Two-Hole Bound States from an Effective Field Theory for Magnons and Holes in an Antiferromagnet on the Honeycomb Lattice

Masterarbeit

der Philosophisch-naturwissenschaftlichen Fakultät
der Universität Bern

vorgelegt von

Marcel Wirz

2009

Leiter der Arbeit

Prof. Dr. Uwe-Jens Wiese
Institut für Theoretische Physik, Universität Bern
Abstract

In this thesis a systematic low-energy effective field theory for magnons and holes in an antiferromagnet on the honeycomb lattice is constructed analogous to baryon chiral perturbation theory (BχPT). The Hubbard model serves as an underlying microscopic model. We show that the leading action of the pure magnon sector is the same as in the square lattice case. Using the effective theory, we derive the one-magnon exchange potentials. With these potentials, we investigate the Schrödinger equation describing the relative motion of two holes in an otherwise undoped antiferromagnet. We derive the radial solution of this Schrödinger equation for a special case analytically and find that the magnon-mediated forces lead to two-hole bound states under a condition on the low-energy constants.

Also the weak coupling limit of the Hubbard model is investigated. In this context we derive the energy-momentum relation in the zero coupling limit, where massless Dirac fermions arise. In addition to deriving their velocity, we construct the leading terms of the corresponding effective Lagrangian.
## Contents

1 Introduction 1

2 The Honeycomb Lattice 5  
   2.1 A Bipartite Non-Bravais Lattice .......................... 5  
   2.2 Symmetries of the Honeycomb Lattice ......................... 7  
      2.2.1 Shift Symmetries $D_i$ .......................... 7  
      2.2.2 Rotation $O$ and Reflection $R$ Symmetries .............. 7  

3 The underlying Microscopic Models and their Symmetries 9  
   3.1 The Hubbard Model ........................................... 9  
   3.2 The $t$-$J$ Model ............................................ 10  
   3.3 The Quantum Heisenberg Model ............................... 10  
   3.4 The Strong Coupling Limit of the Hubbard Model and how it leads to Anti-ferromagnetism ............................................ 11  
   3.5 Symmetries of the Hubbard Model ............................. 11  
      3.5.1 $SU(2)_s$ Spin Rotation Symmetry ......................... 11  
      3.5.2 $U(1)_Q$ Fermion Number Symmetry ......................... 12  
      3.5.3 Discrete Symmetries $D_i$, $O$, $O'$, and $R$ ...... 12  
      3.5.4 Non-Abelian Extension of the $U(1)_Q$ Symmetry to $SU(2)_Q$ 13  
   3.6 Manifestly $SU(2)_s \otimes SU(2)_Q$ Invariant Formulation of the Hubbard Model 13  

4 Investigation of the Free Fermion Model 15  
   4.1 The Weak Coupling Limit of the Hubbard Model and how it leads to Massless Dirac Fermions ............................................ 15  
   4.2 Effective Field Theory for Dirac Fermions ....................... 19  
      4.2.1 Fermion Fields ............................................ 19  
      4.2.2 Effective Lagrangian ...................................... 21  

5 Magnons 25  
   5.1 Spontaneous Symmetry Breaking ................................ 25  
   5.2 Effective Theory for Magnons ................................ 26  
   5.3 Non-linear Realization of the $SU(2)_s$ Symmetry ............... 28  
   5.4 Composite Magnon Field $v_\mu(x)$ ............................ 30  

6 From Microscopic Operators to Effective Fields for Holes 35  
   6.1 Fermion Operators with a Sublattice Index ..................... 35  
   6.2 Fermion Fields with a Sublattice Index ........................ 36
6.3 Fermion Fields with a Sublattice and Momentum Index 38
6.4 Hole Fields 40

7 Effective Field Theory for Magnons and Holes 43
7.1 Effective Action for Magnons and Holes 43
7.2 Accidental Emergent Symmetries 45
   7.2.1 Galilean Boost Symmetry \( G \) 45
   7.2.2 Continuous \( O(\gamma) \) Rotation Symmetry 46

8 One-Magnon Exchange Potentials 47
8.1 One-Magnon Action 47
8.2 Kinematics 48
8.3 Transforming to Momentum Space 49
8.4 Principle of Stationary Action 50
8.5 Potentials in Momentum Space 51
8.6 Potentials in Position Space 52

9 Two Hole Bound States 55
9.1 Corresponding Schrödinger Equation 55

10 Conclusions and Outlook 59

Acknowledgements 61

Bibliography 63
Chapter 1

Introduction

The ultimate motivation of this thesis is to contribute to the understanding of high temperature superconductivity. Ordinary superconductivity, which was discovered in 1911, is described by the Bardeen-Cooper-Schrieffer (BCS) theory. It results from Cooper pair formation of two electrons. An attractive interaction mediated by phonon exchange may overcome the Coulomb repulsion. The condensation of the Cooper pairs then leads to superconductivity.

High temperature superconductivity was discovered in 1986 by Bednorz and Müller [12]. The responsible mechanism is still not known and the BCS theory does not apply, since in ordinary superconductors the Cooper pairs are coupled weakly, while in high temperature superconductors (HTS) they are coupled strongly. For high temperature superconductivity one assumes that phonons alone can not provide a mechanism for Cooper pair formation.

Beside new iron-based materials, most known HTS result from hole- (missing electrons) or electron-doped layered cuprates (copper-oxides). Before doping, the systems are antiferromagnetic insulators. As most of the known materials come with a square lattice structure, we first discuss them. They have a common basic structure. Two-dimensional CuO$_2$ layers are separated by insulating layers. They can be doped by substituting ions in the insulating layers, with the result that the additional electrons or holes reside in the cuprate layers. As first understood by Anderson [23], the CuO$_2$ planes are responsible for high temperature superconductivity. Since the cuprate layers are coupled very weakly, the relevant physics is two-dimensional and therefore we will work in two dimensions in the following.

In fig. 1.1, the antiferromagnetic and the superconducting phases of an electron- and a hole-doped material on square lattices are shown. For materials with a honeycomb lattice one also finds such antiferromagnetic and superconducting phases. One can see that the antiferromagnetic phases only exist at sufficiently low temperatures and at zero or light doping. Caused by very small couplings between the different layers, the antiferromagnetic correlation length remains infinite at low non-zero temperatures in contrast to the case of an exactly two-dimensional antiferromagnet, which we consider in this thesis. The superconducting phases only arise at doping rates at which the antiferromagnetic order has disappeared.

Most of what we discuss in this thesis has already been done for the square lattice case in [1–8]. However, there are also HTS with other lattices, for example with a honeycomb lattice, which we investigate in this thesis. For example, the dehydrated variant of Na$_x$CoO$_2$·yH$_2$O at $x = 1/3$ shows honeycomb structure. Its physics is similar to the one of the cuprates with the difference that there are CoO$_2$ instead of CuO$_2$ layers. In fig. 1.2, its structure is illustrated. Another antiferromagnetic material with a honeycomb lattice is InCu$_{2/3}$V$_{1/3}$O$_3$, ...
Figure 1.1: Schematic phase diagram of electron- (left) and hole-doped (right) cuprates, showing antiferromagnetism (AF) and superconductivity (SC). (Figure taken from [40].)

again with CuO$_2$ layers. As actual materials with honeycomb structure are hole doped, we restrict ourselves to the hole doped sector. However, the procedure for the electron doped sector would be analogous. When we speak about holes in the following, we mean doped holes relative to a half-filled system (one electron per lattice site on average).

Figure 1.2: Structural views of Na$_{0.7}$CoO$_2$ (left) and Na$_x$CoO$_2$$\cdot$$y$H$_2$O (right), where Na and H$_2$O sites are partially occupied. (Figure take from [39].)

As two-dimensional quantum antiferromagnets are not yet completely understood even before they turn into HTS upon doping, we investigate their low-energy physics in this thesis for materials with a honeycomb lattice. There exist minimal microscopic models like the Hubbard or the $t$-$J$ model, which describe their physics. It is probably not possible to solve these models analytically and except for the undoped, the one-hole, and the one-electron sector, they can not even be solved numerically because of a severe fermion sign problem. Also the exact ground state is not known. Therefore we proceed in another way and construct a systematic low-energy effective field theory for magnons and holes in an antiferromagnet
on the honeycomb lattice analogous to baryon chiral perturbation theory (BχPT) in this thesis. Then we use this theory to investigate the Schrödinger equation for the relative motion of two holes. Also other applications like spirals in the staggered magnetization can be investigated [9, 11].

A characteristic feature of quantum antiferromagnets is the spontaneous symmetry breaking of the global \( SU(2)_s \) spin rotation symmetry down to the subgroup \( U(1)_s \). According to Goldstone’s theorem, the result are two Goldstone bosons, the magnons or antiferromagnetic spin waves. Because they are massless, the low-energy physics is dominated by their dynamics.

In the antiferromagnetic phase, the fermion number \( Q \) is a conserved quantity. This, together with the spontaneously broken \( SU(2)_s \) spin symmetry, allows the construction of a low-energy effective field theory for magnons and holes analogous to BχPT. BχPT and the effective field theory for magnons and holes are compared in [1–4, 7].

In Quantum Chromodynamics (QCD), which describes the strong interactions of quarks and gluons, one is also confronted with the problem that it is probably not analytically solvable. Therefore, a systematic effective field theory, BχPT was developed, which describes the low-energy physics of QCD.

Spontaneous symmetry breaking also occurs in QCD and results in three Goldstone bosons, the pions \( \pi^+, \pi^0, \pi^- \), which dominate the low-energy physics of QCD. Since the baryon number \( B \) is conserved in QCD, each baryon sector can be investigated separately. For the pure pionic sector (\( B = 0 \)), a low-energy effective field theory known as chiral perturbation theory (χPT) was developed in [14, 17]. For the case \( B \neq 0 \) the theory was extended to baryon chiral perturbation theory (BχPT) [18–22].

The effective theory for magnons and holes is used to investigate the low-energy physics of antiferromagnets. Undoped antiferromagnets are governed by magnons. Doped antiferromagnets are of particular interest. At low energy, the dynamics of holes is dominated by long-range magnon-mediated forces. In this thesis we investigate the leading process, one-magnon exchange. Since HTS result from doped antiferromagnets, processes like magnon exchange might be important for Cooper pair formation.

One may ask whether the effective theory for magnons and holes is applicable to HTS. Since the antiferromagnetism has disappeared, the \( SU(2)_s \) symmetry is no longer broken spontaneously. Therefore the perturbative treatment of the effective theory breaks down. However, the effective theory itself does not as long as the magnons, now with a finite correlation length, and the holes with the index structure of the antiferromagnetic phase, remain among the relevant degrees of freedom. In this thesis we limit ourselves to perturbative calculations in the antiferromagnetic phase.

We will now describe what a low-energy effective field theory is. Most microscopic models which describe the physics of a system up to high energies can probably not be solved analytically. What one can do is to catch the relevant degrees of freedom at low energies and describe only those. Since such a theory contains only the relevant low-energy physics, it is easier to handle, and therefore called effective. Of course, such an effective theory is only valid up to a certain energy scale, but below it it is equivalent to the underlying microscopic theory.

For the construction of an effective theory one first has to work out all symmetries of the underlying theory. Then all relevant degrees of freedom at low energies and their transformation behaviour under the various symmetries must be worked out. At last, as Weinberg stated in [14], one has to construct the most general Lagrangian consisting of all terms which are
invariant under all symmetries. These terms consist of the appropriate field degrees of freedom and their derivatives. Derivatives correspond to momenta. Therefore, the Lagrangian of the effective theory is constructed as a derivative expansion, where with each order further corrections are taken into account. Since we are interested in the low-energy physics, we only have to construct the leading orders, i.e. terms with a small number of derivatives. Thus, the goal is to write down the leading terms of the Euclidean action, used in a path integral.

Each term is endowed with a low-energy constant which determines the coupling strength of the corresponding interaction. The numerical values of these low-energy constants can not be determined in the framework of the effective theory, but have to be determined by experiment or numerical simulations. The high-energy physics of the underlying model is absorbed in these low-energy constants. Since short distances correspond to high momenta, the effective theory is insensitive to the microscopic details of the underlying model. Thus, the effective theory is the same for all underlying models sharing the same symmetries. Different models just have different values of the low-energy constants.

Besides fundamental principles of field theory like locality and unitarity, the effective theory for magnons and holes constructed in this thesis relies on three inputs. First, the Hubbard model serves as an underlying microscopic model. (As mentioned, except for the numerical values of the low-energy constants, the effective theory remains the same for all microscopic models which have the same symmetries as the Hubbard model.) The second input is that the global SU(2) spin symmetry is spontaneously broken down to U(1). And the third input is that the holes reside in momentum space pockets centered around $(0, 4\pi/(3\sqrt{3}a))$ and $(0, -4\pi/(3\sqrt{3}a))$ where $a$ is the spacing between two neighbouring lattice sites. The rest of the construction is analogous to BχPT. Apart form these inputs, the construction is only based on symmetries, which the effective theory inherits from the underlying model. This shows the strength and importance of symmetries.

The effective theory is only valid for low energies. In the context of the Hubbard model, low energies are small compared to the parameters $t$ and $U$ which set the energy scales in this model. These energy parameters are incorporated in the low-energy constants of the effective theory. Thus, low energy in the context of the effective theory means small compared to a low-energy constant like the spin stiffness $\rho_s$.

In the microscopic theory, the electrons are coupled strongly. What makes the effective theory so powerful, is the fact that the holes are derivatively coupled to the magnons. Therefore, the long-range forces mediated by magnon exchange between the holes can be investigated using perturbation theory.

Since the microscopic models are defined on a lattice, the Poincaré-invariance is explicitly broken and so the underlying models and with them the effective theory are nonrelativistic. In addition, because of this explicit symmetry breaking, the models and the effective theory do not contain phonons. In real materials phonons are the Goldstone bosons of the spontaneously broken symmetries caused by the formation of the crystal lattice.

I have done this Master thesis in close collaboration with Bänz Bessire who wrote his thesis about the same effective theory, however, with applications to spiral phases of the staggered magnetization [9]. For the square lattice case, such an effective theory has been developed and also the two-hole bound states as well as the spiral phases have been investigated. We used the corresponding theses and papers and adapted everything to the honeycomb lattice. Thus, this thesis closely follows especially [1] as well as [2–8]. We work in natural units, i.e. $\hbar = 1$ in the whole thesis.
Chapter 2

The Honeycomb Lattice

In this thesis we investigate strongly correlated electron systems on an infinitely extended honeycomb lattice with a lattice spacing $a$ between two neighbouring sites. As mentioned in the introduction, the effective theory will inherit all symmetries of the underlying model and with this also the ones of the honeycomb lattice. This chapter discusses some important facts concerning the honeycomb lattice and its symmetry properties.

2.1 A Bipartite Non-Bravais Lattice

The honeycomb lattice is bipartite, which means that it can be divided into two sublattices $A$ and $B$ such that all sites of $A$ only have nearest neighbours on $B$ and vice versa. This will become important later as symmetry transformations can map each sublattice on itself or $A$ on $B$ and vice versa. The two sublattices are illustrated in fig. 2.1. Every site has three nearest neighbours, thus the coordination number is three, which differs from the coordination number of the square lattice, which is four. This fact explains the difference of some low-energy constants, see section 5.2.

Later we will become interested in the first Brillouin zone. This can only be constructed from a Bravais lattice, which the honeycomb lattice is not. A definition of a Bravais lattice can be found for example in [42] and reads: "A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed." Taking a look at fig. 2.1, it is clear that the points on sublattice $A$ look different than those on $B$. However, the two triangular sublattices $A$ and $B$ are Bravais lattices and we can construct a Brillouin zone for each of them. This is what we will do now. Both sublattices are spanned by the primitive lattice vectors

\[ a_1 = \left( \frac{3}{2}a, \sqrt{3}a \right), \quad a_2 = \left( 0, \sqrt{3}a \right), \]

and with the relation

\[ g_i \cdot a_j = 2\pi \delta_{ij}, \]

we can calculate the primitive lattice vectors of the reciprocal lattices

\[ g_1 = \left( \frac{4\pi}{3a}, 0 \right), \quad g_2 = \left( \frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a} \right). \]

As illustrated in fig. 2.2, we see that the reciprocal sublattices are again triangular, but rotated by 30 degrees with respect to the ones in position space. The figure also shows the
first Brillouin zone, which is a regular hexagon. For the first Brillouin zone of the honeycomb lattice this means that it looks like the one of a triangular sublattice, but it is doubly-covered as we have one Brillouin zone for the $A$ and one for the $B$ sublattice. In the following $A$ and $B$ will appear as quantum numbers in addition to spin and momentum. Hence, a momentum state may be occupied by an electron with spin up from lattice $A$, one from $B$ and with a spin down electron from $A$ and one from $B$.

An electron or a hole with a momentum $k$ exactly behaves like one with momentum $k'$, when $k$ and $k'$ only differ by a lattice vector of the reciprocal lattice. For physical quantities which depend on the momentum, this means that only the values in the first Brillouin zone are needed. This periodicity in momentum space implies that for such quantities there are only two corners of the first Brillouin zone of the honeycomb lattice which are different. Which ones are equivalent is shown in fig. 2.3. The coordinates of the first Brillouin zone’s corners
are
\[ k_1 = \left( \frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a} \right), \quad k_2 = \left( 0, \frac{4\pi}{3\sqrt{3}a} \right), \quad k_3 = \left( \frac{-2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a} \right), \]
\[ k_4 = \left( \frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a} \right), \quad k_5 = \left( 0, \frac{-4\pi}{3\sqrt{3}a} \right), \quad k_6 = \left( \frac{-2\pi}{3a}, \frac{-2\pi}{3\sqrt{3}a} \right). \] (2.4)
And its area is given by
\[ A_{BZ} = \frac{8\sqrt{3}\pi^2}{9a^2}. \] (2.5)

\[ \begin{align*}
&k_1, \quad k_2, \\
&k_3, \quad k_4, \\
&k_5, \quad k_6
\end{align*} \]

Figure 2.3: Equivalent corners of the first Brillouin zone.

2.2 Symmetries of the Honeycomb Lattice

Later, when constructing the effective theory, we will search terms which respect all symmetries of the underlying model. First of all, we are interested in a minimal generating system of all symmetry transformations, and now we are looking for such a system including all symmetries of the lattice. As mentioned before, it will become important whether the transformations map the sublattices on themselves or \( A \) is mapped on \( B \) and vice versa.

2.2.1 Shift Symmetries \( D_i \)
Looking at fig. 2.1, we see that a minimal generating system of shift symmetries is given by the drawn translation vectors
\[ a_1 = \left( \frac{3}{2}a, \frac{\sqrt{3}}{2}a \right), \quad a_2 = \left( 0, \sqrt{3}a \right). \] (2.6)
We call the vectors \( a_1 \) and \( a_2 \) and the transformations \( D_1 \) and \( D_2 \). In contrast to the square lattice, where the shift symmetries map \( A \) on \( B \) and vice versa, here the sublattices are mapped onto themselves.

2.2.2 Rotation \( O \) and Reflection \( R \) Symmetries
The six rotations by a multiple of 60 degrees around a center of a hexagon leave the lattice invariant. In addition, the three lines going through the edges of a hexagon and the three perpendicular bisectors of a hexagon side can be viewed as reflection axes. Point reflections at
a midpoint of a hexagon are the same as a reflection at an axis parallel to the $x_1$-axis and one parallel to the $x_2$-axis, thus they don’t have to be considered. These six rotations and six reflections form the so called dihedral group $D_6$. From this we know that the minimal generating system consists of the rotation of 60 degrees and the reflection at the $x_1$-axis. Together with the shift transformations we have a minimal generating system which covers all symmetries. The rotation $O$ turns a lattice point $x = (x_1, x_2)$ into $Ox = (1/2 x_1 - \sqrt{3}/2 x_2, \sqrt{3}/2 x_1 + 1/2 x_2)$ and the reflection $R$ turns it into $Rx = (x_1, -x_2)$. Again in contrast to the square lattice, where the rotation maps the sublattices onto themselves, here the $A$ lattice is mapped to the $B$ and vice versa.
Chapter 3

The underlying Microscopic Models and their Symmetries

As in BχPT, our effective field theory inherits the symmetries from the underlying model. In this chapter we introduce the Hubbard model, which serves as a concrete underlying microscopic model for a quantum antiferromagnet. It shares the important symmetries with the actual materials and is supposed to contain the relevant physics. We also introduce the \( t-J \) and the Heisenberg model as limiting cases of the Hubbard model. By working with such models, we populate the lattice with electrons. First we briefly introduce the three models and explain some important facts. Then we perform a detailed symmetry analysis of the Hubbard model, as this serves as underlying model for the effective theory.

3.1 The Hubbard Model

We first write down the second quantized Hamiltonian which defines the Hubbard model

\[
H = -t \sum_{\langle xy \rangle} (c_x^\dagger c_y + c_y^\dagger c_x) + \frac{U}{2} \sum_x (c_x^\dagger c_x - 1)^2 - \mu \sum_x (c_x^\dagger c_x - 1),
\]

(3.1)

where \( \langle xy \rangle \) denotes a pair of nearest neighbour sites \( x \) and \( y \). The spins at a site \( x = (x_1, x_2) \) are represented by fermion creation operators \( c_{xs}^\dagger \) and annihilation operators \( c_{xs} \) in spinor notation

\[
c_{xs}^\dagger = \begin{pmatrix} c_{x \uparrow}^\dagger, c_{x \downarrow}^\dagger \end{pmatrix}, \quad c_{xs} = \begin{pmatrix} c_{x \uparrow}, c_{x \downarrow} \end{pmatrix},
\]

(3.2)

whose components obey the standard anticommutation relations, which incorporate the Pauli principle

\[
\{c_{xs}^\dagger, c_{ys}\} = \delta_{xy} \delta_{ss'}, \quad \{c_{xs}, c_{ys}^\dagger\} = \{c_{xs}^\dagger, c_{ys}^\dagger\} = 0.
\]

(3.3)

Spin up or down is indicated by arrows \((\uparrow, \downarrow)\) or \( s \) and \( s' \), respectively. This model was introduced to describe the transition from conducting to insulating behaviour of strongly correlated materials. It has the simplest Hamiltonian which describes mobile interacting electrons on a lattice and includes two competing processes: the hopping of the electrons between nearest neighbour lattice sites (if not forbidden by the Pauli principle) and the localization of the electrons on the sites, the latter caused by the Coulomb repulsion between the electrons. Each hop costs a certain amount of energy, which is determined by the hopping
parameter $t$. The interaction between the electrons is simply described by the on-site Coulomb repulsion. If two electrons sit on the same site, this costs an energy $U > 0$. In addition, $\mu$ is the chemical potential for fermion number relative to half-filling (on average one electron per lattice site, $\mu = 0$) which allows us to dope the system with electrons or holes.

### 3.2 The $t$-$J$ Model

Another simple description of mobile interacting electrons which is supposed to describe quantum antiferromagnets, is the $t$-$J$ model. It is defined by the Hamiltonian

$$\mathcal{H} = P \left\{ -t \sum_{\langle xy \rangle} (c_x^\dagger c_y^\dagger + c_y^\dagger c_x) + J \sum_{\langle xy \rangle} \vec{S}_x \cdot \vec{S}_y - \mu \sum_x \left( c_x^\dagger c_x - 1 \right) \right\} P. \quad (3.4)$$

The spin operator at the lattice site $x$ is given by

$$\vec{S}_x = \frac{1}{2} \vec{\sigma}_x,$$

where $\vec{\sigma}$ are the Pauli matrices. As in the Hubbard model, $t$ is the hopping parameter, $\mu$ is the chemical potential for fermion number relative to half-filling, and $J$ describes the coupling between neighbouring spins. Also in this model only nearest neighbour interactions are taken into account. $P$ is a projection operator which restricts the Hilbert space by eliminating doubly occupied sites, such that only singly occupied or empty sites are allowed. Therefore the $t$-$J$ model can solely be doped with holes, while the Hubbard model describes both, the electron and the hole sector. It has the same symmetries as the Hubbard model except for a non-Abelian $SU(2)_Q$ extension of the fermion number symmetry (which we will introduce later). This symmetry is not present in the $t$-$J$ model, because it describes only the hole doped sector. During the construction of the effective theory this additional symmetry of the Hubbard model is broken, such that in both cases we have the same set of symmetries. In [10], for the simulations of mobile holes for the single hole sector, the $t$-$J$ model is used.

### 3.3 The Quantum Heisenberg Model

The quantum Heisenberg model describes magnetism in spin systems on a lattice. In contrast to the previous models, the spins are fixed to a specific site. It has the simplest Hamiltonian describing spin interactions which is defined by

$$\mathcal{H} = J \sum_{\langle xy \rangle} \vec{S}_x \cdot \vec{S}_y,$$

where $J$ is again the exchange coupling constant. The spin operator at site $x$ is given by

$$\vec{S}_x = \frac{1}{2} \vec{\sigma}_x.$$

Whether the sign of $J$ is positive or negative defines if parallel or antiparallel spin alignment is favored. We are interested in antiferromagnetism, thus $J > 0$. 
3.4 The Strong Coupling Limit of the Hubbard Model and how it leads to Antiferromagnetism

In the strong coupling limit \((U \gg t)\) for \(\mu \neq 0\), the Hubbard model goes over in the \(t\)-\(J\) model relating the parameters of the two models by \(t^2/U = J/2\). For \(\mu = 0\) it simplifies further to the antiferromagnetic Heisenberg model relating the parameters by \(J = 2t^2/U > 0\).

As we are interested in antiferromagnetism, we will now describe how the Hubbard model leads to the antiferromagnetic Heisenberg model and put \(U \gg t\) and \(\mu = 0\). This situation can be analyzed by a second order perturbation calculation in \(t/U\), where the Coulomb part of the Hubbard Hamiltonian from which we know the eigenstates, is the unperturbed Hamiltonian while the kinetic term is the perturbation. Since we have \(U \gg t\), doubly occupied sites become energetically very unfavourable. At leading order \((t = 0)\), i.e. neglecting the kinetic term, we get a ground state with one fermion per site. There are infinitely many such ground states for \(t = 0\), as each spin can arbitrarily point up or down. When we take into account corrections due to hopping, this enormous degeneracy disappears. The first order correction is zero, because after one hop we do not return to a ground state. At second order, a fermion can first virtually hop to a nearest neighbour and then, one of them can hop back. Because hops to nearest neighbours with parallel spin orientation are forbidden by the Pauli principle and because the corrections of second order are negative, this leads to antiparallel spin alignment. This perturbation calculation results in the antiferromagnetic Heisenberg Hamiltonian with \(J\) related to the parameters of the Hubbard model by \(J = 2t^2/U > 0\) [43].

Therefore we have to work in the strong coupling limit and at half-filling to describe a Heisenberg antiferromagnet. As we also want to describe moving electrons and holes, it is not enough to take the Heisenberg model where the particles are fixed to the lattice, but we have to use the Hubbard model. Looking at fig. 1.1, we see that an antiferromagnet does not get destroyed immediately by doping. Hence, also at low doping we deal with an antiferromagnet.

3.5 Symmetries of the Hubbard Model

Since we want to describe an antiferromagnet on the honeycomb lattice with the Hubbard model, it should also have all symmetries of the underlying lattice which we figured out in section 2.2. In this section we show that the Hubbard model does so and that it has additional symmetries.

3.5.1 \(SU(2)_s\) Spin Rotation Symmetry

The total \(SU(2)_s\) spin operator (the subscript \(s\) stands for spin) is given by

\[
\vec{S} = \sum_x \vec{S}_x = \sum_x c^\dagger_x \frac{\vec{\sigma}}{2} c_x.
\]

Later we need to know how the spinors transform under the various transformations as we will introduce an operator which consists of them (see eq. (3.17)). Here it also serves to show that the discussed transformations are really symmetry transformations. To see how the spinors transform, we need the unitary operator which implements the global spin rotation in the Hilbert space of the theory

\[
V = \exp \left(i \vec{\eta} \cdot \vec{S} \right).
\]
Then the transformed spinors look like

\[ c'_x = V^\dagger c_x V = \exp \left( i\eta \cdot \vec{\sigma} \right) c_x = gc_x, \quad \text{with} \quad g = \exp \left( i\eta \cdot \vec{\sigma} \right) \in SU(2)_s. \]  

(3.10)

One can see that the Hamiltonian is left invariant under spin rotation, i.e. \([\mathcal{H}, \vec{S}] = 0\), which means that the total spin is conserved.

### 3.5.2 \(U(1)_Q\) Fermion Number Symmetry

The \(U(1)_Q\) fermion number operator is defined by

\[ Q = \sum_x Q_x = \sum_x \left( c_x^\dagger c_x - 1 \right) = \sum_x \left( c_x^\dagger c_x^1 + c_x^1 c_x^\dagger - 1 \right), \]  

(3.11)

and counts the fermions relative to half-filling (due to the subtraction of the constant 1). Again we look at the unitary operator which implements the symmetry transformation in the Hilbert space of the theory

\[ W = \exp \left( i\omega Q \right), \]  

(3.12)

to see how the spinors transform

\[ Q c_x = W^\dagger c_x W = \exp \left( i\omega \right) c_x, \quad \text{with} \quad \exp \left( i\omega \right) \in U(1)_Q. \]  

(3.13)

It is easy to see that the Hamiltonian is left invariant under this transformation, i.e. \([\mathcal{H}, Q] = 0\). This means that the fermion number and with it the electric charge is conserved. Also in actual antiferromagnets this symmetry is unbroken until a superconducting phase is reached.

### 3.5.3 Discrete Symmetries \(D_i, O, O', \text{ and } R\)

The spinors transform in the following ways

\[ D_i : \quad D_i c_x = D_i^\dagger c_x D_i = c_{x+a_i}, \]

\[ O : \quad O c_x = O^\dagger c_x O = c_{Ox}, \]

\[ R : \quad R c_x = R^\dagger c_x R = c_{Rx}. \]  

(3.14)

For our purpose it is not important to know how the unitary operators look like that implement the transformations in the Hilbert space. By redefining the sum over lattice points, one can see that the Hubbard Hamiltonian is left invariant and the three transformations are indeed symmetries. In non-relativistic theories orbital angular momentum and spin are separately conserved, the spin plays the role of an internal quantum number. This means that spatial rotations do not affect the spin and \(SU(2)_s\) transformations can be applied independent of \(O\).

For later convenience it is useful to introduce a combination of the rotation with a special \(SU(2)_s\) transformation \(g = i\sigma_2\), which we call \(O'\). It acts on the spinors as

\[ O' c_x = O'^\dagger c_x O' = (i\sigma_2) c_{Ox}. \]  

(3.15)

In the square lattice case we had a \(D'\) instead of an \(O'\). The Hubbard Model also has a time-reversal symmetry \(T\). Since this is implemented by an antiunitary operator on the spinors, we will implement time-reversal later.
3.5.4 Non-Abelian Extension of the $U(1)_Q$ Symmetry to $SU(2)_Q$

Yang and Zhang noted that on bipartite lattices at half-filling the Hubbard model possesses an $SU(2)_Q$ symmetry, which is an extension of the $U(1)_Q$ symmetry discussed before [26, 27]. Away from $\mu = 0$ the $SU(2)_Q$ symmetry is explicitly broken down to $U(1)_Q$. Often it is called a pseudospin symmetry and it is generated by the three operators

$$Q^+ = \sum_x (-1)^x c_x^\dagger c_x^\uparrow, \quad Q^- = \sum_x (-1)^x c_x^\dagger c_x^\downarrow,$$

$$Q^3 = \sum_x \frac{1}{2} (c_x^\dagger c_x^\uparrow + c_x^\dagger c_x^\downarrow - 1) = \frac{1}{2} Q.$$  \hspace{1cm} (3.16)

The factor $(-1)^x$ is defined to be 1 for $x \in A$ and $-1$ for $x \in B$. In [2] it is discussed that $SU(2)_Q$ is indeed a symmetry of the Hubbard model and there one can also see that next-to-nearest neighbour hopping breaks it. Explicitly it describes a particle-hole symmetry, which means that the positive energy spectrum (for electrons) is the same as the negative one (for holes). Doping ($\mu \neq 0$) induces a shift in this spectrum and destroys the symmetry. In actual materials this symmetry is not realized, but it helps to construct the effective theory and will be broken down explicitly to $U(1)_Q$ in this process, such that it is not included in the effective theory.

3.6 Manifestly $SU(2)_s \otimes SU(2)_Q$ Invariant Formulation of the Hubbard Model

As presented in eq. (3.1), the Hubbard Hamiltonian is not manifestly $SU(2)_Q$ invariant. It turns out to be useful to introduce a matrix-valued fermion operator

$$C_x = \begin{pmatrix} c_x^\dagger & (-1)^x c_x^\dagger \\ c_x^\dagger & -(-1)^x c_x^\dagger \end{pmatrix}. \hspace{1cm} (3.17)$$

A detailed derivation of this operator can be found in [2]. With its help it is possible to write the Hubbard Hamiltonian in a manifestly $SU(2)_s \otimes SU(2)_Q$ invariant form. The unitary operator of the $SU(2)_Q$ transformation acting on the matrix-valued fermion operator reads

$$W = \exp \left( i\vec{\omega} \cdot \vec{Q} \right), \hspace{1cm} (3.18)$$

and the transformation yields

$$\vec{Q} C_x = W^\dagger C_x W = C_x \Omega^T, \quad \text{with} \quad \Omega = \exp \left( i\vec{\omega} \cdot \frac{\vec{\sigma}}{2} \right) \in SU(2)_Q. \hspace{1cm} (3.19)$$

Using the transformation rules of $c_x$ the remaining ones for $C_x$ can be derived to be

$$SU(2)_s : \quad C'_x = g C_x, \quad D_i : \quad D_i C_x = C_{x+i_i}, \quad O : \quad O C_x = C_{Ox} \sigma_3, \quad O' : \quad O' C_x = (i\sigma_2) C_{Ox} \sigma_3, \quad R : \quad R C_x = C_{Rx}. \hspace{1cm} (3.20)$$
When we make an $SU(2)_s$ as well as an $SU(2)_Q$ transformation, we get
\[ \tilde{Q}C'_x = gC_x \Omega^T. \] (3.21)

Since $SU(2)_s$ acts from the left and $SU(2)_Q$ from the right, one can see that the two transformations commute. This makes it possible to formulate the Hubbard Hamiltonian for $\mu = 0$ in the manifestly $SU(2)_s \otimes SU(2)_Q$ invariant form
\[ H = -t \sum_{\langle xy \rangle} \text{Tr} \left[ C^\dagger_x C_y + C^\dagger_y C_x \right] + \frac{U}{12} \sum_x \text{Tr} \left[ C^\dagger_x C_x C^\dagger_x C_x \right] - \frac{\mu}{2} \sum_x \text{Tr} \left[ C^\dagger_x C_x \sigma_3 \right]. \] (3.22)
Chapter 4

Investigation of the Free Fermion Model

In this chapter we take a look at the weak coupling limit of the Hubbard model at half filling. For $U = 0$, i.e. describing free fermions, the corresponding Hamiltonian can be diagonalized analytically. This yields the energy-momentum relation and we will see that the low-energy excitations of such a system are free, relativistic, massless Dirac fermions. Also an analytic expression for their velocity is derived. As there is no spontaneous breaking of a continuous symmetry, in this case there are no Goldstone bosons. We then construct the leading terms of the corresponding effective Lagrangian for the Dirac fermions. This is possible although there is no spontaneous breaking of a continuous symmetry as in $\chi PT$. One only has to include all relevant degrees of freedom in the effective theory which are present at low energies and here these are only the Dirac fermions.

Graphene, a single sheet of graphite, i.e. carbon atoms arranged on a honeycomb lattice, is described by the Hubbard model in the weak coupling limit at half filling. If some variants of graphene exist at stronger coupling, one eventually expects a phase transition at some critical value of $U$, separating graphene’s unbroken phase from a strong coupling antiferromagnetic phase, in which the $SU(2)_s$ spin symmetry is spontaneously broken to $U(1)_s$. The Hubbard model for the square lattice case does not have such a phase transition as this describes an antiferromagnet for arbitrarily small values of $U$.

4.1 The Weak Coupling Limit of the Hubbard Model and how it leads to Massless Dirac Fermions

In this section we investigate the weak coupling limit ($U \ll t$) of the Hubbard model at half-filling ($\mu = 0$). This will allow us to derive the energy-momentum relation in this limit. For $U \ll t$ the interaction is only a very weak perturbation such that the fermions will behave almost free. Thus in the following we treat the free case and put $U = 0$. By doing this, the Hubbard Hamiltonian reduces to the kinetic part

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_t' = -t \sum_{\langle x,y \rangle} \left( c_x^\dagger c_y + c_y^\dagger c_x \right) - t' \sum_{\langle\langle x,y \rangle\rangle} \left( c_x^\dagger c_y + c_y^\dagger c_x \right), \quad (4.1)$$

where we also included a next-to-nearest neighbour hopping term proportional to $t'$ which explicitly breaks the $SU(2)_Q$ symmetry for $t' \neq 0$. The symbol $\langle\langle x,y \rangle\rangle$ indicates the sum
over the next-to-nearest neighbours. Because we neglect the interaction part, we can diagonalize the Hamiltonian by going to momentum space and derive the energy-momentum relation. First we decompose the sum over the nearest and next-to-nearest neighbours into sums over the sublattices and appropriate vectors connecting the sites, such that we catch each connection exactly once

\[ H = -t \sum_{j} \sum_{x} \left( c_{x+ji}^{A \dagger} c_{x}^{B} + c_{x+j_i}^{B \dagger} c_{x}^{A} \right) \]

\[ -t' \sum_{j_i} \left[ \sum_{x} \left( c_{x+ji}^{A \dagger} c_{x+j_i}^{A} + c_{x+j_i}^{B \dagger} c_{x}^{A} \right) \right] \quad \text{(4.2)} \]

with \( A \) and \( B \) on the spinors indicating whether the fermions are created or annihilated on the \( A \) or \( B \) sublattice. The vectors

\[ j_1 = (a, 0), \quad j_2 = \left( -\frac{1}{2}a, \frac{\sqrt{3}}{2}a \right), \quad j_3 = \left( -\frac{1}{2}a, -\frac{\sqrt{3}}{2}a \right), \]

connect the nearest neighbours and

\[ j'_1 = \left( \frac{3}{2}a, \frac{\sqrt{3}}{2}a \right), \quad j'_2 = (0, \sqrt{3}a), \quad j'_3 = \left( \frac{3}{2}a, -\frac{\sqrt{3}}{2}a \right), \]

connect the next-to-nearest neighbours. In the following, one must take into account that the position space is discrete because we work on a lattice. We use the relations

\[ \frac{1}{A_{BZ}} \sum_{x} \exp (i(k - k')x) = \delta^{(2)}(k - k'), \quad \frac{1}{A_{BZ}} \int_{BZ} d^2k \exp (ik(x - x')) = \delta_{x,x'}, \]

and for the spinors

\[ c_{x}^{X} = \frac{1}{A_{BZ}} \int_{BZ} d^2k \exp (ikx) c_{k}^{X}, \quad X \in \{ A, B \}, \]

which we found by studying the square lattice case described in [43]. The components of the spinors in momentum space \( c_{X}^{k} \) and \( c_{X}^{k \dagger} \) still obey the standard anticommutation relations. \( A_{BZ} \) is the area of the first Brillouin zone (BZ) which is given in eq. (2.5). By replacing the creation and annihilation operators in eq. (4.2) by the ones in momentum space and using the other relations we get

\[ H = -\frac{1}{A_{BZ}} \int_{BZ} d^2k \left( \begin{array}{c} c_{k}^{A \dagger} \\ c_{k}^{B \dagger} \end{array} \right) \mathcal{H}(k) \left( \begin{array}{c} c_{k}^{A} \\ c_{k}^{B} \end{array} \right), \]

with

\[ \mathcal{H}(k) = \left( \begin{array}{cc} t' f(k) & t g(k) \\ t g^*(k) & t' f(k) \end{array} \right), \]

and

\[ f(k) = 4 \cos \left( \frac{3}{2}k_1 a \right) \cos \left( \frac{\sqrt{3}}{2}k_2 a \right) + 2 \cos \left( \frac{\sqrt{3}}{2}k_2 a \right), \]

\[ g(k) = \cos (k_1 a) + i \sin (k_1 a) + 2 \cos \left( \frac{\sqrt{3}}{2}k_2 a \right) \left[ \cos \left( \frac{1}{2}k_1 a \right) - i \sin \left( \frac{1}{2}k_1 a \right) \right]. \]
4.1 The Weak Coupling Limit of the Hubbard Model and how it leads to Massless Dirac Fermions

When we diagonalize the Hamiltonian of eq. (4.8), we get the energy-momentum relation for free fermions

\[
E_{\pm}(k) = t' f(k) \pm t g(k) = t' f(k) \pm t \sqrt{3 + f(k)}
\]

\[
= t' \left[ 4 \cos \left( \frac{3}{2} k_1 a \right) \cos \left( \frac{\sqrt{3}}{2} k_2 a \right) + 2 \cos \left( \sqrt{3} k_2 a \right) \right] \pm t \sqrt{3 + 4 \cos \left( \frac{3}{2} k_1 a \right) \cos \left( \frac{\sqrt{3}}{2} k_2 a \right) + 2 \cos \left( \sqrt{3} k_2 a \right)}. \tag{4.11}
\]

The upper solution corresponds to the conduction and the lower to the valence band. Fig. 4.1 shows the energy-momentum relation for \( t = 1 \) and \( t' = 0 \). In this case the \( SU(2)_Q \) symmetry is not broken and the two bands are symmetric with respect to the plane with zero energy.

At zero temperature, since we are at half-filling, all states with energies in the valence band are covered, while all in the conduction band are empty. The two bands touch each other at the corners of the first Brillouin zone at the height of zero energy, which explains the semimetallic behaviour of graphene. These six points, known as Dirac points, represent the Fermi surface at \( E_F = 0 \) for \( t' = 0 \). When only \( t \) varies, the energy scale changes but the shape of the bands remains the same. From eq. (4.11) it is clear that for \( t = 0 \) the bands degenerate for all values of \( t' \). If \( t' \) is nonzero, the \( SU(2)_Q \) symmetry is explicitly broken, the two bands are not symmetric anymore and the energy value where the two bands touch, is shifted. Two examples with \( t' \neq 0 \) are shown in fig. 4.2. For some values of \( t \) and \( t' \), some energy region is covered by both bands, which implies that the Fermi surface is not at the Dirac points anymore. We showed that the two bands touch at the six Dirac points for all values of \( t \) and \( t' \).

Now we expand the energy-momentum relation of eq. (4.11) at each Dirac point in a Taylor series up to first order. This yields

\[
E_{\pm}(p) = \pm \frac{3t a}{2} \sqrt{p_1^2 + p_2^2} - 3t' + \mathcal{O}(p^2), \tag{4.12}
\]

with the momenta \( p_1 \) and \( p_2 \) now measured relative to the corresponding Dirac point. Because this is a cone and because this is exactly the relativistic energy-momentum relation of a
massless, free particle with velocity \( c \) (up to an irrelevant shift \( -3t' \))

\[
E_{\pm}(p) = \pm c|p| = \pm c\sqrt{p_1^2 + p_2^2}, \tag{4.13}
\]

they are called Dirac cones. (This is also the reason why the points are called Dirac points.) Hence, when the Dirac points are the Fermi surface, at low energies the microscopic theory predicts massless, free, relativistic fermions having a velocity

\[
v_F = \frac{3ta}{2}. \tag{4.14}
\]

It is astonishing that the velocity does not depend on the momentum of the particle. Its value is about \(10^6\) m/s \cite{35}. These strange massless Dirac fermions are a product of the geometry of the honeycomb lattice, which is incorporated in the energy-momentum relation via the vectors in eq. (4.3).

Free relativistic fermions with zero mass in two space dimensions are described by the Dirac Hamiltonian

\[
\mathcal{H}_D(p) = \alpha pc = (-\sigma_2p_1 + \sigma_1p_2)c, \tag{4.15}
\]

with \( \alpha_i = \gamma_0\gamma_i \), where we have chosen the gamma matrices to be

\[
\gamma_0 = \sigma_3, \quad \gamma_1 = i\sigma_1, \quad \gamma_2 = i\sigma_2, \tag{4.16}
\]

satisfying

\[
\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}\mathbb{1}_{2\times2}, \quad \mu, \nu \in \{0, 1, 2\}, \quad \text{with} \quad g_{\mu\nu} = \begin{pmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & -1
\end{pmatrix}. \tag{4.17}
\]

Here \( c \) denotes the velocity of the particle. We have shown in addition to the above derivation that expanding eq. (4.8) with \( t' = 0 \) up to first order yields exactly the above Dirac Hamiltonian. The set of gamma matrices may differ in each corner by an unitary transformation.
4.2 Effective Field Theory for Dirac Fermions

Now we will construct a low-energy effective field theory for the Dirac fermions for \( t' = 0 \). For simplicity we ignore spin because in the free case it just represents a trivial irrelevant label. As we do not consider spin, we do not have the \( SU(2)_S \) symmetry. In addition, the generators \( Q^+ \) and \( Q^- \) of the \( SU(2)_Q \) symmetry are not defined and instead we have the \( U(1)_Q \) and an additional \( Z(2) \) symmetry, which represents a discrete particle-hole symmetry, a remnant of the \( SU(2)_Q \) symmetry. It will be interesting to see that mass terms are forbidden because of symmetries alone.

With the following procedure we change from a Hamiltonian to a Lagrangian formulation used in a Euclidean path integral. We will deal with fermion fields represented by Grassmann numbers defined in the space-time continuum and no longer with microscopic operators defined on the lattice. From now on \( x \) means a Euclidean space-time point \( x = (x_1, x_2, t) \). Before we can formulate the effective theory, we have to identify the correct fermion fields and derive their transformation behaviour under the various symmetry transformations.

4.2.1 Fermion Fields

With the help of the energy-momentum relation, we can conclude that at half-filling the lowest energy states are in the circular shaped neighbourhoods of the corners of the first Brillouin zone in momentum space, which are called pockets. Hence, the effective theory has to describe fermions living in these pockets. As already mentioned in section 2.1, there are only two inequivalent corners of the Brillouin zone. The transformation rules of the fermion fields turn out to be simple, when we chose the corners

\[
k_2 = k^\alpha = \left(0, \frac{4\pi}{3\sqrt{3}a}\right), \quad \text{and} \quad k_5 = k^\beta = \left(0, -\frac{4\pi}{3\sqrt{3}a}\right), \tag{4.18}
\]

which we call \( k^\alpha \) and \( k^\beta \) in the following. Their circular shaped neighbourhoods are denoted as the \( \alpha \) and \( \beta \) pocket. For completeness we also have to include the origin \( \Gamma \). In order to address these points in momentum space, we introduce further sublattices in position space which are superimposed with the already introduced \( A \) and \( B \) sublattices, see fig. 4.3. A fermion at space-time point \( x \) is represented by \( \psi^{X_i}(x) \), where \( X_i \) denotes one of the sublattices introduced above. The discrete lattice in position space and the Brillouin zone are connected by a Fourier transformation. With these new fields it is possible to define fermion fields with a momentum index by a discrete Fourier transformation connecting the three points of the corresponding sublattice in position space with the three desired points in momentum space. (As we are not interested to describe fermions at \( \Gamma \), we do not consider the corresponding field.)

\[
\begin{align*}
\psi^{A,f}(x) & = \frac{1}{\sqrt{3}} \sum_{j=1}^{3} \exp \left(-ik^j v_j \right) \psi^{A_j}(x), \\
\psi^{B,f}(x) & = \frac{1}{\sqrt{3}} \sum_{j=1}^{3} \exp \left(-ik^j w_j \right) \psi^{B_j}(x), \tag{4.19}
\end{align*}
\]
with the “flavour” \( f \in \{\alpha, \beta\} \) and the vectors \( v_j \) and \( w_j \) (see also fig. 4.4)

\[
\begin{align*}
v_1 &= -\frac{1}{2}a, -\frac{\sqrt{3}}{2}a, \\
v_2 &= (a, 0), \\
v_3 &= -\frac{1}{2}a, \frac{\sqrt{3}}{2}a, \\
w_1 &= \frac{1}{2}a, -\frac{\sqrt{3}}{2}a, \\
w_2 &= (-a, 0), \\
w_3 &= \frac{1}{2}a, \frac{\sqrt{3}}{2}a. \\
\end{align*}
\] (4.20)

These fields now describe fermions living in the \( \alpha \) and \( \beta \) pocket and the indices \( A \) and \( B \) represent an additional quantum number. To summarize, we have the fields

\[
\begin{align*}
\psi^{A,\alpha}(x) &= \frac{1}{\sqrt{3}} \left( \exp(i\frac{2\pi}{3})\psi^{A_1}(x) + \psi^{A_2}(x) + \exp(-i\frac{2\pi}{3})\psi^{A_3}(x) \right), \\
\psi^{A,\beta}(x) &= \frac{1}{\sqrt{3}} \left( \exp(-i\frac{2\pi}{3})\psi^{A_1}(x) + \psi^{A_2}(x) + \exp(i\frac{2\pi}{3})\psi^{A_3}(x) \right), \\
\psi^{B,\alpha}(x) &= \frac{1}{\sqrt{3}} \left( \exp(i\frac{2\pi}{3})\psi^{B_1}(x) + \psi^{B_2}(x) + \exp(-i\frac{2\pi}{3})\psi^{B_3}(x) \right), \\
\psi^{B,\beta}(x) &= \frac{1}{\sqrt{3}} \left( \exp(-i\frac{2\pi}{3})\psi^{B_1}(x) + \psi^{B_2}(x) + \exp(i\frac{2\pi}{3})\psi^{B_3}(x) \right). \\
\end{align*}
\] (4.21)
The corresponding conjugate fields $\psi^{X,f\dagger}(x)$ are obtained by a dagger operation. However, one must keep in mind that the conjugate Grassmann fields are independent (in contrast to the microscopic operators in Hilbert space).

Next we derive the transformation properties. Due to the different nature of the microscopic theory and the effective theory, it is not possible to derive a connection between the two formulations in a rigorous way. Our connection between the two is to demand that the Grassmann fields inherit the transformation properties of the microscopic operators, which we have already worked out in section 3.5. Hence, the fields on the right hand side of eq. (4.21) transform exactly like the corresponding microscopic operators $c^X_i$ (without spin). How the sublattices $X_i$ change under the geometric symmetries can be seen by considering how the sublattices map onto each other. We already mentioned the $Z(2)$ symmetry, which acts on the microscopic operators as

$Z(2)c^A_i x = c^A_i x$, $Z(2)c^{A\dagger}_i x = c^{A\dagger}_i x$, $Z(2)c^B_i x = -c^B_i x$, $Z(2)c^{B\dagger}_i x = -c^{B\dagger}_i x$.

The effective theory is valid only at low energies. As short distances correspond to high momenta, it does not care about distances of the order of the lattice spacing and we thus no longer distinguish between the points $x$ and $x + a_i$ under shift transformations in the framework of the effective theory. Time-reversal is realized on the Grassmann fields in the usual manner. Thus we get the following transformation rules of the fermion fields

\[
Z(2) : \psi^{A,f}(x) = \psi^{A,f\dagger}(x), \\
Z(2) : \psi^{B,f}(x) = -\psi^{B,f\dagger}(x), \\
U(1)_Q : Q\psi^{X,f}(x) = \exp(i\omega)\psi^{X,f}(x), \\
D_i : D_i\psi^{X,f}(x) = \exp(ik^f a_i)\psi^{X,f}(x), \\
O : O\psi^{A,\alpha}(x) = \exp(-i\frac{2\pi}{3})\psi^{B,\beta}(Ox), \\
O : O\psi^{B,\alpha}(x) = \exp(i\frac{2\pi}{3})\psi^{A,\beta}(Ox), \\
O : O\psi^{B,\alpha}(x) = \exp(i\frac{2\pi}{3})\psi^{A,\beta}(Ox), \\
R : R\psi^{X,f}(x) = \psi^{X,f}(Rx), \\
T : T\psi^{X,f}(x) = -\psi^{X,f\dagger}(Tx), \\
T \psi^{X,f\dagger}(x) = \psi^{X,f\dagger}(Tx),
\]

with $f'$ being the flavour other than $f$ and $X \in \{A,B\}$. Again, apart from time-reversal, one gets the conjugate fields by a dagger operation. $O$, $R$ and $T$ act on a space-time point as

\[
Ox = \left(\frac{1}{2}x_1 - \frac{\sqrt{3}}{2}x_2, \frac{\sqrt{3}}{2}x_1 + \frac{1}{2}x_2, t\right), \\
Rx = (x_1, -x_2, t), \\
Tx = (x_1, x_2, -t).
\]

### 4.2.2 Effective Lagrangian

Since the appropriate fermion fields are found and their transformation rules are derived, we are now ready to construct the leading terms of the systematic low-energy effective Lagrangian
for the Dirac fermions. More concretely, this means that we systematically investigate all possible terms consisting of the fermion fields with momentum index, their conjugate partners, and derivatives. As mentioned in the introduction, we only need the lowest order of the derivative expansion to describe the low-energy physics. Since the fermions to be described have a relativistic energy-momentum relation \( E \propto p \) at low energies, temporal and spatial derivatives count the same. This will be different when we construct the effective theory for magnons and holes in the antiferromagnet. Then all terms which are invariant under all symmetry transformations are endowed with a low-energy constant and form together the desired Lagrangian which has all symmetries of the underlying Hubbard Hamiltonian. We categorize the terms according to the number of derivatives and the number of fields \( n_\psi \) they consist of. The number of fields and derivatives does not change under the transformations. Thus we can investigate each class of terms separately. Because of the \( U(1)_Q \) symmetry, only terms with the same number of undaggered and daggered fields are possible, otherwise there would remain a general phase \( \exp(\pm i\omega) \) when applying the transformation. One must take care that the remaining terms are independent. For example, by partial integration (in the action), from \( \partial_t \psi^X,f\psi^X,f \) one gets \( -\psi^X,f\partial_t \psi^X,f \) and a boundary term which is zero as the fields go to zero at infinity. Therefore one may take only one of the two terms. In the framework of free Dirac fermions (still for \( \mu = 0 \) and \( t' = 0 \)) we limit ourselves to the Lagrangian with two fermion fields and up to one derivative

\[
\mathcal{L}^{\text{free}}_2 = \sum_{f=\alpha,\beta}^{X=A,B} \left[ \psi^X,f\partial_t \psi^X,f + v_F \left( \sigma_X \psi^X,f\partial_t \psi^X,f + i\sigma_f \psi^X,f\partial_1 \psi^X,f \right) \right],
\]  

(4.25)

with \( X' \) being the sublattice index different from \( X \) and

\[
\sigma_X = \begin{cases} 1 & \text{for } X = A, \\ -1 & \text{for } X = B. \end{cases} \quad \text{and} \quad \sigma_f = \begin{cases} 1 & \text{for } f = \alpha, \\ -1 & \text{for } f = \beta. \end{cases}
\]  

(4.26)

This Lagrangian describes the kinetic energy up to first order of a massless, free Dirac fermion living at the \( \alpha \) or \( \beta \) pocket. Here the low-energy constant of the term with the temporal derivative is normalized to one and the only low-energy constant is the fermion velocity \( v_F \). As we see, the above Lagrangian contains no mass terms as predicted by the underlying Hubbard model, which shows the strength of the effective theory which is just based on a symmetry analysis.

In semimetallic graphene the fermions are, of course, not completely free but coupled weakly. Hence, to describe graphene, in addition to including the spin, one would also have to construct the leading terms with more than two fermion fields which describe contact interactions, like the 4-Fermi terms. But terms with identical fermion fields vanish because of the Pauli principle and since we have eight different fields, terms with more than eight fields and without derivatives do not exist.

Massless, free fermions are described by the Dirac Lagrangian without mass terms (here using a \( (2 + 1) \)-dimensional Euclidean metric)

\[
\mathcal{L}_D = c\bar{\Psi} \gamma_\mu \partial_\mu \Psi,
\]  

(4.27)

c denotes again the velocity of the particle and the gamma matrices are given by

\[
\gamma_j = i\sigma_j.
\]  

(4.28)
Our Lagrangian can be brought in this form in the following way. First one puts the fields into the spinors

$$\Psi^\alpha(x) = \begin{pmatrix} \psi_{A,\alpha}(x) \\ \psi_{B,\alpha}(x) \end{pmatrix}, \quad \Psi^\beta(x) = \begin{pmatrix} \psi_{A,\beta}(x) \\ \psi_{B,\beta}(x) \end{pmatrix}. \quad (4.29)$$

When we then multiply both Lagrangians with $1/v_F$ and $1/c$, respectively, there exists a unitary transformation of the gamma matrices such that our Lagrangian assumes the form of the Dirac Lagrangian under the condition $c = -v_F$. Using eq. (4.14), we see that a sign change of $v_F$ implies a sign change of the hopping amplitude $t$. This interchanges particles and holes (see eq. (3.1)), which does not change the physics. Therefore the Lagrangian can be written in the form of the Dirac Lagrangian with one term for the $\alpha$ and one term for the $\beta$ pocket

$$\mathcal{L}_2^{\text{free}} = v_F \left( \bar{\Psi}^\alpha \gamma_\mu \partial_\mu \Psi^\alpha + \bar{\Psi}^\beta \gamma_\mu \partial_\mu \Psi^\beta \right). \quad (4.30)$$

Here a temporal derivative also includes a factor $1/v_F$. 
Chapter 5

Magnons

Now we return to the strong coupling limit, i.e. to antiferromagnets. A characteristic feature of quantum antiferromagnets is the spontaneous breaking of the $SU(2)_s$ symmetry to the subgroup $U(1)_s$, which gives rise to two massless Goldstone bosons, the magnons. Since they are, apart from the holes, the only relevant degrees of freedom at low-energies, their low-energy physics can be described by an effective field theory analogous to $B\chi$PT with or without holes.

This and the next chapter include all additional preparations for the construction of the effective theory for magnons and holes in an antiferromagnet on the honeycomb lattice, which will be developed in chapter 7. In this chapter we first describe the spontaneous symmetry breaking. Then the leading terms of the Euclidean action for the pure magnon sector (corresponding to the pure pion sector of QCD) are derived. Finally, as in $B\chi$PT, we construct a non-linear realization of the spontaneously broken $SU(2)_s$ symmetry, which will be used to couple the magnon fields to the hole fields later. By doing all this, we develop step by step the adequate magnon fields and derive their transformation rules under the various symmetries of the Hubbard model.

5.1 Spontaneous Symmetry Breaking

First we take a look at the interesting phenomenon of spontaneous symmetry breaking. We have seen in section 3.4, that an antiferromagnet is already described by the Heisenberg model. For the ground state of the antiferromagnetic Heisenberg Hamiltonian on the honeycomb lattice we would naively expect all spins on the $A$ sublattice to point up and all spins on the $B$ sublattice to point down or vice versa. This is the classical antiferromagnetic Néel state, which can be written as

$$|N\rangle = \prod_{x \in A} c_{x\uparrow}^\dagger \prod_{x \in B} c_{x\downarrow}^\dagger |0\rangle. \quad (5.1)$$

It motivates the definition of the staggered magnetization vector

$$\vec{M}_s = \sum_x (-1)^x \vec{S}_x, \quad (5.2)$$

which is an order parameter. Note that in the Néel state the ordinary uniform magnetization is zero. We already defined the factor $(-1)^x$ to be 1 for $x \in A$ and $-1$ for $x \in B$. When defined the other way round, the staggered magnetization would point in the opposite direction, but
the physics remained the same. The existence of a non-vanishing order parameter indicates a spontaneous symmetry breaking. Indeed, the Heisenberg Hamiltonian has an $SU(2)_s$ spin symmetry, which can be seen by calculating

$$[\mathcal{H}, \vec{S}] = 0,$$

where $\vec{S}$ is the operator of the total spin

$$\vec{S} = \sum_x \vec{S}_x. \quad (5.4)$$

Instead of this $SU(2)_s$ symmetry, the classical Néel state is invariant only under $U(1)_s$ spin rotations around the spontaneously selected direction of the staggered magnetization.

Taking a closer look, one can see that the classical Néel state is not an eigenstate of the Heisenberg Hamiltonian. It can also be shown that the ground state is an $SU(2)_s$ singlet [41], which is not true for the classical Néel state. Therefore it can not be the ground state. As already mentioned, the true ground state is not known analytically, but it is known that there are also spin fluctuations in addition to the strict antiparallel spin alignment.

Because we do not know the ground state analytically, it is not obvious that there is a spontaneous symmetry breaking. It has been shown by numerical simulations that the antiferromagnetic Heisenberg model indeed shows a spontaneous symmetry breaking $SU(2)_s \to U(1)_s$, where the staggered magnetization is the appropriate order parameter. In $B\chi PT$ there is also such a spontaneous breaking of a continuous symmetry and it is possible to describe the Hubbard model at low energies with an effective theory analogous to $B\chi PT$.

### 5.2 Effective Theory for Magnons

As just discussed, in quantum antiferromagnets there occurs a spontaneous symmetry breaking from the group $G = SU(2)_s$ to the subgroup $H = U(1)_s$. For such a case Goldstone’s theorem [13] predicts $\dim(G) - \dim(H) = 3 - 1 = 2$ massless bosons, here two magnons, also called antiferromagnetic spin waves. They can be interpreted as two linearly independent excitation directions of spin waves. The Goldstone bosons are described by fields in the coset space $G/H$. In our case, the magnons are described by a classical unit-vector field $\vec{e}(x)$, living in the coset space

$$G/H = SU(2)_s/U(1)_s \equiv S^2, \quad (5.5)$$

$$\vec{e}(x) = (e_1(x), e_2(x), e_3(x)), \quad \vec{e}(x)^2 = 1, \quad (5.6)$$

with $x$ again being a Euclidean space-time point. One can view the $\vec{e}(x)$ field as representing the local staggered magnetization. As already mentioned, the effective theory does not care about distances of the order of a lattice spacing, as such distances correspond to high momenta. For the same reason the $\vec{e}(x)$ field represents an average over a lot of spins. Due to the different nature of the $\vec{e}(x)$ field and the microscopic staggered magnetization $\vec{M}_s$, the relation between them can not be derived in a rigorous way.

In order to derive a magnon action, we must know how the $\vec{e}(x)$ field transforms under the various symmetries of the Hubbard model. Since it corresponds to the staggered magnetization of the microscopic model, for the geometric transformations one only has to check whether the sublattices are interchanged or not. An $SU(2)_s$ spin rotation is realized on $\vec{e}(x)$ by a $R \in SO(3)_s$ transformation, where the $SU(2)_s$ transformation defines the corresponding
one in $SO(3)$. How time-reversal is realized on $\vec{e}(x)$, can be derived as follows. The $\vec{e}(x)$ field corresponds to the staggered magnetization and this to spin operators. Spin is a form of angular momentum $\vec{L} = \vec{r} \times \vec{p}$ and under time-reversal the momentum changes sign. Therefore one concludes that the $\vec{e}(x)$ field changes sign under time-reversal.

Because the $SU(2)_Q$ and $U(1)_Q$ symmetries act non-trivially only on fermions, not on bosons, the $\vec{e}(x)$ field and the following magnon field representations are invariant under these transformations. To summarize, we have the following transformation properties

$$SU(2)_S : \quad \vec{e}(x)' = R \vec{e}(x),$$

$$D_1 : \quad D_1 \vec{e}(x) = \vec{e}(x),$$

$$O : \quad O \vec{e}(x) = -\vec{e}(Ox),$$

$$R : \quad R \vec{e}(x) = \vec{e}(Rx),$$

$$T : \quad T \vec{e}(x) = -\vec{e}(Tx),$$

with $Ox$, $Rx$, and $Tx$ as in eq. (4.24). As already mentioned, spatial and spin rotations do not affect each other. Especially the spin rotation does not affect the space-time point $x$. In section 2.2 we pointed out that the sublattices change under rotation, thus we get a minus sign, and they don’t change under a shift. This is different in the square lattice case.

Now we can construct the leading terms of the Euclidean action for the pure magnon sector as we did for the Dirac fermions. They describe the low-energy physics of an undoped antiferromagnet. Antiferromagnetic magnons have a relativistic energy-momentum relation ($E \propto p$) at low energies. Therefore spatial and temporal derivatives count the same. Terms like $\vec{e}(x) \cdot \vec{e}(x)$ are constant and thus irrelevant, while terms like $\vec{e}(x) \cdot \partial_\mu \vec{e}(x)$ are zero. We find exactly the same action as in the square lattice case [24, 28–30]

$$S[\vec{e}] = \int d^2x dt \mathcal{L}_0 = \int d^2x dt \frac{\rho_s}{2} \left( \partial_i \vec{e} \cdot \partial_i \vec{e} + \frac{1}{c^2} \partial_t \vec{e} \cdot \partial_t \vec{e} \right),$$

where the index $i \in \{1, 2\}$ (summation) stands for the two spatial directions. The Euclidean time direction is compactified to a circle $S^1$ of circumference $\beta = 1/T$, where $T$ is the temperature of the system. The spin stiffness $\rho_s$ and the spin wave velocity $c$ are material-dependent low-energy constants. For energy values small compared to $\rho_s$, the low-energy expansion is valid. The values of the low-energy constants can not be derived in the framework of the effective theory. They have to be determined by either experiments or numerical simulations. The two constants $\rho_s$ and $c$ have been determined very precisely by fitting Monte Carlo data to predictions of the effective theory in [25] for the square and in [10] for the honeycomb lattice and are given in tab. 5.1. As mentioned in section 2.1, the coordination number of the honeycomb lattice is three, while for the square lattice it is four, which explains the smaller values for the honeycomb lattice as the spins are more weakly coupled.

In [32–34] it is shown, that there is no spontaneous symmetry breaking for systems in two dimensions. Together with time, we are working in $2+1$ dimensions, where the extent of the time dimension is inversely proportional to the temperature $T$. Thus, at zero temperature we are dealing with three dimensions, where spontaneous symmetry breaking may occur. At non-zero temperatures, the extent of the time dimension is finite and the magnons pick up a mass which is exponentially small in the inverse temperature [30]. The effective theory remains valid as long as the described particles are the lightest and remain the relevant degrees of freedom in the low-energy spectrum.
Lattice | $\rho_s$ | $c$
--- | --- | ---
Square | 0.1808(4)$J$ | 1.6585(10)$Ja$
Honeycomb | 0.102(2)$J$ | 1.297(16)$Ja$

Table 5.1: Numerical values for the low-energy constants $\rho_s$ and $c$. $J$ is the exchange coupling constant of the Heisenberg model and $a$ the corresponding lattice spacing.

Instead of working with the vector field representation $\vec{e}(x)$ of the magnon field, it will turn out to be more convenient to use a $2 \times 2$ matrix representation $P(x)$ defined by

$$P(x) = \frac{1}{2}(1 + \vec{e}(x) \cdot \vec{\sigma}) = \frac{1}{2} \begin{pmatrix} 1 + e_3(x) & e_1(x) - ie_2(x) \\ e_1(x) + ie_2(x) & 1 - e_3(x) \end{pmatrix},$$

(5.9)

with $P(x) \in \mathbb{CP}(1) \cong S^2$ having the properties

$$P(x)^\dagger = P(x), \quad \text{Tr} P(x) = 1, \quad P(x)^2 = P(x),$$

(5.10)

i.e. it is a Hermitian projection matrix. On the matrix representation $P(x)$, the $SU(2)_s$ transformation is again realized by an element $g \in SU(2)_s$ as shown below. The behaviour of $P(x)$ under the other transformations can be derived from the transformation rules of the $\vec{e}(x)$ field. For later convenience we also introduce a $O'$ and a $T'$ transformation which are the ordinary rotation and time-reversal transformations combined with a special $SU(2)_s$ transformation $g = i\sigma_2$. Then we obtain the following transformation behaviour

$$SU(2)_s: \quad P(x)' = g P(x) g^\dagger, \quad D_i: \quad D_i P(x) = P(x), \quad O: \quad O P(x) = 1 - P(Ox), \quad O': \quad O' P(x) = P(Ox)^*, \quad R: \quad R P(x) = P(Rx),$$

$$T: \quad T P(x) = 1 - P(Tx) = O P(O^{-1}Tx), \quad T': \quad T' P(x) = P(Tx)^* = O' P(O^{-1}Tx).$$

(5.11)

The transformed objects have the same properties as $P(x)$. Written in terms of $P(x)$, the magnon action reads

$$S[P] = \int d^2x \, dt \, \rho_s \text{Tr} \left[ \partial_i P \partial_i P + \frac{1}{c^2} \partial_t P \partial_t P \right].$$

(5.12)

5.3 Non-linear Realization of the $SU(2)_s$ Symmetry

Since $SU(2)_s$ is spontaneously broken, global $SU(2)_s$ transformations on the hole fields will be realized by a local, non-linear symmetry transformation in the unbroken subgroup $U(1)_s$. This concept, where a spontaneously broken symmetry group is represented by a non-linear realization in a continuous subgroup, is used in $B\chi$PT and can be generalized to arbitrary compact, connected, semi-simple Lie groups [15, 16]. With this procedure, the magnon fields
can be coupled to the hole fields. The non-linear realization is constructed from the global transformation \( g \in SU(2)_s \) and \( P(x) \). In a first step, we uniquely represent the magnon field by a local \( SU(2)_s \) field \( u(x) \) which diagonalizes \( P(x) \) by a unitary transformation
\[
 u(x)P(x)u(x)^\dagger = \frac{1}{2}(1 + \sigma_3) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad u_{11}(x) \geq 0. \tag{5.13}
\]

To obtain a well-defined diagonalizing field \( u(x) \), we demand that \( u_{11} \) is real and non-negative. Otherwise it would be defined only up to a \( U(1)_s \) phase. A detailed derivation of \( u(x) \) can be found in [2]. One gets
\[
 u(x) = \frac{1}{\sqrt{2(1 + e_3(x))}} \begin{pmatrix} 1 + e_3(x) & e_1(x) - ie_2(x) \\ -e_1(x) - ie_2(x) & 1 + e_3(x) \end{pmatrix} = \begin{pmatrix} \cos(\frac{\theta(x)}{2}) & \sin(\frac{\theta(x)}{2}) \exp(-i\varphi(x)) \\ -\sin(\frac{\theta(x)}{2}) \exp(i\varphi(x)) & \cos(\frac{\theta(x)}{2}) \end{pmatrix}. \tag{5.14}
\]

For the second equality spherical coordinates are used
\[
 \vec{c}(x) = (\sin(\theta(x) \cos(\varphi(x)), \sin(\theta(x) \sin(\varphi(x)), \cos(\theta(x))). \tag{5.15}
\]

As the diagonalizing field rotates an arbitrary magnon field configuration \( P(x) \) at each space-time point in the constant configuration of eq. (5.13), which corresponds to \( \vec{c}(x) = (0, 0, 1) \), it contains the same information as \( P(x) \) or \( \vec{c}(x) \).

With \( u(x) \) we have an \( SU(2)_s \) representation of the magnon field. Now we are looking for the local non-linear symmetry transformation \( h(x) \) in the unbroken subgroup \( U(1)_s \). It results from the behaviour of \( u(x) \) under global \( SU(2)_s \) transformations. We demand
\[
 u(x)^\dagger P(x)^\dagger u(x)^\dagger = u(x)P(x)u(x)^\dagger = \frac{1}{2}(1 + \sigma_3). \tag{5.16}
\]

Since \( P(x) \) transforms under an \( SU(2)_s \) transformation as \( gP(x)g^\dagger \), one might think that the transformed \( u(x) \) takes the form \( u(x)^\dagger = u(x)g^\dagger \). However, then the uniqueness of \( u(x) \) after the transformation is again not guaranteed as \( u_{11} \) may pick up a \( U(1)_s \) phase. In order to make it unique also after the transformation, we must introduce a local non-linear symmetry transformation \( h(x) \), which makes \( u_{11} \) real and non-negative. It has the form
\[
 h(x) = \exp(i\alpha(x)\sigma_3) = \begin{pmatrix} \exp(i\alpha(x)) & 0 \\ 0 & \exp(-i\alpha(x)) \end{pmatrix} \in U(1)_s. \tag{5.17}
\]

Then the diagonalizing field \( u(x) \) transforms under \( SU(2)_s \) as
\[
 u(x)^\dagger = h(x)u(x)g^\dagger, \quad u_{11}(x)^\dagger \geq 0, \tag{5.18}
\]

which implicitly defines \( h(x) \). The \( x \)-dependence of \( h(x) \) arises because it depends on \( P(x) \). However this does not mean that the \( SU(2)_s \) transformation has become truly local. With non-linearity is meant, that \( h(x) \) depends on the magnon field. In the special case that \( g \) is in the unbroken subgroup \( (g = \text{diag}(\exp(i\beta), \exp(-i\beta)) \in U(1)_s) \), \( h(x) \) reduces to \( h(x) = h = g \) i.e. it becomes global and linearly realized.
It remains to show that the $SU(2)_s$ group structure is properly inherited by the non-linear $U(1)_s$ realization. This is the case when a composite $SU(2)_s$ transformation $g = g_2g_1$ leads to a composite transformation $h(x) = h_2(x)h_1(x)$. The first transformation $g_1$ defines $h_1$

$$ P(x)' = g_1P(x)g_1^\dagger, \quad u(x)' = h_1(x)u(x)g_1^\dagger. \quad (5.19) $$

Then the second transformation $g_2$ defines $h_2$

$$ P(x)'' = g_2P(x)g_2^\dagger = g_2g_1P(x)(g_2g_1)^\dagger = gP(x)g^\dagger, \quad u(x)'' = h_2(x)u(x)g_2^\dagger = h_2(x)h_1(x)u(x)(g_2g_1)^\dagger = h(x)u(x)g^\dagger. \quad (5.20) $$

Indeed $h(x) = h_2(x)h_1(x)$ and thus the group structure is properly inherited.

Now we know how the $SU(2)_s$ transformation is realized on the diagonalizing field $u(x)$. Under the other transformations one finds

$$ D_1 : \quad D_1u(x) = u(x),$$
$$ O : \quad O^u(x) = \tau(Ox)u(Ox),$$
$$ O' : \quad O'u(x) = u(Ox)^*,$$
$$ R : \quad Ru(x) = u(Rx),$$
$$ T : \quad T_u(x) = \tau(Tx)u(Tx) = O^u(O^{-1}Tx),$$
$$ T' : \quad T'u(x) = u(Tx)^* = O'^u(O^{-1}Tx), \quad (5.21) $$

with

$$ \tau(x) = \frac{1}{\sqrt{e_1(x)^2 + e_2(x)^2}} \begin{pmatrix} 0 & -e_1(x) + ie_2(x) \\ e_1(x) + ie_2(x) & 0 \end{pmatrix} = \begin{pmatrix} \exp(i\varphi(x)) & -\exp(-i\varphi(x)) \\ \exp(i\varphi(x)) & 0 \end{pmatrix} \in U(1). \quad (5.22)$$

One can see that the transformations, under which the $\vec{e}(x)$ field changes sign ($O$ and $T$), are also spontaneously broken as they are realized in a non-linear manner ($\tau(x)$ depends on the magnon field). The combined transformations $O'$ and $T'$ are realized in a linear manner (independent of the magnon field) and are thus not spontaneously broken. We introduced them because they are easier to handle, as their transformation behaviour is simpler. They are used instead of $O$ and $T$ to facilitate the construction of terms in the effective Lagrangian. In the square lattice case, instead of the rotation, the shift symmetry is spontaneously broken. As already mentioned, this is because on the square lattice the sublattices $A$ and $B$ are interchanged by a shift, while on the honeycomb they are interchanged under rotation.

The above transformation rules can be derived from the transformations of the $\vec{e}(x)$ field. For the combined transformations one first applies $O$ or $T$, respectively, and then the special $SU(2)_s$ transformation, where $h(x)$ takes the form $h(Ox) = (i\sigma_2)\tau(Ox)^\dagger$ or $h(Tx) = (i\sigma_2)\tau(Tx)^\dagger$, respectively.

### 5.4 Composite Magnon Field $v_\mu(x)$

All still in analogy to B\chi PT, we introduce the anti-Hermitian composite magnon field $v_\mu(x)$

$$ v_\mu(x) = u(x)\partial_\mu u(x)^\dagger. \quad (5.23)$$
As it is constructed from the diagonalizing field $u(x)$, it is just another magnon field representation. One finds the transformation rules of $v_\mu(x)$ using those of $u(x)$

\begin{align}
SU(2)_s : \quad & v_\mu(x)' = h(x)[v_\mu(x) + \partial_\mu]h(x)^\dagger, \\
D_i : \quad & D_i v_\mu(x) = v_\mu(x), \\
O : \quad & O v_1(x) = \tau(Ox)^\dagger v_1(Ox) + \partial_1 + \sqrt{3}v_2(Ox) + \sqrt{3}\partial_2 \tau(Ox)^\dagger, \\
& O v_2(x) = \tau(Ox)^\dagger (-\sqrt{3}v_1(Ox) - \sqrt{3}\partial_1 + v_2(Ox) + \partial_2) \tau(Ox)^\dagger, \\
& O v_t(x) = \tau(Ox)(v_t(Ox) + \partial_t) \tau(Ox)^\dagger, \\
O' : \quad & O' v_1(x) = \frac{1}{2} (v_1(Ox)^* + \sqrt{3}v_2(Ox)^*), \\
& O' v_2(x) = \frac{1}{2} (-\sqrt{3}v_1(Ox)^* + v_2(Ox)^*), \\
& O' v_t(x) = v_t(Ox)^*, \\
R : \quad & R v_1(x) = v_1(Rx), \\
& R v_2(x) = -v_2(Rx), \\
& R v_t(x) = v_t(Rx), \\
T : \quad & T v_1(x) = \tau(Tx)(v_1(Tx) + \partial_1) \tau(Tx)^\dagger, \\
& T v_2(x) = -\tau(Tx)(v_2(Tx) + \partial_2) \tau(Tx)^\dagger, \\
& T v_t(x) = v_t(Tx)^*, \\
T' : \quad & T' v_1(x) = v_1(Tx)^*, \\
& T' v_2(x) = -v_2(Tx)^*. \quad (5.24)
\end{align}

Since the composite magnon field is anti-Hermitian and traceless, we can decompose it into the Pauli matrices

\begin{align}
v_\mu(x) = iv_\mu^a(x)\sigma_a = i \left( \begin{array}{cc} v_\mu^3(x) & v_\mu^1(x) \\ v_\mu^{-1}(x) & -v_\mu^3(x) \end{array} \right), \quad a \in \{1, 2, 3\}, \quad v_\mu^a(x) \in \mathbb{R}, \quad (5.25)
\end{align}

where the factor $i$ makes $v_\mu(x)$ anti-Hermitian. The components $v_\mu^a(x)$ are given by

\begin{align}
v_\mu^a(x) = \frac{1}{2i} \text{Tr}[v_\mu(x)\sigma_a]. \quad (5.26)
\end{align}

They do not represent independent degrees of freedom as they are all built from the magnon field. For convenience we also define the fields

\begin{align}
v_\mu^{\pm}(x) = v_\mu^1(x) \mp iv_\mu^3(x). \quad (5.27)
\end{align}

The $v_\mu^3(x)$ and the $v_\mu^{\pm}(x)$ fields will finally be used. Let us first investigate their behaviour under $SU(2)_s$ transformations. With the eqs. (5.24), (5.25), and (5.17) (where $\alpha(x)$ stems from) one finds

\begin{align}
v_\mu^3(x)' &= v_\mu^3(x) - \partial_\mu \alpha(x), \\
v_\mu^{\pm}(x)' &= \exp(\pm 2i\alpha(x))v_\mu^{\pm}(x). \quad (5.28)
\end{align}

The transformation rule for $v_\mu^3(x)$ looks like the one of an Abelian $U(1)_s$ gauge field, while the $v_\mu^{\pm}(x)$ show the behaviour of vector fields charged under $U(1)_s$. Although the spin rotation symmetry disguises itself as a gauge-like symmetry, one should stress that the spin symmetry
is not really gauged. In fact, the gauge field nature of \( v_{\mu}^3(x) \) results from the non-linear \( U(1)_s \) realization of the global \( SU(2)_s \) symmetry.

Under the other transformations using eqs. (5.24) and (5.25) one finds the following behaviour of the \( v_{\mu}^3(x) \) and \( v_{\mu}^+(x) \) fields (\( \varphi(x) \) stems from the diagonalizing field \( u(x) \))

\[
D_i : \quad D_i v_{\mu}^3(x) = v_{\mu}^+(x), \\
O : \quad O v_{\mu}^3(x) = \frac{1}{2} \left( -v_{\mu}^3(Ox) + \partial_1 \varphi(Ox) - \sqrt{3} v_{\mu}^3(Ox) + \sqrt{3} \partial_2 \varphi(Ox) \right), \\
O v_{\mu}^+(x) = \frac{1}{2} \left( \sqrt{3} v_{\mu}^+(Ox) - \sqrt{3} \partial_1 \varphi(Ox) - v_{\mu}^3(Ox) + \partial_2 \varphi(Ox) \right), \\
O v_{\mu}^-(x) = -v_{\mu}^3(Ox) + \partial_1 \varphi(Ox), \\
O' : \quad O' v_{\mu}^3(x) = -\frac{1}{2} \left( v_{\mu}^3(Ox) + \sqrt{3} v_{\mu}^3(Ox) \right), \\
O' v_{\mu}^+(x) = \frac{1}{2} \left( \sqrt{3} v_{\mu}^+(Ox) - v_{\mu}^3(Ox) \right), \\
O' v_{\mu}^-(x) = -v_{\mu}^3(Ox), \\
R : \quad R v_{\mu}^3(x) = v_{\mu}^+(Rx), \\
R v_{\mu}^+(x) = -v_{\mu}^3(Rx), \\
R v_{\mu}^-(x) = v_{\mu}^3(Rx), \\
T : \quad T v_{\mu}^3(x) = -v_{\mu}^3(Tx) + \partial_1 \varphi(Tx), \\
T v_{\mu}^+(x) = v_{\mu}^3(Tx) - \partial_1 \varphi(Tx), \\
T' : \quad T' v_{\mu}^3(x) = -v_{\mu}^3(Tx), \\
T' v_{\mu}^+(x) = v_{\mu}^3(Tx), \quad (5.29)
\]

\[
D_i : \quad D_i v_{\mu}^+(x) = v_{\mu}^+(x), \\
O : \quad O v_{\mu}^+(x) = -\exp(\mp 2i \varphi(Ox)) \frac{1}{2} \left( v_{\mu}^+(Ox) + \sqrt{3} v_{\mu}^+(Ox) \right), \\
O v_{\mu}^-(x) = \exp(\mp 2i \varphi(Ox)) \frac{1}{2} \left( \sqrt{3} v_{\mu}^+(Ox) - v_{\mu}^+(Ox) \right), \\
O v_{\mu}^+(x) = -\exp(\mp 2i \varphi(Ox)) v_{\mu}^+(Ox), \\
O' : \quad O' v_{\mu}^+(x) = -\frac{1}{2} \left( v_{\mu}^+(Ox) + \sqrt{3} v_{\mu}^+(Ox) \right), \\
O' v_{\mu}^-(x) = \frac{1}{2} \left( \sqrt{3} v_{\mu}^+(Ox) - v_{\mu}^+(Ox) \right), \\
O' v_{\mu}^+(x) = -v_{\mu}^+(Ox), \\
R : \quad R v_{\mu}^+(x) = v_{\mu}^+(Rx), \\
R v_{\mu}^-(x) = -v_{\mu}^+(Rx), \\
R v_{\mu}^+(x) = v_{\mu}^+(Rx), \\
T : \quad T v_{\mu}^+(x) = -\exp(\mp 2i \varphi(Tx)) v_{\mu}^+(Tx), \\
T v_{\mu}^-(x) = \exp(\mp 2i \varphi(Tx)) v_{\mu}^+(Tx), \\
T' : \quad T' v_{\mu}^+(x) = -v_{\mu}^+(Tx), \\
T' v_{\mu}^-(x) = v_{\mu}^+(Tx), \quad (5.30)
\]

It is shown in [2], how the magnon action can be formulated in terms of the composite magnon
field which then reads

\[ S[v_{\mu}^\pm] = \int d^2x dt \ 2\rho_s \left( v_i^+ v_i^- + \frac{1}{c^2} v_i^+ v_i^- \right). \]  

(5.31)

As the fields contain a derivative, the terms in the action are kinetic terms and not mass terms.
Chapter 6

From Microscopic Operators to Effective Fields for Holes

Since we also want to describe doped holes, we have to derive the corresponding hole fields and their transformation properties. In the following procedure there are again parallels to the case of the Dirac fermions, but it is a little more complicated because of the non-linear realization of the $SU(2)_s$ symmetry. A priori, the fermion operators or fields we will use in the following sections describe a combination of electrons and holes, which is why we refer them to as fermion operators or fields, respectively. The finally used hole fields are identified in the last section of this chapter.

6.1 Fermion Operators with a Sublattice Index

In [10] the single hole sector of the $t$-$J$ model is investigated with a loop-cluster algorithm. There the energy-momentum relation is simulated (fig. 6.1). It shows that at low energies the holes live at the corners of the first Brillouin zone, i.e. in the same pockets as the Dirac fermions in the weak coupling limit. Hence, the effective theory has to describe holes living

![Figure 6.1: Energy-momentum relation $E(k)/t$ for a single hole in an antiferromagnet on the honeycomb lattice in the $t$-$J$ model for $J/t = 2$. (Figure taken from [10].)
in these pockets. To address the pockets we use the same sublattices as in section 4.2.1. Also here, the connection between the microscopic operators and the Grassmann fields can not be derived in a rigorous way because of the different nature of the microscopic theory and the effective theory. Now we also have to take the spontaneous symmetry breaking into account. As an intermediate step, we introduce fermionic lattice operators by multiplying the diagonalizing field \( u(x) \) of eq. (5.14) and the microscopic operator \( C_x \) of eq. (3.17)

\[
\Psi^X_x = u(x)C_x = u(x) \begin{pmatrix} \psi^X_{x,1} \psi^X_{x,1}^\dagger \\ \psi^X_{x,-1}^\dagger \psi^X_{x,-1} \end{pmatrix}, \tag{6.1}
\]

where \( x \in X \) stands for a discrete lattice site and \( X \in \{ A_1, A_2, A_3, B_1, B_2, B_3 \} \) for a sublattice. For the even \( A \) and odd \( B \) sublattices we have

\[
\Psi^X_x = u(x) \begin{pmatrix} \psi^X_{x,1} \psi^X_{x,1}^\dagger \\ \psi^X_{x,-1}^\dagger \psi^X_{x,-1} \end{pmatrix}, \quad x \in X \land X \in \{ A_1, A_2, A_3 \}, \tag{6.2}
\]

\[
\Psi^Y_x = u(x) \begin{pmatrix} \psi^Y_{x,1} \psi^Y_{x,1}^\dagger \\ \psi^Y_{x,-1}^\dagger \psi^Y_{x,-1} \end{pmatrix}, \quad x \in X \land X \in \{ B_1, B_2, B_3 \}.
\]

Besides addressing the sublattices, this definition is the connection between the microscopic model and the effective theory. It also guarantees that the global \( SU(2)_s \) transformations are realized non-linearly in the subgroup \( U(1)_s \) on the fermionic degrees of freedom (see eq. (6.3)). Since \( SU(2)_s \) is spontaneously broken, the spin along the \( x_3 \)-axis is not a good quantum number any more. Instead we measure the spin of each fermion relative to the local staggered magnetization. Doing so, we indicate spin no longer with an arrow, but with a plus or minus sign, indicating parallel or antiparallel alignment with respect to the local staggered magnetization. The operators \( \psi^X_{x, \pm} \) obey standard anticommutation relations. Using the transformation rules of \( u(x) \) and \( C_x \) one finds the ones for \( \Psi^X_x \)

\[
SU(2)_s: \quad \Psi^X_x' = h(x)\Psi^X_x,
\]

\[
SU(2)_Q: \quad \tilde{Q}\Psi^X_x = \Psi^X_x \Omega^T_x,
\]

\[
D_1: \quad D_1 \Psi^X_x = \Psi^{D_1X}_x,
\]

\[
O: \quad O\Psi^X_x = \tau(Ox)\Psi^{OX}_x \sigma_3,
\]

\[
O': \quad O'\Psi^X_x = (i\sigma_2)\Psi^{OX}_x \sigma_3,
\]

\[
R: \quad R\Psi^X_x = \Psi^{RX}_x.
\tag{6.3}
\]

\( D_1X, OX, \) and \( RX \) are the sublattices after the corresponding transformation. Since we are now dealing with fermions, here the \( SU(2)_Q \) symmetry acts non-trivially. As for \( C_x \), we do not list the transformation rule under time-reversal \( T \) and \( T' \) as this is implemented by an antiunitary operator. However, time-reversal will be implemented afterwards on the effective fields.

### 6.2 Fermion Fields with a Sublattice Index

Again we change from the Hamiltonian to the Lagrangian formalism used in a Euclidean path integral. With this we change from the microscopic operators to Grassmann fields living in
the space-time continuum. We connect the two formulations by identifying matrix-valued fermion fields with the fermionic lattice operators of eq. (6.2), similar as we did for the Dirac fermions

\[
\Psi^X(x) = \begin{pmatrix}
\psi^X_+(x) & \psi^X_1(x) \\
\psi^X_- (x) & -\psi^X_1(x)
\end{pmatrix}, \quad X \in \{A_1, A_2, A_3\},
\]

\[
\Psi^X(x) = \begin{pmatrix}
\psi^X_+(x) & -\psi^X_- (x) \\
\psi^X_- (x) & \psi^X_1(x)
\end{pmatrix}, \quad X \in \{B_1, B_2, B_3\}. \tag{6.4}
\]

Doing so, the matrix-valued fermion fields inherit the transformation rules from the microscopic operators. The conjugate matrix-valued fields read

\[
\Psi^X_\dag(x) = \begin{pmatrix}
\psi^{X\dag}_+(x) & \psi^{X\dag}_1(x) \\
\psi^{X\dag}_- (x) & \psi^{X\dag}_1(x)
\end{pmatrix}, \quad X \in \{A_1, A_2, A_3\},
\]

\[
\Psi^X_\dag(x) = \begin{pmatrix}
\psi^{X\dag}_+(x) & -\psi^{X\dag}_1 (x) \\
-\psi^{X\dag}_- (x) & \psi^{X\dag}_1(x)
\end{pmatrix}, \quad X \in \{B_1, B_2, B_3\}. \tag{6.5}
\]

To avoid confusion with relativistic theories, we do not denote the conjugate fields by \(\bar{\psi}^X_\pm(x)\).

In contrast to their components (Grassmann fields), the matrix-valued fields \(\Psi^X_\dag(x)\) and \(\Psi^X(x)\) are not independent as they consist of the same fields. For the matrix-valued fermion fields we have the following transformation rules

\[
SU(2)_s : \quad \Psi^X(x)' = h(x)\Psi^X(x),
\]

\[
SU(2)_Q : \quad \bar{Q}\Psi^X(x) = \Psi^X(x)Q^T,
\]

\[
D_i : \quad D_i\Psi^X(x) = \Psi^{D_i X}(x),
\]

\[
O : \quad O\Psi^X(x) = \tau(Ox)|\Psi^{OX}(Ox)\sigma_3,
\]

\[
O' : \quad O'\Psi^X(x) = (i\sigma_2)|\Psi^{OX}(Ox)\sigma_3,
\]

\[
R : \quad R\Psi^X(x) = \Psi^{RX}(Rx),
\]

\[
T : \quad T\Psi^X(x) = \tau(Tx)(i\sigma_2)\left[\Psi^{X\dag}(Tx)^T\right]\sigma_3,
\]

\[
T\Psi^X_\dag(x) = -\sigma_3 \left[\Psi^X(Tx)^T\right] (i\sigma_2)^\dagger \tau(Tx)^\dagger,
\]

\[
T' : \quad T'\Psi^X(x) = -\left[\Psi^{X\dag}(Tx)^T\right]\sigma_3,
\]

\[
T'\Psi^X_\dag(x) = \sigma_3 \left[\Psi^X(Tx)^T\right]. \tag{6.6}
\]

An upper index \(T\) on the right denotes transpose, while on the left it denotes time-reversal. Here we now list the transformation behaviour under time-reversal \(T\) and \(T'\). Time-reversal in the effective theory with nonlinearly realized \(SU(2)_s\) symmetry follows from the usual form of time-reversal in the path integral of a nonrelativistic theory in which the spin symmetry is linearly realized. The fermion fields in the two formulations just differ by a factor \(u(x)\).
From the transformation rules above one can read off the ones of the components

\[
\begin{align*}
SU(2)_s : & \quad \psi^X_\pm(x)' = \exp(\pm i\alpha(x))\psi^X_\pm(x), \\
U(1)_Q : & \quad \Omega \psi^X_\pm(x)' = \exp(i\omega)\psi^X_\pm(x), \\
D_i : & \quad D_i \psi^X_\pm(x)' = \psi^{D_i X}_\pm(x), \\
O : & \quad O \psi^X_\pm(x)' = \pm \exp(\mp i\varphi(Ox))\psi^{OX}_\pm(Ox), \\
O' : & \quad O' \psi^X_\pm(x)' = \pm \psi^{OX}_\pm(Ox), \\
R : & \quad R \psi^X_\pm(x) = \psi^{RX}_\pm(Rx), \\
T : & \quad T \psi^X_\pm(x)' = \exp(\mp i\varphi(Tx))\psi^{X1}_\pm(Tx), \\
T' : & \quad T' \psi^X_\pm(x)' = -\psi^X_\pm(Tx), \\
T'' : & \quad T'' \psi^X_\pm(x) = \psi^X_\pm(Tx).
\end{align*}
\] (6.7)

Since the $SU(2)_Q$ symmetry acts simply only on the matrix-valued fields, we only consider the $U(1)_Q$ symmetry on the level of the component Grassmann fields. Under time-reversal, both the spin and the staggered magnetization change their sign. As a result, the projection of the spin on the staggered magnetization does not change.

### 6.3 Fermion Fields with a Sublattice and Momentum Index

To describe the fermions living in the $\alpha$ and $\beta$ pocket, we make the same discrete Fourier transformation as for the Dirac fermions of eq. (4.19) with the matrix-valued fields of eq. (6.4). Then we obtain matrix-valued fermion fields with a momentum index composed of the same linear combinations as we had for the Dirac fermions

\[
\begin{align*}
\Psi^{A,\alpha}(x) &= \frac{1}{\sqrt{3}} (\exp(i\frac{2\pi x}{3})\Psi^{A1}(x) + \Psi^{A2}(x) + \exp(-i\frac{2\pi x}{3})\Psi^{A3}(x)), \\
\Psi^{A,\beta}(x) &= \frac{1}{\sqrt{3}} (\exp(-i\frac{2\pi x}{3})\Psi^{A1}(x) + \Psi^{A2}(x) + \exp(i\frac{2\pi x}{3})\Psi^{A3}(x)), \\
\Psi^{B,\alpha}(x) &= \frac{1}{\sqrt{3}} (\exp(i\frac{2\pi x}{3})\Psi^{B1}(x) + \Psi^{B2}(x) + \exp(-i\frac{2\pi x}{3})\Psi^{B3}(x)), \\
\Psi^{B,\beta}(x) &= \frac{1}{\sqrt{3}} (\exp(-i\frac{2\pi x}{3})\Psi^{B1}(x) + \Psi^{B2}(x) + \exp(i\frac{2\pi x}{3})\Psi^{B3}(x)).
\end{align*}
\] (6.8)

They take the form

\[
\Psi^{A,f}(x) = \begin{pmatrix} \psi^{A,f}_1(x) & \psi^{A,f\dagger}_1(x) \\ \psi^{A,f}_2(x) & -\psi^{A,f\dagger}_2(x) \end{pmatrix}, \quad \Psi^{B,f}(x) = \begin{pmatrix} \psi^{B,f}_1(x) & \psi^{B,f\dagger}_1(x) \\ \psi^{B,f}_2(x) & \psi^{B,f\dagger}_2(x) \end{pmatrix},
\] (6.9)

and their conjugate counterparts are

\[
\Psi^{A,f\dagger}(x) = \begin{pmatrix} \psi^{A,f\dagger}_1(x) & \psi^{A,f\dagger}_2(x) \\ \psi^{A,f\dagger}_1(x) & -\psi^{A,f\dagger}_2(x) \end{pmatrix}, \quad \Psi^{B,f\dagger}(x) = \begin{pmatrix} \psi^{B,f\dagger}_1(x) & -\psi^{B,f\dagger}_2(x) \\ \psi^{B,f\dagger}_2(x) & \psi^{B,f\dagger}_1(x) \end{pmatrix}.
\] (6.10)
Their transformation rules are

\[
SU(2)_s : \quad \Psi^{X,f}(x)' = h(x)\Psi^{X,f}(x),
\]

\[
SU(2)_Q : \quad \tilde{Q}\Psi^{X,f}(x) = \Psi^{X,f}(x)\Omega^T,
\]

\[
D_i : \quad D_i\Psi^{X,f}(x) = \exp(ik^i a_i)\Psi^{X,f}(x),
\]

\[
O : \quad O\Psi^{A,\alpha}(x) = \exp(-i\frac{2\pi}{3})\tau(Ox)\Psi^{B,\beta}(Ox)\sigma_3,
\]

\[
O\Psi^{A,\beta}(x) = \exp(i\frac{2\pi}{3})\tau(Ox)\Psi^{A,\alpha}(Ox)\sigma_3,
\]

\[
O\Psi^{B,\beta}(x) = \exp(-i\frac{2\pi}{3})\tau(Ox)\Psi^{B,\alpha}(Ox)\sigma_3,
\]

\[
O' : \quad O'\Psi^{A,\alpha}(x) = \exp(-i\frac{2\pi}{3})(i\sigma_2)\Psi^{B,\beta}(Ox)\sigma_3,
\]

\[
O'\Psi^{A,\beta}(x) = \exp(i\frac{2\pi}{3})(i\sigma_2)\Psi^{A,\alpha}(Ox)\sigma_3,
\]

\[
O'\Psi^{B,\beta}(x) = \exp(-i\frac{2\pi}{3})(i\sigma_2)\Psi^{B,\alpha}(Ox)\sigma_3,
\]

\[
R : \quad R\Psi^{X,f}(x) = \Psi^{X,f'}(Rx),
\]

\[
T : \quad T\Psi^{X,f}(x) = \tau(Tx)(i\sigma_2) \left[\Psi^{X,f\dagger}(Tx)^T\right] \sigma_3,
\]

\[
T\Psi^{X,f\dagger}(x) = -\sigma_3 \left[\Psi^{X,f}(Tx)^T\right] \sigma_3,
\]

\[
T' : \quad T'\Psi^{X,f}(x) = -\left[\Psi^{X,f\dagger}(Tx)^T\right] \sigma_3,
\]

\[
T'\Psi^{X,f\dagger}(x) = \sigma_3 \left[\Psi^{X,f'}(Tx)^T\right].
\]

From them one can again read off the transformation rules for the components

\[
SU(2)_s : \quad \psi^{X,f}(x)' = \exp(\pm i\alpha(x))\psi^{X,f}(x),
\]

\[
U(1)_Q : \quad Q\psi^{X,f}(x) = \exp(i\omega)\psi^{X,f}(x),
\]

\[
D_i : \quad D_i\psi^{X,f}(x) = \exp(ik^i a_i)\psi^{X,f}(x),
\]

\[
O : \quad O\psi^{A,\alpha}(x) = \mp \exp(-i\frac{2\pi}{3} + i\varphi(Ox))\psi^{B,\beta}(Ox),
\]

\[
O\psi^{A,\beta}(x) = \mp \exp(i\frac{2\pi}{3} + i\varphi(Ox))\psi^{B,\alpha}(Ox),
\]

\[
O\psi^{B,\beta}(x) = \mp \exp(-i\frac{2\pi}{3} + i\varphi(Ox))\psi^{A,\alpha}(Ox),
\]

\[
O' : \quad O'\psi^{B,\beta}(x) = \pm \exp(-i\frac{2\pi}{3})\psi^{B,\alpha}(Ox),
\]

\[
O'\psi^{B,\alpha}(x) = \pm \exp(i\frac{2\pi}{3})\psi^{A,\beta}(Ox),
\]

\[
O'\psi^{B,\beta}(x) = \pm \exp(-i\frac{2\pi}{3})\psi^{A,\alpha}(Ox),
\]

\[
R : \quad R\psi^{X,f}(x) = \psi^{X,f'}(Rx),
\]

\[
T : \quad T\psi^{X,f}(x) = \exp(\mp i\varphi(Tx))\psi^{X,f\dagger}(Tx),
\]

\[
T\psi^{X,f\dagger}(x) = -\exp(\pm i\varphi(Tx))\psi^{X,f'}(Tx),
\]

\[
T' : \quad T'\psi^{X,f}(x) = -\psi^{X,f\dagger}(Tx),
\]

\[
T'\psi^{X,f\dagger}(x) = \psi^{X,f'}(Tx).
\]
6.4 Hole Fields

As already mentioned in the introduction of this chapter, the fermion fields may describe a combination of electron and hole fields. In this section we will now identify the final hole fields. Using the matrix-valued fermion fields we are able to write down a Lagrangian which is $SU(2)_Q$ invariant. However, this would be necessary only for the Hubbard model at half-filling, where electrons and holes are present at the same time. Real materials and also the t-J model do not contain both. This means that the effective Lagrangian which we will construct only has to be $U(1)_Q$ invariant. Hence, we should break the $SU(2)_Q$ symmetry explicitly.

The hole fields can be identified by first writing down all mass terms with the matrix-valued fermion fields with momentum index of eq. (6.9). Second, after writing the mass terms in spinor notation, one has to diagonalize the obtained mass matrices. Then the entries in the diagonals are the masses of the fermions.

The trace notation used for the matrix-valued fermion fields has several difficulties. One never knows whether one has found all terms, it is much harder to see linear dependencies, and terms may be zero (for more details see [4]). Because of that, we also constructed all mass terms in component notation. From this we then knew that there are two linearly independent mass terms. They read

\begin{equation}
\sum_{f=\alpha,\beta} \frac{1}{2} \text{Tr}[M(\Psi^A,f^\dagger \sigma_3 \Psi^A,f - \Psi^B,f^\dagger \sigma_3 \Psi^B,f) + m(\Psi^A,f^\dagger \Psi^A,f + \Psi^B,f^\dagger \Psi^B,f)]
\end{equation}

\begin{equation}
= \sum_{f=\alpha,\beta} \left[ M(\psi^A_+ f^\dagger \psi^A_+ - \psi^A_- f^\dagger \psi^A_- + \psi^B_+ f^\dagger \psi^B_- - \psi^B_- f^\dagger \psi^B_+ )
\right.
\end{equation}

\begin{equation}
+ m(\psi^A_+ f^\dagger \psi^A_+ + \psi^A_- f^\dagger \psi^A_- + \psi^B_+ f^\dagger \psi^B_- + \psi^B_- f^\dagger \psi^B_+ )]
\end{equation}

\begin{equation}
= \sum_{f=\alpha,\beta} \left[ (\psi^A_+ f^\dagger \psi^B_+ f^\dagger) \begin{pmatrix} M + m & 0 \\ 0 & -M + m \end{pmatrix} \begin{pmatrix} \psi^A_+ f^\dagger \\ \psi^B_+ f^\dagger \end{pmatrix}
\right.
\end{equation}

\begin{equation}
+ (\psi^A_+ f^\dagger , \psi^B_+ f^\dagger) \begin{pmatrix} -M + m & 0 \\ 0 & M + m \end{pmatrix} \begin{pmatrix} \psi^A_+ f^\dagger \\ \psi^B_+ f^\dagger \end{pmatrix}
\end{equation}

The term proportional to $M$ is invariant under $SU(2)_Q$ transformations while the one proportional to $m$ is only invariant under $U(1)_Q$ and breaks $SU(2)_Q$ explicitly. Since the obtained matrices are already diagonal, we don’t have to diagonalize them. Without the $SU(2)_Q$-breaking term (i.e. for $m = 0$), the eigenvalues of the mass matrices, and with this the masses of the fermions, are $\pm M$ and we have a perfect symmetry. When we also take the $SU(2)_Q$-breaking term into account, these masses are shifted to $\pm M + m$. The hole fields correspond to the lower eigenvalue $-M + m$ and are identified as the corresponding eigenvectors

\begin{equation}
\psi^{B,\alpha}_+(x), \quad \psi^{B,\beta}_+(x), \quad \psi^{A,\alpha}_-(x), \quad \psi^{A,\beta}_-(x).
\end{equation}

In contrast to the square lattice case, where the mass matrices are not automatically diagonal, we do not obtain linear combinations but only identify the four correct fields. As we remove the electrons, the electron-hole symmetry is broken explicitly and the Lagrangian describing doped holes has to be invariant only under the remaining $U(1)_Q$ fermion number symmetry. However, the $SU(2)_Q$ symmetry was important to identify the hole fields. Electron fields could be identified in the same way as the hole fields. The notation of the four remaining
fields can be simplified as \( B \) is always combined with + and \( A \) with −. Thus in the following we drop the sublattice index and we obtain the final hole fields
\[
\psi_{+}^{\alpha}(x) = \psi_{+}^{B,\alpha}(x), \quad \psi_{+}^{\beta}(x) = \psi_{+}^{B,\beta}(x), \quad \psi_{-}^{\alpha}(x) = \psi_{-}^{A,\alpha}(x), \quad \psi_{-}^{\beta}(x) = \psi_{-}^{A,\beta}(x),
\]
and their conjugated counterparts. Finally, we list their transformation rules, which are the same as in eq. (6.12), but with the simpler notation
\[
SU(2)_{s}: \quad \psi_{\pm}^{f}(x) = \exp(\pm i\alpha(x))\psi_{\pm}^{f}(x),
\]
\[
U(1)Q: \quad Q\psi_{\pm}^{f}(x) = \exp(\pm i\alpha(x))\psi_{\pm}^{f}(x),
\]
\[
D_{1}: \quad D_{1}\psi_{\pm}^{f}(x) = \exp(\pm ik_{a}x)\psi_{\pm}^{f}(x),
\]
\[
O: \quad O\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(x), \quad O\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(x),
\]
\[
O': \quad O'\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(x), \quad O'\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(x),
\]
\[
Q': \quad Q'\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(x), \quad Q'\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(x),
\]
\[
R: \quad R\psi_{\pm}^{f}(x) = \psi_{\pm}^{f}(Rx),
\]
\[
T: \quad T\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(Tx), \quad T\psi_{\pm}^{f}(x) = \exp(\pm i\alpha x)\psi_{\pm}^{f}(Tx),
\]
\[
T': \quad T'\psi_{\pm}^{f}(x) = -\psi_{\pm}^{f}(Tx), \quad T'\psi_{\pm}^{f}(x) = -\psi_{\pm}^{f}(Tx).
\]
(6.16)
They are mapped on themselves under the various symmetry transformations and the spontaneously broken \( SU(2)_{s} \) symmetry is realized in a non-linear way on the hole fields.
Chapter 7

Effective Field Theory for Magnons and Holes

In chapter 5 we derived the effective magnon action for an undoped antiferromagnet. A pure antiferromagnet is the ground state or vacuum of our theory and corresponds to the half-filled system in the Hubbard model. It is like the Dirac sea in a relativistic quantum field theory and it is a charge neutral state. When we remove electrons from the half-filled system, we get doped holes. In this chapter we want to extend the action to describe also doped holes in addition to the magnons. We do this again in a similar way as for the Dirac fermions. At the end we discuss some accidental emergent symmetries.

7.1 Effective Action for Magnons and Holes

One can write the effective action for magnons and holes as

$$S\left[\psi_f^\dagger, \psi_f, \vec{e}\right] = \int d^2x \, dt \sum_{n_\psi} \mathcal{L}_{n_\psi},$$

(7.1)

where $n_\psi$ stands for the number of hole fields. The partition function takes the form

$$Z = \int D\psi_f^\dagger D\psi_f D\vec{e} \exp\left(-S\left[\psi_f^\dagger, \psi_f, \vec{e}\right]\right).$$

(7.2)

For completeness we again write down the leading terms of the low-energy effective magnon Lagrangian

$$\mathcal{L}_0 = \frac{\rho_s}{2} \left( \partial_i \vec{e} \cdot \partial_i \vec{e} + \frac{1}{c^2} \partial_t \vec{e} \cdot \partial_t \vec{e} \right) = 2\rho_s \left( v_i^+ v_i^- + \frac{1}{c^2} v_t^+ v_t^- \right).$$

(7.3)

Before we can begin with the construction of the effective Lagrangian describing holes, which consists of derivatives, hole fields and the magnon fields $v_\mu^\sigma(x)$ and $v_\mu^\pm(x)$, we have to consider how the number of derivatives is counted. As mentioned, the magnons have a relativistic energy-momentum relation ($E \propto p$) at low energies. Therefore, both, spatial and temporal derivatives on magnon fields correspond to first order. The holes on the other side, have a non-relativistic energy-momentum relation ($E \propto p^2$) at low energies. Thus a temporal derivative acting on a hole field corresponds to second order while a spatial derivative corresponds to first order. This causes problems as derivatives can be shifted around by partial integration. For example a temporal derivative may act first on a hole field and after a partial integration...
on a magnon field. To solve this problem completely, which is necessary when one wants to do loop-calculations, one would have to develop a power counting scheme. This is nontrivial and since we are only interested in the leading order, we don’t need it for our purposes. Therefore we won’t develop such a power counting scheme at the moment. Instead we make the convention that we always let temporal derivatives act on the hole fields if such exist in a given term. In the following we will go up to second order in the expansion to also include temporal derivatives.

One has to keep in mind, that the magnon fields also contain a derivative. As we did in the case of the Dirac fermions, we characterize the parts of the Lagrangian by the number of hole fields they contain. We argued that always as many daggered as undaggered hole fields are needed in a term. Up to second order, the contribution \( L_2 \) which describes a single \( \alpha \) or \( \beta \)-hole doped in the antiferromagnet and its interactions with magnons reads

\[
L_2 = \sum_{s=+,+} \left[ M \psi_s^f \psi_s^f + \psi_s^f D_t \psi_s^f + \frac{1}{2M^f} D_t \psi_s^f D_t \psi_s^f \right.
+ \Lambda \psi_s^f \left( i s v_1^f + \sigma_f v_2^f \right) \psi_s^f + i K \left( \left[ (D_1 + i \sigma_f D_2) \psi_s^f \right] (v_1^f + i \sigma_f v_2^f) \psi_s^f 
- \left( v_1^f + i \sigma_f v_2^f \right) \psi_s^f \left( (D_1 + i \sigma_f D_2) \psi_s^f \right) \right.
+ \sigma_f \tilde{v}_1^f \psi_s^f \left. \right] + i \sigma_f N_2 \left( \psi_s^f \psi_s^f \right. \psi_s^f + i s v_2^f \psi_s^f \psi_s^f \left. \right) - \psi_s^f \psi_s^f \psi_s^f \psi_s^f \right],
\]  

(7.4)

with the field strength tensor of the composite Abelian ”gauge” field defined by

\[
f^3_{ij}(x) = \partial_i v^3_j(x) - \partial_j v^3_i(x).
\]  

(7.5)

\( \sigma_f \) is still + for \( f = \alpha \) and – for \( f = \beta \). As already mentioned, the \( SU(2)_s \) symmetry is not really gauged, it just acts on the hole fields as a local \( U(1)_s \) gauge-like symmetry. To make the Lagrangian invariant, we introduced the covariant derivatives

\[
D_t \psi_{\pm}^f(x) = \left[ \partial_t \pm i v_1^f(x) - \mu \right] \psi_{\pm}^f(x),
\]

\[
D_t \psi_{\pm}^f(x) = \left[ \partial_t \mp i v_1^f(x) + \mu \right] \psi_{\pm}^f(x),
\]

\[
D_t \psi_{\pm}^f(x) = \left[ \partial_t \pm i v_3^f(x) \right] \psi_{\pm}^f(x),
\]

\[
D_t \psi_{\pm}^f(x) = \left[ \partial_t \mp i v_3^f(x) \right] \psi_{\pm}^f(x).
\]  

(7.6)

The chemical potential \( \mu \) enters the covariant time-derivative like an imaginary constant vector potential for the fermion number symmetry \( U(1)_Q \).

All low-energy constants in \( L_2 \) are real. \( M \) is the rest mass and \( M' \) the kinetic mass of a hole. Since we deal with a non-relativistic theory, they don’t have to be the same. Terms including magnon fields describe hole-magnon interactions. As we will see in chapter 8, \( v_{\pm}^f(x) \) corresponds to one magnon and \( v_3^f(x) \) to two magnons. The terms proportional to \( \Lambda \) are the leading hole-one-magnon interaction terms and are thus dominant. There is an \( M'^{\prime} \)-term but no \( L \)-term in the square lattice case. In fact, the two terms are similar but because of a minus sign in case of the \( L \)-term, some contributions cancel and it can be written in a simpler form. The factor \( i \) in front of the \( K \) and \( N_2 \)-term ensures that the corresponding Hamiltonian is Hermitian. Also here \( \rho_s \) defines the energy scale below which the low-energy expansion is valid, i.e. for energy values small compared to \( \rho_s \). In addition to the spin stiffness \( \rho_s \) and the spin wave velocity \( c \) (see tab. 5.1), also the value of the kinetic mass \( M' \) has been determined in [10]. Its value is \( 4.1(1)/ta^2 \), with \( t \) from the \( t-J \) model.

From eq. (7.4) one can derive a single hole energy-momentum relation

\[
E^f(p) = M + \frac{p_0^2}{2M^f} + O(p^4),
\]  

(7.7)
where the momentum is relative to the center of the corresponding hole pocket. This is the energy-momentum relation of a free, nonrelativistic particle and it describes circular shaped hole pockets, which is in agreement with the simulation mentioned in section 6.1.

Terms with more than two hole fields are contact terms and therefore describe short-range interactions. Because we are most interested in the long-range interactions, we only construct $L_4$ without derivatives in addition to $L_2$. It reads

$$L_4 = \sum_{s=+,-} \left[ \frac{G_1}{2} (\psi^\alpha_s \psi^\alpha_s \psi^\beta_s \psi^\beta_s + \psi^\beta_s \psi^\beta_s \psi^\alpha_s \psi^\alpha_s) + G_2 \psi^\alpha_s \psi^\alpha_s \psi^\beta_s \psi^\beta_s + G_3 \psi^\alpha_s \psi^\alpha_s \psi^\beta_s \psi^\beta_s \right].$$  \hfill (7.8)

All low-energy constants are real. As already mentioned in the case of the Dirac fermions, terms with identical fermion fields vanish due to the Pauli principle and thus also terms with more than eight fermion fields and without derivatives again do not exist.

## 7.2 Accidental Emergent Symmetries

The fundamental forces underlying condensed matter physics are Poincaré-invariant. By the formation of a crystal lattice, some of the space-time symmetries are spontaneously broken. The Goldstone bosons resulting from this spontaneous symmetry breaking are the phonons. They arise in the low-energy spectrum, but it is expected that they alone can not provide a mechanism for Cooper pair formation. In the Hubbard model, and hence in our effective theory, these symmetries are broken explicitly as the lattice is given from the outset. Therefore the Hubbard model and the effective theory don’t contain phonons. In this context of a non-relativistic theory, in addition to the breakdown of the continuous translation and rotation symmetries to their discrete counterparts, also the Galilean boost invariance is broken. This provides a preferred rest frame and because of that, magnon-mediated forces between a pair of holes may depend on the center of mass momentum of the pair.

If phonons were important, one could construct an effective theory of spontaneously broken $SU(2)_s$ and Galilean symmetry, which then would include magnons and phonons. We assume in this thesis that phonons do not play an important role. Hence it is legitimate to break the Galilean symmetry by hand, thus excluding phonons.

In the following two sections we show that some leading terms of the effective Lagrangian show accidentally emergent symmetries which are broken by higher orders in the expansion.

### 7.2.1 Galilean Boost Symmetry $G$

Ignoring the higher order $K$-term, the $L_2$ (of eq. (7.4)) shows an accidental Galilean boost symmetry $G$ acting on the different fields as

$$G : \quad G P(x) = P(Gx), \quad Gx = (x_1 - v_1 t, x_2 - v_2 t, t),$$

$$G \psi^f_\pm(x) = \exp(-p^f_i x_i + \omega^f t) \psi^f_\pm(Gx),$$

$$G \psi^f_{\mp}(x) = \exp(p^f_i x_i - \omega^f t) \psi^f_{\mp}(Gx),$$

$$G v^3_i(x) = v^3_i(Gx),$$

$$G v^2_i(x) = v^2_i(Gx) - v_i v^3_i(Gx),$$

$$G v^+_i(x) = v^+_i(Gx) - v_i v^+_i(Gx)$$

$$G v^-_i(x) = v^-_i(Gx) - v_i v^-_i(Gx),$$  \hfill (7.9)
with
\[ p_1' = M'v_1, \quad p_2' = M'v_2, \]
and the energy-momentum relation
\[ \omega' = \frac{(p'_1)^2}{2M'}. \]

Here the \( v_i \) denote the boost velocity. By means of this accidental Galilean boost symmetry, the magnon-mediated forces between two holes don’t depend on the total momentum and it is possible to investigate the hole pair in their rest frame without loss of generality as long as only the leading \( \Lambda \)-term is involved (see chapter 9).

### 7.2.2 Continuous \( O(\gamma) \) Rotation Symmetry

Again ignoring the higher order \( K \)-term, \( \mathcal{L}_2 \) also has an accidental continuous \( O(\gamma) \) rotation symmetry which acts on the fields as

\[
\begin{align*}
O(\gamma)\psi \pm (x) &= \exp(is\sigma_{\frac{\gamma}{2}})\psi \pm (O(\gamma)x), \\
O(\gamma)v_1(x) &= \cos\gamma v_1(O(\gamma)x) + \sin\gamma v_2(O(\gamma)x), \\
O(\gamma)v_2(x) &= -\sin\gamma v_1(O(\gamma)x) + \cos\gamma v_2(O(\gamma)x),
\end{align*}
\]

with
\[
O(\gamma)x = O(\gamma)(x_1, x_2, t) = (\cos\gamma x_1 - \sin\gamma x_2, \sin\gamma x_1 + \cos\gamma x_2, t).
\]

Here the \( v_i \) stand for the composite magnon field of eq. (5.23). The \( \Lambda \)-term also has this symmetry. This implies that, in contrast to the square lattice case, where no such accidental rotation symmetry occurs, spirals in the staggered magnetization can point in an arbitrary direction. This is discussed in [9, 11].
Chapter 8

One-Magnon Exchange Potentials

At low energies, the long-range dynamics is dominated by one-magnon exchange between holes. Since we are interested in possible long-range attractive forces between hole pairs as potential mechanisms for Cooper pair formation, we will focus on them. Hence, in the following we are going to use the effective theory to investigate the one-magnon exchange between a pair of holes. For this purpose we first derive the one-magnon exchange potentials between an isolated pair of holes in an otherwise undoped antiferromagnet in this chapter. The system is considered undoped as two additional holes do not cause a finite hole density. It is also possible to investigate a system with finite hole density, which is done in [9, 11] in the context of spiral phases. In the following by ”one-magnon physics” we mean processes in which a single magnon couples to holes. After deriving the potentials, in the next chapter we will write down the corresponding Schrödinger equation and discuss it. In this chapter we deal with two-dimensional space vectors and three-dimensional space-time vectors. To distinguish them, from now on two-dimensional space vectors are denoted with a vector arrow while the three-dimensional space-time vectors are not.

8.1 One-Magnon Action

Aiming at the potentials, we will first derive the one-magnon action, which is the reduced action only describing a single magnon propagating and coupling to holes. For this we now do some preparation. In the ground state of an antiferromagnet, the staggered magnetization points in the same direction at every space-point. Without loss of generality, we can choose the ordered configuration to point in the $x_3$-direction, i.e. $\vec{e}(x) = (0, 0, 1)$. To include magnons, we allow small fluctuations in the local staggered magnetization. We expand the magnon fluctuations $m_1(x)$ and $m_2(x)$ around the ordered staggered magnetization up to first order

$$\vec{e}(x) = \left( \frac{m_1(x)}{\sqrt{\rho_s}}, \frac{m_2(x)}{\sqrt{\rho_s}}, 1 \right) + \mathcal{O}(m^2).$$

The $L_0$ from eq. (7.3) expanded in the magnon fluctuations reads

$$L_0 = \frac{1}{2} \left( \partial_i m_a \partial_i m_a + \frac{1}{c^2} \partial_i m_a \partial_t m_a \right) + \mathcal{O}(m^4),$$

with a sum over the repeated indices. It describes the propagation of a magnon, therefore contains two fields, and is thus quadratic in the fluctuations. The magnons are coupled to the
holes through the $v^3_\mu(x)$ and $v^\pm_\mu(x)$ fields. We also expand them in the magnon fluctuations

$$v^+_\mu(x) = \frac{1}{2\sqrt{\rho_s}} \partial_\mu [m_2(x) \pm im_1(x)] + O(m^3),$$

$$v^3_\mu(x) = \frac{1}{4\rho_s} [m_1(x) \partial_\mu m_2(x) - m_2(x) \partial_\mu m_1(x)] + O(m^4).$$

One can see that $v^\pm_\mu(x)$ is linear in the fluctuations and thus describes one magnon, while $v^3_\mu(x)$ is quadratic and describes two magnons. Using the combination

$$m(x) = m_1(x) + im_2(x),$$

we can write them in a more compact form

$$v^+_\mu(x) = \frac{i}{2\sqrt{\rho_s}} \partial_\mu m^*(x), \quad v^-_\mu(x) = -\frac{i}{2\sqrt{\rho_s}} \partial_\mu m(x).$$

Now we will extract the one-magnon physics from $\mathcal{L}_0$ and $\mathcal{L}_2$ (eqs. (7.3) and (7.4)). Thus, apart from the propagator, we only take contributions up to first order in the fluctuations into account. This means that the $v^\pm_\mu(x)$ fields drop out. The low-energy effective action relevant for one-magnon exchange then reads

$$S[\psi^f_\pm, \psi^f_\mp, m] = \int d^2x \, dt \left\{ \frac{1}{2} \left( \partial_\mu m^* \partial_\mu m + \frac{1}{c^2} \partial_\mu m^* \partial_\mu m \right) - \frac{1}{2\sqrt{\rho_s}} \sum_{f=\alpha,\beta} \sum_{j=1}^4 \left[ \Lambda \left( \psi^{f+}_\mu (\partial_1 m^* + i\sigma_2 m^*) \psi^j_- + \psi^{j+}_\mu (\partial_1 m - i\sigma_2 m) \psi^j_+ \right) + K \left( \partial_1 - i\sigma_2 \partial_2 \right) \psi^{f+}_\mu (\partial_1 m^* - i\sigma_2 m^*) \psi^j_- - (\partial_1 m^* - i\sigma_2 \partial_2 m^*) \psi^{j+}_\mu (\partial_1 m - i\sigma_2 m) \psi^j_+ + (\partial_1 m + i\sigma_2 \partial_2 m) \psi^{j+}_\mu (\partial_1 + i\sigma_2 \partial_2 m) \psi^j_+ \right) + O(m^2)\mathcal{L}_2 + O(m^4)\mathcal{L}_0 \right\}. \quad (8.6)$$

We dropped the terms describing only holes. From the hole-magnon interaction terms only the $\Lambda$ and parts of the $K$-term describe one-magnon couplings. One can see that a hole undergoes a spin flip by emitting or absorbing a magnon. The magnon carries the spin difference one in the sense of a flavour quantum number. This implies that only holes with opposite spin can exchange a magnon.

### 8.2 Kinematics

We now discuss the kinematics of one-magnon exchange at tree level. The corresponding Feynman diagram is shown in fig. 8.1. The $\vec{p}_\pm$ are the momenta of the incoming and the $\vec{p}'_\pm$ the momenta of the outgoing holes, while the momentum carried by the exchanged magnon is denoted by $\vec{q}$. Here $f = \alpha, \beta$ and $\bar{f} = \alpha, \beta$ stand for the flavour of the incoming spin $+$ and $-$ hole, respectively. The incoming and outgoing holes are asymptotically free with the energy-momentum relation from eq. (7.7)

$$E^f(\vec{p}) = M + \frac{p^2}{2M} + O(p^4).$$

(8.7)
8.3 Transforming to Momentum Space

\[
\begin{align*}
\vec{p}_+ & \quad \rightarrow \quad \vec{p}_- \\
\vec{p}_+ & \quad \rightarrow \quad \vec{p}_+ \\
\vec{p}_- & \quad \rightarrow \quad \vec{p}_- \\
\vec{f}_+ & \quad \rightarrow \quad \vec{f}_- \\
\vec{f}_- & \quad \rightarrow \quad \vec{f}_+ \\
\vec{q} & \quad \rightarrow \quad \vec{q}
\end{align*}
\]

Figure 8.1: Tree-level Feynman diagram for one-magnon exchange between two holes. (Figure taken from [5].)

Momentum conservation at the vertices implies
\[
\vec{p}_+ = \vec{q} + \vec{p}_-^\prime, \quad \text{and} \quad \vec{p}_- = \vec{p}_+^\prime - \vec{q}. \quad \Rightarrow \quad \vec{p}_+ + \vec{p}_- = \vec{p}_+^\prime + \vec{p}_-^\prime,
\]
where we can identify the total momentum \( \vec{P} \) of the hole pair
\[
\vec{P} = \vec{p}_+ + \vec{p}_- = \vec{p}_+^\prime + \vec{p}_-^\prime.
\]

Energy conservation at the vertices implies
\[
E^f(\vec{p}_+) = q_0 + E^f(\vec{p}_-^\prime), \quad \text{and} \quad E^f(\vec{p}_-) = E^f(\vec{p}_+^\prime) - q_0,
\]
where \( q_0 \) stands for the energy of the magnon. Solving these two equations for \( q_0 \) gives
\[
q_0 = \frac{1}{2M^f}(\vec{p}_+^2 - \vec{p}_-^2), \quad q_0 = \frac{1}{2M^f}(\vec{p}_+^2 - \vec{p}_-^2).
\]

In the following we will use the energy-momentum vectors
\[
p = (\vec{p}, E^f(\vec{p})), \quad q = (\vec{q}, q_0).
\]

The actual form of \( q_0 \) will not be used in the following. From the eqs. (8.11) we only want to note that \( q_0 \propto \vec{p}^2 \). The following calculations will always involve \( q^2 \), never just \( q \). Because \( q_0^2 \) is proportional to \( \vec{p}^4 \) and since we work only up to order \( \vec{p}^2, \vec{q}^2 \) and \( \vec{q}^2 \) are actually the same.

8.3 Transforming to Momentum Space

It is convenient to work in momentum space. Therefore we will transform the action relevant for one-magnon physics from eq. (8.6) into momentum space. The Fourier transformations of the hole fields and the magnon fluctuations take the form
\[
\begin{align*}
\psi^f_{\pm}(x) &= \frac{1}{(2\pi)^3} \int d^3p \psi^f_{\pm}(p) \exp(-ipx), \\
\psi^{f\dagger}_{\pm}(x) &= \frac{1}{(2\pi)^3} \int d^3p \psi^{f\dagger}_{\pm}(p) \exp(ipx), \\
m(x) &= \frac{1}{(2\pi)^3} \int d^3q m(q) \exp(iqx), \\
m^*(x) &= \frac{1}{(2\pi)^3} \int d^3q m^*(q) \exp(-iqx).
\end{align*}
\]

(8.13)
With these we can construct the combinations arising in the action

\[
\int d^3x \partial_\mu m^*(x) \partial_\mu m(x) = \frac{1}{(2\pi)^3} \int d^3q \, m(q) m^*(q) q_\mu^2, \quad \text{(no sum over } \mu),
\]

\[
\int d^3x \psi_{+}^f(x) \partial_j m^*(x) \psi_{-}^f(x) = -i \int d^3p_- \int d^3q \, \psi_{+}^f(p_- + q) m^*(q) \psi_{-}^f(q) j_j,
\]

\[
\int d^3x \psi_{-}^f(x) \partial_j m(x) \psi_{+}^f(x) = \frac{i}{(2\pi)^6} \int d^3p_+ \, d^3q \, \psi_{-}^f(p_+ - q) m(q) \psi_{+}^f(p_+ + q) j_j,
\]

\[
\int d^3x \partial_i \psi_{+}^f(x) \partial_j m(x) \psi_{-}^f(x) = \frac{1}{(2\pi)^3} \int d^3p_+ \, d^3q \, \psi_{-}^f(p_+ - q) m(q) \psi_{+}^f(p_+) j_j (p_+ - q),
\]

\[
\frac{1}{(2\pi)^3} \int d^3p_+ \, d^3q \, \psi_{-}^f(p_+ - q) m(q) \psi_{+}^f(p_+) j_j (p_+ - q),
\]

By means of these relations we obtain the one-magnon action in momentum space

\[
S[\psi_{\pm}^f, m] = \int d^3q \sum_{f=\alpha, \beta} \left\{ \frac{1}{(2\pi)^3} \frac{1}{2} m^* q^2 
\right. \\
+ \frac{1}{(2\pi)^6} \frac{\Lambda}{\sqrt{2} \rho_s} \left[ \int d^3p_- \, \psi_{+}^f m^* \psi_{-}^f (iq_1 + \sigma f q_2) - \int d^3p_+ \, \psi_{+}^f m \psi_{+}^f (iq_1 - \sigma f q_2) \right] \\
+ \frac{iK}{(2\pi)^6} \frac{\Lambda}{\sqrt{2} \rho_s} \left[ \int d^3p_- \, \psi_{+}^f m^* \psi_{-}^f (iq_1 (p_- + q_1) - i q_2 (p_- + q_2)) \\
- \sigma f (q_1 (p_- + q_2) + q_2 (p_- + q_1)) + p_- q_2 + p_- q_1 + i p_- q_1 - i p_- q_2 \right] \\
+ \int d^3p_+ \, \psi_{+}^f m \psi_{+}^f (iq_1 (p_+ + q_1) - i q_2 (p_+ + q_2)) \\
\left. + \sigma f (q_1 (p_+ + q_2) + q_2 (p_+ + q_1)) + p_+ q_2 + p_+ q_1 + i p_+ q_1 - i p_+ q_2 \right \} \right\}. \quad (8.14)
\]

The term proportional to $1/c^2$ in the magnon propagator disappeared because it is proportional to $p_0^2$ and thus proportional to $p^4$. Note that the arguments of the fields are always the same and that we drop them when writing down a Lagrangian.

### 8.4 Principle of Stationary Action

Since we consider the magnon exchange only at tree level, the physics is of non-quantum nature and thus we can use the principle of stationary action. Therefore we extremize the action in momentum space with respect to the magnon fluctuations $m^*(q)$ and $m(q)$ with the
help of the Euler-Lagrange equations. This results in

\[ m(q) = -\frac{1}{(2\pi)^3 \sqrt{\rho_s q^2}} \int d^3p_- \sum_{f=\alpha,\beta} \left\{ \Lambda \psi_+^f (p_- + q) \psi_-^f (p_-) (iq_1 + \sigma_f q_2) \\
- K \psi_+^f (p_- + q) \psi_-^f (p_-) (q_1 + i\sigma_f q_2) \\
\times (q_1 + 2p_{-1} + i\sigma_f (2p_{-2} + q_2)) \right\}, \quad (8.16) \]

and

\[ m^*(q) = -\frac{1}{(2\pi)^3 \sqrt{\rho_s q^2}} \int d^3p_+ \sum_{f=\alpha,\beta} \left\{ \Lambda \psi_-^f (p_+ - q) \psi_+^f (p_+) (iq_1 - \sigma_f q_2) \\
- K \psi_-^f (p_+ - q) \psi_+^f (p_+) (q_1 - i\sigma_f q_2) \\
\times (q_1 - 2p_{+1} + i\sigma_f (2p_{+2} - q_2)) \right\}. \quad (8.17) \]

When we plug the obtained expressions for \( m^*(q) \) and \( m(q) \) back into the action, the magnon fields are integrated out and we obtain

\[ S[\psi_\pm^f, \psi_\pm^f]_{\text{stat}} = -\frac{1}{(2\pi)^\nu} \int d^3p \, d^3p_+ \, d^3p_- \sum_{f=\alpha,\beta} \frac{1}{2\rho_s} \\
\left\{ \Lambda^2 \left[ \psi_+^f \psi_-^f \psi_-^f \psi_+^f - \psi_+^f \psi_-^f \psi_-^f \psi_+^f \frac{1}{q^2} (iq_1 + \sigma_f q_2)^2 \right] \\
+ K^2 \left[ \psi_+^f \psi_-^f \psi_-^f \psi_+^f (2p_{+1} - q_1 - i\sigma_f (2p_{+2} - q_2)) (2p_{-1} + q_1 + i\sigma_f (2p_{-2} + q_2)) \\
+ \frac{1}{q^2} \psi_+^f \psi_-^f \psi_-^f \psi_+^f (q_1 + i\sigma_f q_2)^2 (2p_{+1} - q_1 + i\sigma_f (2p_{+2} - q_2)) (2p_{-1} + q_1 + i\sigma_f (2p_{-2} + q_2)) \right] \\
- K \Lambda \left[ \frac{1}{q^2} \psi_+^f \psi_-^f \psi_-^f \psi_+^f (q_1 - i\sigma_f q_2)^2 (i(2p_{+1} - q_1) + \sigma_f (2p_{+2} - q_2)) \\
+ \psi_+^f \psi_-^f \psi_-^f \psi_+^f (i(2p_{+1} - q_1) - \sigma_f (2p_{+2} - q_2)) \right] \\
+ \Lambda K \left[ \frac{1}{q^2} \psi_+^f \psi_-^f \psi_-^f \psi_+^f (q_1 + i\sigma_f q_2)^2 (i(2p_{-1} + q_1) - \sigma_f (2p_{-2} + q_2)) \\
+ \psi_+^f \psi_-^f \psi_-^f \psi_+^f (i(2p_{-1} + q_1) - \sigma_f (2p_{-2} + q_2)) \right] \right\}. \quad (8.18) \]

The ordering of the low-energy constants indicates which term (\( \Lambda \) or \( K \)) is responsible for the upper and the lower vertex, respectively, in the Feynman diagram in fig. 8.1. Note that the sign of the exchange potentials (see next section) depends on the ordering of the hole fields. The above ordering, i.e. \( \psi_+^f \psi_-^f \psi_+^f \psi_-^f \), leads to the correct over-all sign.

### 8.5 Potentials in Momentum Space

From the stationary action we can read off the resulting potentials for the various combinations. In momentum space they take the form

\[ \langle \tilde{p}_+^f \tilde{p}_-^f | V_{FG}^{ff} | \tilde{p}_+^f \tilde{p}_-^f \rangle = V_{FG}^{ff} (q^2) \delta(\tilde{p}_+^f + \tilde{p}_-^f - \tilde{p}_+^f - \tilde{p}_-^f), \quad F, G \in \{ \Lambda, K \}, \quad (8.19) \]
8. One-Magnon Exchange Potentials

with

\[ V_{\Lambda\Lambda}^{ff}(q) = -\frac{\Lambda^2}{2\rho_s}, \quad V_{\Lambda\Lambda}^{ff}(q) = \frac{\Lambda^2}{2\rho_s q^2}(i\sigma_1 - \sigma_3 q^2)^2, \]

\[ V_{KK}^{ff}(q) = -\frac{K^2}{2\rho_s q^2}(2(p_{+1} - i\sigma_fp_{+2}) - q_1 + i\sigmafq_2)(2(p_{-1} + i\sigma_fp_{-2}) + q_1 + i\sigmafq_2), \]

\[ V_{KK}^{ff}(q) = -\frac{K^2}{2\rho_s q^2}(q_1 - i\sigmafq_2)^2(2(p_{+1} - i\sigma_fp_{+2}) - q_1 + i\sigmafq_2)(2(p_{-1} - i\sigma_fp_{-2}) + q_1 - i\sigmafq_2), \]

\[ V_{kk}^{ff}(q) = -\frac{i\Lambda K}{2\rho_s q^2}(q_1 + i\sigmafq_2)^2(2(p_{-1} + i\sigma_fp_{-2}) + q_1 + i\sigmafq_2), \]

\[ V_{\Lambda\Lambda}^{ff}(q) = -\frac{i\Lambda}{2\rho_s}(2(p_{-1} - i\sigma_fp_{-2}) + q_1 - i\sigmafq_2), \]

\[ V_{KK}^{ff}(q) = -\frac{i\Lambda K}{2\rho_s}(2(p_{+1} - i\sigma_fp_{+2}) - q_1 + i\sigmafq_2), \]

\[ V_{kk}^{ff}(q) = -\frac{i\Lambda K}{2\rho_s}(2(p_{+1} - i\sigma_fp_{+2}) - q_1 + i\sigmafq_2). \] (8.20)

Here the first low-energy constant and the first flavour correspond to the upper vertex, while the second low-energy constant and the second flavour correspond to the lower vertex in the Feynman diagram in fig. 8.1.

### 8.6 Potentials in Position Space

We already noted that the \( \Lambda \)-term is the leading contribution in one-magnon interactions. In the next chapter we will investigate the Schrödinger equation for the relative motion of two holes. For this we will only use the leading contribution, i.e. only the \( \Lambda\Lambda \)-potentials. Hence, we have to transform these back into position space. The other potentials could also be transformed into position space. This is a little more complicated but can be done along the lines of [1]. For the transformation of the potentials with mixed flavours we use the integrals

\[ \int d^2\vec{q} \frac{q_j^2}{q^2} \exp(i\vec{q} \cdot \vec{x}) = 2\pi \left( \frac{1}{x^2} - 2\frac{x_j^2}{x^4} \right) + \int f \delta^{(2)}(\vec{x}), \quad \text{(no sum over } j), \]

\[ \int d^2\vec{q} \frac{q_1 q_2}{q^2} \exp(i\vec{q} \cdot \vec{x}) = -4\pi \frac{x_1 x_2}{x^4} + g \delta^{(2)}(\vec{x}), \quad f, g \in \mathbb{R}, \] (8.21)

which can be solved by using

\[ \frac{1}{q^2} = \int_0^\infty d\lambda \exp(-\lambda q^2). \] (8.22)

Then the \( \Lambda\Lambda \)-potentials in position space read

\[ \langle \vec{r}_+ \vec{r}_- | V_{\Lambda\Lambda}^{ff} | \vec{r}_+ \vec{r}_- \rangle = V^{ff}_{\Lambda\Lambda}(\vec{r}) \delta^{(2)}(\vec{r}_+ - \vec{r}_-) \delta^{(2)}(\vec{r}_- - \vec{r}_+), \] (8.23)

with

\[ V^{ff}_{\Lambda\Lambda}(\vec{r}) = -\Lambda^2 \delta^{(2)}(\vec{r}), \quad V^{ff}_{\Lambda\Lambda}(\vec{r}) = \frac{\Lambda^2}{2\rho_s} \exp(2i\sigma_f \varphi). \] (8.24)

The \( V^{ff}_{\Lambda\Lambda}(\vec{r}) \) potentials would also have additional short-distance \( \delta \)-function contributions resulting from eq. (8.21), which we dropped. Since we will model the short-distance repulsion
by a hard core radius, $\delta$-function contributions will not be used in the following. Therefore we will also not use the $V_{\Lambda\Lambda}^f(\vec{r})$ potentials. All these contributions add to the 4-fermion contact interactions. Here $\vec{r} = \vec{r}_+ - \vec{r}_-$ denotes the distance vector between the two holes and $\varphi$ is the angle between $\vec{r}$ and the $x_1$-axis. The $\delta$-functions in eq. (8.23) assure that the holes do not change their position during the magnon exchange. Note that although the magnons travel with the finite speed $c$, the potentials are instantaneous. Retardation effects occur only at higher orders. As already mentioned in section 7.2, because of the accidental emergent Galilean boost symmetry, the $\Lambda\Lambda$-potentials do not depend on the total momentum $\vec{P}$ of the hole pair. The $V_{\Lambda\Lambda}^f(\vec{r})$ potentials fall off with $1/r^2$. 
Chapter 9

Two Hole Bound States

In this chapter we investigate the Schrödinger equation for the relative motion of two holes. As mentioned in the last chapter, we only take the leading long-ranged $V^{LL'}(\vec{r})$ potentials into account. The short-distance forces we take into account by imposing a hard core radius, i.e. a boundary condition on the wave function near the origin. We derive the radial solution for a special case analytically and find that the magnon-mediated forces lead to bound states of holes under a condition on some low-energy constants.

9.1 Corresponding Schrödinger Equation

Since the $\Lambda$-term shows an accidental Galilean boost symmetry, we can investigate the hole pair in its rest frame without loss of generality. The kinetic energy of the hole pair is

$$T = \sum_{f=\alpha,\beta} \frac{p^2_f}{2M'} + O(p^4) + \frac{p^2_i}{M'} + O(p^4).$$

(9.1)

We introduce the two probability amplitudes $\Psi_1(\vec{r})$ and $\Psi_2(\vec{r})$ which represent the two flavour-spin combinations $\alpha_+\beta_-$ and $\alpha_-\beta_+$, respectively, where we choose the distance vector $\vec{r}$ to point from the $\beta$ to the $\alpha$ hole. Because the holes undergo a spin flip during the magnon exchange, the two probability amplitudes are coupled through the magnon exchange potentials and the Schrödinger equation describing the relative motion of the hole pair is a two-component equation which reads

$$\begin{pmatrix}
-\frac{1}{M'} \Delta & V_{\Lambda\Lambda}^{\alpha\beta}(\vec{r}) \\
V_{\Lambda\Lambda}^{\alpha\beta}(\vec{r}) & -\frac{1}{M'} \Delta
\end{pmatrix}
\begin{pmatrix}
\Psi_1(\vec{r}) \\
\Psi_2(\vec{r})
\end{pmatrix} = E
\begin{pmatrix}
\Psi_1(\vec{r}) \\
\Psi_2(\vec{r})
\end{pmatrix},$$

(9.2)

with the binding energy $E$. When we plug in the potentials, we obtain

$$\begin{pmatrix}
-\frac{1}{M'} \Delta & \gamma \frac{1}{M'} \exp(-2i\varphi) \\
\gamma \frac{1}{M'} \exp(2i\varphi) & -\frac{1}{M'} \Delta
\end{pmatrix}
\begin{pmatrix}
\Psi_1(\vec{r}) \\
\Psi_2(\vec{r})
\end{pmatrix} = E
\begin{pmatrix}
\Psi_1(\vec{r}) \\
\Psi_2(\vec{r})
\end{pmatrix},$$

(9.3)

with

$$\gamma = \frac{\Lambda^2}{2\pi \rho_s}.$$  

(9.4)
Since we are mostly interested in the radial part of the solution, we make the separation ansatz
\[ \Psi_1(r, \varphi) = R_1(r) \exp(i m_1 \varphi), \quad \Psi_2(r, \varphi) = R_2(r) \exp(i m_2 \varphi), \] (9.5)
with \( r = |\vec{r}| \). Inserting the ansatz, we get the two coupled equations
\[
- \frac{1}{M'} \Delta (R_1(r) \exp(i m_1 \varphi)) + \gamma \frac{R_2(r)}{r^2} \exp(-2i \varphi) \exp(i m_2 \varphi) = E R_1(r) \exp(i m_1 \varphi),
\]
\[
- \frac{1}{M'} \Delta (R_2(r) \exp(i m_2 \varphi)) + \gamma \frac{R_1(r)}{r^2} \exp(2i \varphi) \exp(i m_1 \varphi) = E R_2(r) \exp(i m_2 \varphi). \] (9.6)

By using the Laplace operator in polar coordinates
\[
\Delta \Psi(\vec{r}) = \frac{\partial^2 \Psi(\vec{r})}{\partial r^2} + \frac{1}{r} \frac{\partial \Psi(\vec{r})}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Psi(\vec{r})}{\partial \varphi^2},
\] (9.7)
and after a multiplication of the first equation with \( M' \exp(-i m_1 \varphi) \) and of the second with \( M' \exp(-i m_2 \varphi) \), we obtain
\[
- \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{1}{r^2} m_1^2 \right) R_1(r) + \gamma M' \frac{R_2(r)}{r^2} \exp(-i \varphi(2 + m_1 - m_2)) = M' E R_1(r),
\]
\[
- \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{1}{r^2} m_2^2 \right) R_2(r) + \gamma M' \frac{R_1(r)}{r^2} \exp(i \varphi(2 + m_1 - m_2)) = M' E R_2(r). \] (9.8)

To separate the radial from the angular equations the relation
\[ 2 + m_1 - m_2 = 0 \] (9.9)
has to be fulfilled. Therefore we introduce the parameter \( m \)
\[ m_1 = m - 1, \quad m_2 = m + 1. \] (9.10)

Then we obtain the radial equations
\[
- \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{1}{r^2} (m - 1)^2 \right) R_1(r) + \gamma M' \frac{R_2(r)}{r^2} = M' E R_1(r),
\]
\[
- \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{1}{r^2} (m + 1)^2 \right) R_2(r) + \gamma M' \frac{R_1(r)}{r^2} = M' E R_2(r). \] (9.11)

In this thesis we content ourselves with the case \( m = 0 \), for which the two equations decouple and can be solved analytically. The other cases would have to be investigated numerically. Now with \( m = 0 \), we first add the second equation to the first and then subtract the second from the first. Then we obtain the two equations
\[
\left[ - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \frac{1}{r^2} \right) \right] (R_1(r) + R_2(r)) = M' E (R_1(r) + R_2(r)),
\]
\[
\left[ - \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \frac{1}{r^2} \right) \right] (R_1(r) - R_2(r)) = M' E (R_1(r) - R_2(r)). \] (9.12)

Because the two equations are different, but the energy \( E \) is the same, one of the equations has a zero solution. In the first equation the potential always has a positive sign and is thus
9.1 Corresponding Schrödinger Equation

repulsive. In the second equation on the other hand, the potential has a negative sign and is therefore attractive when the low-energy constants obey the relation

\[ 1 - \frac{M'\Lambda^2}{2\pi\rho_s} \leq 0. \]  

(9.13)

Thus, magnon-mediated forces can only lead to bound states if the low-energy constant \( \Lambda \) is larger than the critical value

\[ \Lambda_c = \sqrt{\frac{2\pi\rho_s}{M'}}. \]  

(9.14)

The same critical value arises in the investigation of the spiral phases, see [9]. Hence we are interested in the solution of the system where the first equation has a zero solution and the second a non-zero one. Then we have

\[ R_1(r) + R_2(r) = 0. \]  

(9.15)

Therefore the second equation simplifies to

\[ -\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) + (1 - \gamma M') \frac{1}{r^2} R(r) = M' E R(r), \]  

(9.16)

and we are now looking for the radial wave function \( R(r) \) between the two holes. The same equation occurred in the square lattice case and we can solve it in the same way (see [1]). It is ill-defined because the \( 1/r^2 \) potential is too singular at the origin. However, we have not yet included the short-range interactions. We model the short-range repulsion by a hard core radius \( r_0 \), i.e. we require \( R(r_0) = 0 \) for \( r \leq r_0 \).

Next we multiply the equation with \( -r^2 \) and write \( E = -|E| \), since we are now looking for bound states with \( E < 0 \). Thus we get

\[ r^2 \frac{d^2 R(r)}{dr^2} + r \frac{dR(r)}{dr} + (\gamma M' - 1 - r^2 M'|E|) R(r) = 0. \]  

(9.17)

By introducing the dimensionless parameters \( z = \sqrt{M'|E|r} \) and \( \nu = i\sqrt{\gamma M' - 1} \), we can bring the equation in the form of a Bessel differential equation (see [44])

\[ z^2 \frac{d^2 R(z)}{dz^2} + z \frac{dR(z)}{dz} - (z^2 + \nu^2) R(z) = 0. \]  

(9.18)

This equation is solved by the modified Bessel function \( K_{\nu}(z) \). Thus we obtain the radial wave function of the two holes

\[ R(r) = AK_{\nu}\left(\sqrt{M'|E|r}\right), \quad \nu = i\sqrt{\gamma M' - 1}, \]  

(9.19)

where \( A \) is a normalization constant. Demanding that the solution vanishes at the hard core radius gives a quantization condition for the bound state energy. The quantum number \( n \) then labels the \( n \)-th excited state. For large \( n \), the binding energy is given by

\[ E_n \sim -\frac{1}{M' r_0^2} \exp\left(-\frac{2\pi n}{\sqrt{\gamma M' - 1}}\right). \]  

(9.20)

Like every quantity calculated with the effective theory, the binding energy depends on low-energy constants. The binding is exponentially small in \( n \) and there are infinitely many bound
states. While the highly excited states have exponentially small energy and exponentially large size, for sufficiently small $r_0$ the ground state could have a small size and be strongly bound. However, as already mentioned, for short-distance physics the effective theory should not be trusted quantitatively. If the holes were really tightly bound, one could construct an effective theory which incorporates them as explicit low-energy degrees of freedom. As long as the binding energy is small compared to the relevant high-energy scales such as $\rho_s$, our result is valid and receives only small corrections from higher-order effects.
Chapter 10

Conclusions and Outlook

In this thesis we developed a systematic low-energy effective field theory for magnons and holes in an antiferromagnet on the honeycomb lattice analogous to BχPT. As an underlying microscopic model we used the Hubbard model. Apart from different values of the low-energy constants, the effective theory remains the same for other underlying models which have the same symmetries as the Hubbard model. We have shown that the leading action of the pure magnon sector is the same as in the square lattice case. The main part of this thesis was the construction of the leading terms of the effective Lagrangian describing magnons and holes. Most of the terms are similar to the ones in the square lattice case. However, there is an $M''$-term but no $L$-term in the square lattice case. In fact, the two terms are similar but because of a minus sign in case of the $L$-term, some contributions cancel and it can be written in a simpler form. There is also a second order $K$-term in case of the honeycomb lattice. The important leading $A$-term also occurs. The leading terms of the effective Lagrangian show an accidental emergent Galilean boost symmetry and an accidental emergent continuous rotation symmetry.

By means of the effective theory for magnons and holes we derived the one-magnon exchange potentials. Using these potentials, we investigated the Schrödinger equation describing the relative motion of two holes in an otherwise undoped antiferromagnet. We solved the radial part of this Schrödinger equation for a special case analytically and showed that under a condition on the low-energy constants the magnon-mediated forces lead to two hole bound states.

We also investigated the weak coupling limit of the Hubbard model. In this context we derived the energy-momentum relation in the zero coupling limit, where massless Dirac fermions arise. For these we constructed the leading terms of the corresponding effective Lagrangian and derived an analytic expression for their velocity.

It would be interesting to solve the radial differential equations (9.11) numerically for the cases $m \neq 0$ in further studies and to see whether this leads to two-hole bound states. In a further step, one could also take into account higher order potentials in the Schrödinger equation.

One knows that in real antiferromagnets, doped charge carriers get localized on impurities, which occur in every real antiferromagnet. Actually also doping, which is achieved by substituting ions in the insulating layers, causes impurities. This localization might be a reason for the separation of the antiferromagnetic and the superconducting phases. It would also be possible to include impurities in the effective theory, to investigate their influence on
the low-energy physics of antiferromagnets. In this thesis we have laid the groundwork for such future investigations.
Acknowledgments

First I would like to thank Professor Uwe-Jens Wiese for his excellent support although he was not in Bern all the time during this Master thesis. He always found time to answer a lot of questions, was understanding our difficulties and cared for a pleasant working atmosphere. I’m also grateful for his careful proof-reading.

Special thanks go to my mate Bänz Bessire, with whom I did all work of his and my Master thesis in close collaboration, for the excellent teamwork. It was a pleasure to work with such a committed physicist.

Many thanks are addressed to Dr. Florian Kämpfer who took, especially at the beginning, often time to answer our questions. This thanks also go to all the other people who helped us or we had discussions with, especially Dr. Fu-Jiung Jiang, Dr. Christoph Brügger, Professor Christoph Hofmann, and Urs Gerber.

Another big thanks is directed to my parents who made my studies possible although it was my second education.

Last but not least, I thank Esther Fiechter, Ruth Bestgen, Ottilia Hänni, and Kathrin Weyeneth for taking good care of all administrative issues.
Bibliography


Erklärung
gemäss Art. 28 Abs. 2 RSL 05

Name/Vorname: Wirz Marcel
Matrikelnummer: 04-125-936
Studiengang: Physik
Bachelor ☐ Master ☒ Dissertation ☐
Titel der Arbeit: Two-Hole Bound States from an Effective Field Theory for Magnons and Holes in an Antiferromagnet on the Honeycomb Lattice
Leiter der Arbeit: Prof. Dr. Uwe-Jens Wiese


Bern, den 18. Februar 2009

M. Wirz