

Schwinger-Boson Approach to Quantum Spin Systems: Gaussian Fluctuations in the “Natural” Gauge

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We compute the Gaussian-fluctuation corrections to the saddle-point Schwinger-boson results using collective coordinate methods. Concrete application to investigate the frustrated J_1 - J_2 antiferromagnet on the square lattice shows that, unlike the saddle-point predictions, there is a quantum nonmagnetic phase for $0.53 \lesssim J_2/J_1 \lesssim 0.64$. This result is obtained by considering the corrections to the spin stiffness on large lattices and extrapolating to the thermodynamic limit, which avoids the infinite-lattice infrared divergencies associated with Bose condensation. The very good agreement of our results with exact numerical values on finite clusters lends support to the calculational scheme employed. [S0031-9007(97)02739-7]

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In recent years there has been a lot of interest in the properties of quantum magnetic systems [1], particularly frustrated quantum antiferromagnets (AF). Although this interest was initially related to the possible connections between magnetism and superconductivity in the ceramic compounds, the current activity in the area is now well beyond this original motivation.

Among the analytical methods used to study quantum spin systems, the Schwinger-boson approach [2] is one of the most elegant and successful techniques. Contrary to standard spin-wave theory, it does not rely on having a magnetized ground state, which leads to nice rotational properties of the results and to the possibility of describing ordered and disordered phases in a unified treatment. However, this theory has the drawback of being defined in a constrained bosonic space, with unphysical configurations being allowed when this constraint is treated as a soft (average) restriction. This drawback can be in principle corrected by including local fluctuations of the boson chemical potential [3].

Despite the widespread use in the literature of the Schwinger-boson representation of quantum spin operators, we are not aware of a complete calculation of Gaussian corrections to saddle-point results. In particular, for frustrated quantum AF such calculations have been sketched several times [2,4,5], but never fully undertaken. In this work we fill up this gap by presenting the general calculation of Gaussian fluctuations in the Schwinger-boson approach. Since the theory presents a local U(1) symmetry, we use collective coordinate methods—as developed in the context of relativistic lattice gauge theories [6]—to handle the infinitely many zero modes associated to the local symmetry breaking in the saddle-point expansion. As a concrete application, we study the existence and location of the nonmagnetic quantum phase predicted to occur as a consequence of quantum fluctuations and frustration in the J_1 - J_2 model [7].

We will consider a general Heisenberg Hamiltonian, $H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$, where $\langle ij \rangle$ are links on a lattice. We write spin operators in terms of Schwinger bosons [5]: $\vec{S}_i = \frac{1}{2} \mathbf{a}_i^\dagger \cdot \vec{\sigma} \cdot \mathbf{a}_i$, where $\mathbf{a}_i^\dagger = (a_{i\uparrow}^\dagger, a_{i\downarrow}^\dagger)$ is a bosonic spinor, $\vec{\sigma}$ is the vector of Pauli matrices, and there is a boson-number restriction $\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} = 2S$ on each site. With this faithful representation of the spin algebra, the rotational invariant spin-spin interaction can be written as $\vec{S}_i \cdot \vec{S}_j =: B_{ij}^\dagger B_{ij} : - A_{ij}^\dagger A_{ij}$. We defined the SU(2) invariants $A_{ij} = \frac{1}{2} \sum_\sigma \sigma a_{i\sigma} a_{j\bar{\sigma}}$ and $B_{ij}^\dagger = \frac{1}{2} \sum_\sigma a_{i\sigma}^\dagger a_{j\sigma}$ ($\bar{\sigma} = -\sigma$, $\sigma = \pm$), and the notation $:O:$ indicates the normal order of operator O .

Using boson coherent states to formulate the partition function, we formally integrate the Schwinger bosons by decoupling the quartic terms in H using two complex Hubbard-Stratonovich fields $W_{ij}^r(\tau)$ ($r = 1, 2$ correspond, respectively, to the fields that couple to the ferromagnetic B and antiferromagnetic A channels). This leads to $Z = \int [\mathcal{D}\bar{W}\mathcal{D}W][\mathcal{D}\lambda] e^{-\mathcal{A}}$, where the measure $[\mathcal{D}\bar{W}\mathcal{D}W] = \prod_{\langle ij \rangle, r, \tau} (J_{ij}/2\pi i) d\bar{W}_{ij}^r(\tau) dW_{ij}^r(\tau)$ and $[\mathcal{D}\lambda] = \prod_{i, \tau} d\lambda_i(\tau)/2\pi$. Here \bar{W} is the complex conjugate of W and the effective action

$$\mathcal{A} = \int_0^\beta d\tau \left(\sum_{\langle ij \rangle, r} J_{ij} \bar{W}_{ij}^r(\tau) W_{ij}^r(\tau) + i2S \sum_i \lambda_i(\tau) \right) + \mathcal{F}_b(\bar{W}, W, \lambda). \quad (1)$$

The integration on λ comes from the integral representation of the δ functions which force the boson number restriction on each site. In (1) $\mathcal{F}_b(\bar{W}, W, \lambda)$ is the free energy of a boson gas coupled to \bar{W}, W . In a compact notation where site (i), Nambu (s), and Matsubara (τ) indices are summed over in the trace (Tr) operation, we have $\mathcal{F}_b(\bar{W}, W, \lambda) = \text{Tr} \ln \mathcal{M}(\bar{W}, W, \lambda)$. The dynamical

matrix $\mathcal{M}_{ij}^{ss'}(\tau)$ is given by

$$\begin{aligned}\mathcal{M}_{ij}^{11} &= \partial_\tau + i\lambda_i \delta_{ij} - \frac{J_{ij}}{2}(W_{ij}^1 - \overline{W}_{ji}^1) = -\mathcal{M}_{ij}^{22}, \\ \mathcal{M}_{ij}^{12} &= \frac{J_{ij}}{2}(W_{ij}^2 - W_{ji}^2) = \overline{\mathcal{M}}_{ij}^{21},\end{aligned}$$

where we have suppressed the τ dependences to simplify notation. It is important to stress that this formal result for \mathcal{F}_b must be understood as the limit of a discrete- τ mesh [8]. In the functional formulation such a procedure picks up the zero-point contributions to the energy coming from the Bogoliubov transformation in the canonical approach.

The action \mathcal{A} is invariant under both local gauge transformations, $W_{ij}^r \rightarrow W_{ij}^r e^{i(\theta_i \pm \theta_j)}$ ($-$ for $r = 1$, $+$ for $r = 2$), $\lambda_i \rightarrow \lambda_i - \partial_\tau \theta_i$, and global SU(2) rotations of the original bosonic spinors. Consequently, it would be convenient to include external sources $\overline{\eta}, \eta$ which explicitly break the global SU(2) invariance: $\mathcal{F}_b \rightarrow \mathcal{F}_b - \overline{\eta} \mathcal{M}^{-1} \eta$. They are useful to study the spontaneous breaking of this symmetry at $T = 0$ as a consequence of Bose condensation, which signals the onset of magnetic long-range order in the ground state [5]. However, in order to avoid the infrared divergencies associated to this symmetry breaking, in what follows we approach the thermodynamic limit by extrapolation of results on large but finite lattices.

Up to this point all the manipulations are exact. To proceed further we resort, as usual, to a saddle-point expansion. Using the collective notation for the fields $\vec{\varphi}^\dagger \equiv (\overline{W}, W, \lambda)$, the (static) saddle-point values $\overline{W}_{ij}^r, W_{ij,0}^r$ and $\lambda_{i,0}$ are obtained from the extremal equations

$$\left. \frac{\partial \mathcal{A}}{\partial \vec{\varphi}} \right|_{\text{SP}} = \vec{\psi}_0^\dagger + \text{Tr} \left(\mathcal{G}_0 \frac{\partial \mathcal{M}_0}{\partial \vec{\varphi}_0} \right) = 0, \quad (2)$$

where $\vec{\psi}_0^\dagger = (J\overline{W}_0, JW_0, 2Si)$ and $\mathcal{G}_0 = \mathcal{M}_0^{-1}$ is the bosonic Green function at saddle-point order [9]. After expanding \mathcal{A} to second order in the field fluctuations around these saddle-point values, we end up with

$$Z \cong e^{-\mathcal{A}_0} \int [D\vec{\varphi}^\dagger D\vec{\varphi}] e^{-\frac{1}{2} \Delta \vec{\varphi}^\dagger \cdot \mathcal{A}^{(2)} \cdot \Delta \vec{\varphi}}. \quad (3)$$

In this equation $\mathcal{A}_0 = \beta \sum_{\langle ij \rangle} J_{ij} (|W_{ij,0}^1|^2 - |W_{ij,0}^2|^2)$ is the effective action evaluated at the saddle point, and $\Delta \vec{\varphi}$ are the field fluctuations. The matrix $\mathcal{A}^{(2)}$ is given by

$$\mathcal{A}^{(2)} \equiv \left. \frac{\partial^2 \mathcal{A}}{\partial \vec{\varphi}^\dagger \partial \vec{\varphi}} \right|_{\text{SP}} = J - \text{Tr} \left(\mathcal{G}_0 \frac{\partial \mathcal{M}_0}{\partial \vec{\varphi}_0^\dagger} \mathcal{G}_0 \frac{\partial \mathcal{M}_0}{\partial \vec{\varphi}_0} \right),$$

where J is a diagonal matrix containing the exchange couplings J_{ij} along the diagonal, except for the entries corresponding to λ - λ derivatives that are zero.

We stress that the saddle-point expansion of the effective action breaks the gauge invariance of the theory. Although the spontaneous breaking of a local symmetry is strictly forbidden by Elitzur's theorem [10], a possible jus-

tification of this procedure has been given in the context of relativistic lattice gauge theories [11]: The existence of saddle-point solutions connected by the continuous U(1) gauge group makes the $\mathcal{A}^{(2)}$ matrix to have infinitely many zero modes, which are the Goldstone bosons associated to the spurious local symmetry breaking. In particular, for translational-invariant saddle-point values $W_{ij,0}^r = W_{i-j,0}^r, \lambda_{i,0} = \lambda_0$, transforming to momentum-frequency space there is a zero mode $\vec{\varphi}_0^R(\mathbf{k}, \omega) = \delta \vec{\varphi}(\theta) / \delta \theta_{\mathbf{k}\omega} |_{\text{SP}}$ in every \mathbf{k} - ω subspace. Here $\vec{\varphi}(\theta)$ is the vector of gauge-transformed fields (notice that $\vec{\varphi}_0^R$ is a *right* eigenvector of the non-Hermitian matrix $\mathcal{A}^{(2)}$). To avoid the infinities associated to these modes without restoring forces—which correspond to local symmetry transformations—we introduce collective coordinates along the gauge orbit. Exact integration of these coordinates eliminates the zero modes and restores the gauge symmetry (in the sense that noninvariant operators average to zero) [11]. This program can be carried out by enforcing in (3) the so-called background gauge condition or “natural” gauge [6], $\vec{\varphi}(\theta)^\dagger \cdot \vec{\varphi}_0^R = 0$. This condition can be introduced into the functional measure by means of the Fadeev-Popoff trick, and restricts the integration to field fluctuations which are orthogonal to the collective coordinates. At $T = 0$, after carrying out the remaining integrations in (3) on the genuine fluctuations, we obtain the one-loop correction to the ground-state energy *per site*,

$$E_1 = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \sum_{\mathbf{k}} \ln \left(\frac{\Delta_{\text{FP}}(\mathbf{k}, \omega)}{|\omega| \sqrt{\det \mathcal{A}_\perp^{(2)}(\mathbf{k}, \omega)}} \right). \quad (4)$$

Here the Fadeev-Popoff determinant $\Delta_{\text{FP}}(\mathbf{k}, \omega) = |\vec{\varphi}_0^L(\mathbf{k}, \omega) \cdot \vec{\varphi}_0^R(\mathbf{k}, \omega)|$ ($\vec{\varphi}_0^L(\mathbf{k}, \omega)$ is the *left* zero mode of $\mathcal{A}^{(2)}$ in the \mathbf{k} - ω subspace), and $\mathcal{A}_\perp^{(2)}$ is the projection of $\mathcal{A}^{(2)}$ in the subspace orthogonal to the collective coordinates.

We have particularized these results for a matrix J_{ij} which couples a given site to its first (J_1) and second (J_2) neighbors on a square lattice. This model with frustrating $J_1, J_2 > 0$ has been much studied in recent years in connection with the physics of the lightly doped CuO₂ planes (see [12], and references therein). The main problems under discussion are the location and physical properties of a possible nonclassical phase for intermediate frustration $\alpha = J_2/J_1 \sim 1/2$. In the ordered phases of this model [with magnetic wave vectors $\mathbf{Q} = (\pi, \pi)$ for small α and $\mathbf{Q} = (\pi, 0)$ for $\alpha \sim 1$] the Bose condensate breaks the global SU(2) symmetry and its density gives the local magnetization [5]. The associated physical Goldstone modes at $\mathbf{k} = 0, \mathbf{Q}$ lead to serious infrared divergencies of intermediate quantities, which have to be cured by standard renormalization prescriptions. In order to avoid these problems we have computed physical quantities (which are free of these divergencies) on large but finite lattices, and finally

extrapolated these values to the thermodynamic limit. In particular, we considered lattices of up to 60×60 sites, and checked that the extrapolated values had no sensible errors up to the digits presented. However, this procedure requires a careful numerical treatment, since finite results are obtained by cancellations among products of the very large entries of the matrix $\mathcal{A}^{(2)}$.

Equations (2)–(4) lead to a ground-state energy $E_{GS} = E_0 + E_1$ as shown in Fig. 1. Figure 1 contains the result for the infinite lattice and also for finite lattices of 16 and 36 sites, which allow a comparison with exact results obtained by numerical diagonalization [13]. The addition of the Gaussian correction E_1 [Eq. (4)] slightly improves the already very good saddle-point value E_0 . At saddle-point order the theory predicts a first order transition between the two magnetic ground states at some intermediate frustration ($\alpha \approx 0.6$), with no intervening disordered phase. This is in contradiction with numerical studies [14] and series expansion results [15], which found a disordered purely quantum phase somewhere in the range $0.3 \leq \alpha \leq 0.6$. However, it has been recently shown that these finite-lattice studies probably did not reach the scaling region where the required extrapolation can be trusted [16]. In our case, the existence or not of magnetic long-range order was investigated by considering the spin-stiffness tensor $\rho_s = \partial^2 E(\mathbf{Q}) / \partial \mathbf{Q} \partial \mathbf{Q}$, where $E_{GS}(\mathbf{Q})$ is the ground-state energy with twisted boundary conditions [14,16]. In particular, the corrections to the saddle-point values obtained in [16] lead to the results shown in Fig. 2. It gives the stiffness along one of the lattice directions in the $\mathbf{Q} = (\pi, \pi)$ phase at saddle-point and one-loop order, on lattices of 16 and 20 sites (according to numerical studies [14] the tilted 20-site lattice has a stiffness closer to the thermodynamic limit than regular clusters). The comparison with exact re-

sults [13] shows a good agreement, especially for the 20-site lattice. The extrapolation to the thermodynamic limit leaves a window $0.53 \leq \alpha \leq 0.61$, where the stiffness vanishes and the magnetic order is melted by the combined action of quantum fluctuations and frustration (see Fig. 3). This result is in fairly good agreement with the second-order modified spin wave calculation of [17], which predicts a quantum disordered phase in the range (0.52–0.57). Notice that our theory—valid also in the disordered region—predicts that for $0.61 \leq \alpha \leq 0.64$ the short-range AF order is energetically more favorable than the weak collinear order (see dotted line in Fig. 1). However, the characterization of the true ground state in this region requires the consideration of possible nonmagnetic ordered states [4]. Finally, we have computed the spin-wave velocity c_s in the Néel phase using the finite-size formula $E_{GS}(N) \sim E_{GS} - a/N^{3/2}$ and the relation $a = 1.4372c_s$ [18]. For $J_2 = 0$ we obtained $c_s \approx 1.52J_1$ at saddle-point order, and $c_s \approx 1.37J_1$ including the Gaussian fluctuations. These values should be compared to the result of exact diagonalization [13], $c_s \approx 1.28 - 1.44J_1$, which depends on the cluster sizes considered to extrapolate. In Fig. 3 we plot the scaling coefficient a as a function of frustration (in the collinear phase this coefficient should be proportional to some anisotropy-averaged velocity). In the Néel phase the spin-wave velocity vanishes at $\alpha \approx 0.54$, slightly above the point where the stiffness goes to zero. In the collinear phase the averaged velocity never vanishes, and actually it blows up at $\alpha \approx 0.58$. Notably, this is the value where the stronger stiffness in the AF direction of the collinear order vanishes. More details and a further discussion of these results will be given elsewhere.

Before closing, it is worth mentioning a few side questions we have considered while performing these calculations. First, since the Hamiltonian commutes with the local boson-number restrictions, we considered imposing them only through τ -independent Lagrange multipliers λ_i . This reduces the local gauge symmetry

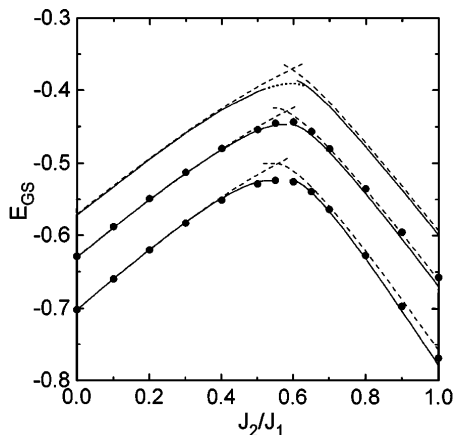


FIG. 1. Ground-state energy *per site* E_{GS} as a function of J_2/J_1 for lattices of (from top to bottom) $N = \infty$, 36, and 16 sites. The full and dashed lines give the fluctuation-corrected and saddle-point results, respectively. Points are exact results from Ref. [13]. The dotted line in the range $0.53 \leq J_2/J_1 \leq 0.64$ indicates the region without long-range magnetic order. Notice that for clarity the curves corresponding to $N = \infty$ and 36 have been shifted upwards in 0.1 and 0.05, respectively.

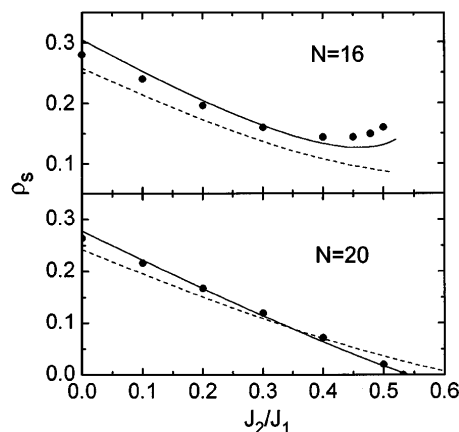


FIG. 2. Spin stiffness ρ_s in the Néel phase for (a) a 16-site lattice, and (b) a tilted 20-site lattice. Symbols and line types are the same as in Fig. 1.

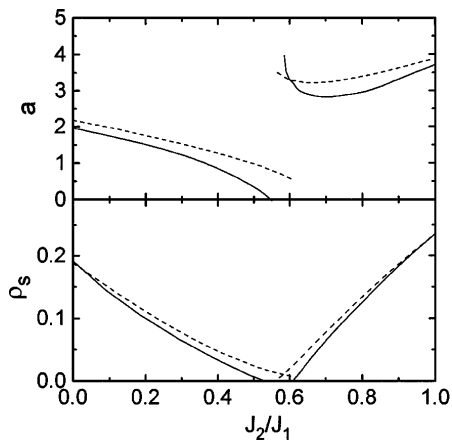


FIG. 3. Scaling coefficient a proportional to the spin-wave velocity (top panel) and spin stiffness ρ_s (bottom panel) extrapolated to the thermodynamic limit. Line types are the same as in Fig. 1.

to static transformations and, consequently, $\mathcal{A}^{(2)}$ contains zero modes only in the $\omega = 0$ subspace. For the calculation of the ground-state energy—which involves an integration over ω —it is then allowed to simply forget about these modes and compute $E_1 = \frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega \sum_{\mathbf{k}} \ln \det \mathcal{A}_{\text{trunc}}^{(2)}(\mathbf{k}, \omega)$, where $\mathcal{A}_{\text{trunc}}^{(2)}$ is equal to $\mathcal{A}^{(2)}$ with the column and row corresponding to the (static) λ fluctuations deleted. In this case there is no need for Δ_{FP} and (4) is equivalent to the RPA result for the bosonic theory with λ_0 taken as a chemical potential. We checked that this procedure gives the same result as (4), although the numerical evaluation requires extra care because of the divergencies near $\omega = 0$. Second, in most works in the literature on Schwinger bosons the identity $:B_{ij}^\dagger B_{ij}: + A_{ij}^\dagger A_{ij} \equiv S^2$ (which holds because of the constraint) is used to simplify the Hamiltonian, leaving only the ferromagnetic B or the antiferromagnetic A channel in the formulation. In a previous publication [19] we warned that at saddle-point order this produces large errors in the ground-state energy, since the above identity is largely violated when the constraint is imposed only on average. We proved that this remains true even after the inclusion of fluctuations, with the contributions of both channels being important. Third, in (4) we can write $\ln \det \mathcal{A}_{\perp}^{(2)} \equiv \text{Tr} \ln \mathcal{A}_{\perp}^{(2)} = -\sum_{n=1}^{\infty} \frac{1}{n} \text{Tr}(I - \mathcal{A}_{\perp}^{(2)})^n$. If only the first term ($n = 1$) is added to the saddle-point energy E_0 , the result is equivalent to the energy obtained in a full Hartree-Fock-Bogoliubov decoupling of the quartic boson interactions in H . Moreover, it can be proved that $E_{\text{HFB}} = E_0 + E_{n=1} = \frac{3}{2}E_0$. That is, a fully self-consistent treatment takes advantage of the unphysical enlargement of Fock space to lower the energy too much. The inclusion of terms with $n \geq 2$ corrects E_{HFB} in nearly 50%.

In conclusion, we have computed the Gaussian-fluctuation corrections to the Schwinger-boson saddle-

point results using collective coordinate methods. As a concrete application, we investigated the ground-state structure of the J_1 - J_2 model. By considering the spin stiffness of this model we showed that, contrary to the saddle-point predictions, there is a quantum nonmagnetic phase that intervenes between the Néel (π, π) and collinear $(\pi, 0)$ orders, as suggested by numerical methods. Its stability region is, however, smaller than predicted by these methods. Moreover, the comparison with exact results on finite lattices lends support to our calculations, which, in addition, have the advantage of a well-defined thermodynamic limit. Finally, the theory developed here can be easily extended to spiral phases, [19] which would allow one to investigate, for instance, the ground-state order in triangular [20] and *kagomé* lattices [21]. Work in this direction is in progress.

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