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Theoretical Tools for Spin Models in Magnetic Systems

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Chapter 5

Schwinger bosons

The spin-wave formalism is very useful when we have a magnetically ordered ground state. However, there are a lot of circumstances when this is not the case. For instance, when we want to treat quantum states which are rotationally symmetric. In these cases, one can use the parton formalism (which does not impose any preferred spin direction) where the spin operators are decomposed into two (or more) kinds of partons that can be either bosonic or fermionic. In this chapter, I start studying the bosonic operators called Schwinger bosons. One of the advantages of the boson formalism over the fermion is that it can give a ground state with Néel order. I also will briefly discuss the fermion operator formalism and study valence bond lattices.

5.1 Schwinger bosons

The Schwinger boson technique can describe different ground-state structures in a unified formalism, without biasing the calculation toward the existence or non-existence of long-range magnetic order. That is, we have a formalism capable of describing any possible ground state. In this approach, there is no need to partition the lattice into different sublattices (although it can be done) or perform any spin operator rotation to a local reference axis, as is customarily done in the standard spin-wave theory.

If $|0\rangle$ represents the Schwinger bosons vacuum, we introduce two operators a and b by

$$|\uparrow\rangle = a^{\dagger}|0\rangle, \quad |\downarrow\rangle = b^{\dagger}|0\rangle, \tag{5.1}$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are spin-1/2 states. The operators a and b satisfy the standard bosonic commutation relations: $[a, a^{\dagger}] = 1$, $[b, b^{\dagger}] = 1$. We have also

$$\begin{aligned} &a|0\rangle = 0, \quad b|0\rangle = 0, \quad a^{\dagger}|\uparrow\rangle = 0, \\ &a|\uparrow\rangle = |0\rangle, \quad b|\downarrow\rangle = |0\rangle, \quad b^{\dagger}|\downarrow\rangle = 0, \end{aligned} \tag{5.2}$$

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$a^\dagger$ and $b^\dagger$ create spin ½ particles called spinons. The spin operators are represented by

$$S^+ = S^x + iS^y = a^\dagger b, \qquad S^- = S^x - iS^y = b^\dagger a, \tag{5.3}$$

$$S^z = \frac{1}{2}(a^\dagger a - b^\dagger b). \tag{5.4}$$

We can verify that the commutation relations are satisfied:

$$\begin{aligned}
[S^x, S^y] &= \frac{i}{2}[S^+, S^-] = \frac{i}{2}[a^\dagger b, b^\dagger a] = \frac{i}{2}(a^\dagger a - b^\dagger b) = iS^z \\
[S^z, S^x] &= \frac{1}{2}[S^z, S^+ + S^-] = \frac{1}{4}[a^\dagger a - b^\dagger b, a^\dagger b + b^\dagger a] \\
&= \frac{1}{2}(a^\dagger b - b^\dagger a) = iS^y, \\
[S^y, S^z] &= \frac{1}{2i}[S^+ - S^-, S^z] = \frac{1}{4i}[a^\dagger b - b^\dagger a, a^\dagger a - b^\dagger b] \\
&= \frac{i}{2}(a^\dagger b + b^\dagger a) = iS^x.
\end{aligned} \tag{5.5}$$

We also have

$$\begin{aligned}
S(S+1) &= S^xS^x + S^yS^y + S^zS^z = \frac{1}{2}(S^+S^- + S^-S^+) + S^zS^z \\
&= \frac{1}{2}[(a^\dagger b)^2 + (b^\dagger a)^2] + \frac{1}{4}(a^\dagger a - b^\dagger b)^2 \\
&= \frac{1}{2}(a^\dagger a + b^\dagger b)\left[1 + \frac{1}{2}(a^\dagger a + b^\dagger b)\right],
\end{aligned} \tag{5.6}$$

i.e.,

$$S = \frac{1}{2}(a^\dagger a + b^\dagger b). \tag{5.7}$$

The relations (5.2) enlarge the on-site Hilbert space. To remain within the physical space, one has to satisfy (5.7).

A singlet $\uparrow\downarrow$ in the sites (i, j) is given by

$$|\alpha\rangle_{ij} = \frac{1}{\sqrt{2}}\left(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle\right), \tag{5.8}$$

and so

$$|\alpha\rangle_{ij} = \frac{1}{\sqrt{2}}\left(a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger\right)|0\rangle. \tag{5.9}$$

A general spin state $|S, m\rangle$ is generated by the relation

$$|S, m\rangle = \frac{(a^\dagger)^{S+m}(b^\dagger)^{S-m}}{\sqrt{(S+m)!}\sqrt{(S-m)!}}|0\rangle. \tag{5.10}$$

We can verify that

(a) If $S = ½$, $m = \pm ½$

$$|1/2, 1/2\rangle = a^\dagger|0\rangle, \qquad |1/2, -1/2\rangle = b^\dagger|0\rangle. \tag{5.11}$$

(b) If $S = 1$, $m = 1, 0, -1$

$$|1, 1\rangle = \frac{(a^\dagger)^2}{\sqrt{2}}|0\rangle, \qquad |1, -1\rangle = \frac{(b^\dagger)^2}{\sqrt{2}}|0\rangle, \quad |1, 0\rangle = a^\dagger b^\dagger|0\rangle. \tag{5.12}$$

(c) If $S = 2$, $m = 2, 1, 0, -1, -2$

$$\begin{aligned} |2, 2\rangle &= \frac{(a^\dagger)^4}{\sqrt{4!}}|0\rangle, \qquad |2, -2\rangle = \frac{(b^\dagger)^4}{\sqrt{4!}}|0\rangle, \\ |2, 1\rangle &= \frac{(a^\dagger)^3 b^\dagger}{\sqrt{3!}}|0\rangle \qquad |2, -1\rangle = \frac{a^\dagger(b^\dagger)^3}{\sqrt{3!}}|0\rangle, \\ |2, 0\rangle &= \frac{(a^\dagger)^2(b^\dagger)^2}{2}|0\rangle. \end{aligned} \tag{5.13}$$

Note that the condition (5.7) implies that the physical space is given by $n_a + n_b = 2S$, where $n_a = a^\dagger a$ and $n_b = b^\dagger b$. If a Schwinger boson, say a, condenses in some particular mode because it carries a spin index, such a condensate state spontaneously breaks the SU(2) symmetry. In this case, we can eliminate the a boson using the constraint (5.7)

$$b \leftrightarrow b, \qquad a \leftrightarrow \sqrt{2S - b^\dagger b}\,, \tag{5.14}$$

and we get the Holstein–Primakoff representation.

Let us define the bond operators

$$\hat{A}_{ij} \equiv \frac{1}{2}(a_i b_j - b_i a_j), \qquad \hat{B}_{ij} \equiv \frac{1}{2}\left(a_i^\dagger a_j + b_i^\dagger b_j\right). \tag{5.15}$$

We have then the identity

$$\vec{S}_i \cdot \vec{S}_j = :\hat{B}_{ij}^\dagger \hat{B}_{ij}: - \hat{A}_{ij}^\dagger \hat{A}_{ij}, \tag{5.16}$$

where :: denotes normal ordering. Both operators (5.15) are rotationally invariants. That is, they are invariant under any transformation SU(2) of the spinors $\begin{pmatrix} a_i \\ b_i \end{pmatrix}$. We can easily show that

$$\hat{B}_{ij}^{\dagger}\hat{B}_{ij} = 2(\vec{S}_i + \vec{S}_j)^2, \qquad \hat{A}_{ij}\hat{A}_{ij} = 2(\vec{S}_i - \vec{S}_j)^2, \tag{5.17}$$

revealing the character ferromagnetic and antiferromagnetic, respectively, of each term. Note that

$$\hat{A}_{ij} = -\hat{A}_{ji}. \tag{5.18}$$

$\hat{A}_{ij}^{\dagger}$ creates a spin-singlet in the oriented bond ij (it is called the valence bond (VB) order parameter, see section 5.8), and $\hat{B}_{ij}^{\dagger}$ implies a hopping of Schwinger bosons from site to site. $\hat{A}_{ij}^{\dagger}\hat{A}_{ij}$ is proportional to the number (0 or 1) of a singlet between sites i and j. The constraint (5.7) allows us to write

$$:\hat{B}_{ij}^{\dagger}\hat{B}_{ij}: + \hat{A}_{ij}^{\dagger}\hat{A}_{ij} = S^2. \tag{5.19}$$

So, we can eliminate one of the terms if it is of interest. The Hamiltonian

$$H = \pm J\sum_{\langle ij\rangle}\vec{S}_i \cdot \vec{S}_j, \tag{5.20}$$

can be written as

$$H = \pm J\sum_{\langle ij\rangle}\left(\hat{B}_{ij}^{\dagger}\hat{B}_{ij} - \hat{A}_{ij}^{\dagger}\hat{A}_{ij}\right) + \sum_i \lambda_i(a_i^{\dagger}a_i + b_i^{\dagger}b_i - 2S). \tag{5.21}$$

This Hamiltonian preserves the SU(2) spin-rotation invariance. The last term, where λ_i is a site-dependent Lagrange multiplier, restricts the number of bosons per site following the constraint (5.7). To proceed, we need to decouple the four operator terms in (5.21). By a judicious choice of decoupling, we can, in principle, describe any sort of ordered or disordered structure in the ground state of (5.21). The possibility of long-range magnetic order is incorporated in the theory by allowing the Schwinger bosons to condense.

5.2 Mean-field approximation

In the mean-field approximation (MFA) we take λ_i to be site-independent and use the decoupling

$$\hat{A}_{ij}^{\dagger}\hat{A}_{ij} \to \hat{A}_{ij}^{\dagger}\langle\hat{A}_{ij}\rangle + \langle\hat{A}_{ij}^{\dagger}\rangle\hat{A}_{ij} - |\langle\hat{A}_{ij}^{\dagger}\rangle|^2, \tag{5.22}$$

and a similar expression for the B term. The averages are taken in the mean-field state. In the MFA, we neglect bond operator fluctuations and replace $\langle\hat{A}_{ij}\rangle$ and $\langle\hat{B}_{ij}\rangle$ by complex bond parameters A_{ij} and B_{ij}. If we do not consider flux phases (see section 5.5 for the definition of flux), we can take the parameters to be real. The decoupling can also be done using the Hubbard–Stratonovich transformation [1]. The final result is the same.

A general Schwinger boson mean-field Hamiltonian with explicit global SU(2) symmetry must be of the form

$$H_{MF} = \sum_{\langle ij \rangle} J_{ij}\left(-A_{ij}^{*}\hat{A}_{ij} + B_{ij}^{*}\hat{B}_{ij} + h.c.\right) + \sum_{\langle ij \rangle} J_{ij}\left(|A_{ij}|^2 - |B_{ij}|^2\right) + \lambda \sum_{i}\left(a_i^{\dagger}a_i + b_i^{\dagger}b_i - \kappa\right), \tag{5.23}$$

where the complex numbers $A_{ij} = -A_{ji}$, $B_{ij} = B_{ji}^{*}$ are the parameters of the mean-field ansatz (the set of parameters A_{ij}, B_{ij} appearing in the mean-field Hamiltonian is called an ansatz). The parameter κ can be continuously varied to interpolate between the classical limit ($\kappa = \infty$) and the extreme quantum limit ($\kappa \to 0$). Fixing $\kappa = 2S$ to study a spin S model is not necessarily the best choice. Note that A_{ij} is antisymmetric with respect to the interchange $i \to j$. So, for instance, in the Fourier transform along the x-direction of $a_i b_j$ we get (+) to the right and (−) to the left, which leads to: $e^{ik_x} - e^{-ik_y} = 2i \sin k_x$. We write

$$A_{ij} = \langle \hat{A}_{ij} \rangle, \qquad B_{ij} = \langle \hat{B}_{ij} \rangle. \tag{5.24}$$

At the mean field, the local constraint (5.7) is enforced only on the average via the Lagrange multiplier λ. Note that the present formalism does not impose any preferred spin direction: giving a finite expectation value $A_{ij} \neq 0$ to the operator $\hat{A}_{ij}$ does not break the SU(2) symmetry.

One of the most used approaches is searching for an optimal A_{ij} and B_{ij} self-consistently solving for stationary points of the mean-field free energy. The mean-field energy of a gas of bosons is given by

$$F_{MF} = N\beta^{-1}\sum_{k} \ln\left(1 - e^{-\beta\omega_k}\right) + E_g, \tag{5.25}$$

where E_g is the ground-state energy of the Hamiltonian (5.23). The conditions (5.24) should be obeyed to enforce self-consistency, which is equivalent to

$$\frac{\partial F_{MF}}{\partial A_{ij}} = 0, \text{ and } \qquad \frac{\partial F_{MF}}{\partial B_{ij}} = 0,$$

together with the condition $\langle \hat{n}_i \rangle = \kappa \leftrightarrow \frac{\partial F_{MF}}{\partial \lambda} = 0$.

As is often the case with mean-field theory, the self-consistent equations possess several solutions. To compare the various solutions, one can, at a first approximation, compare the mean-field energies (but note that these energies are not variational).

As was said before, we can use $\hat{A}_{ij}$ or $\hat{B}_{ij}$, and keeping only $\hat{A}_{ij}$ is a widespread practice in the literature. However, Mezio *et al* [2] have shown that using only $\hat{A}_{ij}$ gave incorrect results to the triangular lattice. Even on the square lattice, the simultaneous use of both operators improved the result for the ground-state energy [3]. In frustrated

systems where disordered phases could appear, the use of both operators is more convenient [4, 5].

Auerbach [1] extended the SU(2) Schwinger boson representation to SU($\mathcal{N}$) with $\mathcal{N}$ large by increasing the number of Schwinger boson flavors from 2 to $\mathcal{N}$. The bond operator is generalized to: $\hat{A}_{ij} = \sum_{\alpha=1}^{N} a_{i\alpha} a_{j\alpha}$. The mean-field theory is strictly valid only in the $\mathcal{N} \to \infty$ limit, as we show below. We have the exact result

$$\hat{A}_{ij}^{\dagger} \hat{A}_{ij} = \hat{A}_{ij}^{\dagger} \langle \hat{A}_{ij} \rangle + \left\langle \hat{A}_{ij}^{\dagger} \right\rangle \hat{A}_{ij} - \left\langle \hat{A}_{ij}^{\dagger} \right\rangle \langle \hat{A}_{ij} \rangle + \left(\hat{A}_{ij}^{\dagger} - \left\langle \hat{A}_{ij}^{\dagger} \right\rangle \right) (\hat{A}_{ij} - \langle \hat{A}_{ij} \rangle).$$

All terms except the last one are of order $\mathcal{N}^2$. By the central limit theorem, the last term is a product of terms of order square root of $\mathcal{N}$, and thus, one order less than the others. In the large $\mathcal{N}$ limit, it can be neglected, and we get the mean-field result (5.22). However, the mean-field theory can be used as an analytic approach even for $S = ½$, since it captures various disordered and exotic ground states. The large $\mathcal{N}$ approach handles strong local interactions in terms of constraints, and at the mean-field level, the constraints are enforced only on average. Higher-order corrections systematically reintroduce their effects in $1/\mathcal{N}$, including the disordering effects of quantum fluctuations. We can treat the last term in the exact expansion in perturbation theory, and the $1/\mathcal{N}$ corrections to the mean-field theory can be calculated using Feynman diagrams, which describe interactions between the free quasiparticles of the mean-field theory. Finding a large-$\mathcal{N}$ ground state amounts to solving a classical minimization problem. However, it is rather difficult to include the effect of fluctuations beyond the mean-field approximation. Although we will not consider the implications of $1/\mathcal{N}$ corrections, they present a way to extend the mean-field results significantly when the mean-field theory predicts pathological behavior.

The SU($\mathcal{N}$) approach proposed by Auerbach [1] is valid only for ferromagnets. Bipartite antiferromagnets can also be studied in SU($\mathcal{N}$) by performing a special transformation on one sublattice. Read and Sachdev [6] extended the theory by duplicating $\mathcal{N}$ times the two species of bosons at each site to the group Sp($\mathcal{N}$), called the symplectic group, which is a subgroup of SU($\mathcal{N}$). In the group Sp($\mathcal{N}$) the elements reverse sign under time reversal, just like the SU(2) spins. The generalized bond operator is now written as $\hat{A}_{ij} = \frac{1}{2} \sum_{\alpha=1}^{N} (a_{i\alpha} b_{j\alpha} - b_{i\alpha} a_{j\alpha})$. For a definition of the group Sp($\mathcal{N}$) see appendix A. For $\mathcal{N} = 1$, the theory becomes the Heisenberg model with SU(2) symmetry. I will not use the large $\mathcal{N}$ theory in this book, and the presentation above was to give some information to the reader. For further details, one should consult the references.

5.3 Ferromagnet

This case is trivial. We use the operator $\hat{B}$. From (5.16) and (5.19) we have

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{\langle ij \rangle} \left(2 : \hat{B}_{ij}^{\dagger} : B_{ij} - S^2 \right) \tag{5.26}$$

$$H_{MF} = -2J\sum_{\langle ij\rangle}\left[\frac{B}{2}\left(a_i a_j^{\dagger} + a_i^{\dagger}a_j + b_i b_j^{\dagger} + b_i^{\dagger}b_j\right) - B^2\right] + \lambda\sum_i (a_i^{\dagger}a_i + b_i^{\dagger}b_i - 2S). \tag{5.27}$$

Or

$$H_{MF} = -JB\sum_{\langle ij\rangle}\left(a_i a_j^{\dagger} + a_i^{\dagger}a_j + b_i b_j^{\dagger} + b_i^{\dagger}b_j\right) + \lambda\sum_i\left(a_i^{\dagger}a_i + b_i^{\dagger}b_i\right) + NzJB^2 - 2N\lambda S, \tag{5.28}$$

where N is the number of sites. Fourier transforming (5.28) we get

$$H_{MF} = \sum_k \omega_k (a_k^{\dagger}a_k + b_k^{\dagger}b_k) + NzB^2 - 2N\lambda S, \tag{5.29}$$

where

$$\omega_k = \lambda - zJB\gamma_k. \tag{5.30}$$

Equation (5.25) is here written as

$$F_{MF} = N\beta^{-1}\sum_k \ln(1 - e^{-\beta\omega_k}) + NzJB^2 - 2N\lambda S. \tag{5.31}$$

Minimizing (5.31) with respect to λ and B we obtain:

$$\frac{1}{N}\sum_k n_k = S, \tag{5.32}$$

$$\frac{1}{N}\sum_k n_k\gamma_k = B. \tag{5.33}$$

In the thermodynamic limit, we take $N \to \infty$, and integrals can substitute the sums. As we take $T \to 0$, the Bose function vanishes for all $\vec{k} \neq 0$. There must be a macroscopic occupation at $\vec{k} = 0$ to satisfy the constraint (5.32):

$$S \approx \frac{1}{N}n_0. \tag{5.34}$$

That is, there is a Bose condensation at $T = 0$ at $\vec{k} = 0$. The Bose condensation is complete because all available Schwinger boson density ($2S$ per site) is accumulated in that single mode. Auerbach [1] showed that in the limit $T \to 0$ the dispersion relation ω_k reduces to the one for the ferromagnetic spin waves: $\omega_k = zJS(1 - \gamma_k)$.

Note that the boson condensation occurs only when the number of bosons is conserved, as is the case with Schwinger bosons. Since they cannot disappear, they condense in the ground state at $T = 0$. That does not happen with magnons of the

Holstein–Primakoff representation since there is no conservation rule for them. If there is a gap in the dispersion relation, equation (5.32) can be satisfied without the necessity of condensation. As we saw before, if there is a gap in the Heisenberg model's excitation spectrum, the ground state must be disordered.

Equation (5.30) can be written as

$$\omega_k = zB\left(1 - \gamma_k + \frac{1}{4z}\kappa^2\right), \qquad \kappa^2 = 4z\left(\frac{\lambda}{zB} - 1\right). \tag{5.35}$$

In general, we must solve the self-consistent equations numerically. For the Heisenberg ferromagnet and antiferromagnet in one and two dimensions, Auerbach [1] obtained some analytical expressions, and I will not present his result here. However, I would like to address just one point: the calculation of the correlation length. The standard spin-wave theories can be used only in the ordered phase and therefore give infinite correlation length (although the correlation length can be estimated for the disordered phase with some suppositions). We can get analytical expressions for the correlation length in disordered phases in just a few cases. Since the Schwinger boson formalism can be used in disordered phases, it is a convenient tool for this kind of calculation. Here, I will follow Auerbach [1] to calculate the ferromagnet's correlation length in two dimensions. He has shown that in this case, one has

$$\kappa \approx \sqrt{16\pi}\exp\left(-\frac{2\pi JS^2}{T}\right), \qquad B = JS + O(T/JS). \tag{5.36}$$

The free boson expression gives the mean-field spin correlation function

$$\left\langle S_i^+ S_j^- \right\rangle = \left\langle a_i^\dagger b_i b_j^\dagger a_j \right\rangle = |R_{ij}|^2 + S\delta_{ij}, \tag{5.37}$$

where

$$R_{ij} = \frac{1}{N}\sum_k n_k e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}. \tag{5.38}$$

For small values of $\vec{k}$ we have $n_k \approx T/\omega_k$, $\gamma_k \approx 1 - k^2/4$ and so we can write (5.38) as

$$R_{ij} \approx \frac{T}{JS}\int \frac{d^2\vec{k}}{(2\pi)^2}\frac{e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}}{\kappa^2/4 + k^2}. \tag{5.39}$$

At large distances, we get

$$R_{ij} \propto \left(|\vec{r}_i - \vec{r}_j|/\xi\right)^{-1/2}\exp\left(-|\vec{r}_i - \vec{r}_j|\kappa/2\right)\left(1 + \frac{2}{|\vec{r}_i - \vec{r}_j|\kappa} + \cdots\right). \tag{5.40}$$

Inserting (5.40) into (5.37) we find

$$\left\langle S_i^+ S_j^- \right\rangle \propto \frac{\xi}{|\vec{r}_i - \vec{r}_j|} e^{-|\vec{r}_i - \vec{r}_j|/\xi}, \tag{5.41}$$

where $\xi = \kappa^{-1}$ is the spin correlation length. We see that, in agreement with the Mermin–Wagner theorem, there is no long-range order at $T > 0$.

5.4 Antiferromagnet

There is more than one way to treat the problem. First, I will follow Auerbach [1] and consider the antiferromagnet on a bipartite lattice with sublattices A and B and nearest-neighbor interactions and use only the operator $\hat{A}_{ij}$. As I said before, this operator is antisymmetric to the interchange of $i \to j$. As we know, one has a Néel order in the ground state (at least in 2d and 3d). So, we apply a spin rotation by π about the y-axis on sublattice B, which changes

$$a_j \to -b_j, \qquad b_j \to a_j. \tag{5.42}$$

This transformation preserves the constraint (5.7). The bond operator transforms into a symmetric operator

$$A_{ij} \to A_{ij} = \frac{a_i a_j + b_i b_j}{2}. \tag{5.43}$$

The Hamiltonian is then written as

$$H = -J \sum_{\langle ij \rangle} \left(2 \hat{A}_{ij}^\dagger \hat{A}_{ij} - S^2 \right). \tag{5.44}$$

The mean-field Hamiltonian becomes

$$\begin{aligned} H_{MF} = JA \sum_{\langle ij \rangle} \left(a_i^\dagger a_j^\dagger + a_i a_j + b_i^\dagger b_j^\dagger + b_i b_j \right) \\ + \lambda \sum_i (a_i^\dagger a_i + b_i^\dagger b_i) + NzJA^2 - 2NS\lambda. \end{aligned} \tag{5.45}$$

Fourier transforming, we get

$$\begin{aligned} H_{MF} = \sum_k \lambda \left(a_k^\dagger a_k + b_k^\dagger b_k \right) \\ + \frac{JzA}{2} \sum_k \gamma_k \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k} + b_k^\dagger b_{-k}^\dagger + b_k b_{-k} \right) \\ + NJzA^2 - 2NS\lambda. \end{aligned} \tag{5.46}$$

Using the Bogoliubov transformation

$$a_k = \cosh \theta_k \alpha_k + \sinh \theta_k \alpha_{-k}^\dagger, \qquad b_k = \cosh \theta_k \beta_k + \sinh \theta_k \beta_{-k}^\dagger, \tag{5.47}$$

we write (5.46) as

$$
\begin{aligned}
H_{MF} \;=\; & \frac{1}{2}\sum_k (\lambda \cosh 2\theta_k + zJA\gamma_k \sinh 2\theta_k)\left(\alpha_k^\dagger \alpha_k + \alpha_k \alpha_k^\dagger + \beta_k^\dagger \beta_k + \beta_k \beta_k^\dagger\right) \\
& (\lambda \sinh 2\theta_k + zJA\gamma_k \cosh 2\theta_k)\left(\alpha_k^\dagger \alpha_{-k}^\dagger + \alpha_k \alpha_{-k} + \beta_k^\dagger \beta_{-k}^\dagger + \beta_k \beta_{-k}\right) \\
& + NzJA^2 - 2N\left(S + \frac{1}{2}\right)\lambda.
\end{aligned} \tag{5.48}
$$

The condition that the anomalous term should vanish leads to

$$
\tanh 2\theta_k = -\frac{zJA\gamma_k}{\lambda}. \tag{5.49}
$$

The final result is

$$
H_{MF} = \sum_k \omega_k \left(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k + \frac{1}{2}\right) + NzJA^2 - 2N\left(S + \frac{1}{2}\right)\lambda, \tag{5.50}
$$

where

$$
\omega_k = \sqrt{\lambda^2 - (zJA\gamma_k)^2}\,. \tag{5.51}
$$

Using $\ln(1 - e^{-x}) = \ln e^{-x/2}(e^{x/2} - e^{-x/2}) = -x/2 + \ln 2 \sinh (x/2)$, we can write the mean-field energy as

$$
F_{MF} = \beta^{-1} \sum_k 2 \ln \left[2 \sinh \left(\frac{\beta\omega_k}{2}\right)\right] - 2N\left(S + \frac{1}{2}\right)\lambda + NzJA^2. \tag{5.52}
$$

Minimizing (5.52) with relation to λ and A gives

$$
\frac{1}{N}\sum_k \frac{\lambda}{\omega_k}\left(n_k + \frac{1}{2}\right) = S + \frac{1}{2}, \tag{5.53}
$$

$$
\frac{1}{N}\sum_k \frac{z^2 JA\gamma_k^2}{\omega_k}\left(n_k + \frac{1}{2}\right) = zA. \tag{5.54}
$$

The excitations in the Schwinger boson approach are not the conventional magnons of the spin-wave theory. The Schwinger boson Hamiltonian is quartic in Bose operators so that magnon–magnon interactions are incorporated into the theory already at the mean-field order. The problem was well discussed by Auerbach [1]. He shows that the Schwinger boson mean-field ground state for the nearest-neighbor model is disordered in one dimension and has long-range order in two and three dimensions. The Schwinger boson mean-field theory fails for half-odd integer spin chains. As mentioned before, the one-dimensional antiferromagnet is a complex problem.

Yoshioka [7] treated the same problem using only the VB order parameter $\hat{A}_{ij}$ without applying the spin rotation at sublattice B (he did not use a bipartite lattice). He commented that it is not strange that the Néel order appears in the ground state, since the VB state can, in general, express any spin-singlet state, and the Néel order is such a state. When Auerbach divided the lattice into two sublattices, there was an implicit assumption of the Néel order's existence. For the case of the square lattice, this assumption is reasonable and justified. For other lattices, the nature of the long-range order (if it exists) is not clear.

Now I will use the two operators to describe the same model. For a pedagogical purpose, I will treat the nearest-neighbor problem at zero temperature. However, the procedure is more useful when we have, for instance, second and even third nearest-neighbor spins. Using both operators, we write the Hamiltonian, after the mean-field decoupling, as

$$\begin{aligned} H = J\sum_{\langle ij\rangle}\Big[\Big(B_{ij}^{*}\hat{B}_{ij} - A_{ij}^{*}\hat{A}_{ij} + h.c.\Big) + \Big(-B_{ij}^{*}B_{ij} + A_{ij}^{*}A_{ij} + h.c.\Big)\Big] \\ + \lambda\sum_{i}(a_i^{\dagger}a_i + b_i^{\dagger}b_i - 2S). \end{aligned} \tag{5.55}$$

After a Fourier transformation, we get

$$\begin{aligned} H_{MF} = \sum_{k}\Big[B(k) + \lambda\Big]\Big(a_k^{\dagger}a_k + b_k^{\dagger}b_k\Big) \\ - i\sum_{k}A(k)\Big(a_k b_{-k} + a_k^{\dagger}b_{-k}^{\dagger}\Big) - 2\lambda NS + 2N(A^2 - B^2), \end{aligned} \tag{5.56}$$

where

$$A(\vec{k}) = \frac{J}{2}\sum_{\delta}\sin(\vec{k}\cdot\vec{\delta})A_{\delta}, \qquad B(\vec{k}) = \frac{J}{2}\sum_{\delta}\cos(\vec{k}\cdot\vec{\delta})B_{\delta}, \tag{5.57}$$

and the sums are performed over the $\vec{\delta}$ vectors connecting the pair of sites coupled by J.

We have: $A_{-\vec{\delta}} = -A_{\vec{\delta}}$, $B_{-\vec{\delta}} = B_{\vec{\delta}}$. After a Bogoliubov transformation

$$\alpha_k^{\dagger} = \cosh\theta_k a_k^{\dagger} - \sinh\theta_k b_{-k}, \qquad \beta_k^{\dagger} = \cosh\theta_k b_k^{\dagger} - \sinh\theta_k a_{-k}, \tag{5.58}$$

with

$$\tanh\theta_k = -\frac{A(\vec{k})}{B(\vec{k}) + \lambda}, \tag{5.59}$$

we get

$$H_{MF} = \sum_{k}\omega_k\Big(\alpha_k^{\dagger}\alpha_k + \beta_k^{\dagger}\beta_k + 1\Big) - N\lambda(1 + 2S), \tag{5.60}$$

where

$$\omega_k = \sqrt{[B(\vec{k}) + \lambda]^2 - A^2(\vec{k})}\,. \tag{5.61}$$

Minimizing F_{MF} at zero temperature, we find

$$\frac{1}{2N}\sum_k \frac{A(\vec{k})}{\omega_k}(1 + 2n_k)\sin(\vec{k}\cdot\vec{\delta}) = A_{\vec{\delta}}, \tag{5.62}$$

$$\frac{1}{2N}\sum_k \frac{B(\vec{k}) + \lambda}{\omega_k}(1 + 2n_k)\cos(\vec{k}\cdot\vec{\delta}) = B_{\vec{\delta}}, \tag{5.63}$$

$$\frac{1}{2N}\sum_k \frac{B(\vec{k}) + \lambda}{\omega_k}(1 + 2n_k) = \frac{1}{2} + S. \tag{5.64}$$

These equations were solved numerically by Ceccato *et al* [3]. They found $B = 0$ and the ground-state energy $E_g = -0.335$ in agreement with quantum Monte Carlo calculation. The value using the Auerbach [1] approach is $E_g = -0.420$.

5.5 Gauge transformation

In this section, I will indicate the Schwinger bosons by b_α, with $b_1 = a$, $b_2 = b$. Let us consider the local U(1) gauge transformation $b_{n\alpha} \to e^{i\theta_n} b_{n\alpha}$. The Hamiltonian remains invariant if we perform the transformation

$$A_{ij} \to e^{i(\theta_i+\theta_j)} A_{ij}, \qquad B_{ij} \to e^{i(-\theta_i+\theta_j)_i} B_{ij}. \tag{5.65}$$

If a gauge transformation connects two mean-field ansatzes after a symmetry operation, the two ansatzes will describe the same physical state and should be considered identical. The set of all transformations that leave a mean-field ansatz invariant is called the projective symmetry group (PSG). Some elements of the PSG are a pure local transformation of the kind (5.65). The set of such elements form a subgroup of the PSG called the invariant gauge group (IGG). If A_{ij} and B_{ij} are both non-zero, the IGG group has elements: identity and $b_{i\alpha} \to -b_{i\alpha}$. That is the Z_2 group. If the B_{ij} are non-zero while all A_{ij} vanish, the IGG will be a U(1) group $b_{i\alpha} \to e^{i\varphi} b_{i\alpha}$ where φ is a site-independent constant. The sum of the phases of an operator around a plaquette is called *flux*. If an operator is written as $\chi_{ij} = \chi_0 e^{i\theta_{ij}}$, the flux is defined as $\theta_{ij} + \theta_{jk} + \theta_{kl} + \theta_{li}$ in the plaquette *ijkl*.

5.6 Frustration

Before continuing with the Schwinger bosons, I will briefly discuss the concept of frustration, which will be useful in the following. An excellent reference in the subject is Schmidt and Thalmeier [8]. There are two types of spin-exchange frustration. First, one has geometric frustration when only antiferromagnetic

nearest-neighbor (n. n.) bonds are present, and the exchange bonds cannot be simultaneously minimized because of local geometric constraints, enforced by the lattice coordination as, e. g., in the triangular or kagome lattice. The other case is the frustration due to competition when the n. n. interaction themselves are unfrustrated, as in the square lattice. Still, the exchange bonds to the next nearest (n. n. n.) or further neighbors introduce a conflict of spin orientation. In the quantum Heisenberg model, one has the simultaneous influence of frustration and quantum fluctuations (zero-point motion of spin waves) at zero temperature complemented by thermal fluctuations (thermally excited spin-wave modes) at finite temperature. Frustration and competition between interactions is a highly debated issue in the field of quantum magnetism. A good review paper on this topic is Misguich [9].

Suppose the ground state of a classical Heisenberg model has no long-range magnetic order because of frustration. In that case, it does not necessarily imply that this remains true at $T > 0$ or for the quantum version of the model [10]. The spectrum of fluctuations generally depends on the ground state. That can lead to a selection mechanism known as *order by disorder* that can lead to long-range magnetic order.

One model of great interest is the two-dimensional square lattice frustrated spin-1/2 Heisenberg antiferromagnet, commonly referred to as the J_1–J_2 model. This model has been studied extensively by various analytical and numerical techniques [9]. For $J_2 = 0$, the ground state is antiferromagnetically ordered at zero temperatures as was said before. The next nearest-neighbor interaction J_2 (along the diagonals) induces frustration and breaks the antiferromagnetic order.

In the classical or mean-field picture of the magnetic order, the spin structure is uniquely determined by minimizing the mean-field ground-state energy $E_{cl} = NS^2J(\vec{Q})$ where $\vec{Q}$ is the modulation vector of the magnetic phase and $J(\vec{k})$ is given by $J(\vec{k}) = J_1(\cos k_x + \cos k_y) + 2J_2 \cos k_x \cos k_y$.

Minimizing E_{cl} with relation to $\vec{Q}$ leads to three possible magnetic phases: Ferromagnet (FM): $\vec{Q} = (0, 0)$, Néel antiferromagnet (NAF) $\vec{Q} = (\pi, \pi)$ and collinear antiferromagnet (CAF) $\vec{Q} = (\pi, 0)$ or $\vec{Q} = (0, \pi)$, where the neighboring spins align ferromagnetically along one axis of the square lattice and antiferromagnetically along with the other (see table 5.1). In fact, the classical ground state is infinitely degenerate for $J_2/J_1 > 1/2$, and the energy is independent of the angle between the spins on the two sublattices. Quantum fluctuations lead to the collinear

Table 5.1. The condition of existence of the three magnetic phases

Phase	Condition
Ferromagnet	$J_1 \leqslant 0,\ J_2/\lvert J_1\rvert \leqslant 1/2$
Antiferromagnet	$J_1 \geqslant 0,\ J_2/\lvert J_1\rvert \leqslant 1/2$
Collinear AF	$J_2 \geqslant 0,\ J_2/\lvert J_1\rvert \geqslant 1/2$

ground state. At zero temperature, the spin orientations of the three types of classical ground-state configurations exhibited by the model are shown in figure 5.1.

The interplay of quantum fluctuations and frustration will strongly modify the classical picture. It has been found that for small $\eta = J_2/J_1$, the ground state is still Néel ordered, but it undergoes a second-order quantum phase transition at a certain $\eta = \eta_{1C}$ from the Néel to a magnetically disordered state. For η larger than another critical value η_{2C}, one has a collinear ordered state. There is substantial evidence that the ground state of the quantum disordered phase has no long-range magnetic order for $0.4 < \eta < 0.6$ for S = ½. There is, however, a good deal of disagreement over the exact positions of the critical points, and the nature of the magnetically disordered region is still under debate.

It happens that the simple form of the J_1–J_2 model is rarely fully adequate to treat realistic systems. In particular, lattice distortions may lead to further anisotropies of the exchange interactions. The spin–orbit interactions can also cause anisotropies of the symmetric exchange [8].

As was mentioned before, the spin-wave formalism cannot be used to study magnetically disordered phases. Still, it can be applied to the ordered phases of frustrated systems, and it can indicate the transition to the disordered ones.

In the study of frustrated magnets, it is usual to plot χ^{-1} as a function of temperature, which at high temperature has the linear form $\chi^{-1} \propto (T - \theta_{CW})$, where the Curie–Weiss constant θ_{CW} indicates the magnet's sign and strength of interactions. θ_{CW} is negative in an antiferromagnet. In the absence of frustration, magnetic order appears below the Néel temperature $T_N \sim |\theta_{CW}|$. Geometrically frustrated magnets do not order at T_N. Instead, they remain in the paramagnetic phase to a much lower temperature at $T_C \ll |\theta_{CW}|$ (a large value for $f \equiv |\theta_{CW}|/T$ is a signature of frustration). These magnets are strongly correlated in the region $T_C \ll T \ll T_N$. However, long-range order is absent. A remarkable characteristic of frustrated magnets is the large accidental degeneracy of ground states, which manifests as zero modes that are not associated with any symmetry breaking (distinct from the Goldstones modes). In most cases, it is not easy to treat these zero modes analytically since spin configurations in the classical ground states do not have long-range order, and we should resort to numerical calculations.

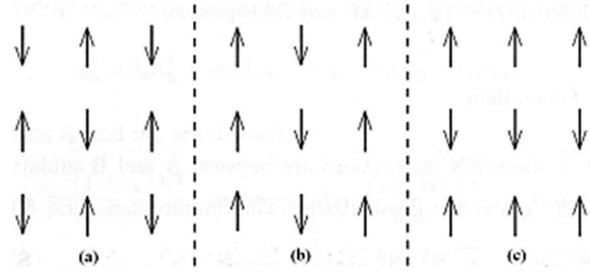

Figure 5.1. Classical ground states for the model studied in this paper: (a) Néel (π, π), (b) collinear (π, 0), (c) collinear (0, π).

5.7 Schwinger boson and the J_1–J_2 model

Following Yang and Wang [11], I will study the square lattice J_1–J_2 antiferromagnetic Heisenberg model, mentioned in the last section, using the Schwinger boson formalism. The Hamiltonian is

$$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j. \tag{5.66}$$

As was mentioned in the last section, the ground state of this model is the Néel state for $J_2/J_1 \leqslant 0.4$ and shows a collinear order for $J_2/J_1 \geqslant 0.6$. It is not the goal of this section to study the disordered region, but only to present an example of the use of the Schwinger bosons. Several mean-field ansatzes are treated in the literature, and here I will show only one for pedagogical purposes.

As before, we will write the mean-field Hamiltonian as

$$H_{MF} = \sum_{ij} J_{ij}\left(-A_{ij}^{*}\hat{A}_{ij} + B_{ij}^{*}\hat{B}_{ij} + h \cdot c\right) + \sum_{ij} J_{ij}\left(|A_{ij}|^2 - |B_{ij}|^2\right) - \lambda \sum_i (\hat{n}_i - \kappa), \tag{5.67}$$

where $\langle \hat{n}_i \rangle \equiv \kappa = 2S$. We use an ansatz where A_1 and B_2 are real, and B_1 is pure imaginary. The ansatz is given by

$$\begin{aligned} A_{(x,\,y)(x+1,\,y)} &= -A_{(x,\,y)(x,\,y+1)} = A_1, \qquad B_{(x,\,y)(x+1,\,y)} = -B_{(x,\,y)(x,\,y+1)} = B_1 \\ B_{(x,\,y)(x+1,\,y+1)} &= -B_{(x,\,y)(x-1,\,y+1)} = B_2. \end{aligned} \tag{5.68}$$

After a Fourier transformation, H_{MF} is written as

$$H_{MF} = \sum_k \psi_k^{\dagger} D_k \psi_k + N\Big[\lambda(1 + 2S) + 2J_1\left(|A_1|^2 - |B_1|^2\right) - 2J_2\,|B_2|^2\Big], \tag{5.69}$$

where $\psi_k = (a_k,\, b_{-k}^{\dagger})^T$ and

$$D_k = (-2J_2B_2\,f_1 - \lambda)I - J_1A_1\,f\sigma_y - \mathrm{Im}(J_1B_1)f\sigma_z, \tag{5.70}$$

where

$$f_1 = \sin k_x \sin k_y, \qquad f = \sin k_x - \sin k_y. \tag{5.71}$$

Performing a Bogoliubov transformation, we get

$$H_{MF} = \sum_k \omega_k\left(\alpha_k^{\dagger}\alpha_k + \beta_k^{\dagger}\beta_k + 1\right) + N[\lambda(1 + \kappa) + 2J_1(|A_1|^2 - |B_1|^2) - 2J_2\,|B_2|^2], \tag{5.72}$$

where

$$\omega_{k\pm} = \sqrt{(2J_2B_2\,f_1 + \lambda)^2 - (J_1A_1\,f)^2} \pm J_1\mathrm{Im}(B_1\,f). \tag{5.73}$$

The self-consistent equations at $T = 0$ are

$$\begin{aligned} 1 + \kappa &= -\int_{BZ} \frac{1}{2}\left(\frac{\partial\omega_{k+}}{\partial\lambda} + \frac{\partial\omega_{k-}}{\partial\lambda}\right)d^2k, \\ 4A_1 &= -\int_{BZ} \frac{1}{2}\left(\frac{\partial\omega_{k+}}{\partial A_1} + \frac{\partial\omega_{k-}}{\partial A_1}\right)d^2k, \\ 4|B_1| &= \int_{BZ} \frac{1}{2}\left(\frac{\partial\omega_{k+}}{\partial|B_1|} + \frac{\partial\omega_{k-}}{\partial|B_1|}\right)d^2k, \\ 4B_2 &= -\int_{BZ} \frac{1}{2}\left(\frac{\partial\omega_{k+}}{\partial B_2} + \frac{\partial\omega_{k-}}{\partial B_2}\right)d^2k. \end{aligned} \tag{5.74}$$

Yang and Wang [11], using different ansatzes, found six spin-liquid states that could be relevant to the J_1–J_2 Heisenberg model (for more details, the reader should consult their paper).

5.8 Valence bonds

In some magnetic models with frustrated interactions, low spin quantum numbers, and especially in small dimensions, long-range magnetic order (defined as we saw before as the existence of a non-zero on-site magnetization) is not the most general situation. Although we cannot find the exact quantum ground state of the antiferromagnetic Heisenberg model in many cases, it is sometimes possible to find a good approximation from a suitable variational ansatz when the spin-wave formalism does not work very well. Generalizing the exact result of the four site spin antiferromagnetic Heisenberg model discussed in chapter 1, we might expect that the ground state is given by a superposition of many possible singlet configurations. Many such systems can be represented in terms of spin paired into rotationally invariant singlets, called *valence bonds* (VB) [1, 12–14]. The VB on a pair of sites i and j is given by

$$|(ij)\rangle \equiv \left(a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger\right)|0\rangle, \tag{5.75}$$

where a_i and b_i are Schwinger bosons on site i and $|0\rangle$ is the vacuum state without any bosons. This state minimizes the energy of the antiferromagnetic coupling between the two spins

$$\langle(ij)|\vec{S}_i \cdot \vec{S}_j\,|(ij)\rangle = -3/4. \tag{5.76}$$

Note that we can still have long-range order at $T = 0$. Two neighboring spins first pair themselves in a singlet, forming a valence bond (which we call dimers). These dimers can then order among themselves, creating a valence bond solid (VBS), which breaks translational symmetry. As in the Néel order, this phase can be described by a local order parameter (figure 5.2).

If we assign a VB to each pair of a given partition of the set of sites of an antiferromagnetic lattice, we can define a variational wave function as

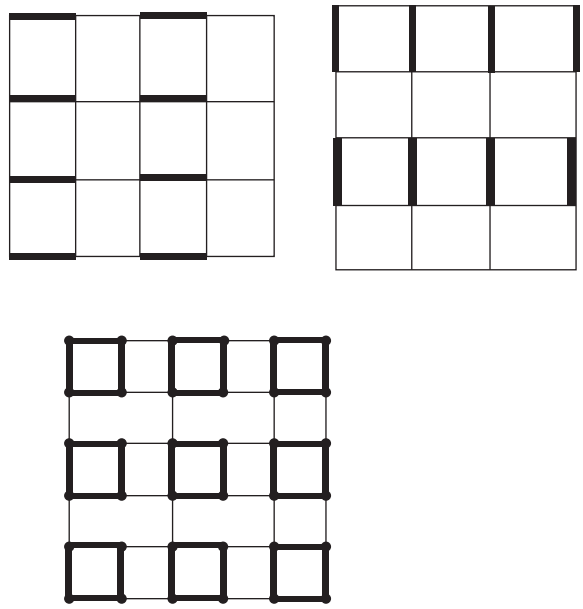

Figure 5.2. A VBS breaks lattice symmetry.

$$|VB\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle, \tag{5.77}$$

where c_α are variational parameters,

$$|\alpha\rangle = \prod_{(ij)\in\Lambda_\alpha} |(ij)\rangle, \tag{5.78}$$

and Λ_α is a particular configuration of bonds (ij) on the lattice such that exactly $2S$ bonds end at each lattice site. One sees that every term in $|\alpha\rangle$ contains exactly $2S$ creation operators at each site, i.e. $|\alpha\rangle$ satisfies the constraint $a_i^\dagger a_i + b_i^\dagger b_i = 2S$ for local spin quantum number S and is thus (generally not normalized) an appropriate state of the Heisenberg model with spin S. Like $|\alpha\rangle$, the superposition (5.77) is a spin-singlet.

Note that although $|VB\rangle$ is a singlet, the nature of the spin correlations depends on the weight c_α. In particular, if this state has significant weight for a configuration Λ_α, the spin correlation can even be long-ranged ordered (Néel ordered). If the weight can be neglected when the valence bond exceeds a finite $\xi \sim O(1)$ length, the spin correlations are expected to decay exponentially.

Even if we allow only nearest-neighbor valence bonds, many possible dimers covering the entire lattice are possible. For each dimer covering of the lattice, there is a valence bond basis state. The Hamiltonian flips a pair of vertical bonds on a plaquette to a pair of horizontal ones and vice-versa. If this is the case, the resulting ground state would not have a long-range order. Such states were called *resonance valence bond* (RVB) states by Anderson (figure 5.3).

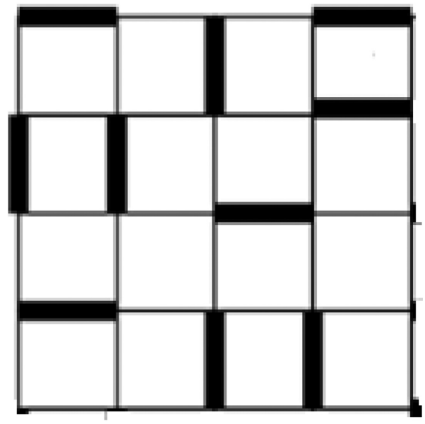

Figure 5.3. The RVB state is a superposition of different partitioning of spins into valence bond.

In a paramagnetic phase, a distinction should be made between spin systems that possess long-range order (LRO) in the VB arrangements (the valence bond crystals mentioned above) and spin systems that do not develop long-range order in any local order parameter at any temperature. The latter systems are called *spin liquids.* Such systems have no LRO in spin, dimer, or any (finite) higher-order correlation functions. The spinons excitations are deconfined. In inelastic neutron scattering experiments, spinons are created in pairs because a neutron changes S^z_{tot} by ± 1. The two spinons of a given pair can then propagate independently. We will return to spin liquids in chapter 10.

Let us consider the case of spin ½, on a bipartite valence bond configuration Λ_α, i.e., $(ij) \in \Lambda_\alpha$ only if $i \in A$ and $j \in B$ or $i \in B$ and $j \in A$ for sublattices A and B. Without loss of generality, we assume $i \in A$ and $j \in B$.

The state $|\alpha\rangle$ can then be written as

$$|\alpha\rangle = \prod_{(ij)\in\Lambda_\alpha} \frac{|\uparrow\rangle_i|\downarrow\rangle_j - |\downarrow\rangle_i|\uparrow\rangle_j}{\sqrt{2}}. \tag{5.79}$$

The spin correlation function in this state is given by

$$\langle\alpha|\vec{S}_k \cdot \vec{S}_l|\alpha\rangle - \langle\alpha|\vec{S}_k|\alpha\rangle.\ \langle\alpha|\vec{S}_l|\alpha\rangle. \tag{5.80}$$

For $k = l$ we have $\langle\alpha|\vec{S}_k \cdot \vec{S}_l|\alpha\rangle = S(S+1) = 3/4$. In the following, we assume $k \neq l$. For $S = ½$, any site belongs only to a single bond in Λ_α. If k and l do not belong to the same bond, $|\alpha\rangle$ does not contain any correlation between $\vec{S}_k$ and $\vec{S}_l$ and then

$$\langle\alpha|\vec{S}_k \cdot \vec{S}_l|\alpha\rangle - \langle\alpha|\vec{S}_k|\alpha\rangle \cdot \langle\alpha|\vec{S}_l|\alpha\rangle = 0. \tag{5.81}$$

If k and l belong to the same bond, we have for $k \in A$ and $l \in B$ (without loss of generality):

$$\begin{aligned}\langle\alpha|\vec{S}_k\cdot\vec{S}_l|\alpha\rangle &= \frac{\langle\downarrow|_l\langle\uparrow|_k-\langle\uparrow|_l\langle\downarrow|_k}{\sqrt{2}}\left(\frac{S_k^+S_l^-+S_k^-S_l^+}{2}+S_k^zS_l^z\right)\\ &\quad\times\frac{|\uparrow\rangle_k|\downarrow\rangle_l-|\downarrow\rangle_k|\uparrow\rangle_l}{\sqrt{2}}\\ &= \frac{1}{2}\langle\downarrow|_l\langle\uparrow|_k\,S_k^zS_l^z\,|\uparrow\rangle_k|\downarrow\rangle_l-\frac{1}{4}\langle\downarrow|_l\langle\uparrow|_k\,S_k^+S_l^-\,|\downarrow\rangle_k|\uparrow\rangle_l\\ &\quad-\frac{1}{4}\langle\uparrow|_l\langle\downarrow|_k\,S_k^-S_l^+\,|\uparrow\rangle_k|\downarrow\rangle_l-\frac{1}{2}\langle\uparrow|_l\langle\downarrow|_k\,S_k^zS_l^z\,|\downarrow\rangle_k|\uparrow\rangle_l\\ &= -\frac{1}{8}-\frac{1}{4}-\frac{1}{4}-\frac{1}{8}=-\frac{3}{4}.\end{aligned}\tag{5.82}$$

So, we have the result

$$\langle\alpha|\vec{S}_k\cdot\vec{S}_l|\alpha\rangle-\langle\alpha|\vec{S}_k|\alpha\rangle\cdot\langle\alpha|\vec{S}_l|\alpha\rangle=\begin{cases}3/4 & \text{if } k=l\\ -3/4 \text{ if } (kl)\in\Lambda_\alpha \text{ or } (lk)\in\Lambda_\alpha.\\ 0 & \text{otherwise}\end{cases}\tag{5.83}$$

If all bonds in Λ_α are of short range. i.e., if there is a length ξ so that Λ_α does not contain bonds (ij) with $|\vec{r}_i-\vec{r}_j|\geqslant\xi$, the spin correlation in $|\alpha\rangle$ is of short range. Then any superposition of such states also has only a short-range spin correlation. States of this type are spin-liquid states. Note that, although any state $|\alpha\rangle$ breaks translational symmetry, the valence bond state $|\mathrm{VB}\rangle$ can restore this symmetry.

It is challenging to prove directly that an RVB state is realized for a given spin-1/2 model because it requires performing numerical simulations on enormous clusters.

Up to now, we have considered systems with fixed interactions. However, we can obtain impressive results in varying one or more parameters. For instance, let us consider the antiferromagnetic Heisenberg model on a square lattice shown in figure 5.4, with nearest-neighbor exchange interactions equal to J and J/λ with $\lambda\geqslant 1$. At $\lambda=1$ one has the isotropic Heisenberg model which, as we know, has a ground state with Néel order. For $\lambda\gg 1$, the ground state can be considered to be a product of nearest-neighbor singlet valence bonds on the J links, and this state is not smoothly connected to the Néel state. Quantum Monte Carlo simulations have shown a direct quantum phase transition between the two states at a critical value of λ (quantum phase transitions will be studied in section 6.2).

5.9 VBS ground states for spins larger than 1/2

One way to construct a VBS ground state with spin $S=1$ is to associate two spins ½ at each lattice site and create the spin one state by symmetrizing them [15, 16]. To avoid the formation of spin $S=2$, we antisymmetrize states between different neighbor lattice sites. The graph representing the VBS ground state in one dimension is presented in figure 5.5. In the same way, we can get VBS states for higher values of

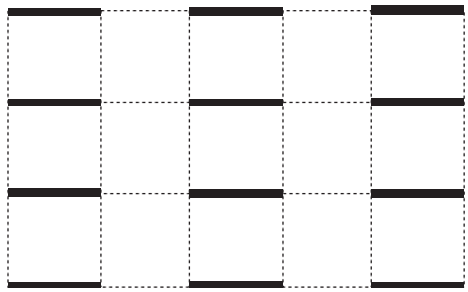

Figure 5.4. The full lines represent the exchange interaction J. The dashed lines represent the exchange J/λ.

Figure 5.5. Small solid circles are spins ½. Lines represent antisymmetrization and circles symmetrization.

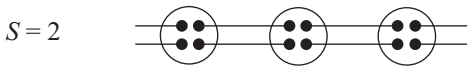

Figure 5.6. The graph for spin $S = 2$.

spins. In figure 5.6 I show the graph for $S = 2$. In terms of Schwinger bosons, the VBS ground state is given by

$$|\text{VBS}\rangle = \prod_{i=0}^{L} \left(a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger\right)^S |0\rangle. \tag{5.84}$$

5.10 Fermion operators

In this section, I introduce a SU(2) fermionic representation. The fermionic representation does not display magnetically ordered phases and tends to favor dimerized states. As in the case of Schwinger bosons, two spin ½ charge-neutral spinon operators $f_{i\alpha}$ ($\alpha = 1, 2$) are introduced. These operators satisfy anticommutation relations, and the spin operator $\vec{S}_i$ is represented by [17]

$$\vec{S}_i = \frac{1}{2} f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta}, \tag{5.85}$$

or

$$S_i^+ = f_{i\alpha}^\dagger f_{i\beta}, \qquad S_i^- = f_{i\beta}^\dagger f_{i\alpha}, \qquad S_i^z = \frac{1}{2}\left(f_{i\alpha}^\dagger f_{i\alpha} - f_{i\beta}^\dagger f_{i\beta}\right). \tag{5.86}$$

The Hamiltonian

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j, \tag{5.87}$$

is then written as

$$H = -\frac{1}{2}\sum_{\langle ij\rangle} J_{ij} f^{\dagger}_{i\alpha} f_{j\alpha} f^{\dagger}_{j\beta} f_{i\beta} + \sum_{\langle ij\rangle} J_{ij}\left(\frac{1}{2}n_i - \frac{1}{4}n_i n_j\right). \tag{5.88}$$

The second term in (5.88) is a constant and can be dropped. As before, we impose the constraint

$$f^{\dagger}_{i1} f_{i1} + f^{\dagger}_{12} f_{i2} = 1 (= 2S). \tag{5.89}$$

This representation is limited to $S = 1/2$ due to the Pauli principle. We obtain a mean-field ground state at zero-order using the following approximations. First, we impose the constraint on the average using a site-dependent and time-independent Lagrange multiplier $\lambda_i(f^{\dagger}_{i\alpha} f_{i\alpha} - 1)$. Second, we replace the operator $f^{\dagger}_{i\alpha} f_{j\alpha}$ by its ground-state expectation value $\langle f^{\dagger}_{i\alpha} f_{j\alpha}\rangle = \chi_{ij}$. The MF Hamiltonian is then given by

$$H_{MF} = -\frac{1}{2}\sum_{\langle ij\rangle} J_{ij}\left[\left(f^{\dagger}_{i\alpha} f_{j\alpha}\chi_{ji} + h.c.\right) - |\chi_{ij}|^2\right] + \sum_i \lambda_i\left(f^{\dagger}_{i\alpha} f_{i\alpha} - 1\right). \tag{5.90}$$

The excitations in the zeroth-order mean-field theory are free spinons described by $f_{i\alpha}$. The term χ_{ij} has two kinds of fluctuations, amplitude fluctuations and phase fluctuations. The amplitude fluctuations can be neglected since they have a finite energy gap. The phase fluctuation a_{ij} around the mean-field ansatz $\bar{\chi}_{ij}$ can be taken into account writing

$$\chi_{ij} = \bar{\chi}_{ij} e^{-ia_{ij}}. \tag{5.91}$$

We can then write the mean-field Hamiltonian as

$$H = -\sum_{\langle ij\rangle} J_{ij}\left(f^{\dagger}_{i\alpha} f_{j\alpha}\bar{\chi}_{ji} e^{-ia_{ji}} + h.c.\right) - \sum_{i,\alpha}\lambda_i\left(f^{\dagger}_{i\alpha} f_{i\alpha} - 1\right), \tag{5.92}$$

where we have included fluctuations in λ. Equation (5.92) was called the first-order mean-field Hamiltonian by Wen [17]. The Hamiltonian is invariant under the gauge transformation:

$$a_{ij} \to a_{ij} + \theta_i - \theta_j, \qquad f_i \to f_i e^{i\theta_i}, \tag{5.93}$$

and the spinons are coupled to a U(1) gauge field (λ_i, a_{ij}). The original Heisenberg model was an interacting spin model with boson excitations. In the above procedure, the bosonic spin operator was split into a product of two fermionic operators. Then a gauge field was introduced to glue the spinons back into a bosonic spin. It is expected then that the first-order mean-field theory could work if the gauge field is in a confining phase, where the spinons interact with each other through a linear potential and never appear as free quasiparticles at low energies.

As an example, I will discuss the π-flux state (defined in section 5.5) for the nearest-neighbor Heisenberg model. This state is given by the ansatz [17]:

$$\chi_1 = \chi_{j,j+\hat{e}_x}, \quad \chi_2 = \chi_{j+\hat{e}_x,j+\hat{e}_y}, \quad \chi_3 = \chi_{j+\hat{e}_x+\hat{e}_y,j+\hat{e}_y}, \quad \chi_4 = \chi_{j+\hat{e}_y,j}, \quad \lambda_i = 0. \tag{5.94}$$

We have two nonequivalent sites on sublattices A and B. Let us write $\bar{f}_j$ when $j \in B$. The Hamiltonian can be written as

$$\begin{aligned} H = &- J \sum_{j\in A} \sum_{\alpha} \left(\chi_1 \bar{f}^{\dagger}_{j+\hat{e}_x,\alpha} f_{j\alpha} + \chi_4^* \bar{f}^{\dagger}_{j+\hat{e}_y} f_{j\alpha} + h.c. \right) \\ &- J \sum_{j\in B} \sum_{\alpha} \left(\chi_3^* f^{\dagger}_{j+\hat{e}_x,\alpha} \bar{f}_{j\alpha} + \chi_2 f^{\dagger}_{j+\hat{e}_y,\alpha} \bar{f}_{j\alpha} + h.c. \right) \\ &+ JN\left(|\chi_1|^2 + |\chi_2|^2 + |\chi_3|^2 + |\chi_4|^2 \right). \end{aligned} \tag{5.95}$$

Taking

$$\chi_1 = |\chi|, \quad \chi_2 = i|\chi|, \quad \chi_3 = |\chi|, \quad \chi_4 = i|\chi|, \tag{5.96}$$

into H and Fourier transforming, we get

$$H = J \sum_k \sum_{\alpha} |\chi| \left\{ f^{\dagger}_{k\alpha} \bar{f}_{k\alpha} (\cos k_x + i \cos k_y) + \bar{f}^{\dagger}_{k\alpha} f_{k\alpha} (\cos k_x - i \cos k_y) \right\}. \tag{5.97}$$

We can write

$$H = J \sum_{k,\alpha} \begin{pmatrix} f^{\dagger}_{k\alpha} & \bar{f}^{\dagger}_{k\alpha} \end{pmatrix} \begin{pmatrix} 0 & |\chi|(\cos k_x + i \cos k_y) \\ |\chi|(\cos k_y - i \cos k_y) & 0 \end{pmatrix} \begin{pmatrix} f_{k\alpha} \\ \bar{f}_{k\alpha} \end{pmatrix}, \tag{5.98}$$

and we get the spinon spectrum

$$E_{\pm}(k) = \pm J|\chi| \sqrt{\cos^2 k_x + \cos^2 k_y}. \tag{5.99}$$

The excitations are gapless Dirac fermions with spin ½ and electrically neutral. Because there are two inequivalent sublattices, the dispersion relation has two branches. We can see that the gap vanishes at $\vec{k} = (\pm\pi, \pm\pi)$.

The flux in each plaquette is $\theta_{12} + \theta_{23} + \theta_{34} + \theta_{41} = \pi \pmod{2\ \pi}$. Since $(i)^2 = -1 = e^{i\pi}$ we have a π-flux (figure 5.7). The function χ is obtained by minimizing the ground-state mean-field energy. To calculate the ground-state energy, we must sum the energies of the lower branch (since the band is half-filled) and then add the term quadratic in χ. That gives

$$E_g = -\sum_k J|\chi| \sqrt{\cos^2 k_x + \cos^2 k_y} + J\,|\chi|^2 N. \tag{5.100}$$

We have then

$$|\chi| = \frac{1}{4} \int \frac{d^2\vec{k}}{(2\pi)^2} \sqrt{\cos^2 k_x + \cos^2 k_y}. \tag{5.101}$$

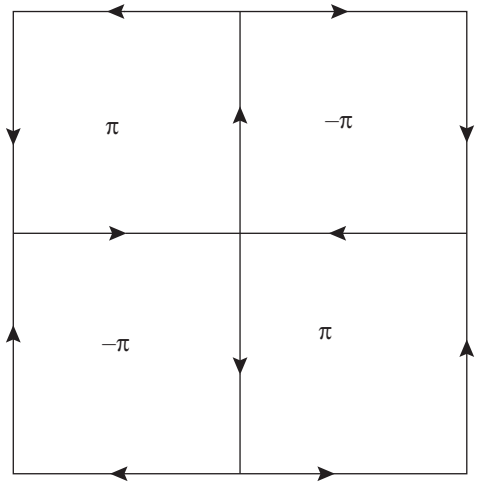

Figure 5.7. The mean-field ansatz of the π-flux state.

At the mean-field level, the π-flux state contains gapless spin excitations, which correspond to the particle-hole excitations. In addition to these excitations, the mean-field theory also has U(1) gauge fluctuations (a_{ij}, λ_i). The interaction between the spin excitations and gauge fluctuations is discussed in detail by Wen [17] in his excellent book, where also several ansatzes for spin liquids are presented.

5.11 Holons

Let us consider a lattice of dimers (each dimer has spin 0, so the ground state has spin 0). As was mentioned before, the elementary magnetic excitations involve replacing one of the singlets by a triplet state. Fractionalization of the triplet means that the two spin-1/2 excitations (spinons with charge zero) can propagate independently. If we remove a single electron, its removal results in breaking one of the dimers, leaving an empty state (called a *holon*) and a free spin (spinon) on the same bond. If the dimers can change their positions by quantum fluctuations, the holon and the spinon can move on the lattice. The electron will have fractionalized into the spinon carrying spin ½ and the holon with spin-zero and electric charge $+e$. This effect is called spin-charge separation.

We can define a set of Bose and Fermi operators b_i and $f_{\alpha i}$, at each site i, satisfying the constraint at each site [13]:

$$b_i^\dagger b_i + f_{\alpha i}^\dagger f_{\alpha i} = 1 \quad \text{(no sum in } i\text{)}. \tag{5.102}$$

Let $|\bar{0}\rangle$ be the reference state for these operators and define the states $|h\rangle, |\uparrow\rangle$ and $|\downarrow\rangle$ representing a holon with charge $+e$ and spin-zero and spinons $|\uparrow\rangle$ with spin up and $|\downarrow\rangle$ with spin down and zero charges:

$$|h\rangle \equiv |e, 0\rangle = b^\dagger\,|\bar{0}\rangle, \quad |\uparrow\rangle \equiv |0, \uparrow\rangle = f_\uparrow^\dagger\,|\bar{0}\rangle \quad |\downarrow\rangle \equiv |0, \downarrow\rangle = f_\downarrow^\dagger\,|\bar{0}\rangle. \tag{5.103}$$

The operator $c^{\dagger}_{\sigma i}$, which creates a fermion of charge e and spin σ at each site i, is given by

$$c^{\dagger}_{\sigma i} = b_i f^{\dagger}_{\sigma i} \text{ (no sum in } i). \tag{5.104}$$

5.12 The dimer order parameter

In this section, I will introduce the dimer order parameter for a one-dimensional spin 1/2 system described by the Hamiltonian [18]

$$H = \sum_{l=1}^{N} (J_1 \vec{S}_l \cdot \vec{S}_{l+1} + J_2 \vec{S}_l \cdot \vec{S}_{l+2}), \tag{5.105}$$

with $J_2/J_1 = 1/2$ and periodic boundary conditions. The system has a pure dimer order in the ground state

$$\left|\phi_1^{D}\right\rangle = [1, 2][3, 4]\ldots[N-1, N], \qquad \left|\phi_2^{D}\right\rangle = [2, 3][4, 5]\ldots[N, 1]. \tag{5.106}$$

The dimer order parameter is given by the operator

$$D = \frac{1}{N}\sum_{l=1}^{N} (-1)^l D_l, \qquad D_l = S_l^+ S_{l+1}^- + S_l^- S_{l+1}^+. \tag{5.107}$$

Dimer order manifests itself in the four-spin correlation function $\langle D_l D_{l+n}\rangle$. We have

$$\langle D_l D_{l+n}\rangle - \langle D_l\rangle\langle D_{l+n}\rangle = \frac{1}{4}(-1)^n. \qquad n \neq 0. \tag{5.108}$$

We can generalize the dimer order parameter for two dimensions. In general, we cannot calculate this parameter analytically, but it is useful in numerical calculations [19].

5.13 The Shastry–Sutherland lattice

The Shastry–Sutherland lattice (figure 5.8) for spin ½ was studied by Shastry and Sutherland [20] as an example of a frustrated quantum spin system with an exact ground state. It is described as a square lattice with J' antiferromagnetic coupling between nearest neighbors and J antiferromagnetic couplings between next nearest-neighbors in every second square along the diagonals. In the classical limit, when $S \to \infty$ the ground state is Néel ordered if $J/J' \leqslant 1$ and is helically ordered otherwise, where the twist between one spin and its nearest neighbor is given by $q = \cos^{-1}(-J'/J)$ [21]. Shastry and Sutherland [20] have shown that the dimer state (built from singlets) is an exact eigenstate of the Hamiltonian for any J, J' and that it is the exact ground state for $J/J' > 2$. Numerical calculations have shown that for $J'/J \geqslant 1.55 \pm 0.05$ the model has a gap in the spectrum of excitations and is in a dimerized valence bond crystal. For $J'/J \leqslant 1.55 \pm 0.05$ the system exhibits Néel

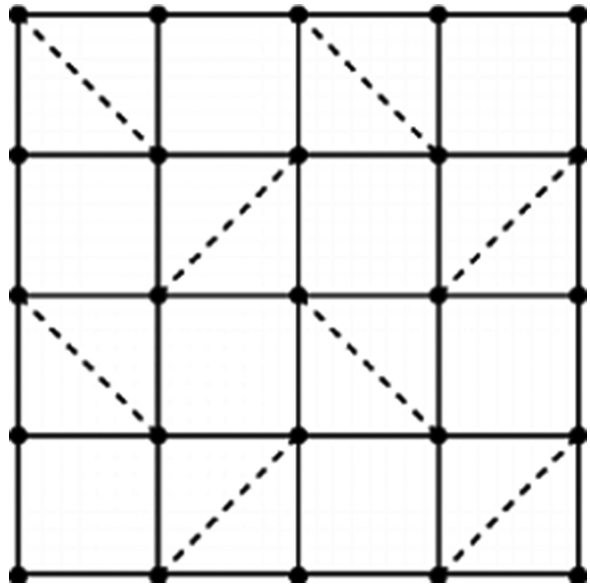

Figure 5.8. The exchange J' acts along the horizontal and vertical lines, while the exchange J acts along the diagonal dashed lines.

order. The possibility of an intermediate phase, possibly with short-range helical correlations, has been discussed in the literature [22].

5.14 Exercises

5.1. Show that the state (5.10) is an eigenstate of the total spin $\vec{S}^2$ and S^z operators with the correct eigenvalues $S(S+1)$ and m, respectively.

5.2. Find the self-consistent equations for the ferrimagnetic chain, introduced in problem 2.1, using the mean-field Schwinger boson formalism (see [23]).

5.3. Find the self-consistent equations for the antiferromagnetic Heisenberg model on a triangular lattice in the presence of a magnetic field using the mean-field Schwinger boson formalism. Note: when we use the Schwinger boson technique, we do not need to rotate the axis in the presence of a magnetic field, as was done in the case of the spin-wave theory (see [24]).

5.4. The two-dimensional square lattice anisotropic Heisenberg antiferromagnet is described by the following Hamiltonian

$$h = J_x \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_y \sum_{\langle l,m \rangle} \vec{S}_l \cdot \vec{S}_m,$$

where the sums $\langle i, j \rangle$ and $\langle l, m \rangle$ are defined for the nearest neighbors along the x- and y-directions, respectively. Using the Schwinger boson mean-field theory find the self-consistent equations for the parameters (see [25]).

5.5. Consider the spin ½ Majundar–Ghosh Hamiltonian

$$H = \frac{4|J|}{3}\sum_{n=1}^{N}\left(\vec{S}_n \cdot \vec{S}_{n+1} + \frac{1}{2}\vec{S}_n \cdot \vec{S}_{n+2}\right) + \frac{N|J|}{2},$$

where the total number of sites N is even, and $\vec{S}_{N+1} = \vec{S}_1$. Show that the dimer (or valence bond) states:

$$|\Omega_{\pm}\rangle = \prod_{n=1}^{N/2}\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{2n} \otimes |\downarrow\rangle_{2n\pm1} - |\downarrow\rangle_{2n} \otimes |\uparrow\rangle_{2n\pm1}\right)$$

are exact ground states, i.e., $|\Omega_{+}\rangle$ describes the state where neighboring spins on sites $2n$ and $2n + 1$ are in a total singlet ($S = 0$) state (note: write the Hamiltonian in terms of the total spin of a triad: $\vec{J}_n = \vec{S}_{n-1} + \vec{S}_n + \vec{S}_{n+1}$) (see [1])).

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