Quantum Magnets with an $SO(n)$ symmetry

by

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Submitted to the Department of Physics
in partial fulfillment of the requirements for the degree of

Science Bachelor in Physics

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

June 1998

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Abstract

In this thesis the theory of quantum antiferromagnetism is developed in the $SO(n)$-symmetric formulation of the vector Heisenberg model. A brief review of the traditional techniques applied to the Heisenberg model and the results thereof is followed by the treatment of the generalized $SU(n)$ models of ferromagnetism and antiferromagnetism, and the generalized $SO(n)$ tensor model of antiferromagnetism. In the limit of large n, all of these models lead to mean field theories, which can be used to obtain the low-energy excitation spectra of the ground state.

The generalized $SO(n)$ vector model is introduced by embedding $SO(n)$ into $SO(n+1)$. The $n(n+1)/2$ generators of $SO(n+1)$ are split into two groups, $n(n-1)/2$ generators of $SO(n)$ and the remaining n coset generators of $SO(n+1)$. The latter transform as an n-vector under the $SO(n)$ rotations and can thus be used to define the $SO(n)$ exchange interaction. The nearest-neighbor Heisenberg Hamiltonian is written in terms of real Majorana fermions in the spinor representation of $SO(n+1)$. The path-integral formulation of the partition function leads to a saddle-point approximation in the large n limit, from which the mean field Hamiltonian and the gap equations are obtained.

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Acknowledgments

I am greatly indebted to Uwe Wiese for his patience in guiding me along the thorny paths of science, and to Sonya for everything else.

Contents

Chapter 1

Introduction

1.1 Magnetic materials

It is an empirical fact that for relatively small magnetic fields the response of the material is linear, $\mathbf{M} = \chi\mathbf{H}$, where $\mathbf{M}$ is the magnetization, $\mathbf{H}$ is the magnetic field, and χ is the magnetic susceptibility of the material. When $\mathbf{M}$ is parallel to $\mathbf{H}$ ($\chi > 0$), the material is called paramagnetic, and when $\mathbf{M}$ and $\mathbf{H}$ are antiparallel to each other ($\chi < 0$), the material is called diamagnetic. However, there are exceptions to this rule. Most notably, the linear dependence is broken in some materials without applied field, in which case they may exhibit non-zero magnetization. Such materials are called ferromagnetic. It has been established that a phase transition occurs in all ferromagnets at a certain critical temperature (also called the Curie temperature T_c, fixed for the given material), which turns a ferromagnet into a paramagnet.

It was proved by Bohr in 1911 and by van Leeuwen in 1919[1] that for any statistical ensemble of classical electrons the net magnetization must always identically vanish (the Bohr-van Leeuwen theorem); it follows, that there can be no explanation of magnetism in the framework of classical physics. Yet the semi-classical approach of Bohr's old quantum theory is able to explain to some extent the properties of magnetic materials.

In quantum physics, however, magnetism emerges naturally due to the permutation antisymmetry of the wavefunction which gives rise to the exchange term in the interaction between two electrons. To first order of the perturbation expansion for the energy, the

[1] For details, see [11] and references therein.

electrons are assumed to be strictly localized, and the exchange interaction (in this case called *direct* or *potential exchange*) is found to favor a parallel configuration of neighboring spins. Therefore all spins in a ferromagnetic ground state tend to align themselves parallel to each other, resulting in the macroscopic phenomena of spontaneous magnetization. When the temperature rises beyond the material-specific Curie point, the ferromagnetic order is destroyed by the thermal fluctuations, and the ferromagnet becomes a paramagnet.

To second order, the so-called *kinetic exchange* arises from the electrons being allowed to hop between the neighboring lattice sites. Unlike the potential exchange, the kinetic exchange tends to orient the neighboring spins antiparallel to each other, thus promoting the *antiferromagnetic order*. In real materials both the potential and the kinetic exchange are present; the dominating term determines whether the material is ferromagnetic or antiferromagnetic.

Antiferromagnets proved to be a hard nut to crack, both analytically and experimentally. The experimental discovery of antiferromagnets was delayed by the fact that they exhibit no macroscopic spontaneous magnetization and are, in that respect, indistinguishable from ordinary paramagnets. On the analytical side, the exact ground state was found only for the case of one spatial dimension; even the two-dimensional case proved exceedingly difficult for exact analysis.

The discovery of the high-temperature cuprate superconductors in 1986 [2] motivated a new wave of interest in the properties of 2-dimensional quantum antiferromagnets. High T_c superconductivity was originally discovered in $La_{2-x}Ba_xCuO_4$, the undoped precursor of which, La_2CuO_4, is an insulator with strong spin interactions between holes located at the copper sites in CuO_2 planes. It is widely believed that the antiferromagnetic spin interactions in the CuO_2 layers play an important role in shaping the superconducting properties of the doped copper oxides, while rare-earth doping ions merely stabilize the 2D layered structure and provide charge carriers. Thus the study of the planar antiferromagnets bears foremost importance to the study of high-temperature superconductivity.

1.2 Heisenberg model

One of the simplest models for electronic interactions in solids is the spin-1/2 Hubbard model,

$$\mathcal{H} = \sum_{\mathbf{x},\mathbf{y}} \sum_{\sigma} b_{\mathbf{xy}} (c^{\dagger}_{\mathbf{x}\sigma} c_{\mathbf{y}\sigma} + c^{\dagger}_{\mathbf{y}\sigma} c_{\mathbf{x}\sigma}) + U \sum_{\mathbf{x},\sigma} c^{\dagger}_{\mathbf{x}\sigma} c_{\mathbf{x}\sigma} c^{\dagger}_{\mathbf{x},-\sigma} c_{\mathbf{x},-\sigma}.$$

Note, that everywhere in the subsequent discussion we will neglect the edge effects by assuming the lattice to be sufficiently large, which is justified in the thermodynamic limit. Since even in the nearest-neighbor approximation the Hubbard Hamiltonian is too complicated for direct analysis, a number of simplifications have been introduced. In the strong-coupling limit ($U \gg b$) and for half-filling[2] the electrons are strictly localized on the lattice with the exchange interaction governed by a single effective exchange integral $J_{\mathbf{xy}}$ which takes into account the effects of both direct and kinetic exchange. (In the opposite limit of weak coupling the electrons are considered entirely itinerant.) In that case, the only remaining degrees of freedom are spins, and for half-filling the Hubbard model reduces to the spin Heisenberg model.

The effective exchange energy is written in terms of the spin exchange operator $\mathcal{P} = J_{\mathbf{xy}} \mathbf{S}_{\mathbf{x}} \cdot \mathbf{S}_{\mathbf{y}}$, where $\mathbf{S}_{\mathbf{x}}$ and $\mathbf{S}_{\mathbf{y}}$ are spin operators at the lattice sites $\mathbf{x}$ and $\mathbf{y}$ respectively. The above form of the exchange operator is reminiscent of the classical expression for the interaction energy of two coupled magnetic moments.

Sometimes, to account for the anisotropy of the crystal, the isotropic exchange interaction is replaced by $J_{\mathbf{xy}}[f(S_{1\mathbf{x}}S_{1\mathbf{y}} + S_{2\mathbf{x}}S_{2\mathbf{y}}) + gS_{3\mathbf{x}}S_{3\mathbf{y}}]$. In the latter case, two specific approximations have gained most popularity. If $g \gg f$, the z-part of the interaction dominates the x- and y- parts, which permits us to neglect the latter compared to the former. The resulting model is called the *Ising model.* If, on the other hand, $f \gg g$, the z-axis contribution can be neglected, yielding the XY-model. Both the Ising and the XY models can, under certain assumptions, serve as crude approximations to the Heisenberg Hamiltonian, but they also play an important role in condensed-matter physics as self-contained descriptions of such quantum statistical systems as binary alloys, lattice gas, etc.

The Heisenberg Hamiltonian on a d-dimensional lattice is defined in terms of the exchange interactions on the lattice,

[2]The filling factor signifies how many spins are located at each lattice site. The highest possible filling factor is 2; thus, half-filling corresponds to filling factor 1.

$$\mathcal{H}_H = \mp \sum_{\mathbf{x},\mathbf{y}} J_{\mathbf{xy}} \mathbf{S}_\mathbf{x} \cdot \mathbf{S}_\mathbf{y},$$

where $J_{\mathbf{xy}} > 0$, the upper sign corresponds to the ferromagnetic case, the lower sign corresponds to the antiferromagnetic case, and the sum is taken over all pairs of mutually interacting spins. Although significantly simpler than the Hubbard model, this Hamiltonian is still too complicated for the analytic treatment, and therefore further simplifications are usually introduced. In particular, the spin exchange may be considered sufficiently short-ranged to treat it in the nearest neighbor approximation. We can also assume the magnetic material to be isotropic and homogeneous, so that the exchange integral $J_{\mathbf{xy}}$ becomes independent of $\mathbf{x}$ and $\mathbf{y}$. Then the resulting Hamiltonian can be rewritten as

$$\mathcal{H} = \mp J \sum_{<\mathbf{x},\mathbf{y}>} \mathbf{S}_\mathbf{x} \cdot \mathbf{S}_\mathbf{y}, \tag{1.1}$$

the sum $\sum_{<\mathbf{x},\mathbf{y}>}$ being taken over all pairs of nearest neighbors. The Hamiltonian (1.1) is known as the nearest-neighbor isotropic Heisenberg Hamiltonian.

1.3 Long-range order

In the ferromagnetic ground state all spins are known to align themselves parallel to each other; this alignment causes spontaneous magnetization, and, in general, a nonlinear response of a ferromagnet to the applied magnetic field. The antiferromagnetic ground state is, however, much more complicated and is exactly known only for one-dimensional antiferromagnets. A good candidate for the antiferromagnetic ground state is the so-called *Néel state* in which the lattice is said to be comprised of two sublattices A and B with mutually antiparallel magnetizations, all nearest neighbors of a spin in sublattice A being in sublattice B, and vice versa. However, the Néel state is not an eigenstate of the Heisenberg Hamiltonian, and therefore can serve only as a trial ground state for variational purposes.

Although in both cases the interaction is essentially short-ranged, there exists a correlation between spins located at lattice sites separated by distances much greater than the effective distance of the nearest neighbor interaction. Such correlations characterize *long-range order* and are responsible for the macroscopic properties of the (anti)ferromagnetic

samples (for instance, the nonlinear response to the applied magnetic field, mentioned earlier). One of the most remarkable properties of the states with long-range order is the fact that the symmetry of the ground state is usually lower than the symmetry of the Hamiltonian. For instance, the Heisenberg Hamiltonian is $SO(3)$ invariant, but the ferromagnetic ground state has a preferred direction corresponding to the direction of the spontaneous magnetization. Therefore the original $SO(3)$ symmetry of the Hamiltonian is broken down to the the $SO(2)$ symmetry of the ground state.

The phenomenon described above is in fact very general and is known under the name of *spontaneous symmetry breaking.* It can be shown that a spontaneously broken symmetry implies the existence of long-range order in the thermodynamic limit (see [1], Chapter 6). As the measure of long-range order in quantum magnets, the spin-spin correlation length is generally used. The correlation length shows the effective distances at which the correlation between two spins is non-zero. In the ordered phase, the correlation length is infinite, but as the temperature increases, thermal fluctuations seek to destroy the ground state ordering, and the correlation length becomes finite. At high temperatures the spins become essentially uncorrelated, and therefore we expect an order-disorder phase transition to occur at some critical temperature T_c.

It must be noted, that although the three-dimensional ferromagnets and antiferromagnets exhibit spontaneous symmetry breaking and long-range order at finite temperatures, in lower dimensions it is not so. Hohenberg proved in 1967 that superfluidity is impossible in one and two dimensions at $T > 0$ [10], and Mermin and Wagner showed that under the same condition no long-range order exists in 1D and 2D quantum magnets with short-range interactions [12]. It turns out that in 1D and 2D cases $T_c = 0$, so even at infinitesimal temperatures the correlation length is finite, consistent with the Mermin-Wagner theorem. Yet while in 2D there is long-range order at $T = 0$, in 1D no long-range order is possible even at zero temperature, as shown by Bethe in 1931 [3].

The broken symmetry has very important consequences for the ground state. In particular, the Goldstone theorem states that spontaneous breaking of a continuous symmetry implies that the low-energy excitations of the ground state can be viewed as massless bosons known as *Goldstone bosons* or *Goldstone modes.* In quantum magnets, the Goldstone bosons are called *magnons* or *spin waves*; their spectrum for the spin-1/2 antiferromagnetic chain was calculated by des Cloizeaux and Pearson following Bethe's approach [5].

Chapter 2

Generalized models

One of the possible ways to deal analytically with the spin models in general and the Heisenberg model in particular is the so-called *large n approximation.* The gist of this method consists in assigning to each lattice site an internal symmetry characterized by a (large) parameter n. For example, taking $SU(n)$ or $SO(n)$ as the symmetry group and sending n to infinity, we can hope that a useful approximation emerges. Essentially, the $n \to \infty$ limit yields a mean field theory, which can be extended for the case of finite n by expanding in powers of $1/n$. In the next section and section 3.1 we briefly review the treatment of the $SU(n)$ Heisenberg model in [1], Chapters 16 and 18. The definition of the $SO(n)$ model is given in section 2.2, and the mean field approximation is discussed in section 3.2. We refer the reader to [1] for the details and the bibliography on the $1/n$ expansion.

2.1 $SU(n)$ models

Below we outline two possible $SU(n)$ generalizations of the usual $SU(2)$ Heisenberg model, the Schwinger boson models of a ferromagnet and an antiferromagnet.

2.1.1 Ferromagnet

The usual nearest-neighbor $SU(2)$ Heisenberg ferromagnetic model is defined as

$$\mathcal{H} = -J \sum_{<\mathbf{x},\mathbf{y}>} \sum_{k=1}^{3} S_{k\mathbf{x}} S_{k\mathbf{y}} = -J \sum_{<\mathbf{x},\mathbf{y}>} \left(\frac{S^+_{\mathbf{x}} S^-_{\mathbf{y}} + S^+_{\mathbf{y}} S^-_{\mathbf{x}}}{2} + S_{3\mathbf{x}} S_{3\mathbf{y}} \right), \tag{2.1}$$

where J is the ferromagnetic exchange constant, $J > 0$. For spin-1/2, the representation of the angular momentum S_k is given by

$$S_{k\mathbf{x}} = \frac{1}{2} \sum_{i,j=1}^{2} a^{\dagger}_{i\mathbf{x}} \sigma_k^{ij} a_{j\mathbf{x}}, \tag{2.2}$$

where σ_k are the Pauli matrices, and a_i are bosonic creation and annihilation operators with the usual commutation relations,

$$\begin{aligned} [a_{i\mathbf{x}}, a_{j\mathbf{y}}] &= [a^{\dagger}_{i\mathbf{x}}, a^{\dagger}_{j\mathbf{y}}] = 0, \\ [a_{i\mathbf{x}}, a^{\dagger}_{j\mathbf{y}}] &= \delta_{ij}\delta_{\mathbf{xy}}. \end{aligned} \tag{2.3}$$

The local spin constraint is enforced by the equation $\sum_{i=1}^{2} a^{\dagger}_{i\mathbf{x}} a_{i\mathbf{x}} = 1 = 2 \cdot 1/2$. Substitution of (2.2) into (2.1) yields the second-quantized Heisenberg Hamiltonian.

Generalization to $SU(n)$ proceeds as follows. Instead of spin components S_k we now use the non-hermitian generators of $SU(n)$. This may be justified by noting that in the case of $SU(2)$ components of angular momentum may themselves serve as the generators of the symmetry group. However, in the generalized case it is more convenient to use combinations of the hermitian generators of $SU(n)$ J_{ij}, which are split into S_{ij}, symmetric in ij, and A_{ij}, antisymmetric in ij. It is easy to check that $T_{ij} \equiv (S_{ij} + iA_{ij})/2$ satisfy the commutation relations[1]

$$[T_{ij}, T_{kl}] = \delta_{jk} T_{il} - \delta_{il} T_{kj}. \tag{2.4}$$

For $n = 2$, the definition for T_{ij} reduces to the spherical basis for $SU(2)$ ($T_{12} \to S^{+}$, $T_{21} \to S^{-}$, $T_{11} \to S + S_z$, and $T_{22} \to S - S_z$). Analogously to the ordinary $SU(2)$ case (2.1), the $SU(n)$ exchange interaction can be written in terms of the "generalized spherical basis" T_{ij} as well as in terms of the more common cartesian basis J_{ij}. For convenience, we choose the former.

The second quantized representation is given by defining n boson flavors a_i, $i = 1, \ldots, n$ at each lattice site. We represent the "generalized spherical basis" of $SU(n)$ as $T_{ij} = a^{\dagger}_i a_j$; it is easily checked that such generators do obey the commutation relations (2.4). The spin

[1]The commutation relations for the standard Hermitian basis of $SU(n)$ are $[J_{ij}, J_{kl}] = -i(\delta_{jk} J_{il} - \delta_{il} J_{kj})$.

constraint generalizes to

$$\sum_{k=1}^{n} a_{k\mathbf{x}}^{\dagger} a_{k\mathbf{x}} = nS, \tag{2.5}$$

where S determines the generalized "spin size". The $SU(n)$ Heisenberg Hamiltonian is now given, up to a constant, by

$$\mathcal{H} = -\frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} \sum_{i,j=1}^{n} T_{ij,\mathbf{x}} T_{ji,\mathbf{y}} = -\frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} :\mathcal{B}_{\mathbf{xy}}^{\dagger} \mathcal{B}_{\mathbf{xy}}:, \tag{2.6}$$

where $\mathcal{B}_{\mathbf{xy}} = \sum_{k=1}^{n} a_{k\mathbf{x}}^{\dagger} a_{k\mathbf{y}}$ is the bond operator between the nearest-neighbor lattice sites $\mathbf{x}$ and $\mathbf{y}$. Since by construction $[\sum_{\mathbf{x}} S_{ij,\mathbf{x}}, \mathcal{H}] = [\sum_{\mathbf{x}} A_{ij,\mathbf{x}}, \mathcal{H}] = 0$, the Hamiltonian is manifestly $SU(n)$-symmetric.

2.1.2 Antiferromagnet

In the case of an antiferromagnet, it is customary to work on a bipartite lattice with the nearest-neighbor interaction between the sublattices A and B. The $SU(2)$ antiferromagnetic Hamiltonian is identical to (2.1), but with the plus sign. The sign change is due to the antiferromagnetic coupling, which tends to put all pairs of nearest neighbors in a spin singlet state. In the $SU(n)$ case it corresponds to choosing the representations on the two sublattices to be Hermitian conjugates of each other. The spin constraint (2.5) remains intact. The $SU(n)$ antiferromagnetic bosonic Hamiltonian is thus, up to a constant,

$$\mathcal{H}_B = -\frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} \sum_{i,j=1}^{n} T_{ij,\mathbf{x}} \tilde{T}_{ji,\mathbf{x}} = -\frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} :B_{\mathbf{xy}}^{\dagger} B_{\mathbf{xy}}:, \tag{2.7}$$

where $\mathcal{B}_{\mathbf{xy}} = \sum_{k=1}^{n} a_{k\mathbf{x}} a_{k\mathbf{y}}$ is the bond operator, and $\tilde{T}_{ij,\mathbf{x}} = a_{j\mathbf{x}}^{\dagger} a_{i\mathbf{x}}$ correspond to the "spherical basis" of the conjugate representation on sublattice B. Note, that in this case the Hamiltonian is invariant not under general $SU(n)$ transformation, but rather under staggered conjugate $SU(n)$ transformations on the two sublattices.

2.2 $SO(n)$ models

Another possible way to generalize the $SU(2)$ model is to use the well-known fact that groups $SU(2)$ and $SO(3)$ are homomorphic. Thus, an $SU(2)$ symmetric model can also be

viewed as an $SO(3)$ symmetric model, which can be generalized to $SO(n)$ for arbitrary n.

The group $SO(n)$ is a group of all proper rotations of n-dimensional Euclidean space $\mathbb{R}^n$. The dimension of its Lie algebra is $n(n-1)/2$. The generator, generating rotation in the ij-plane, is expressed as

$$J_{ij} = -i(x_i\partial_j - x_j\partial_i). \tag{2.8}$$

This formula is essentially a generalization of the usual definition of the 3-dimensional angular momentum generators, $\mathbf{J} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$. It follows directly from the definition (2.8) that the J_{ij} are antisymmetric, $J_{ij} = -J_{ji}$ and $J_{ii} = 0$. For $n > 2$ the group $SO(n)$ is non-abelian. The commutation relations between its generators are [9]

$$[J_{ij}, J_{kl}] = -i(\delta_{il}J_{jk} + \delta_{jk}J_{il} - \delta_{ik}J_{jl} - \delta_{jl}J_{ik}). \tag{2.9}$$

2.2.1 Tensor $SO(n)$ model

It is possible to generalize the $SO(3)$ Heisenberg model to $SO(n)$ for arbitrary n in a number of ways. In the tensor $SO(n)$ model [7], the $SO(n)$ exchange interaction is defined as

$$\mathbf{J}_\mathbf{x} \cdot \mathbf{J}_\mathbf{y} = \sum_{i>j} J_{ij,\mathbf{x}} J_{ij,\mathbf{y}}. \tag{2.10}$$

Then the antiferromagnetic $SO(n)$ Heisenberg Hamiltonian is

$$\mathcal{H} = \frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} \sum_{i>j} J_{ij,\mathbf{x}} J_{ij,\mathbf{y}}, \tag{2.11}$$

where the factor of $1/n$ preserves the finite scale of the interaction in the large n limit. It is easily seen that for $n = 3$ the Hamiltonian (2.11), properly rescaled, reduces to (2.1).

To represent the $SO(n)$ spin operators we use real or Majorana fermions [6], [7], [14]. We define n Majorana fermions at each lattice site with the following properties. First, the creation and annihilation operators for Majorana fermions are hermitian, and second, they satisfy the following anticommutation relations [6], [7], [14]:

$$\eta^\dagger_{j\mathbf{x}} = \eta_{j\mathbf{x}}, \text{ and } \{\eta_{j\mathbf{x}}, \eta_{k\mathbf{y}}\} = \delta_{\mathbf{xy}}\delta_{jk}. \tag{2.12}$$

In particular, it follows from (2.12), that

$$\eta_{j\mathbf{x}}^2 = \frac{1}{2} \tag{2.13}$$

The commutators (2.8) are expressed via the Majorana fermions at each lattice site as

$$J_{ij,\mathbf{x}} = -\frac{i}{2}[\eta_{i\mathbf{x}}, \eta_{j\mathbf{x}}] = \begin{cases} -i\eta_{i\mathbf{x}}\eta_{j\mathbf{x}}, & i \neq j, \\ 0, & i = j. \end{cases} \tag{2.14}$$

The expression (2.14) is recognized as the $2^{[(n-1)/2]}$-dimensional spinor representation of $SO(n)$ [8], [9]. Calculating the square of the angular momentum in this representation we obtain, using (2.13),

$$\mathbf{J}_{\mathbf{x}}^2 = \sum_{i>j}^{n} J_{ij,\mathbf{x}} J_{ij,\mathbf{x}} = \frac{1}{2} \sum_{i,j=1}^{n} J_{ij,\mathbf{x}} J_{ij,\mathbf{x}} = \frac{n^2 - n}{8}.$$

The spinor representation of $SO(3)$ is equivalent to the two-dimensional representation by the Pauli matrices, or spin-1/2 representation [6]:

$$\mathbf{J}_{\mathbf{x}} = -\frac{i}{2}\vec{\eta}_{\mathbf{x}} \times \vec{\eta}_{\mathbf{x}}, \qquad \mathbf{J}_{\mathbf{x}}^2 = \frac{3}{4} = \frac{1}{2}\Big(1 + \frac{1}{2}\Big).$$

Using (2.12) and (2.13), the Hamiltonian (2.11) may be rewritten in Majorana representation as

$$\mathcal{H} = \frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} \left[\frac{n}{8} + \frac{1}{2} \left(\sum_{i=1}^{n} \eta_{i\mathbf{x}} \eta_{i\mathbf{y}} \right)^2 \right]. \tag{2.15}$$

2.2.2 Vector $SO(n)$ model

Our treatment of the $SO(n)$ model is largely based on the fact that $SO(n+1)$ contains $SO(n)$ as a proper subgroup. After choosing $n(n-1)/2$ generators of $SO(n)$ as generators of $SO(n+1)$, we are left with n degrees of freedom, which we will call the coset generators, denoting them with the first subscript 0. (Thus J_{jk} for $j \neq 0$ is a generator of both $SO(n+1)$ and $SO(n)$, but J_{0l} is a generator of $SO(n+1)$ and not a generator of $SO(n)$.)

It follows from the equation (2.9) that a commutator of a generator of $SO(n)$ and a coset generator is a linear combination of coset generators only and thus belongs to the

subspace of the Lie algebra of $SO(n+1)$ generated by the coset generators:

$$[J_{ij}, J_{0l}] = -i(\delta_{jl} J_{0i} - \delta_{il} J_{0j}).$$

(Note, however, that the subspace in question is not a subalgebra of $so(n+1)$, since it is not closed under the commutator, $[J_{0j}, J_{0l}] = iJ_{jl}$.) Thus, the n coset generators of $SO(n+1)$ transform as n components of an n-vector in $\mathbb{R}^n$ under the $SO(n)$ transformations. This analogy permits us to define the exchange interaction between two "$SO(n)$ spins" as the dot product of the n-component spin-"vectors" of the form $\mathbf{J} \equiv (J_{01}, \ldots, J_{0n})$. Such a model may be called a *vector $SO(n)$ Heisenberg model*, and its antiferromagnetic Hamiltonian is given by

$$\mathcal{H} = \frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} \sum_{k=1}^{n} J_{0k,\mathbf{x}} J_{0k,\mathbf{y}}, \tag{2.16}$$

where, as before, the factor of $1/n$ preserves the finite scale of the interaction for $n \to \infty$. Since the commutator of the Hamiltonian with the lattice spin operator $[\mathcal{H}, J_{ij}] \equiv [\mathcal{H}, \sum_{\mathbf{x}} J_{ij}(\mathbf{x})] = 0$ for $i, j = 0, \ldots, n$, the Hamiltonian is readily seen to be $SO(n)$-invariant.

It is instructive to see what becomes of our model in the case of the $SO(3)$ symmetry. For $n = 3$ we denote the subgroup generators of $SO(3) \subset SO(4)$ as $S_1 = J_{23}$, $S_2 = J_{31}$, $S_3 = J_{12}$, and the coset generators as $T_i = J_{0i}$. Then, while the subgroup generators satisfy the usual $so(3) = su(2)$ algebra, $[S_i, S_j] = i\varepsilon_{ijk} S_k$, the commutation relations between the coset generators may be written as $[T_i, T_j] = i\varepsilon_{ijk} S_k$, and between the subgroup generators and the coset generators as $[S_i, T_j] = i\varepsilon_{ijk} T_k$. Let us now define the following operators, $A_i^{\pm} \equiv (S_i \pm T_i)/2$. Then it is easily seen that $[A_i^{\pm}, A_j^{\pm}] = i\varepsilon_{ijk} A_k^{\pm}$ and $[A_i^{+}, A_j^{-}] = 0$. Therefore, $\{A_i^{+}\}$ and $\{A_i^{-}\}$ generate two orthogonal $so(3)$ subalgebras of $so(4) = so(3) \otimes so(3)$. From the definition of $A_i^{\pm}$, $T_i = A_i^{+} - A_i^{-}$, and the $SO(3)$ exchange interaction may be rewritten in terms of $A_i^{\pm}$ as

$$\mathbf{J}_{\mathbf{x}} \cdot \mathbf{J}_{\mathbf{y}} = \sum_{i=1}^{3} T_{i\mathbf{x}} T_{i\mathbf{y}} = \sum_{i=1}^{3} (A_{i\mathbf{x}}^{+} A_{i\mathbf{y}}^{+} - A_{i\mathbf{x}}^{+} A_{i\mathbf{y}}^{-} - A_{i\mathbf{x}}^{-} A_{i\mathbf{y}}^{+} + A_{i\mathbf{x}}^{-} A_{i\mathbf{y}}^{-}).$$

We see that for $n = 3$ the Hamiltonian (2.16) cannot be reduced to the Heisenberg Hamiltonian (2.1) and therefore it is not a true $SO(n)$ generalization of the Heisenberg Hamiltonian. Nevertheless, it is symmetric under simultaneous staggered rotations from the two $SO(3)$

subgroups of $SO(4)$.

Using the Majorana representation (2.12), we first of all calculate the analog of the square of the angular momentum:

$$\mathbf{J}_{\mathbf{x}}^2 = \sum_{k=1}^{n} J_{0k,\mathbf{x}} J_{0k,\mathbf{x}} = \frac{n}{4}. \tag{2.17}$$

For $n = 3$ the above equation yields $\mathbf{J}^2 = 3/4$. Therefore we conclude that our vector model of $SO(n)$ exchange describes interaction between two "generalized spin-1/2" particles.

Finally, the vector $SO(n)$ Heisenberg Hamiltonian in Majorana representation is

$$\mathcal{H} = \frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} \sum_{k=1}^{n} \eta_{0\mathbf{x}} \eta_{0\mathbf{y}} \eta_{k\mathbf{x}} \eta_{k\mathbf{y}}. \tag{2.18}$$

Chapter 3

Mean field approximation

3.1 $SU(n)$

The partition function is expressed as a coherent state path integral [1],

$$\mathcal{Z} = \mathrm{Tr}\, P_S\, e^{-\beta\mathcal{H}} = \int \mathcal{D}^2\mathbf{z}\, \mathcal{D}\mu\, \exp\left(-\int_0^\beta d\tau \mathcal{L}(z^*, z)\right),$$

where P_S is the spin projector defined according to the equation (2.5), z^* and z are Grassmann variables for the fermionic path integral and complex numbers for the bosonic path integral, and the Lagrangian $\mathcal{L}(z^*, z)$ incorporates the spin constraint using a Lagrange multiplier $\mu_{\mathbf{x}}$.

3.1.1 Ferromagnet

In this case the Lagrangian reads,

$$\mathcal{L}(\tau) = \sum_{k\mathbf{x}} z^*_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau) - \frac{J}{n}\sum_{<\mathbf{x},\mathbf{y}>} Z^*_{\mathbf{x}\mathbf{y}}(\tau) Z_{\mathbf{x}\mathbf{y}}(\tau) + i\sum_{k\mathbf{x}} \mu_{\mathbf{x}}(z^*_{k\mathbf{x}}(\tau) z_{k\mathbf{x}}(\tau) - S),$$

where $Z_{\mathbf{x}\mathbf{y}}(\tau) = \sum_{k=1}^{n} z^*_{k\mathbf{x}}(\tau) z_{k\mathbf{y}}(\tau)$. This Lagrangian contains a biquadratic interaction, which we linearize via the Hubbard-Stratonovich transformation[1],

[1]The Hubbard-Stratonovich transformation is an operator form of the Gaussian integral identity (see Appendix A).

$$e^{\varepsilon A Z^*_{\mathbf{xy}}(\tau) Z_{\mathbf{xy}}(\tau)} = \int\limits_{-\infty}^{\infty} d^2Q \, \exp\left[-\varepsilon\left(Z^* Q_{\mathbf{xy}}(\tau) + Z Q^*_{\mathbf{xy}}(\tau) + \frac{Q^*_{\mathbf{xy}}(\tau) Q_{\mathbf{xy}}(\tau)}{A}\right)\right], \quad (3.1)$$

where $Q_{\mathbf{xy}}(\tau)$ is a complex auxiliary field defined for each nearest neighbor bond at each timestep τ. Using (3.1), we rewrite the partition function as

$$\mathcal{Z} = \int \mathcal{D}^2\mathbf{z}\, \mathcal{D}^2Q\, \mathcal{D}\mu \, \exp\left(-\int\limits_0^\beta d\tau \mathcal{L}(\tau)\right),$$

with the measure $\mathcal{D}^2Q \equiv \prod_{\tau,\mathbf{xy}} d^2Q_{\mathbf{xy}}(\tau)$ and the Lagrangian

$$\begin{aligned}\mathcal{L}(\tau) =& \sum_{k\mathbf{x}} z^*_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau) + \sum_{<\mathbf{x},\mathbf{y}>} (Z^*_{\mathbf{xy}}(\tau) Q_{\mathbf{xy}}(\tau) + Q^*_{\mathbf{xy}}(\tau) Z_{\mathbf{xy}}(\tau)) + \\ &+ i\sum_{k\mathbf{x}} \mu_{\mathbf{x}} z^*_{k\mathbf{x}}(\tau) z_{k\mathbf{x}}(\tau) + \frac{n}{J}\sum_{<\mathbf{x},\mathbf{y}>} |Q_{\mathbf{xy}}(\tau)|^2 - inS\sum_{\mathbf{x}} \mu_{\mathbf{x}} \equiv \\ &\equiv \mathbf{z}^* \hat{G}^{-1} \mathbf{z} + \frac{n}{J}\sum_{<\mathbf{x},\mathbf{y}>} |Q_{\mathbf{xy}}(\tau)|^2 - inS\sum_{\mathbf{x}} \mu_{\mathbf{x}}, \end{aligned} \quad (3.2)$$

where the Green function matrix $\hat{G}$ is defined by $\hat{G}^{-1} = \partial_\tau + \hat{\mu} + \hat{Q}$. Now the z fields can be integrated out of the partition function by virtue of the Gaussian integral identity (A.2). The partition function then becomes

$$\begin{aligned}\mathcal{Z} &= \int \mathcal{D}^2Q\, \mathcal{D}\mu\, e^{-nS}, \quad (3.3)\\ S &= -\frac{1}{n}\mathrm{Tr}_{k\tau\mathbf{x}}(\ln \hat{G}) + \int\limits_0^\beta \left(\sum_{<\mathbf{x},\mathbf{y}>} \frac{|Q_{\mathbf{xy}}(\tau)|^2}{J} - iS\sum_{\mathbf{x}} \mu_{\mathbf{x}}\right) d\tau, \end{aligned}$$

where we have used the well-known identity (A.4).

It follows from (3.3) that if $n \to \infty$, the exponential becomes infinitely large and the value of the integral may be determined by the value of the action at the saddle point. In the zeroth approximation (also called the *mean field* theory), the auxiliary fields $Q_{\mathbf{xy}}(\tau)$ and $\mu_{\mathbf{x}}$ are replaced by their static and uniform mean values (hence the name), and their fluctuations are considered to be suppressed by the exponential growing very large as n approaches infinity. The physical meaning of the procedure of mean field theory consist in choosing a normal quadratic Hamiltonian which contains the mean field as a parameter and which best approximates the behavior of the ground state and the low-energy excitation spectrum of the original problem. However, there are no means of justifying the "mean

field" assumptions *a priori*; one has to solve the problem self-consistently to assure that the fluctuations are indeed negligible. Nevertheless, assuming that the "physical" saddle point, minimizing the free energy $\mathcal{F}(\beta) = -\ln \mathcal{Z}/\beta$, *does* correspond to a static and uniform configuration of auxiliary fields, the partition function may be evaluated and the mean field Hamiltonian may be expressed in terms of the mean field (in our case, in terms of Q and μ). The condition requiring the free energy to be minimal constitutes the *gap*, or *mean field equation*, from which the specific values of Q and μ are determined.

In (3.3), the second term in the full action nS is proportional to n and therefore does indeed grow large when $n \to \infty$. At the first glance, the first term may seem to be independent of n. However, if we consider the Green function $\hat{G}$ more closely, we find that it is comprised of n replica of identical Green functions, each repetition corresponding to one of the n constrained fermion flavors. Thus the trace of its logarithm is n times larger than the trace of each of these n identical Green functions, which are easily seen to be in fact independent of n. Therefore the first term can also be shown to exhibit a linear dependence on n at $n \to \infty$ limit.

After averaging, the Lagrangian (3.2) yields the mean field Hamiltonian,

$$\mathcal{H}_{MF} = -Q \sum_{<\mathbf{x},\mathbf{y}>,k} \left(c^{\dagger}_{k\mathbf{x}} c_{k\mathbf{y}} + c^{\dagger}_{k\mathbf{y}} c_{k\mathbf{x}} \right) + \mu \sum_{k\mathbf{x}} c^{\dagger}_{k\mathbf{x}} c_{k\mathbf{x}} + nN \frac{zQ^2}{2J} - nNS\mu, \qquad (3.4)$$

where Q assumed to be real (it is, in fact, possible to show that Q must be real in order for the mean field Hamiltonian to be physically relevant). In the momentum representation we obtain

$$\mathcal{H} = \sum_{k\mathbf{k}} \varepsilon_{\mathbf{k}} a^{\dagger}_{k\mathbf{k}} a_{k\mathbf{k}} + nN \frac{zQ^2}{2J} - nNS\mu,$$

where N is the number of lattice sites, z is the *coordination number*, equal to the number of the nearest neighbors of each lattice site, $\mathbf{k}$ is the momentum of the lattice excitations, and the dispersion relation is given by

$$\varepsilon_{\mathbf{k}} = \mu - zQ\gamma_{\mathbf{k}}, \quad \gamma_{\mathbf{k}} = \frac{1}{z} \sum_{\hat{\nu}} e^{i\mathbf{k}\hat{\nu}},$$

where $\hat{\nu}$ are the nearest neighbor vectors. The mean field free energy is given by

$$\mathcal{F} = n \sum_{\mathbf{k}} \ln \left(1 - \exp\left(-\beta\varepsilon_{\mathbf{k}}\right)\right) + nN \frac{zQ^2}{2J} - nNS\mu.$$

Minimizing the free energy, we differentiate with respect to μ and Q and obtain the gap equation,

$$\frac{1}{N}\sum_{\mathbf{k}} n_{\mathbf{k}} = S, \tag{3.5}$$

$$\frac{1}{N}\sum_{\mathbf{k}} n_{\mathbf{k}}\gamma_{\mathbf{k}} = \frac{Q}{J}, \tag{3.6}$$

where $n_{\mathbf{k}} = (\exp(\beta\varepsilon_{\mathbf{k}}) - 1)^{-1}$ is the bosonic occupation number.

3.1.2 Antiferromagnet

For the bosonic Hamiltonian (2.7) the partition function reads,

$$\mathcal{L}(\tau) = \sum_{k\mathbf{x}} z^*_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau) - \frac{J}{n}\sum_{<\mathbf{x},\mathbf{y}>} Z^*_{\mathbf{x}\mathbf{y}}(\tau)Z_{\mathbf{x}\mathbf{y}}(\tau) + i\sum_{k\mathbf{x}} \mu_{\mathbf{x}}(z^*_{k\mathbf{x}}(\tau)z_{k\mathbf{x}}(\tau) - S),$$

where $Z_{\mathbf{x}\mathbf{y}}(\tau) = \sum_k z_{k\mathbf{x}}(\tau)z_{k\mathbf{y}}(\tau)$, and z are ordinary complex numbers in this context. Similarly to the fermionic case, we perform the Hubbard-Stratonovich transformation and obtain the bosonic counterpart to (3.2). Recalling that the interactions are defined only between the nearest neighbors belonging to different sublattices, we may write the Lagrangian as

$$\mathcal{L}(\tau) = [\mathbf{z}^*_A, \mathbf{z}_B]\hat{G}^{-1}\begin{bmatrix}\mathbf{z}_A \\ \mathbf{z}^*_B\end{bmatrix} + \int_0^\beta \left(\sum_{<\mathbf{x},\mathbf{y}>}\frac{|Q_{\mathbf{x}\mathbf{y}}(\tau)|^2}{J} - iS\sum_{\mathbf{x}}\mu_{\mathbf{x}}\right)d\tau,$$

$$\hat{G}^{-1} = \begin{bmatrix}\partial_\tau + \hat{\mu} & \hat{Q} \\ \hat{Q}^\dagger & -\partial_\tau + \hat{\mu}\end{bmatrix}.$$

Using (A.1) and (A.4), we integrate over $\mathbf{z}$ and arrive at

$$\mathcal{Z} = \int \mathcal{D}^2 Q\, \mathcal{D}\mu\, e^{-nS}, \tag{3.7}$$

$$S = -\frac{1}{n}\mathrm{Tr}_{k\tau\mathbf{x}}(\ln\hat{G}) + \int_0^\beta \left(\sum_{<\mathbf{x},\mathbf{y}>}\frac{|Q_{\mathbf{x}\mathbf{y}}(\tau)|^2}{J} - iS\sum_{\mathbf{x}}\mu_{\mathbf{x}}\right)d\tau.$$

Similarly to the fermionic case, the large n limit of the action leads to a saddle point which yields a mean field Hamiltonian

$$\mathcal{H} = \sum_{k\mathbf{x}} \mu a^\dagger_{k\mathbf{x}}a_{k\mathbf{x}} + Q\sum_{<\mathbf{x},\mathbf{y}>,k}(a^\dagger_{k\mathbf{x}}a^\dagger_{k\mathbf{y}} + a_{k\mathbf{x}}a_{k\mathbf{y}}) + nN\frac{zQ^2}{2J} - nNS\mu,$$

or, going to the momentum representation,

$$\mathcal{H} = \sum_{k\mathbf{k}} \left[\mu a^\dagger_{k\mathbf{k}} a_{k\mathbf{k}} + \frac{zQ\gamma_\mathbf{k}}{2} (a^\dagger_{k\mathbf{k}} a^\dagger_{k\mathbf{k}} + a_{k\mathbf{k}} a_{k\mathbf{k}}) \right] + nN \frac{zQ^2}{2J} - nNS\mu. \tag{3.8}$$

This Hamiltonian, containing anomalous terms of the form $a^\dagger a^\dagger$ and aa, can be diagonalized by virtue of the generalized Bogoliubov transformation,

$$a_{k\mathbf{k}} = \cosh\theta_\mathbf{k}\, \alpha_{k\mathbf{k}} + \sinh\theta_\mathbf{k}\, \alpha^\dagger_{k,-\mathbf{k}} \quad \text{and} \quad a_{k,-\mathbf{k}} = \cosh\theta_\mathbf{k}\, \alpha_{k-\mathbf{k}} + \sinh\theta_\mathbf{k}\, \alpha^\dagger_{k\mathbf{k}}. \tag{3.9}$$

Substitution of (3.9) into (3.8) yields

$$\begin{aligned} \mathcal{H} = \sum_{k\mathbf{k}} \Big[& (\mu\cosh 2\theta_\mathbf{k} + zQ\gamma_\mathbf{k} \sinh 2\theta_\mathbf{k})(a^\dagger_{k\mathbf{k}} a_{k\mathbf{k}} + a_{k\mathbf{k}} a^\dagger_{k\mathbf{k}}) + \\ & + (\mu \sinh 2\theta_\mathbf{k} + zQ\gamma_\mathbf{k} \cosh 2\theta_\mathbf{k})(a^\dagger_{k\mathbf{k}} a^\dagger_{k-\mathbf{k}} + a_{k\mathbf{k}} a_{k-\mathbf{k}}) \Big] + nN \frac{zQ^2}{2J} - \frac{2S+1}{2} nN\mu. \end{aligned}$$

We can make the coefficient at the anomalous term vanish by setting

$$\tanh 2\theta_\mathbf{k} = -\frac{zQ\gamma_\mathbf{k}}{\mu}.$$

Expressing $\sinh 2\theta_\mathbf{k}$ and $\cosh 2\theta_\mathbf{k}$ via $\tanh 2\theta_\mathbf{k}$, we arrive at the normal diagonal Hamiltonian

$$\mathcal{H} = \sum_{k\mathbf{k}} \varepsilon_\mathbf{k} \left(a^\dagger_{k\mathbf{k}} a_{k\mathbf{k}} + \frac{1}{2} \right) + nN \frac{zQ^2}{2J} - \frac{2S+1}{2} nN\mu,$$

where the dispersion relation is

$$\varepsilon_\mathbf{k} = \sqrt{\mu^2 - (zQ\gamma_\mathbf{k})^2}.$$

The free energy can easily be found as

$$\mathcal{F} = \frac{1}{\beta} \sum_{k\mathbf{k}} \ln \left(2 \sinh \frac{\beta\varepsilon_\mathbf{k}}{2} \right) + nN \frac{zQ^2}{2J} - \frac{2S+1}{2} nN\mu,$$

and the gap equation is

$$\frac{1}{N}\sum_{\mathbf{k}}\frac{\mu}{\varepsilon_{\mathbf{k}}}\left(n_{\mathbf{k}}+\frac{1}{2}\right)=S+\frac{1}{2}, \tag{3.10}$$

$$\frac{1}{N}\sum_{\mathbf{k}}\frac{\mu}{\varepsilon_{\mathbf{k}}}\left(n_{\mathbf{k}}+\frac{1}{2}\right)=\frac{zQ}{J.} \tag{3.11}$$

3.2 $SO(n)$

Analogously to the equation (3.1), the partition function in Majorana fermion representation is given by [14]

$$\mathcal{Z}=\mathrm{Tr}\,e^{-\beta\mathcal{H}}=\int\mathcal{D}z\;e^{-\int_0^\beta d\tau\mathcal{L}(z)},$$

where the z fields are the Grassmann numbers, and the Lagrangian $\mathcal{L}(z)$ is now equal to

$$\mathcal{L}=\frac{1}{2}\sum_{k\mathbf{x}}z_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau)+\frac{J}{2n}\sum_{<\mathbf{x},\mathbf{y}>}\left(\sum_{k=1}^{n}z_{k\mathbf{x}}z_{k\mathbf{y}}\right)^2 \tag{3.12}$$

for the tensor $SO(n)$ model (2.15), and

$$\mathcal{L}=\frac{1}{2}\sum_{k\mathbf{x}}z_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau)+\frac{J}{n}\sum_{<\mathbf{x},\mathbf{y}>}\sum_{k=1}^{n}z_{0\mathbf{x}}z_{0\mathbf{y}}z_{k\mathbf{x}}z_{k\mathbf{y}} \tag{3.13}$$

for the vector $SO(n)$ model (2.18).

3.2.1 Tensor $SO(n)$ model

We rewrite the Lagrangian (3.12) as

$$\mathcal{L}=\frac{1}{2}\sum_{k\mathbf{x}}z_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau)+\frac{J}{n}\sum_{<\mathbf{x},\mathbf{y}>}Z_{\mathbf{xy}}^2(\tau)$$

where $Z_{\mathbf{xy}}(\tau)=\sum_{i=1}^{n}z_{i\mathbf{x}}(\tau)z_{i\mathbf{y}}(\tau)$. According to [14], the Hubbard-Stratonovich transformation of a biquadratic Hamiltonian in the Majorana representation is

$$\exp\left[-\int_0^\beta d\tau\left(\frac{J}{2n}\sum_{<\mathbf{x},\mathbf{y}>} Z_{\mathbf{xy}}^2(\tau)\right)\right] =$$

$$= \int \mathcal{D}Q\ \exp\left[-\int_0^\beta d\tau\left(\frac{2n}{J}\sum_{<\mathbf{x},\mathbf{y}>} Q_{\mathbf{xy}}^2(\tau) - 2i\sum_{<\mathbf{x},\mathbf{y}>} Q_{\mathbf{xy}}(\tau)Z_{\mathbf{xy}}(\tau)\right)\right].$$

We rewrite the partition function as

$$\mathcal{Z} = \int \mathcal{D}z\mathcal{D}Q\ \exp\left(-\int_0^\beta d\tau\mathcal{L}(\tau)\right),$$

$$\mathcal{L}(\tau) = \frac{1}{2}\sum_{k\mathbf{x}} z_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau) - 2i\sum_{<\mathbf{x},\mathbf{y}>} Q_{\mathbf{xy}}(\tau)Z_{\mathbf{xy}}(\tau) + \frac{2n}{J}\sum_{<\mathbf{x},\mathbf{y}>} Q_{\mathbf{xy}}^2(\tau).$$

Defining the Green function by $\hat{G}^{-1} = \partial_\tau + i\hat{Q}$, we may rewrite the Lagrangian as

$$\mathcal{L}(\tau) = \frac{1}{2}z\hat{G}^{-1}z + \frac{2n}{J}\sum_{<\mathbf{x},\mathbf{y}>} Q_{\mathbf{xy}}^2(\tau).$$

Integration over z yields

$$\mathcal{Z} = \int \mathcal{D}Q\ e^{-nS}, \quad S = \frac{1}{2n}\mathrm{Tr}_{k\tau\mathbf{x}}\ln\hat{G}^{-1} + \frac{2}{J}\int_0^\beta d\tau\sum_{<\mathbf{x},\mathbf{y}>} Q_{\mathbf{xy}}^2(\tau).$$

The mean field Hamiltonian, corresponding to the saddle point in the $n \to \infty$ limit, is

$$\mathcal{H} = -2iQ\sum_{<\mathbf{x},\mathbf{y}>,k} \eta_{k\mathbf{x}}\eta_{k\mathbf{y}} + \frac{zQ^2}{J}Nn.$$

Since η are real, $\eta_{\mathbf{x}}^\dagger = \eta_{\mathbf{x}}$, their Fourier images must satisfy $\eta_{\mathbf{k}}^\dagger = \eta_{-\mathbf{k}}$; therefore, momenta $\mathbf{k}$ may be defined on the "positive" half of the Brillouin zone only[2]. Performing the Fourier transform, we arrive at

$$\mathcal{H} = -2iQ\sum_{k\mathbf{k}} \eta_{k\mathbf{k}}^\dagger\eta_{k\mathbf{k}}\sum_{\hat{\nu}} e^{i\mathbf{k}\hat{\nu}} + \frac{zQ^2}{J}Nn = \sum_{k\mathbf{k}>0} \varepsilon_{\mathbf{k}}\eta_{k\mathbf{k}}^\dagger\eta_{k\mathbf{k}} - \frac{2Qz}{\pi}Nn + \frac{zQ^2}{J}Nn,$$

[2]See [14] and [6] for details.

where $\sum_{k\mathbf{k}>0} = \sum_{k=1}^{n} \sum_{\mathbf{k}\in 1/2\ \mathrm{BZ}}$, and the dispersion relation is given by

$$\varepsilon_{\mathbf{k}} = 4Q \sum_{\hat{\nu}} \sin k\hat{\nu} = 2Qz\gamma_{\mathbf{k}}, \text{ where } \gamma_{\mathbf{k}} = \frac{2}{z} \sum_{\hat{\nu}} \sin k\hat{\nu}. \tag{3.14}$$

Note, that the summation $\sum_{\hat{\nu}}$ does not generally run over all nearest neighbors of a lattice site. In most cases, the coordination number is even and for each $\hat{\nu}$ there exists another nearest neighbor vector $\hat{\nu}' = -\hat{\nu}$ (which is the case for a 1-dimensional chain, a square and a hexagonal lattice in 2 dimensions, etc.), and the summation runs only over a half of the nearest neighbors of each lattice site. However, for some lattices (for example, for a hexagonal lattice), the summation runs over all nearest neighbors, as in the $SU(n)$ case, and the spectrum becomes $\varepsilon_{\mathbf{k}} = 4Qz\gamma_{\mathbf{k}}$.

The free energy is now found as

$$\mathcal{F} = -\frac{n}{\beta} \sum_{\mathbf{k}>0} \ln\left(1 + \exp\left(-\beta\varepsilon_{\mathbf{k}}\right)\right) - \frac{2Qz}{\pi} Nn + \frac{zQ^2}{J} Nn,$$

and the gap equation is given by (for the dispersion relation 3.14)

$$\frac{\pi}{N} \sum_{\mathbf{k}>0} n_{\mathbf{k}}\gamma_{\mathbf{k}} = 1 - \pi\frac{Q}{J}, \tag{3.15}$$

where $n_{\mathbf{k}}$ is the fermionic occupation number, $n_{\mathbf{k}} = \left(\exp\left(\beta\varepsilon_{\mathbf{k}}\right) + 1\right)^{-1}$.

3.2.2 Vector $SO(n)$ model

Defining

$$Y_{\mathbf{xy}}(\tau) = z_{0\mathbf{x}}(\tau) z_{0\mathbf{y}}(\tau), \quad Z_{\mathbf{xy}}(\tau) = \sum_{i=1}^{n} z_{i\mathbf{x}}(\tau) z_{i\mathbf{y}}(\tau),$$

we rewrite the Lagrangian (3.13) as

$$\mathcal{L} = \frac{1}{2} \sum_{k\mathbf{x}} z_{k\mathbf{x}}(\tau)\partial_\tau z_{k\mathbf{x}}(\tau) + \frac{J}{n} \sum_{<\mathbf{x},\mathbf{y}>} Y_{\mathbf{xy}}(\tau) Z_{\mathbf{xy}}(\tau).$$

The Hubbard-Stratonovich transformation now reads (see (A.3))

$$\exp\left(-\frac{J}{n}Y_{\mathbf{xy}}(\tau)Z_{\mathbf{xy}}(\tau)\right) =$$

$$= \int \mathcal{D}^2 Q \ \exp\left(-\frac{n}{J}Q^*_{\mathbf{xy}}(\tau)Q_{\mathbf{xy}}(\tau) + Q_{\mathbf{xy}}(\tau)Y_{\mathbf{xy}}(\tau) + Q^*_{\mathbf{xy}}(\tau)Z_{\mathbf{xy}}(\tau)\right),$$

where $Q_{\mathbf{xy}}(\tau)$ is the (complex) auxiliary field. Following the usual routine, we obtain the following mean field Hamiltonian,

$$\mathcal{H} = \sum_{<\mathbf{x},\mathbf{y}>}\left(Q\eta_{0\mathbf{x}}\eta_{0\mathbf{y}} + Q^*\sum_{k=1}^{n}\eta_{k\mathbf{x}}\eta_{k\mathbf{y}} + \frac{Q^*Q}{2J}Nn\right) =$$

$$= \sum_{\mathbf{k}>0}\varepsilon_{\mathbf{k}}\left(\sum_{k=1}^{n}\eta^\dagger_{k\mathbf{k}}\eta_{k\mathbf{k}} - \eta^\dagger_{0\mathbf{k}}\eta_{0\mathbf{k}}\right) - \frac{Pz}{2\pi}N(n-1) + \frac{P^2 z}{2J}Nn, \tag{3.16}$$

where

$$\varepsilon_{\mathbf{k}} = Pz\gamma_{\mathbf{k}} \text{ and } \gamma_{\mathbf{k}} = \frac{2}{z}\sum_{\hat{\nu}}\sin\mathbf{k}\hat{\nu}, \tag{3.17}$$

where we have set $Q = iP$, $P \in \mathbb{R}$ for the spectrum to be real. The mean field free energy is now given by

$$\mathcal{F} = -\frac{1}{\beta}\sum_{\mathbf{k}>0}\left(\ln(1+e^{\beta\varepsilon_{\mathbf{k}}}) + n\ln(1+e^{-\beta\varepsilon_{\mathbf{k}}})\right) - \frac{Pz}{2\pi}N(n-1) + \frac{P^2 z}{2J}Nn,$$

and the gap equation is

$$\frac{2\pi}{N}\sum_{\mathbf{k}>0}n_{\mathbf{k}}\gamma_{\mathbf{k}} = 1 - 2\pi\frac{P}{J}. \tag{3.18}$$

Chapter 4

Conclusion

The large n approximation has been used extensively in both QFT and statistical mechanics for the past several decades. In particular, the quantum theory of magnetism has been studied with several varieties of the large n techniques (see, for example, [1], [4], [7], and the bibliography therein). This thesis suggests another approach to the problem of the quantum antiferromagnetism, namely, a formulation of the vector model possessing an $SO(n)$ symmetry. There exist classical counterparts of such models, and once the gap equation (3.18) is solved and the exact spectrum and the low-temperature dynamics of the Hamiltonian (3.16) is determined, it would be instructive to compare them with the corresponding results of the classical models[1].

The equation (3.18), however, is a transcendental equation and cannot be solved analytically. Thus, to obtain the mean field P, defining the saddle point, one would have to resort to numerical calculations. Once the correct P is obtained, the low-energy excitation spectrum will follow immediately.

Although the Hamiltonian (3.16) and the equation (3.18) were written in the approximation of the homogeneous and uniform mean field, it seems possible that the actual mean field exhibits more complicated spatial dependence. That, however, cannot be told without solving the gap equation itself; however, once the self-consistent solution is found, it should be easy to see if any modifications of the mean field Hamiltonian are necessary.

The next step in investigating the vector $SO(n)$ model would consist in searching for long range order. The most essential long range order parameter for quantum magnets is

[1] See [4].

the spin-spin correlation length; to find it, a generating functional should be constructed, which would couple the ordering magnetic field to the spin at the lattice site $\mathbf{x}$. From it, the spin-spin correlation function $\langle \mathbf{J_x} \cdot \mathbf{J_y} \rangle$ can be derived; its spatial dependence would determine the correlation length ξ and the existence of Goldstone bosons. Specifically, it is hoped that in two dimensions ξ will be infinite at $T = 0$ and proportional to $e^{-1/T}$ at $T > 0$.

The Hamiltonian (3.16) is valid (with only minor modifications), for a large class of antiferromagnetic models, ranging from the well-studied one-dimensional antiferromagnetic chain to a variety of models in two and three dimensions, including the spin-1/2 square lattice, which is relevant to the study of the high T_c superconductors. Therefore, its results should be easy to test experimentally, as the experimental work on Heisenberg antiferromagnets has been quite extensive in the recent years.

Appendix A

Some important formulas

The following identity is a multidimensional generalization of a one-dimensional Poisson integral:

$$\int d^2\mathbf{Z}\, e^{-\mathbf{Z}^* G \mathbf{Z} - \mathbf{Z}_a^* \mathbf{Z} - \mathbf{Z}^* \mathbf{Z}_b} = \det G^{-1} e^{\mathbf{Z}_a^* G^{-1} \mathbf{Z}_b}, \tag{A.1}$$

where $\mathbf{z} = (z_1, \ldots, z_N)$ and the measure is given by

$$d^2\mathbf{z} \equiv \prod_{i=1}^{N} \frac{dx_i dy_i}{\pi}.$$

The identity (A.1) holds for any complex vectors $\mathbf{Z}_a$ and $\mathbf{Z}_b$ and any complex matrix G with the positive Hermitian part (the latter condition is necessary to insure convergence).

Fermionic coherent states are parametrized by Grassmann numbers. The fermionic Gaussian integral is given by

$$\int d^2\mathbf{Z}\, e^{-\mathbf{Z}^* G \mathbf{Z} + \mathbf{Z}_a^* \mathbf{Z} + \mathbf{Z}^* \mathbf{Z}_b} = \det G\, e^{\mathbf{Z}_a^* G^{-1} \mathbf{Z}_b}. \tag{A.2}$$

Note, that here G may be arbitrary since positivity of the Hermitian part of G is not required for the convergence of the Grassmann path integral.

Both (A.1) and (A.2) rely on the following one-dimensional identity,

$$\int dz dz^*\, e^{-Az^* z + a^* z + z^* b} = C e^{a^* b / A}, \tag{A.3}$$

where $A > 0$ and C is some constant. This can be proved as follows (where C absorbs all

constant factors, arising from the change of the integration measure, etc.):

$$\int dzdz^*\ e^{-Az^*z+a^*z+z^*b} = C\int_0^\infty dr^2 \int_0^{2\pi} d\phi\ e^{-Ar^2} e^{a^*re^{i\phi}+bre^{-i\phi}} =$$

$$= C\int_0^\infty dr^2\ e^{-Ar^2} \int_0^{2\pi} d\phi \sum_{m=0}^\infty \sum_{n=0}^\infty \frac{(a^*r)^m e^{im\phi}}{m!} \frac{(br)^n e^{-in\phi}}{n!} =$$

$$= C\sum_{n=0}^\infty \frac{(a^*b)^n}{n!n!} \int_0^\infty d(Ar^2)\ e^{-Ar^2} \frac{(Ar^2)^n}{A^n} = C\sum_{n=0}^\infty \frac{(a^*b/A)^n}{n!n!} \int_0^\infty dt\ e^{-t}t^n =$$

$$= C\sum_{n=0}^\infty \frac{(a^*b)^n}{n!n!}\Gamma(n+1) = C\sum_{n=0}^\infty \frac{(a^*b/A)^n}{n!} = Ce^{a^*b/A}.$$

Another important identity is

$$\det G = e^{\mathrm{Tr}\ln G}, \tag{A.4}$$

which is widely used in both statistical mechanics and QFT. To convince oneself of its validity, one may consider G to be nondegenerate and diagonalizable. Working in the eigenbasis of G and letting λ_i be its eigenvalues, we get $e^{\mathrm{Tr}\ln G} = e^{\sum \ln \lambda_i} = \prod \lambda_i = \det G$.

Bibliography

[1] A. Auerbach, *Interacting electrons and quantum magnetism*, NY, Springer-Verlag, 1994.

[2] J. C. Bednorz and K. A. Müller, Z. Phys. B **64** (1986) 189

[3] H. Bethe, Z. Phys **71**, 205 (1931)

[4] E. Brezin and S. Wadia, *Large N Expansion in Quantum Field Theory and Statistical Mechanics*, World Scientific, Singapore, 1993.

[5] J. des Cloizeaux, J. J. Pearson, Phys. Rev. **128**, 2131 (1962)

[6] P. Coleman, E. Miranda, and A. Tsvelik, Phys. Rev. B **49**, 8955 (1994).

[7] D. Foerster, F. Triozon, Phys. Rev. B **56**, 8069 (1997)

[8] Daniel Z. Freedman, *Group Theory in Physics* lecture notes, unpublished

[9] Howard Georgi, *Lie Algebras in Particle Physics*, Benjamin/Cummings Publishing Company, Inc., 1982.

[10] P. C. Hohenberg, Phys. Rev. **158**, 383 (1967)

[11] Daniel C. Mattis, *The Theory of Magnetism I/II*, Berlin, Springer-Verlag, 1981/1985

[12] N. D. Mermin and D. C. Wagner, Phys. Rev. Lett. **17**, 1133 (1967).

[13] J. W. Negele, H. Orland, *Quantum many-particle systems*, Redwood City, Calif., Addison-Wesley Pub. Co., 1988

[14] A. M. Tsvelik, *Quantum Field Theory of the Condensed Matter Physics*, Cambridge University Press, Cambridge, England, 1995

[15] Kei Yosida, *Theory of Magnetism*, Berlin, Springer-Verlag, 1996