

Bosonic mean-field theory of quantum Heisenberg spin systems: Bose condensation and magnetic order

Sanjoy Sarker

Department of Physics and Astronomy, University of Alabama, P.O. Box 1921, Tuscaloosa, Alabama 35486-1921

C. Jayaprakash

Department of Physics, The Ohio State University, Columbus, Ohio 43210-1106

H. R. Krishnamurthy

Department of Physics, Princeton University, P.O. Box 708, Princeton, New Jersey 08544

Michael Ma

Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221-0011

(Received 13 February 1989)

We discuss the mean-field approach to the quantum Heisenberg ferromagnet and antiferromagnet on bipartite lattices using the Schwinger boson representation, with the constraints imposed on the average. The low-dimensional results of Arovas and Auerbach [Phys. Rev. B. **38**, 316 (1988)] are derived simply by using a Hartree-Fock decomposition and the Peierls variational principle. We study the models below their critical temperatures in three dimensions (and at zero temperature in $d=2$ dimensions) by identifying magnetic ordering with Bose condensation of the Schwinger bosons. This novel interpretation enables us to compute the low-temperature (in the ordered regime) thermodynamic properties and dispersion relations, which agree with the results of spin-wave theory. We also extract critical properties that are related to those of the spherical model. A brief discussion of the limitations of the approach is also presented.

I. INTRODUCTION

There has been considerable recent interest in the study of quantum Heisenberg models¹⁻⁷ motivated by La_2CuO_4 and other compounds related to high- T_c superconductors. Arovas and Auerbach (AA)² have studied an $\text{SU}(N)$ generalization of the Heisenberg model within a large- N approximation. They employed the Schwinger boson representation⁸ to perform a saddle-point approximation to the functional integral representing the partition function and obtained low-temperature thermodynamic² and dynamic⁹ properties. Their results provide a reasonable description of the disordered, though strongly correlated, low-temperature regime (the so-called "spin liquid") in one- and two-dimensional (2D) models, both for the ferromagnetic and antiferromagnetic (AF) cases. For the 2D quantum antiferromagnet, their results are in agreement with those of Chakravarty, Halperin, and Nelson⁴ derived using the nonlinear σ -model representation. The $S = \frac{1}{2}$ quantum spin chain was studied by Takahashi³ who used a variational density-matrix approach and obtained thermodynamic properties in excellent agreement with the exact Bethe-ansatz results.

We have extended the mean-field approach to quantum spin models formulated in the Schwinger boson representation and used in Ref. 2. The primary motivation for our study is the extension of this method to investigate the Heisenberg-Hubbard model.¹⁰ The latter model, important in the study of cuprate superconductors, is

defined by

$$\mathcal{H}_{H-H} = \mathbb{P} \left[-J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) - t \sum_{\langle i,j \rangle, \mu} c_{i\mu}^\dagger c_{j\mu} \right] \mathbb{P},$$

where $c_{i\mu}^\dagger$ creates an electron at site i with spin μ and $\langle ij \rangle$ denotes nearest neighbors on a d -dimensional lattice; $\mathbf{S}_i \equiv \frac{1}{2} c_{i\mu}^\dagger \boldsymbol{\sigma}_{\mu\nu} c_{i\nu}$ and $n_i \equiv c_{i\mu}^\dagger c_{i\mu}$ are the spin and number operators at site i , and \mathbb{P} is the projection operator that eliminates doubly occupied sites. At half filling, the term proportional to t which represents hole hopping is absent ($n_i \equiv 1$) and the Hamiltonian \mathcal{H}_{H-H} reduces to that of the spin- $\frac{1}{2}$ Heisenberg antiferromagnet considered in this paper. A novel mean-field theory for the Heisenberg-Hubbard model based on using Schwinger bosons to describe singly occupied sites or spins and a "slave" fermion to describe the empty sites or holes is discussed elsewhere.¹⁰

In this paper we first show that the low-dimensional results of Arovas and Auerbach (AA) can be obtained easily by a direct Hartree-Fock decomposition of the Heisenberg Hamiltonian into a quadratic form and using the Peierls variational principle;¹¹ the constraint arising from the Schwinger boson representation is imposed on the average. Then, we extend our considerations to the three-dimensional model and show that the same approach can describe (long-range) magnetic ordering at low temperatures ($T < T_c$) in 3D (and at $T=0$ in 2D) if we identify the magnetic ordering with a Bose condensa-

tion of the Schwinger bosons. We show that this approach correctly reproduces spin-wave theory (dispersion relation for spin waves and thermodynamics properties such as magnetization) at low temperatures. However, it yields, not surprisingly, critical exponents for the continuous phase transition which are related to those of the spherical model. We discuss the derivation of these results for the ferromagnetic problem in Sec. II and for the antiferromagnetic model in Sec. III. In the last section we present critical remarks regarding various assumptions made in the mean-field theory; in particular, we discuss the local gauge invariance associated with the representation and the gauge-variant nature of the condensate.

II. FERROMAGNET

In this section we consider the mean-field theory of the ferromagnetic Heisenberg model in the Schwinger boson representation. The spin- S Heisenberg ferromagnet is described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (2.1)$$

where the exchange constant $J > 0$ and the sum is over all nearest-neighbor pairs of a d -dimensional hypercubical lattice with periodic boundary conditions.

A. Mean-field equations

In the Schwinger representation,⁸ each spin variable S_i is replaced by two bosons $b_{i\sigma}$ where $\sigma = \pm 1$ at each lattice site i . The spin operators can be represented as follows:

$$\begin{aligned} S_i^z &= \frac{1}{2}(b_{i\uparrow}^\dagger b_{i\uparrow} - b_{i\downarrow}^\dagger b_{i\downarrow}), \\ S_i^+ &= b_{i\uparrow}^\dagger b_{i\downarrow}, \quad S_i^- = b_{i\downarrow}^\dagger b_{i\uparrow}. \end{aligned} \quad (2.2)$$

In addition, the bosons satisfy the constraint

$$\sum_{\sigma} b_{i\sigma}^\dagger b_{i\sigma} = 2S \quad (2.3)$$

at each lattice site i .

Using the constraints the Hamiltonian in (2.1) can be expressed as a biquadratic form in the boson operators:

$$H = -2J \sum_{\langle i,j \rangle} :B_{ij}^\dagger B_{ij}: + \frac{NzJ}{2} S^2, \quad (2.4)$$

where $B_{ij}^\dagger = \frac{1}{2} \sum_{\sigma} b_{i\sigma}^\dagger b_{j\sigma}$, N is the number of sites in the lattice, z the number of nearest neighbors, and $:$ denotes normal ordering. The rotationally invariant form (2.4) and its $SU(N)$ generalization have been studied by Arovas and Auerbach for the ferromagnetic model. They derived a mean-field theory using the functional integral representation of the partition function and analyzed it in the disordered regime. First we derive the same results by a direct mean-field theory.

A crucial approximation in this mean-field theory, in addition to the neglect of fluctuations, is that the constraints (2.3) are imposed only on the average. The N constraints can, in this approximation, be taken into account by introducing a single Lagrange multiplier λ .

Next, we make a Hartree-Fock decomposition of Eq. (2.4) which leads to the following mean-field Hamiltonian:

$$\begin{aligned} H_{\text{MF}} &= \lambda \sum_i \left[\sum_{\sigma} b_{i\sigma}^\dagger b_{i\sigma} - 2S \right] \\ &\quad - 2J \sum_{\langle i,j \rangle} \{ \langle B_{ij}^\dagger \rangle B_{ij} + \langle B_{ij} \rangle B_{ij}^\dagger \} \\ &\quad + 2J \sum_{\langle i,j \rangle} \langle B_{ij}^\dagger \rangle \langle B_{ij} \rangle + \frac{NzJ}{2} S^2, \end{aligned} \quad (2.5)$$

where $\langle \dots \rangle$ indicates thermal averaging and the Lagrange multiplier λ is determined by requiring that $\langle \sum_{\sigma} b_{i\sigma}^\dagger b_{i\sigma} \rangle = 2S$. Following AA we assume that $\langle B_{ij} \rangle$ is real and uniform, and we define the mean-field amplitude $B = \langle B_{ij}^\dagger \rangle = \langle B_{ij} \rangle$. A nonzero value for B signifies short-range ferromagnetic correlations. Since the b_{\uparrow} and the b_{\downarrow} channels are decoupled the mean-field Hamiltonian can be diagonalized by Fourier transformation:

$$H_{\text{MF}} = \frac{NzJ}{2} S^2 - 2\lambda SN + NzJB^2 + \sum_{\mathbf{k},\sigma} \omega_{\mathbf{k}} b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma}, \quad (2.6)$$

where

$$\omega_{\mathbf{k}} = JBz(\epsilon_{\mathbf{k}} + \Lambda) = JBz(\epsilon_{\mathbf{k}} - 1) + \lambda \quad (2.7)$$

gives the dispersion relation for the Schwinger bosons,

$$\Lambda = \frac{\lambda}{JBz} - 1 \quad (2.8)$$

and

$$\epsilon_{\mathbf{k}} = \frac{1}{z} \sum_{\delta} (1 - e^{i\mathbf{k} \cdot \delta}). \quad (2.9)$$

The energy per site u and the free energy per site f are then given by

$$u = -JzB^2 + \frac{Jz}{2} S^2, \quad (2.10)$$

$$\begin{aligned} f &= -\frac{Jz}{2} S^2 - 2Jz\Lambda SB - Jz(B - S)^2 \\ &\quad - \frac{2}{N_{\beta}} \sum_{\mathbf{k}} \ln(1 + n_{\mathbf{k}}), \end{aligned} \quad (2.11)$$

where $n_{\mathbf{k}} = (e^{\omega_{\mathbf{k}}/k_B T} - 1)^{-1}$ is the Bose occupation factor. The Lagrange multiplier (chemical potential) λ and the mean-field amplitude B are determined by minimizing the free energy:

$$S = \frac{1}{N} \sum_{\mathbf{k}} n_{\mathbf{k}}, \quad (2.12)$$

$$B = S - \frac{1}{N} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}}. \quad (2.13)$$

Equations (2.12) and (2.13) are the fundamental equations of our mean-field theory.

B. Disordered regime

In the disordered regime the sums in Eqs. (2.12) and (2.13) can be converted into integrals over the first Brill-

loun zone of the reciprocal lattice. This yields

$$S = \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta(\epsilon_k + \Lambda)} - 1} \quad (2.14)$$

and

$$B = S - \int \frac{d^d k}{(2\pi)^d} \frac{\epsilon_k}{e^{\beta(\epsilon_k + \Lambda)} - 1}, \quad (2.15)$$

where d is the spatial dimensionality and we have defined the parameter $\beta \equiv JBz/k_B T$. These equations were obtained by AA [Eqs. 3.5(a) and 3.5(b) in Ref. 2] and by Takahashi³ from a mean-field analysis of his modified spin-wave theory.

We now briefly summarize the results of the analysis of Eqs. (2.14) and (2.15) by Takahashi and AA. Note that since $\epsilon_k \geq 0$ we must have $\Lambda \geq 0$. Since the integral in Eq. (2.14) vanishes at $T=0$ there is no zero-temperature solution in any dimension. For $d=1$ and 2 dimensions there is a solution for all $T>0$ which implies that the system is disordered at any nonzero temperature and the symmetry is unbroken since the theory is rotationally invariant. That the system is disordered can be also demonstrated explicitly from the spin-spin correlation function which vanishes exponentially at large distances. Furthermore, in $d=1$, dimension the low-temperature behavior of the free energy and the susceptibility agrees with the exact Bethe-ansatz results, apart from overall numerical factors of 2 and $\frac{3}{2}$, respectively. This numerical discrepancy was attributed by AA to the overcounting of the number of independent boson degrees of freedom: The point is that the constraint requires there be exactly one independent Bose operator per site, whereas relaxing the constraint makes both b_\uparrow and b_\downarrow bosons independent. The problem of overcounting does not arise in the Takahashi³ theory, since the latter is based on the single-component Holstein-Primakoff representation of the spin operators. In fact, the mean-field results of Ref. 3 can be obtained from the Schwinger boson theory by making the replacement $b_{i\uparrow} = b_{i\uparrow}^\dagger = (2S - b_{i\downarrow}^\dagger b_{i\downarrow})^{1/2}$ and expanding the square root. In this way the b_\uparrow component is effectively removed so that the results are in quantitative agreement with the Bethe-ansatz results at low temperatures. The price is that the modified spin-wave theory is not rotationally invariant in contrast to the Schwinger boson mean-field theory.¹²

In two dimensions there are no exact results available for comparison. Nonetheless, it is believed that the theory gives reasonable results at low temperatures. For $d > 2$ there exists a critical temperature T_c such that Eq. (2.14) has no solution for $T < T_c \neq 0$. Arovas and Auerbach have taken this as an indication that the system is ordered below T_c . Of course, for the ferromagnet the ground state and the low-lying excitations are known exactly, and spin-wave theory yields accurate results at low temperatures. The question then arises if this form of mean-field theory can be extended below T_c , and if so, what corresponds to ferromagnetic ordering? What are the critical properties? Furthermore, is the theory capable of reproducing the spin-wave results? Below we ad-

dress these issues. Before investigating the question of ordering we examine the critical behavior of the model as T approaches T_c from above.

C. Critical behavior as $T \rightarrow T_c^+$

For $T > T_c$ Eq. (2.14) has a solution with the chemical potential $\Lambda > 0$ so that the boson dispersion ω_k exhibits a gap for $T > T_c$. As $T \rightarrow T_c^+$, Λ decreases and goes to zero at $T = T_c$. The critical properties are essentially determined by how Λ vanishes as $T \rightarrow T_c$. In one and two dimensions $T_c = 0$ and Λ vanishes as T^2 and $T e^{-\text{const}/T}$, respectively.

For $d > 2$ the critical temperature is obtained from Eqs. (2.14) and (2.15) by setting $\Lambda = 0$ which gives

$$S = \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta_c \epsilon_k} - 1} \quad (2.16)$$

and

$$B_c = S - \int \frac{d^d k}{(2\pi)^d} \frac{\epsilon_k}{e^{\beta_c \epsilon_k} - 1}. \quad (2.17)$$

From (2.16) we determine β_c as a function of S which can be used in (2.17) to obtain B_c . The critical temperature is then found from $k_B T_c / J = z B_c / \beta_c$.

Note that B decreases with increasing T so that for $T > T_c$, $\beta < \beta_c$. For fixed β the integrals in (2.16) and (2.17) are not necessarily analytic functions of Λ . It is convenient to define

$$I(\tilde{\beta}) \equiv \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\tilde{\beta} \epsilon_k} - 1}. \quad (2.18)$$

Clearly $I(\tilde{\beta})$ is analytic in $\tilde{\beta}$ and $I(\tilde{\beta}_c) = S$. Using (2.18) on both sides of Eq. (2.16) we obtain

$$\int \frac{d^d k}{(2\pi)^d} \left[\frac{1}{e^{\tilde{\beta} \epsilon_k} - 1} - \frac{1}{e^{\tilde{\beta}(\epsilon_k + \Lambda)} - 1} \right] = I(\tilde{\beta}) - I(\tilde{\beta}_c). \quad (2.19)$$

For $\tilde{\beta} \lesssim \tilde{\beta}_c$, Λ is small and the main contribution to the integral comes from small values of ϵ . The density of states for small ϵ behaves as $\epsilon^{d/2-1}$. Expanding the denominators we find that the left-hand side of Eq. (2.19) behaves as

$$\sim \frac{\Lambda}{\tilde{\beta}} \int_0^{\epsilon_{\max}} d\epsilon \frac{\epsilon^{d/2-2}}{\epsilon + \Lambda} \sim \begin{cases} \frac{1}{\tilde{\beta}} \Lambda^{d/2-1}, & 2 < d < 4 \\ -\frac{1}{\tilde{\beta}} \Lambda \ln \Lambda, & d = 4 \\ \frac{\Lambda}{\tilde{\beta}}, & d > 4. \end{cases} \quad (2.20)$$

Since the right-hand side is proportional to $\tilde{\beta}_c - \tilde{\beta}$, we find that $\Lambda \sim (\tilde{\beta}_c - \tilde{\beta})^s$ with $s = 2/(d-2)$ for $2 < d < 4$ and $s = 1$ for $d > 4$. At $d = 4$,

$$\Lambda \sim -(\tilde{\beta}_c - \tilde{\beta}) / \ln(\tilde{\beta}_c - \tilde{\beta}).$$

Up to this point the analysis is identical to that for an

ideal Bose gas close to the condensation temperature $\bar{\beta}_c^{-1}$. It should be recalled, however, that we are dealing with an interacting Bose gas, the effect of interaction entering through the quantity B . The parameter $\bar{\beta}$ is a function of both T and B . To find the critical properties we need to analyze the behavior of B close to T_c . Note that $B=B_c$ is finite at T_c . For $T \rightarrow T_c$ the extra factor of ε in the integral in Eq. (2.17) ensures that B is an analytic function of Λ for all $d > 2$. A simple analysis then yields $B - B_c \sim (\bar{\beta}_c - \bar{\beta})$, from which we obtain $(B - B_c) \sim t$, where $t \equiv (T - T_c)/T_c$. Therefore, we have

$$\Lambda \sim t^s \quad (2.21)$$

with $s = 2/(d - 2)$ for $2 < d < 4$.

To find the correlation length and susceptibility exponents we consider the spin-spin correlation function which is given by

$$G(\mathbf{R}) \equiv \langle \mathbf{S}(\mathbf{0}) \cdot \mathbf{S}(\mathbf{R}) \rangle = \frac{3}{2} [S \delta_{\mathbf{R}, \mathbf{0}} + |g(\mathbf{R})|^2], \quad (2.22a)$$

where

$$g(\mathbf{R}) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{i\mathbf{k} \cdot \mathbf{R}}}{e^{\bar{\beta}(\varepsilon_{\mathbf{k}} + \Lambda)} - 1}. \quad (2.22b)$$

Note that for $\mathbf{R} = \mathbf{0}$, it follows from Eq. (2.14) that $g(\mathbf{0}) = S$, and therefore, $G(\mathbf{0}) = (\frac{3}{2})S(S + 1)$; this has the correct spin dependence but is wrong by a factor of $\frac{3}{2}$. As mentioned earlier this discrepancy arises presumably because the constraints are imposed only on the average. Note that since $\varepsilon_{\mathbf{k}} \sim k^2$ for small k , the correlation length ξ diverges as $\xi \sim \Lambda^{-1/2} \sim t^{-\nu}$ with $\nu = 1/(d - 2)$ for $2 < d < 4$ which is identical to the correlation length exponent in the spherical model.

Similarly, the susceptibility can be calculated from Eq. (2.22) and is given by

$$k_B T \chi^{zz}(\mathbf{q}) = \frac{(g_0 \mu_B)^2}{2} \left[S + \int \frac{d^d k}{(2\pi)^d} n_{\mathbf{k}} n_{\mathbf{k} + \mathbf{q}} \right], \quad (2.23)$$

where $n_{\mathbf{k}} = (e^{\omega_{\mathbf{k}}/k_B T} - 1)^{-1}$. Consider $\chi(\mathbf{q} = \mathbf{0})$: By examining the behavior of the integrand in Eq. (2.23) at small ε it is easy to establish that the susceptibility diverges as $t^{-\gamma}$ with $\gamma = (4 - d)/(d - 2)$ for $2 < d < 4$. Finally, since the energy is essentially determined by B^2 [see Eq. (2.10)] the specific heat goes to a constant as $T \rightarrow T_c^+$ as in the ideal Bose gas. To summarize, the critical behavior as $T \rightarrow T_c^+$ is that of a Bose gas close to its condensation temperature. In particular, for $d = 3$, $\nu = 1$, and $\gamma = 1$.

D. Ordered regime

As mentioned earlier, Eq. (2.14) does not have a solution below T_c . However, the preceding analysis suggests that Bose condensation occurs for $T \leq T_c$. This is not surprising since the total number of bosons is fixed. Here we show that the condensation in the Schwinger boson theory corresponds to the breaking of rotational symmetry and ferromagnetic ordering in the spin system. The analysis depends slightly on how one chooses to break the symmetry, although the results do not.

Let us first consider the case in which condensation

occurs in both the b_{\uparrow} and b_{\downarrow} channels in an equivalent fashion. Then $\langle b_{\uparrow}^{\dagger} b_{\uparrow} \rangle = \langle b_{\downarrow}^{\dagger} b_{\downarrow} \rangle = S$, and $\langle S^z \rangle = 0$. We can obtain a solution to the basic equation (2.12) by separating out the $k = 0$ mode and converting the sum over the remaining terms into an integral. This leads to

$$S = \rho + \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\bar{\beta}(\varepsilon_{\mathbf{k}} + \Lambda)} - 1}, \quad (2.24)$$

where $\rho \equiv \langle b_{0\uparrow}^{\dagger} b_{0\uparrow} \rangle / N = 1[N(e^{\bar{\beta}\Lambda} - 1)]$ is the condensate density. Above T_c , $\rho = 0$, whereas for $T < T_c$, ρ acquires a finite value. This can occur if $\bar{\beta}\Lambda$ vanishes as N^{-1} . Note that since $\varepsilon_{\mathbf{k}} = 0$ for the $k = 0$ mode the equation for B remains unchanged. Setting $\Lambda = 0$ we have for $T < T_c$,

$$\rho = S - \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\bar{\beta}\varepsilon_{\mathbf{k}}} - 1} = S - I(\bar{\beta}), \quad (2.25)$$

$$B = S - \int \frac{d^d k}{(2\pi)^d} \frac{\varepsilon_{\mathbf{k}}}{e^{\bar{\beta}\varepsilon_{\mathbf{k}}} - 1}. \quad (2.26)$$

In the condensed region $|b_{0\uparrow}^{\dagger}| = |b_{0\downarrow}^{\dagger}| = |b_{0\downarrow}| = |b_{0\uparrow}| = (N\rho)^{1/2}$. In particular, at $T = 0$, $\rho = S$. If the phases of the Bose fields are chosen to be the same then $\langle S^x \rangle = 1/N |b_{0\uparrow}|^2 = \rho$, $\langle S^y \rangle = 0$. In this case the system is ferromagnetically ordered in the x direction with the magnetization $m = \rho$. A different choice of phase induces a rotation in the x - y plane, but the magnitude of the magnetization remains the same. That the system is ordered in the transverse direction can also be seen by considering the spin-spin correlation function. It is easily shown that in the present case

$$\lim_{R \rightarrow \infty} \langle \mathbf{S}_{\perp}(\mathbf{0}) \cdot \mathbf{S}_{\perp}(\mathbf{R}) \rangle = \rho^2 = m^2,$$

whereas $\langle S^z(\mathbf{0}) S^z(\mathbf{R}) \rangle \rightarrow 0$ as $R \rightarrow \infty$.

At low temperatures, simple power counting shows that for $d > 2$, $B = S - \text{const} T^{d/2+1}$. We can deduce the leading-order result for the magnetization m by setting $B = S$ in Eq. (2.25). The resulting equation for m is identical to that of spin-wave theory. Therefore, we have $m \sim S - \text{const} \times T^{d/2}$. Higher-order results are obtained by systematically expanding Eqs. (2.25) and (2.26). By expanding the integrals in Eqs. (2.25) and (2.26) about $\bar{\beta}_c$, i.e., as T approaches T_c from below, we find that the magnetization vanishes as $|t|$. Hence, the critical exponent $\beta = 1$ which is twice the ordinary mean-field result.

Although, in the preceding analysis rotational symmetry is broken in the transverse direction, the results are equivalent if instead the system is allowed to order along the z axis as we demonstrate now. We add a small magnetic field in the z direction and then let the field go to zero at the end of the calculation. In the ordered region the two channels are not equivalent; in particular, the number density of b_{\uparrow} bosons, $n_{b_{\uparrow}}$, is $S + m$, and the number density of b_{\downarrow} bosons, $n_{b_{\downarrow}}$, is $S - m$. Hence, instead of Eq. (2.12) we have to consider two separate equations for the b_{\uparrow} and b_{\downarrow} channels

$$\langle b_{i\uparrow}^{\dagger} b_{i\uparrow} \rangle = S + m = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{e^{\bar{\beta}(\varepsilon_{\mathbf{k}} + \Lambda - h)} - 1}, \quad (2.27)$$

$$\langle b_{i\downarrow}^\dagger b_{i\downarrow} \rangle = S - m = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} + \Lambda + h)} - 1}, \quad (2.28)$$

where the parameter h is proportional to the magnetic field. Note that the equation for B [Eq. (2.13)] remains unchanged even in the presence of the field. For $h > 0$ only the b_{\uparrow} channel needs to undergo Bose condensation since there is a solution to Eq. (2.28) for the b_{\downarrow} channel without condensation provided the value of the magnetization is chosen appropriately. In the ordered region, set $\Lambda = h$, and convert the sums into integrals after separating out the $\mathbf{k} = 0$ term for the b_{\uparrow} channel (this is the condensate density ρ); then let $h \rightarrow 0$ which yields

$$\rho = S + m - I(\tilde{\beta}), \quad (2.29)$$

and

$$m = S - I(\tilde{\beta}), \quad (2.30)$$

where the integral $I(\tilde{\beta})$ is given by Eq. (2.18). The magnetization is determined by Eq. (2.30) which is the same as Eq. (2.25)

III. ANTIFERROMAGNET

A. Mean-field equations and disordered regime

In contrast to the ferromagnetic model, the ground state and the excitation spectrum of the quantum antiferromagnetic Heisenberg model are not known exactly except in one dimension. The classic paper of Anderson¹³ provides an excellent description of the low-temperature behavior of the quantum antiferromagnet using spin-wave theory. The intimate connection between spin waves and Schwinger bosons suggests that the bosonic representation should be well suited to investigate the AF case also. The Hamiltonian is given by

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (3.1)$$

where $J > 0$. In terms of the Schwinger bosons the above Hamiltonian can be written as

$$H = -2J \sum_{\langle i,j \rangle} A_{ij}^\dagger A_{ij} + \frac{NzJ}{2} S^2, \quad (3.2)$$

where $A_{ij}^\dagger = \frac{1}{2} \sum_{\sigma} \sigma b_{i\sigma}^\dagger b_{j-\sigma}^\dagger$. We will assume that the lattice is bipartite allowing us to make the transformation $b_{j\uparrow} \rightarrow -b_{j\downarrow}$, $b_{j\downarrow} \rightarrow b_{j\uparrow}$, i.e., $S_j^\pm \rightarrow -S_j^\mp$ and $S_j^z \rightarrow -S_j^z$ for sites on one sublattice, say, B . We will denote the transformed bosons by $\tilde{b}_{i\sigma}$. (Note that $A_{ij}^\dagger \rightarrow \tilde{A}_{ij}^\dagger = \frac{1}{2} \sum_{\sigma} \tilde{b}_{i\sigma}^\dagger \tilde{b}_{j\sigma}^\dagger$ if $j \in$ sublattice B .) The constraints on the bosons given by Eq. (2.3) remain unaltered. As in Sec. II we introduce a Lagrange multiplier (chemical potential) λ to impose the constraint on the average, i.e., we ignore the nonzero wavelength components of the constraint. Performing a Hartree-Fock decomposition of the Hamiltonian leads to the following mean-field Hamiltonian:

$$H_{\text{MF}} = E_0 + \lambda \sum_{i,\sigma} \tilde{b}_{i\sigma}^\dagger \tilde{b}_{i\sigma} - 2J\tilde{A} \sum_{\langle i,j \rangle} (\tilde{A}_{ij}^\dagger + \tilde{A}_{ij}), \quad (3.3)$$

where $E_0 = \frac{1}{2} NzJS^2 - 2\lambda NS + J\tilde{A}^2 Nz$, and we have made a specific ansatz for the mean-field amplitude $\langle \tilde{A}_{ij} \rangle = \langle \tilde{A}_{ij}^\dagger \rangle = \tilde{A}$, a real number. A nonzero value for the mean-field amplitude \tilde{A} indicates *short-range* antiferromagnetic order.

In momentum space the mean-field Hamiltonian becomes

$$H_{\text{MF}} = E_0 + \lambda \sum_{\mathbf{k},\sigma} \tilde{b}_{\mathbf{k}\sigma}^\dagger \tilde{b}_{\mathbf{k}\sigma} - \frac{J\tilde{A}z}{2} \sum_{\mathbf{k},\sigma} \gamma_{\mathbf{k}} (\tilde{b}_{\mathbf{k}\sigma}^\dagger \tilde{b}_{-\mathbf{k}\sigma}^\dagger + \text{H.c.}), \quad (3.4)$$

where

$$\gamma_{\mathbf{k}} \equiv \frac{1}{z} \sum_{\delta} e^{i\mathbf{k} \cdot \delta} = 1 - \epsilon_{\mathbf{k}}. \quad (3.5)$$

It is straightforward to diagonalize H_{MF} in Eq. (3.4) using a standard Bogoliubov transformation,

$$\tilde{b}_{\mathbf{k}\uparrow} = \cosh\theta_{\mathbf{k}} \alpha_{\mathbf{k}} + \sinh\theta_{\mathbf{k}} \alpha_{-\mathbf{k}}^\dagger,$$

$$\tilde{b}_{\mathbf{k}\downarrow} = \cosh\theta_{\mathbf{k}} \beta_{\mathbf{k}} + \sinh\theta_{\mathbf{k}} \beta_{-\mathbf{k}}^\dagger,$$

where $\tanh 2\theta_{\mathbf{k}} = J\tilde{A}z\gamma_{\mathbf{k}}/\lambda$. This yields,

$$H_{\text{MF}} = E_0 - \lambda N + \sum_{\mathbf{k}} \omega_{\mathbf{k}} (\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} + 1), \quad (3.6)$$

where

$$\omega_{\mathbf{k}} = [\lambda^2 - (J\tilde{A}z\gamma_{\mathbf{k}})^2]^{1/2} \quad (3.7)$$

specifies the dispersion relation for the Schwinger boson quasiparticles and N is the number of lattice sites.

The self-consistent equations for the chemical potential λ and the mean-field amplitude \tilde{A} can be derived as before and are given by

$$S + \frac{1}{2} = \frac{1}{N} \sum_{\mathbf{k}} \frac{\mu}{(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\beta(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right] \quad (3.8)$$

and

$$\tilde{A} = \frac{1}{N} \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2}{(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\beta(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right], \quad (3.9)$$

where we have defined $\mu \equiv \lambda/(J\tilde{A}z)$ and $\tilde{\beta} \equiv J\tilde{A}z/(k_B T)$. We note that in addition to Eq. (3.9), there is a trivial solution $\tilde{A} = 0$.

Equations (3.8) and (3.9) become identical to those obtained by Auerbach and Arovas from the functional integral method when the sums over \mathbf{k} are converted into integrals over the first Brillouin zone of the reciprocal lattice. Their results at low temperature, for $d=1,2$ are summarized below. First, note that since $\gamma_{\mathbf{k}}^2 \leq 1$, we must have $\mu \geq 1$. If $\mu = 1$ then there is no gap, the gap being given by $(\mu^2 - 1)^{1/2}$. For $d=1$ there is a solution to the equations even at $T=0$ for all S . This means that the ground state is disordered, in contrast to the ferromagnetic case in qualitative agreement with the Bethe-ansatz solution for $S = \frac{1}{2}$. Furthermore, there is a gap in the excitation spectrum which behaves for large S as $\sim Se^{-\pi S}$,

again in qualitative agreement with the Haldane prediction¹⁴ $\sim S^2 e^{-\pi S}$ for integer spins; however, the theory cannot distinguish between integral and half-odd-integral spins and does not predict gaplessness which occurs generically for half-integral spins. In two dimensions, there exists a solution for $T > 0$ so that the system is disordered at finite temperatures. However, unlike the $d = 1$ case, there is no solution at $T = 0$ for any $S > 0.2$. This implies that the system possesses Néel order at $T = 0$. The excitation spectrum for $d = 2$ dimensions is gapless, the gap vanishing as $\sim e^{-4\pi S^2/T}$ as $T \rightarrow 0$.

For $d > 2$, there exists a critical temperature T_N such that there is no solution to the mean-field equations for $T < T_N \neq 0$ again suggesting that Néel order sets in at T_N . For $T > T_N$ the chemical potential $\mu > 1$ so that there is a finite gap in the spectrum. As T approaches T_N from above $\mu \rightarrow 1$ and the gap vanishes at $T = T_N$. The Néel temperature is thus determined by setting $\mu = 1$ in Eqs. (3.8) and (3.9) and converting the sums into integrals over the first Brillouin zone of the reciprocal lattice:

$$S + \frac{1}{2} = \int \frac{d^d k}{(2\pi)^d} \frac{1}{(1 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\tilde{\beta}_c (1 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right], \quad (3.10)$$

$$\tilde{A}_c = \int \frac{d^d k}{(2\pi)^d} \frac{\gamma_{\mathbf{k}}^2}{(1 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\tilde{\beta}_c (1 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right]. \quad (3.11)$$

For large S an approximate analytic expression for the Néel temperature can be obtained in three dimensions by using the Hubbard density of states

$$\rho(\gamma) = \frac{4}{\pi} (1 - \gamma^2)^{1/2}$$

with $0 < \gamma < 1$ and making a high-temperature expansion on the right-hand side. This gives

$$\tilde{A}_c = \frac{S}{2} + \frac{1}{4} - \frac{1}{3\pi}, \quad S + \frac{1}{2} \simeq \frac{2}{\pi} + \frac{2}{\tilde{\beta}_c}$$

from which we obtain

$$\frac{kT_c}{zJ} \simeq \frac{1}{4} \left[S + \frac{1}{2} - \frac{2}{3\pi} \right] \left[S + \frac{1}{2} - \frac{2}{\pi} \right] \simeq \frac{1}{4} S^2.$$

Since T_c scales with S^2 the high-temperature expansion is valid. (In $d = 3$ dimensions, this yields $k_B T_c / J \approx 1.5 S^2$, which agrees with the numerical estimate $k_B T_c / J \approx 1.45 S^2$.)

B. Critical behavior as $T \rightarrow T_N^+$

We now show that although the structure of Eqs. (3.8) and (3.9) is different from that of the corresponding equations for the ferromagnetic case, the critical properties are the same. This is to be expected for bipartite lattices. We convert the sums into integrals to facilitate analysis. The critical behavior is determined by the values of the integrands for γ close to 1, i.e., $\varepsilon = 1 - \gamma$ close to zero.

Expanding the denominator in Eq. (3.8) we find that the integral behaves as

$$\int d\varepsilon \varepsilon^{d/2-1} \left[\frac{1}{\tilde{\Lambda} + 2\varepsilon} \frac{1}{\tilde{\beta}} + \frac{1}{2} \frac{1}{\sqrt{\tilde{\Lambda} + 2\varepsilon}} \right], \quad (3.12)$$

where we have defined $\tilde{\Lambda} = \mu^2 - 1$. An analysis similar to that in the ferromagnetic case yields (for $4 > d > 2$)

$$\tilde{\beta}_c - \tilde{\beta} \simeq \text{const} \times \left[\frac{1}{\tilde{\beta}} \tilde{\Lambda}^{d/2-1} + \frac{1}{2} \tilde{\Lambda}^{d/2-1/2} \right], \quad (3.13)$$

where the second term which corresponds to the second term in Eq. (3.12) is of higher order in $\tilde{\Lambda}$ and can be dropped. Note that this is identical to the result in Eq. (2.20) for the ferromagnetic case. Similarly we find, $\tilde{A}_c - \tilde{A} \simeq \text{const} \Lambda^{d/2-1}$. These results give $\tilde{A}_c - \tilde{A} \sim t$ and $\tilde{\Lambda} \sim t^{2/(d-2)}$ [see Eq. (2.21)]. Therefore, the ferromagnetic and the antiferromagnetic models have the same critical properties.

C. Ordered region: Bose condensation

Below T_N there is no solution to Eq. (3.8) without Bose condensation. The nature of the condensate is somewhat different in the antiferromagnetic case. Because of the anomalous coupling the spectrum only on γ^2 . The condensation occurs in three dimensions at $\mathbf{k} = (0, 0, 0)$ and $\mathbf{k} = (\pi, \pi, \pi)$ mode simultaneously, corresponding to $\gamma = \pm 1$. Precisely at T_N , the chemical potential μ approaches unity and then sticks at this value for all $T < T_N$. Separating the $\gamma = \pm 1$ term in Eq. (3.8) we see that the condensate density is given by

$$\rho = \frac{2}{N\tilde{\Lambda}^{1/2}} \left[\frac{1}{e^{\tilde{\beta}\tilde{\Lambda}^{1/2}} - 1} + \frac{1}{2} \right], \quad (3.14)$$

where, as before, $\tilde{\Lambda} = \mu^2 - 1$. For ρ to be finite we must have $\tilde{\Lambda} = 2/\rho N\tilde{\beta} + O(1/N^2)$. Since $N\tilde{\Lambda}^{1/2} \rightarrow \infty$ in this limit we can drop the second term in Eq. (3.14). For $T < T_N$ Eqs. (3.8) and (3.9) can be written as

$$S + \frac{1}{2} = \rho + \int \frac{d^d k}{(2\pi)^d} \frac{1}{(1 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\tilde{\beta}(1 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right], \quad (3.15)$$

$$A = \rho + \int \frac{d^d k}{(2\pi)^d} \frac{\gamma_{\mathbf{k}}^2}{(1 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\tilde{\beta}(1 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right]. \quad (3.16)$$

For fixed $\tilde{\beta}$ Eq. (3.15) determines the condensate density ρ . We now show that ρ is the sublattice magnetization by considering the spin-spin correlation function:

$$\langle S^x(0) S^x(\mathbf{R}) \rangle = \frac{1}{2} |f(\mathbf{R})|^2 - \frac{1}{2} |g(\mathbf{R})|^2, \quad (3.17)$$

where

$$f(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\mu e^{i\mathbf{k} \cdot \mathbf{R}}}{(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} \left[\frac{1}{e^{\tilde{\beta}(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right]$$

and

$$g(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} e^{i\mathbf{k} \cdot \mathbf{R}} \left[\frac{1}{e^{\beta(\mu^2 - \gamma_{\mathbf{k}}^2)^{1/2}} - 1} + \frac{1}{2} \right].$$

It can be shown that $f(\mathbf{R})$ vanishes for \mathbf{R} odd and $g(\mathbf{R})$ vanishes for \mathbf{R} even. As $\mathbf{R} \rightarrow \infty$, $f(\mathbf{R}) \rightarrow \rho$ for \mathbf{R} even and $g(\mathbf{R}) \rightarrow \rho$ for \mathbf{R} odd. Hence, $\langle S^x(0)S^x(\mathbf{R}) \rangle = \pm \rho^2$ as \mathbf{R} goes to infinity. Therefore, ρ is the sublattice magnetization m_s .

Equations (3.15) and (3.16) correspond to (interacting) spin waves in the ordered region. In particular, the spectrum is gapless and behaves as $\sim k$ at small \mathbf{k} . At $T=0$ we have

$$m_s = S + \frac{1}{2} - \frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \frac{1}{(1 - \gamma_{\mathbf{k}}^2)^{1/2}}. \quad (3.18)$$

At $d=2$ dimensions, $m_s \simeq S - 0.2$. Of course, the system is only ordered at $T=0$. For $d > 2$, elementary power counting at low temperatures leads to the standard spin-wave result:

$$m_s(T) = m_s(0) - \text{const} \times T^{d-1}. \quad (3.19)$$

IV. CONCLUDING REMARKS

In summary, we have extended the bosonic mean-field theory of Arovav and Auerbach for the ferromagnetic and antiferromagnetic Heisenberg models to the ordered regime. We have shown that the condensation of Schwinger bosons corresponds to broken rotational symmetry and can be interpreted as signaling ferromagnetic or antiferromagnetic ordering. In the low-temperature region spin-wave results are reproduced. However, the free energy and the susceptibility are off by factors of 2 and $\frac{2}{3}$. The critical exponents have been obtained and are related to those of a classical spherical model. The critical properties are, not surprisingly, quantitatively inaccurate. Our paper provides a simple derivation of the results which allows a straightforward extension to more complex models. We also note that unlike in many other slave-boson approaches to many-body problems, we have provided a simple and appealing physical interpretation to Bose condensation in these models.

We finally discuss the fact that the Bose condensation is not real although the associated magnetic transitions

are. The Heisenberg Hamiltonian in the bosonic representation has a local gauge invariance, under the transformation $b_{i\mu} \rightarrow b_{i\mu} e^{i\theta_i}$ (θ_i must be the same for up- and down-spin bosons). Our choice of the mean-field amplitudes and the Bose condensation violate this invariance. However, the mean-field free energy is invariant under gauge transformations of the mean-field amplitudes of the form $A_{ij} \rightarrow A_{ij} e^{i(\theta_i + \theta_j)}$ and $B_{ij} \rightarrow B_{ij} e^{i(\theta_i - \theta_j)}$. If one were to average over all these (physically equivalent) gauge-related choices for the amplitudes, non-gauge-invariant quantities would have vanishing expectation values (in agreement with Elitzur's theorem¹⁵). In contrast, physical quantities, such as spin-spin correlations, etc., are gauge invariant, and have the same value for all these gauge-related choices for the mean-field amplitudes. Hence, we believe that conclusions drawn about physical quantities, using a particular choice of gauge for the mean-field amplitudes, are valid in general. The local gauge invariance is intimately tied to the existence of a local constraint $\sum_{\sigma} b_{i\sigma}^{\dagger} b_{i\sigma} = 1$ at each site i . We have imposed the constraint only on the average, thus violating the local gauge invariance. Could imposing the constraint exactly yield results completely at variance with those obtained within the mean-field theory? We note that the Hamiltonian preserves the local constraint and does not connect sectors of the Hilbert space with different values of $\sum_{\sigma} b_{i\sigma}^{\dagger} b_{i\sigma}$. Hence, one expects that the exact ground state with the local constraints satisfied can be projected out of the (presumably multiply degenerate) ground state in the space in which no constraints are imposed; if the mean-field ground state approximates the latter ground state reasonably well, then the physics predicted by the approximation should be good. Indeed, the results are encouraging. However, the approximation does fail to obtain the asymptotic low-temperature results exactly, even though the temperature dependences are correct.

ACKNOWLEDGMENTS

C.J. and H.R.K. acknowledge financial support from the National Science Foundation (Grant No. NSF-DMR-845-1911). The research of H.R.K. and S.S. was supported in part by a grant from U.S. Department of Energy (Division of Materials Research of the office of Basic Energy Sciences).

¹P. W. Anderson, *Science* **235**, 1196 (1987).

²D. P. Arovav and A. Auerbach, *Phys. Rev. B* **38**, 316 (1988).

³M. Takahashi, *Phys. Rev. Lett.* **58**, 168 (1987).

⁴S. Chakravarty, B. I. Halperin, and D. R. Nelson, *Phys. Rev. Lett.* **60**, 1057 (1988).

⁵D. A. Huse and V. Elser, *Phys. Rev. Lett.* **60**, 2531 (1988); D. A. Huse, *Phys. Rev. B* **37**, 2380 (1988); J. D. Reger and A. P. Young, *ibid.* **37**, 5978 (1988).

⁶G. Shirane, Y. Endoh, R. J. Birgeneau, M. A. Kastner, Y. Hidaka, M. Oda, M. Suzuki, and T. Muramaki, *Phys. Rev. Lett.* **59**, 1613 (1987).

⁷A. Aharony, R. J. Birgeneau, A. Coniglio, M. A. Kastner, and

H. E. Stanley, *Phys. Rev. Lett.* **60**, 1330 (1988).

⁸See, for example, D. C. Mattis, *Theory of Magnetism I* (Springer-Verlag, Berlin, 1981).

⁹A. Auerbach and D. P. Arovav, *Phys. Rev. Lett.* **61**, 617 (1988).

¹⁰C. Jayaprakash, H. R. Krishnamurthy, and Sanjoy Sarker (unpublished).

¹¹R. P. Feynman, *Statistical Mechanics* (Benjamin, Reading, 1972).

¹²It must also be stressed that although the number of independent Bose variables is one per site in the Takahashi theory the problem of the constraints is not solved completely since the constraints require that average number of bosons be less

than $2S$ at every site. The mean-field theory allows for any number of bosons to be at a given site as long as the total is fixed. At higher and higher temperatures the theory cannot be valid since more and more of the unphysical part of the

Hilbert space will be included in the partition function.
¹³P. W. Anderson, Phys. Rev. **86**, 694 (1952).
¹⁴F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
¹⁵S. Elitzur, Phys. Rev. D **12**, 3978 (1975).