These authors show how the perturbation of $O(\alpha/c)$ gives the true nature of the ground state for strong repulsion (for infinite repulsion the ground state is highly degenerate); in particular they compute the form of the spin subsystem when the flux is applied.

The microscopic oscillations also affect the overall magnitude of the persistent current. It is attenuated by a factor of $1/N$ because of the many level crossings. This means that the current vanishes to $O(1/L)$ since $N \propto L$ when the density of electrons is constant. Thus strong repulsion can make the persistent current disappear.

4.4 Magnetic impurity in a system of interacting particles

In the previous sections we have treated the non-interacting case with and without a non-magnetic impurity, as well as the δ -function interacting Fermi gas. What we really would like to do next is to treat the case of non-interacting (or interacting) fermions *and* a magnetic impurity. This is a hard problem. The essence of the Kondo effect is that a magnetic impurity induces an effective interaction between the electrons. Due to the extra degree of freedom that the spin of the impurity introduces, the order in which particles scatter off the impurity matters. One way to encode this is to use the Bethe Ansatz solution to the problem [22]. However, when we want to compute the persistent current from this solution we run into some problems. First, using the definition of the persistent current above in (4.4), the linear spectrum gives no variation of the current with the flux. Second, in the ring there are both left- and right-movers. Thus we would need two different kinds of particles, both interacting with the impurity. One way of getting around this problem is to define even and odd parity channels as in [38], with only the even parity channel coupling to the impurity. These authors also use another definition of the persistent current that is supposed to be valid in the case of a linear dispersion. This solution is rather limited, however, because it is valid only in the neighborhood of some discrete values of the flux. What will happen when one moves away from these values of the flux is not clear, although it is argued on physical grounds that the obtained formula is valid for any (small) value of the flux. The effect of level crossings could be very important for the conclusions about the overall magnitude of the

persistent current. The δ -function interacting Fermi gas in the limit of strong coupling discussed in the preceding section illustrates the point.

It would be nice if it was possible to use an arbitrary dispersion instead. Even the simplest case of non-interacting fermions with a magnetic impurity and a quadratic dispersion we don't know how to solve. The electron-electron interaction has to be written down explicitly in the Hamiltonian (as we have done in (2.23)) and can not be induced by the impurity as is the case for the linear dispersion.

Let us now concentrate on the simpler problem of the special cases discussed throughout the thesis with a ferromagnetic impurity in a repulsive δ -function interacting Fermi gas. For these models we already have the explicit Bethe Ansatz solutions; and we can almost immediately write down the result for the persistent current using the finite-size result for the case with an impurity obtained in Section 3.3.

An artifact of the Bethe Ansatz solution in these cases is the presence of the counter-term at the origin (V_{cc} in (2.23)). This is needed because we must require that there is no presence of back-scattering off the impurity for the Bethe Ansatz construction to work. The importance of this term is easily seen in the case of a non-magnetic impurity. As we discussed above the pure δ -function scatterer and that with the additional counter-term give very different behavior for the persistent current in the limit of strong coupling.

Anyway, we can at least solve two special cases with a magnetic impurity and a quadratic dispersion. The easiest case is the one where $J' = -J$. In this case the BAE are given by (2.24):

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{k_j - \Lambda_\gamma + ic/2}{k_j - \Lambda_\gamma - ic/2} \quad (4.21a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \prod_{j=1}^N \frac{\Lambda_\gamma - k_j - ic/2}{\Lambda_\gamma - k_j + ic/2} \left(\frac{\Lambda_\gamma - ic/2}{\Lambda_\gamma + ic/2} \right). \quad (4.21b)$$

Bound electrons would correspond to k 's with an imaginary part. It is easily seen that inserting a k with an imaginary part into these equations cannot give a solution. Thus all the k 's are real and we can conclude that no bound electron states exist.

Now we can apply the results for the finite-size corrections to the ground state energy that we worked out in the last chapter. Again we let $D_c \rightarrow D_c + \varphi_e$ in the finite-size correction formula (3.35). Since $\epsilon_{i\infty}$ is independent of the flux the flux-dependent part of the energy is the same as for the pure δ -function interacting gas above. This implies that the result for the persistent current is again given by (4.20). The only effect of the impurity is to change $D_c \rightarrow D_c + D_{ic}$ and $D_s \rightarrow D_s + D_{is}$. D_{ic} and D_{is} are given by (3.38) where $\vec{\rho}_i$ is computed from (3.11) with the inhomogeneous part given by

$$\vec{\rho}_{i0} = \begin{bmatrix} 0 \\ K_{1/2}(\lambda) \end{bmatrix}.$$

However, since we are working with $k^\pm = \pm k_0$ and $\lambda^\pm = \pm \lambda_0$ we find that $\vec{\rho}_i$ is an even function. This implies (via 3.38 and 3.23) that $D_{ic} = D_{is} = 0$. Hence we can conclude that our impurity does not affect the persistent current.

In the other special case $J' = 3J$, the BAE in (2.24) allows for two complex momenta. Physically this means that two electrons are allowed to bind to the impurity (c.f. [20]). This is also what happens in the ground state since this minimizes the energy of the system. An approximative treatment of these bound electrons correct to order e^{-cL} is to have two complex momenta: $k = \pm ic$. Inserting these into the BAE in (2.24) we arrive at the following BAE for the remaining $(N - 2)$ real momenta:

$$e^{ik_j L} = \prod_{\gamma=1}^M \frac{k_j - \Lambda_\gamma + ic/2}{k_j - \Lambda_\gamma - ic/2} \left(\frac{k_j - ic}{k_j + ic} \right) \quad (4.22a)$$

$$\prod_{\delta=1, \delta \neq \gamma}^M \frac{\Lambda_\gamma - \Lambda_\delta - ic}{\Lambda_\gamma - \Lambda_\delta + ic} = \prod_{j=1}^{N-2} \frac{\Lambda_\gamma - k_j - ic/2}{\Lambda_\gamma - k_j + ic/2} \left(\frac{\Lambda_\gamma - i3c/2}{\Lambda_\gamma + i3c/2} \right). \quad (4.22b)$$

Now we are ready to use the finite-size correction formula. Once again we have a δ -function interacting Fermi gas with impurity terms so the persistent current is given by (4.20).⁴ The contribution from the impurity takes the same form as in the case above. Reading off the contributions from our BAE we find that in this case $\vec{\rho}_i$ is given by the solution to (3.11) when the inhomogeneous part is

$$\vec{\rho}_{i0} = \begin{bmatrix} K_1(k) \\ K_{3/2}(\lambda) \end{bmatrix}.$$

This is also an even function, hence $D_{ic} = D_{is} = 0$. Thus the impurity does not affect the persistent current in this case either.

We can finally conclude that starting with a repulsive δ -function interacting Fermi gas and a quadratic spectrum the inclusion of our kind of impurity does not alter the behavior of the persistent current. Hence the persistent current with or without the impurity is given by

$$I(\varphi) = -\frac{e}{\pi L} (\xi_{11} v_c [\xi_{11} D_c + \xi_{11} \varphi_e + \xi_{12} D_s] + \xi_{21} v_s [\xi_{21} D_c + \xi_{21} \varphi_e + \xi_{22} D_s]). \quad (4.23)$$

4.5 Conclusion

Persistent currents is an interesting effect. There is still a controversy as to the question of what will happen to the persistent current when one couples a magnetic impurity (i.e. a quantum dot in the Kondo regime) to a mesoscopic ring. Different approaches seems to give different results. This is probably due to the smallness of the effect which leads to an extreme sensitivity to approximations employed to compute it.

⁴We ignore the difference between N and $N - 2$ electrons since this just gives a correction of $O(1/N)$ to v_c , v_s and the elements of $\hat{\xi}$. There are no other changes that affects the flux-dependent part of the energy.

In this thesis we have presented the exact Bethe Ansatz solution to a model with a kind of ferromagnetic impurity that is inserted into a repulsive δ -function interacting Fermi gas with a quadratic dispersion relation. We then studied the persistent current in a ring described by this model. The result is that the impurity does not affect the persistent current. The persistent current is the same as for the pure δ -function interacting Fermi gas without the ferromagnetic impurity.

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Appendix A

The Second Euler-Maclaurin Formula

This appendix contains a sketchy derivation of the Second Euler-Maclaurin formula and the form of it that is used to obtain the finite-size corrections in this thesis. The Euler-Maclaurin formula is usually given as (see e.g. [31])

$$\int_a^b f(x)dx = h \left[\frac{1}{2}f(a) + f(a+h) + \dots + f(b-h) + \frac{1}{2}f(b) \right] - \frac{B_2 h^2}{2!} f'(x)|_a^b - \frac{B_4 h^4}{4!} f'''(x)|_a^b - \dots, \quad (\text{A.1})$$

where B_n are the Bernoulli numbers. This form is convenient for approximating an integral with a sum. Note that the series is only asymptotically convergent. In our case we want to approximate a sum with an integral, while having control over the size of the induced error. For this purpose we rewrite the formula with step size h and $h/2$ as

$$h \left[\frac{1}{2}f(a) + f(a+h) + \dots + f(b-h) + \frac{1}{2}f(b) \right] = \int_a^b f(x)dx + \frac{B_2 h^2}{2!} f'(x)|_a^b + \frac{B_4 h^4}{4!} f'''(x)|_a^b + \dots \quad (\text{A.2a})$$

$$\frac{h}{2} \left[\frac{1}{2}f(a) + f(a + \frac{h}{2}) + \dots + f(b - \frac{h}{2}) + \frac{1}{2}f(b) \right] = \int_a^b f(x)dx + \frac{B_2 h^2}{2^2 2!} f'(x)|_a^b + \frac{B_4 h^4}{2^4 4!} f'''(x)|_a^b + \dots \quad (\text{A.2b})$$

Two times the second equation minus the first gives the Second Euler-Maclaurin formula

$$\begin{aligned}
h [f(a + h/2) + f(a + 3h/2) + \dots + f(b - h/2)] = \\
\int_a^b f(x) dx - (1 - \frac{1}{2}) \frac{B_2 h^2}{2!} f'(x)|_a^b - (1 - \frac{1}{2^3}) \frac{B_4 h^4}{4!} f'''(x)|_a^b - \dots \approx \\
\int_a^b f(x) dx - \frac{h^2}{24} f'(x)|_a^b, \quad (\text{A.3})
\end{aligned}$$

where in the last step we have only kept the leading correction and use $B_2 = 1/6$. The sums that we are interested in are of the form

$$\sum_n f(k_n) = \sum_{I_n=I^-}^{I^+} f(z^{-1}(\frac{I_n}{L})).$$

Thus we can take $h = 1/L$ and define k^\pm such that $z(k^\pm) = (I^\pm \pm 1/2)/L$. Then, using $dx = z'(k)dk \equiv \rho(k)dk$ and $\partial_x z^{-1}(x) = 1/z'(x)$, we arrive at the desired form of the formula:

$$\frac{1}{L} \sum_n f(k_n) \approx \int_{k^-}^{k^+} \rho(k) f(k) dk + \frac{1}{24L^2} \left[\frac{f'(k)}{\rho(k)} \right]_{k^+}^{k^-}. \quad (\text{A.4})$$

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