Schwinger-boson calculation for a frustrated antiferromagnet

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The application of the Schwinger-boson transformation to quantum Heisenberg magnets is briefly reviewed, beginning with the derivation of a rotationally invariant mean-field theory. The inclusion of Gaussian fluctuations is discussed in some detail for a general (non-Bravais) lattice, extending available results for simple lattices. Numerical results are presented for the ground-state energy of the Shastry-Sutherland model, and possible future refinements of the method are outlined.

I. INTRODUCTION

The Schwinger-boson method is a versatile means of studying quantum spin systems. It relies on the correspondence between spin and boson degrees of freedom defined by the Schwinger-boson transformation. The introduction of fictitious boson degrees of freedom permits the derivation of simple mean-field theories, with rotationally invariant order parameters which cannot be defined in terms of the original spins. Because the procedure explicitly preserves rotational invariance, spontaneous symmetry breaking need not be assumed, in contrast to standard spin-wave approaches. The method is therefore capable of describing collinear, spiral, and spin-liquid phases within a unified framework, where broken-symmetry phases are represented by Bose-condensed phases of Schwinger bosons. At the mean-field level, early Schwinger-boson calculations produced quantitatively disappointing results. However, small changes in the formalism greatly improve its accuracy without unduly complicating its use. In this paper we briefly review the application of the Schwinger-boson transformation to quantum Heisenberg magnets, beginning with the derivation of a rotationally invariant mean-field theory. We then show in some detail how Gaussian fluctuations around the mean-field solution can be included for arbitrary (non-Bravais) lattices. This generalizes the available results, which treat simple lattices. As an application, we examine the Shastry-Sutherland model, which has been the subject of renewed interest due to its experimental realization in SrCu2(BO3)2.

II. SCHWINGER-BOSON METHOD

The Schwinger-boson transformation is an exact mapping from spin to boson degrees of freedom, given by \( \mathbf{S} \rightarrow \frac{1}{2}(\hat{a}^{\dagger} \hat{b})_m \sigma_{mn}(\hat{a} \hat{b})_n \); here \( m, n = 1, 2 \), and \( \sigma \) is the vector of Pauli matrices. The original spin Hilbert space corresponds not to the full boson Hilbert space but rather to the \((2S + 1)\)-dimensional subspace in which \( \delta n = \hat{a}^{\dagger} \hat{a} + \hat{b}^{\dagger} \hat{b} - 2S = 0 \). Our goal is to evaluate the partition function, \( Z(\beta) = \text{Tr}_{\text{phys}} e^{-\beta \hat{H}} \), where \( \hat{H}(\{\hat{S}_i\}) \rightarrow \hat{H}(\{\hat{a}_i, \hat{b}_i\}) \) is an arbitrary spin Hamiltonian transformed to a boson Hamiltonian, and the trace is restricted to the physical subspace. We can replace the restricted trace with a trace over the full boson Hilbert space using an appropriate projection operator for each spin:

\[
\hat{P}_i = \int \frac{d\lambda_i}{2\pi} \exp \left( -i\lambda_i \delta n_i \right). \tag{1}
\]

Then \( Z = \text{Tr} (\prod_i \hat{P}_i) e^{-\beta \hat{H}} \), which can be rewritten as a functional integral in the usual way. In particular, we obtain

\[
Z(\beta) = \frac{\int D\phi_a D\phi_b D\lambda \delta[\partial_\tau \lambda] \exp (-\mathcal{A}[\phi_a, \phi_b, \lambda])}{\int D\lambda \delta[\partial_\tau \lambda]} \tag{2}
\]

where the Euclidean action is

\[
\mathcal{A} = \int_0^\beta d\tau \left( \mathcal{H}(\{\phi_{ai}, \phi_{bi}\}) + \sum_i i\lambda_i \delta n_i + \sum_{i, \tau} \phi_{ai} \partial_\tau \phi_{ai} \right). \tag{3}
\]

The Lagrange multipliers \( \{\lambda_i\} \) have been promoted to time-dependent variables; the inclusion of \( \delta[\partial_\tau \lambda] \equiv \prod_{i, \tau} \delta(\partial_\tau \lambda_i) \) in the functional measure ensures that \( Z \) remains the same.

The action (3) is invariant under local gauge transformations parametrized by \( \{\theta(\tau)\} \): \( \lambda \rightarrow \lambda - \partial_\tau \theta, \phi \rightarrow e^{i\theta} \phi \). This gauge symmetry is associated with the conservation of total boson number on each site, which holds simply because the magnitude of each spin is constant. The gauge is partially fixed in Eq. (2) by the condition that \( \partial_\tau \lambda = 0 \); the remaining, unfixed, transformations are those where \( \theta \) is time-independent. The action will often have additional symmetries, such as global SU(2) invariance; these depend entirely on the symmetries of the spin Hamiltonian.

We specialize to the Heisenberg Hamiltonian, \( \hat{H} = \sum_{<ij>} J_{ij} \hat{S}_i \cdot \hat{S}_j \). Under the Schwinger-boson transformation \( \hat{S}_i \rightarrow \hat{B}_{ij} \hat{B}_{ij}^\dagger \hat{A}_{ij} \), where \( \hat{A}_{ij} = \frac{1}{2}(\hat{a}_i \hat{b}_j - \hat{b}_i \hat{a}_j) \), \( \hat{B}_{ij} = \frac{1}{2}(\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j) \), and \( \hat{O} \) is the normal-ordered form of \( \mathcal{O} \). The bilinear operators \( \hat{A}_{ij} \) and \( \hat{B}_{ij} \) are invariant under simultaneous SU(2) rotations of spins \( i \) and \( j \), so they may take on vacuum expectation values even without spontaneous rotational symmetry breaking.
This makes them convenient order parameters on which to base a mean-field theory. These operators are not, however, invariant under the U(1) gauge transformations described earlier (since they couple physical and unphysical states), so such theories retain some gauge degrees of freedom. These degrees of freedom become important when the order parameters are allowed to fluctuate around their average values.

We write the Hamiltonian in a form suitable for lattices with several spins per unit cell:

$$\mathcal{H} = \sum_{\mathbf{x} \mu n} J_n \hat{S}_{\mathbf{x}, \mu n} \cdot \hat{S}_{\mathbf{x} + \mathbf{y}, \nu n}.$$  \hspace{1cm} (4)

Here $\mathbf{x}$ labels the unit cell, $\mu$ and $\nu = 1, 2, \ldots, N_{\text{sites}}$ are site labels within a unit cell, and $n = 1, 2, \ldots, N_{\text{bonds}}$ is a bond label. We then formulate a mean-field theory with order parameters $\{A_{\mathbf{x} n}, B_{\mathbf{x} n}\}$ by introducing complex Hubbard-Stratonovich fields $\alpha$ and $\beta$, linearly coupling them to $A$ and $B$, and using them to integrate out the original boson fields $\phi$. This yields a new representation of the partition function,

$$Z(\beta) = \frac{\int D\alpha D\beta D\lambda \delta(\partial_\tau \lambda) \exp (-A_{\text{eff}}[\alpha, \beta, \lambda])}{\int D\alpha D\beta D\lambda \delta(\partial_\tau \lambda) \exp (-A_{\text{HS}}[\alpha, \beta])},$$  \hspace{1cm} (5)

where the effective and Hubbard-Stratonovich actions are

$$A_{\text{eff}} = A_{\text{HS}} + \text{Tr} \ln \hat{M} + \int_0^\beta d\tau \sum_{\mathbf{x} \mu} 2iS_\mu \lambda_{\mathbf{x} \mu},$$  \hspace{1cm} (6a)

$$A_{\text{HS}} = \int_0^\beta d\tau \sum_{\mathbf{x} n} J_n (\alpha^*_{\mathbf{x} n} \alpha_{\mathbf{x} n} + \beta^*_{\mathbf{x} n} \beta_{\mathbf{x} n}).$$  \hspace{1cm} (6b)

The denominator of (5) can be evaluated exactly, but it is convenient for normalization purposes to leave it as it stands. The dynamical matrix $M[\alpha, \beta, \lambda]$, defined in the Appendix, describes the propagation of Schwinger bosons coupled to the Hubbard-Stratonovich fields.

As noted by Trumper et al., the effective action (6a) has a gauge symmetry inherited from the boson action (4). The gauge-fixing functional, given by $\delta(\partial_\tau \lambda)$, can be chosen more or less arbitrarily without changing the value of $Z$; this can be done with the Faddeev-Popov procedure. However, while the exact value of $Z$ is gauge-invariant, the terms in a general perturbative expansion of it are not. We will therefore retain the current gauge-fixing condition in what follows, but observe that this quantitatively affects our results, because the saddle-point expansion we use is not controlled by any gauge-invariant small parameter. By contrast, mean-field theories which take as order parameters either $\{A_{\mathbf{x} n}\}$ or $\{B_{\mathbf{x} n}\}$, but not both, have natural SU(N) generalizations in which the saddle-point expansion is controlled by $1/N$.

Next we look for stationary points of $A_{\text{eff}}$ with respect to its arguments. We consider only static and translationally invariant solutions of the form $\alpha_{\mathbf{x} n} = \alpha^*_{\mathbf{x} n} = \alpha_n$, $\beta_{\mathbf{x} n} = \beta_n$, and $\lambda_{\mathbf{x} \mu} = -i\Lambda_\mu$, where $\alpha$, $\beta$, and $\Lambda$ are real, and we work in the zero-temperature limit. With these restrictions we can derive the desired rotationally invariant mean-field equations. Collectively they take the variational form $\delta E = 0$, where the energy per unit cell is given by

$$\frac{1}{N} E(\alpha, \beta, \Lambda) = \sum_n J_n (\alpha_n^2 - \beta_n^2) - \sum_\mu (2S_\mu + 1)\Lambda_\mu$$

$$+ \frac{1}{N} \sum_{\mathbf{k} \mu} \omega_{\mathbf{k} \mu},$$  \hspace{1cm} (7)

and the quasiparticle energies $\{\omega_{\mathbf{k} \mu}\}$ are defined in the Appendix. This represents a set of $2N_{\text{bonds}} + N_{\text{sites}}$ coupled nonlinear equations, which must be solved numerically for the mean-field parameters $\alpha^{(0)}, \beta^{(0)},$ and $\Lambda^{(0)}$. (There are generally several gauge-equivalent saddle points, differing only in the signs of $\alpha$ and $\beta$; which one of these is chosen as the mean-field solution is irrelevant.) The resulting boson propagator $\hat{g}^{(0)} = (M^{(0)})^{-1}$ enters into the calculation of fluctuation corrections. The ground-state energy per unit cell can be rewritten as

$$\frac{1}{N} E^{(0)} = \sum_n J_n (\beta_n^2 - (\alpha_n^2)^2).$$

Finally, we include fluctuations around the saddle point in the usual way, by expanding the action in a power series:

$$A_{\text{eff}} = A^{(0)} + \frac{1}{2} \Psi^\dagger \frac{\partial^2 A_{\text{eff}}}{\partial \Psi \partial \Psi^\dagger} \bigg|^{\Psi = \cal O(\Psi^2)}}$$  \hspace{1cm} (8)

where the fluctuation fields $\Psi^\dagger = (\alpha^*, \alpha, \beta^*, \beta) = (\alpha^*, \alpha, \beta^*, \beta)^{(0)}$ do not include $\lambda$ due to our choice of gauge. The matrix of second derivatives, which is block-diagonal in reciprocal space, determines the Gaussian correction to the ground-state energy:

$$E^{(1)} = \int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \sum_{\mathbf{k}} \text{Tr} \ln \left( \mathbb{1} - \hat{D}(\mathbf{k}, \omega) \right),$$  \hspace{1cm} (9)

where

$$D_{\mathbf{a} m, b n}(\mathbf{k}, \omega) = J_m^{-1} \text{Tr} \left( \frac{\partial \hat{M}}{\partial \Psi^*_{\mathbf{a} m, \mathbf{k} n}} \frac{\partial \hat{M}}{\partial \Psi_{\mathbf{b} n, \mathbf{k} n}} \right).$$  \hspace{1cm} (10)

These expressions, together with the details provided in the Appendix, represent our main analytical results. We now discuss the numerical results for a particular lattice.

### III. SHAstry-Sutherland Lattice

The Shastry-Sutherland model is a frustrated 2D antiferromagnet with bonds of two different strengths, as shown in Fig. 2. The relevant physical parameters are the ratio $g \equiv J_2/J_1$ and the spin magnitude $S$. In the
classical limit ($S \to \infty$) the ground state has Néel order for $g \leq 2$ and helical long-range order otherwise. For finite $S$ and sufficiently large $g$, the exact quantum ground state is known: it is fully dimerized, with the two spins on each $J_2$-bond in the singlet state $|1\rangle$. (This is often referred to as a spin-liquid phase due to the lack of long-range order.) The energy of this state is always $-2S(S+1)J_2$ per unit cell. Moreover one expects the Néel order present at $g = 0$ to persist up to some positive $g_c(S)$. We would like to clarify to what extent quantum fluctuations melt the classical spiral ordering. Our main interest is in the case $S = 1/2$. This is the physically relevant case, and the existence of a spiral phase is in the greatest doubt here. A previous Schwinger-boson calculation at the mean-field level showed a spiral phase in the range $1.1 \leq g \leq 1.65$. This result has not been confirmed by exact diagonalization, since the spiral states are only energetically favorable on large lattices. High-order series expansions, starting from both $g = \infty$ and $g = 0$, have been used to locate accurately the energetic crossover between the Néel and spin-liquid phases; however, these calculations provide no evidence for or against an intermediate spiral phase.

When describing helical phases it is common to use “twisted” periodic boundary conditions, where spins along one cluster boundary are rotated with respect to those on the opposite boundary. This procedure breaks rotational invariance and complicates the analysis somewhat, so we do not use it here. The price we pay is that helices with small pitch cannot be accommodated by small clusters with untwisted boundary conditions. We found that helical mean-field solutions exist for clusters with as few as 24 sites, suggesting that finite-size effects probably do not seriously alter our results on larger clusters.

We used the Schwinger-boson method to calculate the ground state energy for $S = 1/2$. The mean-field equations can be solved numerically for the full range of $g$. For small $g$, the solution with lowest energy is purely antiferromagnetic ($\alpha \neq 0$, $\beta = 0$) on the strong $J_1$-bonds and purely ferromagnetic ($\beta \neq 0$, $\alpha = 0$) on the weaker $J_2$-bonds. This solution is unique and has ordering wavevector $\mathbf{Q} = (\pi, \pi)$; we identify it as the Néel state. When $g$ is increased, new solutions with ordering wavevectors $\mathbf{Q} = (\pi \pm \delta q, \pi)$ and $\mathbf{Q} = (\pi, \pi \pm \delta q)$ appear through a bifurcation of the Néel state; we identify these solutions as helical states with pitch along the $x$-axis and $y$-axis respectively. The helical states are degenerate for square lattices. Finally, for sufficiently large $g$, the energy of the helical states exceeds that of the spin-liquid state, and the ground state becomes disordered.

The results for a small cluster ($16$-site, $4 \times 4$) are shown in Fig. 2. The Néel state does not undergo any bifurcation here, due to the small size of the cluster. The Schwinger-boson mean-field estimate exceeds the exact ground state energy by a small and roughly constant amount over the full range of $g$. A second-order perturbative calculation around $g = 0$ (that is, around the Néel state) yields similar results in the displayed range (although naturally perturbation theory is more accurate near $g = 0$). Finally, the inclusion of Gaussian fluctuations in the Schwinger-boson calculation improves the accuracy, but for $g \gtrsim 1.3$ only: for larger $g$ the results deteriorate rapidly.

In Fig. 3 we show the mean-field and Gaussian-order results for a larger, rectangular cluster ($64$-site, $16 \times 4$), for which exact results are unavailable (except for the spin-liquid state). In this case the Néel state bifurcates.

**FIG. 1:** Shastry-Sutherland lattice. Single- and double-line bonds have strengths $J_1$ and $J_2$ respectively. The dashed square contains one unit cell.

**FIG. 2:** Ground-state energy, small cluster. The energy per unit cell is plotted, in units of $J_1$, as calculated by (from top to bottom at figure left) perturbation theory, Schwinger-boson theory (mean field), exact diagonalization, and Schwinger-boson theory (Gaussian order).
The results can be interpreted in two ways. It may be that the very good agreement between the mean-field and exact ground-state energies is simply fortuitous; the partition function may not be dominated by contributions from the neighborhood of the mean-field solution. In that case no refinement of the present saddle-point expansion will yield better results. This is a real possibility; however, since the Schwinger-boson mean-field approach also gives accurate results on a number of other systems, it seems unlikely.

It also may be that we have failed to treat the gauge degrees of freedom properly. As noted earlier, the choice of gauge-fixing condition has a quantitative effect on the order-by-order results of the saddle-point expansion. [13] We worked in a simple but otherwise arbitrary gauge. It would be preferable to control the expansion in a gauge-invariant way. This should be possible along the lines of Ref. [4] (and references therein): allow the number of boson “flavors” to become large, say N, and generalize the fields A, B, and \( d_\theta \) in a natural way to include these new flavors. When this is done correctly, the effective action for \( \alpha, \beta, \) and \( \lambda \) will be proportional to N; the saddle-point expansion will then yield an asymptotic series in 1/N, each term of which is gauge-invariant. This program would put the present work on a sounder theoretical footing, by determining in what limit its results become exact. The key step is to generalize A and B simultaneously; this remains a challenge for the future.

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APPENDIX A: DETAILS OF CALCULATION

This appendix contains details about some aspects of the calculation which, while extraneous to the main body of the paper, are included for the sake of completeness.

The boson action (which was integrated out) has the form \( \langle \phi_\alpha^* \phi_\beta \rangle \cdot \tilde{M} \cdot \langle \phi_\alpha \phi_\beta^* \rangle^T \); i.e., it is anomalous. The
where all fields are Fourier-transformed, with arguments $(\mathbf{k} - \mathbf{k'}, \omega - \omega')$ suppressed, and
\[
(F_{n}^{\pm})_{\mathbf{k}\mu,\mathbf{k'}\mu'} = \frac{1}{2} \mathcal{J}_{n}\left(\delta_{\mu\nu} \delta_{\mu'\nu'} e^{ik \cdot y_n} \pm \delta_{\mu\nu} \delta_{\mu'\nu'} e^{-ik \cdot y_n}\right).
\] (A2)

The differing convergence factors $e^{\pm i\omega}$ in the first term of $\hat{M}$ arise from the anomalous nature of the action. They must be taken into account properly to obtain the correct mean-field energy, Eq. (1), and to evaluate the Gaussian correction given by Eq. (2). However, in the latter equation only the first $(n=1)$ term from the expansion $\text{Tr} \ln(\mathbf{1} - \hat{D}) = -\sum_{n} \frac{1}{n} \text{Tr} \hat{D}^{n}$ needs these factors to force convergence of the $\omega$-integral, and the contribution to $E^{(1)}$ from this term can be shown to equal $\frac{1}{2}E^{(0)}$. For numerical work, then, it is simplest to rewrite the Gaussian correction as
\[
E^{(1)} = \frac{1}{2}E^{(0)} + \int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \sum_{\mathbf{k}} \left(\text{Tr} \hat{D} + \text{Tr} \ln(\mathbf{1} - \hat{D})\right)
\] (A3)

and disregard the convergence factors.

The mean-field dynamical matrix is block-diagonal:
\[
\frac{1}{\beta N} \hat{M}^{(0)}(\mathbf{k}, \omega) = i\omega \mathbf{1} \otimes \sigma_z + \hat{A}(\mathbf{k}) \otimes \mathbf{1} + \hat{B}(\mathbf{k}) \otimes \sigma_y,
\] (A4)

where $\hat{A}$ and $\hat{B}$ are Hermitian matrices obtained from the general expression for $M$. This can be diagonalized using a nonunitary (generalized Bogoliubov) transformation: there is a matrix $\hat{S}(\mathbf{k}) = \hat{G}(\mathbf{k}) \otimes \mathbf{1} + \hat{H}(\mathbf{k}) \otimes \sigma_y$ such that $\hat{S}^{\dagger} = (\mathbf{1} \otimes \sigma_z) \hat{S}^{-1}(\mathbf{1} \otimes \sigma_z)$ and
\[
\frac{1}{\beta N} (\hat{S}^{\dagger} \hat{M}^{(0)} \hat{S})_{\mu\mu'} = \delta_{\mu\mu'} \left(\begin{array}{cc}
i\omega + \omega_{k\mu} & 0 \\
0 & -i\omega + \omega_{k\mu}
\end{array}\right).
\] (A5)

The quasiparticle energies $\{\omega_{k\mu}\}$ are the square roots of the eigenvalues of $(A + B)(A - B)$; these eigenvalues will be real and positive when $A$ is large enough, and the mean-field solutions must be sought in that region. The diagonalizing matrix and the quasiparticle energies are analytically tractable for one- and two-site unit cells; in any case they are easy to obtain numerically. The boson propagator is then
\[
\beta N \hat{G}^{(0)}_{\mu\mu'}(\mathbf{k}, \omega) = \hat{S}_{\mu\nu}(\mathbf{k}) \left(\begin{array}{cc}(i\omega + \omega_{k\nu})^{-1} & 0 \\
0 & (-i\omega + \omega_{k\nu})^{-1}\end{array}\right) \hat{S}^{\dagger}_{\nu\mu'}(\mathbf{k}).
\] (A6)

Finally, the mean-field derivatives of $\hat{M}$ with respect to the fluctuation fields are field- and frequency-independent, and can be read directly from Eq. (A1).

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