Functional integral theories of low-dimensional quantum Heisenberg models

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(Received 25 January 1988)

We investigate the low-temperature properties of the quantum Heisenberg models, both ferromagnetic and antiferromagnetic, in one and two dimensions. We study two different large-N formulations, using Schwinger bosons and $S = \frac{1}{2}$ fermions, and solve for their low-order thermodynamic properties. Comparison with exact solutions in one dimension demonstrates the applicability of this expansion to the physical models at $N = 2$. For the square lattice, we find at the mean-field level a low-temperature correlation length which behaves as $\xi \propto \exp(A/T)$, where A asymptotically approaches $2\pi S^2$ for large spin S, but $A_{S=1/2} \simeq 1.16$ and $A_{S=1} \simeq 5.46$. We mention the relevance of our results to recent experiments in La_2CuO_4.

I. INTRODUCTION

Methods of functional integration have recently been applied to many problems involving strongly interacting quantum systems. In particular, "auxilliary-boson" formalisms in conjunction with $1/N$ expansions have met with much success in describing the strong coupling limits of the Kondo impurity,[1] Anderson lattice,[2,3] and Hubbard[4] models. These theories provide simple and intuitive mean-field descriptions of the excitations and are exact in the limit of large quasiparticle degeneracy N (the number of "flavors"). They also yield systematic approximations (the $1/N$ expansion) to thermodynamic coefficients and finite-temperature dynamical response functions in cases where perturbation theory is not applicable. Since the models of physical interest are primarily those with $N = 2$, the question of validity of low-order calculations has to be addressed by comparing results with those of any available exact solutions.

In this paper, we shall employ analogous methods to investigate the properties of low-dimensional ($d = 1, 2$) Heisenberg models. While the ground state of the quantum ferromagnet is ordered, the Mermin-Wagner theorem guarantees that there is no order at finite temperature for either the quantum ferromagnet (FM) or the quantum antiferromagnet (AFM) in dimensions one and two. Naive spin-wave theory, an expansion in Holstein-Primakoff (HP) bosons about an ordered state, thus leads to divergences and gives limited information. Recently, Takahashi[5,6] has described a theory of low-dimensional ferromagnets using a variational density matrix approach in which the Mermin-Wagner theorem is enforced by hand (e.g., the mean density of HP bosons is fixed at S). Operators such as

$$S^+ = h^\dagger (2S - h^\dagger h)^{1/2}$$

are expanded in $h^\dagger h/2S$, and only quartic terms are kept in the HP representation of $S_i \cdot S_j$. The excellent agreement he obtains with thermodynamic Bethe ansatz results is astonishing because the constraint guarantees that $\langle h^\dagger h/2S \rangle = \frac{1}{2}$, which hardly justifies truncation of the aforementioned expansion. In deriving Takahashi's equations from a large-N expansion, we therefore systematize his approximation and help explain its apparent success.

The physics of one-dimensional antiferromagnetic quantum spin chains is largely understood, much due to the work Haldane,[7,8] and Affleck,[9] who derived an effective field theory for the low-energy sector of the Heisenberg system. The excitation spectrum of integer spin chains is predicted to exhibit a gap, and the ground-state correlation functions should decay exponentially at large distances. The half-odd-integer chains are predicted[10,11] to be gapless and to possess algebraically ($\sim n^{-1}$) decaying correlations; this behavior is typified by that of the $S = \frac{1}{2}$ chain, which has been exactly solved using Bethe's ansatz.[12] The thermodynamic properties of the two classes of systems will differ accordingly. The physics behind the Haldane predictions lies in a mapping to the continuum field theory of the $(1+1)$-dimensional nonlinear σ model. Lorentz invariance of the field theory relates the excitation gap to the correlation length in the ground state of the one-dimensional theory. Though this mapping is valid only for asymptotically large values of the spin S, numerical and experimental work[13] suggests that the essential differences between the integer and half-odd-integer chains (e.g., massless versus massive spectra) survive even for small values of S. However, quantitative analytical predictions regarding the properties of the (nonintegrable) small-S models are still lacking.[14]

The two-dimensional quantum Heisenberg model has received considerable attention in recent literature, perhaps due to the advent of high-temperature superconductivity in the compounds $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-\delta}$. La_2CuO_4, which is thought to be an $S = \frac{1}{2}$ antiferromagnet, has been shown to evidence long-ranged

two-dimensional antiferromagnetic correlations; similar observations have been made on the spin-1 system La_2NiO_4.[15] The continuum-limit mapping relates the (large-S) two-dimensional quantum Heisenberg antiferromagnet to the classical three-dimensional nonlinear σ model. The transition temperature of the classical model reflects on a zero-temperature transition as a function of a parameter which is proportional to both $1/S$ and presumably to frustration in some manner. It is therefore not known whether or not the standard $S = \frac{1}{2}$ model on a square lattice is ordered at $T = 0$, although numerical work suggests that it is ordered.[16] In case it is not, the continuum limit has to be taken more carefully, as demonstrated in one dimension, where topological terms alter the behavior of the classical model. In particular, at present it is not known whether the antiferromagnetic integer and half-odd-integer spin models in two (space) dimensions differ qualitatively as they do in one dimension. This question happens to be intimately connected with the resonating valence bond (RVB) description of superconductivity.[17]

Here we investigate the quantum Heisenberg model by using second quantized bosonic and fermionic representations of the spin algebra. In Sec. II, the Hamiltonian is generalized to that of an SU(N)-invariant model, for which there exists a parameter $1/N$ that controls the expansion around the mean field ($N = \infty$) saddle point. Since the physically interesting limit is at $N = 2$, it is important to assess the significance of the higher-order terms in this expansion by comparing our low-order results to available known solutions. We believe that our formalism is quite powerful in that it leads to simple yet nontrivial approximations for many models of physical interest (e.g., the $S = \frac{1}{2}$ square lattice antiferromagnet).

For the ferromagnetic (FM) chain, our Schwinger boson theory (Sec. III) describes the thermally disordered phase in satisfactory agreement with thermodynamic Bethe Ansatz results for the specific heat and susceptibility. We emphasize that the entropy is overcounted at the mean-field level and we show that the Gaussian fluctuations partially remedy this artifact of the static constraint. We find results similar to those of Takahashi's theory. However, unlike the Takahashi approach, the Schwinger bosons provide a manifestly rotationally invariant theory of the excitations.

For the antiferromagnetic (AFM) chain, the bosonic mean-field theory yields a disordered ground state with the correct size of the Haldane gap for large integer spin S, as given by the renormalization group treatment of the nonlinear sigma model. Half-odd-integer spins are *not* represented correctly by the bosonic large-N limit, since their ground states are known to be at least quasidegenerate. The analogous fermionic mean-field theory for $S = \frac{1}{2}$ was discussed by Baskaran, Zou, and Anderson (BZA) for both one- and two-dimensional systems, and was generalized to large N by Affleck and Marston.[18] It captures some of the essential physics missed by the boson theory in one dimension. The Fermi liquid behavior of the BZA theory is studied in relation to the Bethe Ansatz solution, and the fluctuation corrections, calculated in Appendix B, are shown to be important in enforcing

the Gutzwiller projection. We discuss the fermionic large-N theory in Sec. IV.

In two dimensions, the BZA mean-field theory is unstable toward a novel flux phase discussed by Affleck and Marston,[18] whereas the bosonic theory exhibits Néel order at $T = 0$ even for $S = \frac{1}{2}$. We compute the free energy and spin correlation functions for both cases and mention why our bosonic mean-field results are compatible with recent experiments on La_2CuO_4.

II. SU(N) HEISENBERG MODELS, FUNCTIONAL INTEGRALS, AND THE $1/N$ EXPANSION

The standard SU(2) Heisenberg model is described by the Hamiltonian

$$H = \pm \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad \mathbf{S}^2 = S(S+1) \tag{2.1}$$

where the sum is over all (nearest-neighbor) *bonds* in a lattice, and where the $\pm$ sign is adjusted to describe antiferromagnetic or ferromagnetic coupling. Throughout this paper, we use the Heisenberg exchange constant J as the unit of energy; magnetic field strength is given in terms of J/μ_B. This model may be extended to one with an SU(N) symmetry. The parameter N appears as an overall prefactor in the functional integral action, and systematic corrections to the mean-field theory may be cast in the form of a $1/N$ expansion.

A. The case of the ferromagnet

The Heisenberg $\mathbf{S}_i \cdot \mathbf{S}_j$ interaction may be written as a biquadratic form in terms of the Schwinger boson operators (see Appendix A):

$$\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2} \mathcal{F}_{ij}^\dagger \mathcal{F}_{ij} - S(S+1)$$

$$= \frac{1}{2} : \mathcal{F}_{ij}^\dagger \mathcal{F}_{ij} : -S^2 , \tag{2.2}$$

$$\mathcal{F}_{ij} \equiv (a_i^\dagger a_j + b_i^\dagger b_j) ,$$

with $a_n^\dagger a_n + b_n^\dagger b_n = 2S$ for all sites n, and where $:\mathcal{O}:$ is a normal ordered operator in which annihilation operators are moved to the right. The SU(N) generalization of the Schwinger boson algebra involves N bosons per site $b_{\alpha i}$, where α is an SU(N) index and i is a site index. The generators of the algebra are given by the composite operators

$$\mathcal{S}_\beta^\alpha(i) \equiv b_{\alpha i}^\dagger b_{\beta i} , \tag{2.3}$$

which satisfy the algebra

$$[\mathcal{S}_\beta^\alpha(i), \mathcal{S}_\sigma^\rho(j)] = \delta_\beta^\rho \delta_j^i \mathcal{S}_\sigma^\alpha(i) - \delta_\sigma^\alpha \delta_j^i \mathcal{S}_\beta^\rho(i) \tag{2.4}$$

and are subject to the constraint $\sum_{\alpha=1}^N \mathcal{S}_\alpha^\alpha(i) = NS$; S must be an integer multiple of $1/N$. The generalized Hamiltonian is given by

$$H_F = -\frac{1}{N} \sum_{\substack{\langle i,j \rangle \\ \alpha,\beta}} \mathcal{S}_\beta^\alpha(i) \mathcal{S}_\alpha^\beta(j)$$

$$= -\frac{1}{N} \sum_{\langle i,j \rangle} : \mathcal{F}_{ij}^\dagger \mathcal{F}_{ij} : ,$$

$$\mathcal{F}_{ij} \equiv \sum_\alpha b_{\alpha i}^\dagger b_{\alpha j} . \tag{2.5}$$

Apart from a constant reference energy per site $E_{ref}/\mathcal{N} = \frac{1}{2}zS^2$, the $N = 2$ version of this model reduces to the SU(2) model defined in Eq. (2.2). Note that the *local* SU(N) transformation $b_{\alpha i} \to U^{(i)}_{\alpha\beta} b_{\beta i}$ amounts to a unitary transformation of H, and that H is manifestly invariant under global unitary transformations.

B. The case of the antiferromagnet

For the antiferromagnet, we write

$$\mathbf{S}_i \cdot \mathbf{S}_j = -\tfrac{1}{2}\mathcal{A}^\dagger_{ij}\mathcal{A}_{ij} + S^2 \ ,$$
$$\mathcal{A}_{ij} \equiv a_i b_j - b_i a_j \ ,$$
(2.6)

again with constrained total bose occupation $n_a + n_b = 2S$ at every site. In this case, the interaction is already normal ordered. We now assume that the lattice $\mathcal{L}$ is bipartite and that there is thus no frustration. On one sublattice, we make the unitary transformation $a \to -b$, $b \to a$, i.e., $S^+ = -ab^\dagger$, etc. This effectively decouples the SU(2) indices, sending $\mathcal{A}_{ij} \to a_i a_j + b_i b_j$.

In the SU(N) language, this amounts to defining matrices $\mathcal{S}^\alpha_\beta = b^\dagger_\alpha b_\beta$ generating the fundamental representation on one sublattice, and matrices $\bar{\mathcal{S}}^\alpha_\beta = -b^\dagger_\beta b_\alpha$ generating the conjugate representation on the other sublattice.[19] The generalized Hamiltonian is then

$$H_A = -\frac{1}{N} \sum_{\substack{\langle i,j \rangle \\ \alpha,\beta}} \mathcal{S}^\alpha_\beta(i)\bar{\mathcal{S}}^\beta_\alpha(j)$$

$$= -\frac{1}{N} \sum_{\langle i,j \rangle} :\mathcal{A}^\dagger_{ij}\mathcal{A}_{ij}: \ ,$$

$$\mathcal{A}_{ij} \equiv \sum_\alpha b_{\alpha i} b_{\alpha j} \ ,$$
(2.7)

where in each bond $\langle i,j \rangle$ the site j is taken to be in the second sublattice. As before, we enforce $\sum_{\alpha=1}^N \mathcal{S}^\alpha_\alpha(i) = NS$. When $N = 2$, Eq. (2.7) gives the usual antiferromagnetic Heisenberg Hamiltonian up to the constant E_{ref}. We stress that the resulting Hamiltonian is *not* invariant under a global SU(N) transformation U, but by alternately rotating by U and $U^\dagger$ on different sublattices.

C. Fermion large-N theory for the $S = \frac{1}{2}$ antiferromagnet

Affleck and Marston[18,20] have recently formulated a fermion large-N expansion for the $S = \frac{1}{2}$ antiferromagnet. Writing the Heisenberg interaction as

$$\mathbf{S}_i \cdot \mathbf{S}_j = \tfrac{1}{4} - \tfrac{1}{2}\mathcal{D}^\dagger_{ij}\mathcal{D}_{ij} \ ,$$
$$\mathcal{D}_{ij} = c^\dagger_{i\uparrow}c_{j\uparrow} + c^\dagger_{i\downarrow}c_{j\downarrow} \ .$$
(2.8)

[This decomposition into composite operators $\mathcal{D}_{ij}$ is equivalent to the Baskaran-Zou-Anderson[17] (BZA) resonating valence bond (RVB) decoupling.] One now defines the generalized spin operators

$$\mathcal{S}^\alpha_\beta(i) \equiv c^\dagger_{\alpha i} c_{\beta i} \ ,$$
(2.9)

where α is an SU(N) index; these operators obey the commutation relations of Eq. (2.4). The constraint on the fermion occupation is

$$\sum_{\alpha=1}^N c^\dagger_{\alpha i} c_{\alpha i} = \tfrac{1}{2}N$$
(2.10)

and thus we must take N to be even. The Hamiltonian for the SU(N) model takes the now-familiar form

$$H_{S=1/2} = +\frac{1}{N} \sum_{\substack{\langle i,j \rangle \\ \alpha,\beta}} \mathcal{S}^\alpha_\beta(i)\mathcal{S}^\beta_\alpha(j)$$

$$= -\frac{1}{N} \sum_{\langle i,j \rangle} :\mathcal{D}^\dagger_{ij}\mathcal{D}_{ij}: \ ,$$

$$\mathcal{D}_{ij} \equiv \sum_\alpha c^\dagger_{\alpha i} c_{\alpha j} \ ;$$
(2.11)

apart from the constant term E_{ref}, the $N = 2$ Hamiltonian is that of the $S = \frac{1}{2}$ antiferromagnetic Heisenberg model.

D. Path integral formulation

Each of the above SU(N) models possesses a Hamiltonian of the form

$$H = -\frac{1}{N} \sum_{\langle i,j \rangle} :Z^\dagger_{ij}Z_{ij}: \ ,$$
(2.12)

where Z_{ij} is a composite operator, cf. Eqs. (2.5), (2.7), and (2.11). The partition function is given by the coherent state functional integral:

$$Z = \int \mathcal{D}[a,\bar{a};\lambda]\exp(-\mathcal{J}[a,\bar{a};\lambda]) \equiv \exp(-\mathcal{N}\beta F) \ ,$$

$$\mathcal{J} = \int_0^\beta d\tau \left[\tfrac{1}{2}\sum_{i,\alpha}(\bar{a}_{\alpha i}\dot{a}_{\alpha i} - \dot{\bar{a}}_{\alpha i}a_{\alpha i}) - \frac{1}{N}\sum_{\langle i,j \rangle}\bar{Z}_{ij}Z_{ij} \right.$$
$$\left. + \sum_{i,\alpha}\lambda_i(\bar{a}_{\alpha i}a_{\alpha i} - S) \right] \ ,$$
(2.13)

where $a_{\alpha i}(\tau)$ is a complex or Grassmann field, depending on the model of interest, $\bar{a}_{\alpha i}(\tau)$ it its complex conjugate, N is the number of flavors, and $\mathcal{N}$ is the number of spins in the lattice. The λ_i integral proceeds along the imaginary axis from $-i\infty$ to $+i\infty$.[21] Introducing a complex Hubbard-Stratonovich field Q_{ij} for every bond, the biquadratic interaction term may be decoupled, resulting in

$$Z[j] = \int \mathcal{D}[a,\bar{a};Q,\bar{Q};\lambda]e^{-\mathcal{J}_0 - \mathcal{J}_{source}} \ ,$$

$$\mathcal{J}_0 = \int_0^\beta d\tau \left[\tfrac{1}{2}\sum_{i,\alpha}(\bar{a}_{\alpha i}\dot{a}_{\alpha i} - \dot{\bar{a}}_{\alpha i}a_{\alpha i}) + N\sum_{\langle i,j \rangle}\bar{Q}_{ij}Q_{ij} + \sum_{\langle i,j \rangle}(\bar{Q}_{ij}Z_{ij} + Q_{ij}\bar{Z}_{ij}) + \sum_{i,\alpha}\lambda_i(\bar{a}_{\alpha i}a_{\alpha i} - S) \right] \ ,$$
(2.14)

$$\mathcal{J}_{source} = j\sum_{\substack{\langle i,j \rangle \\ \alpha,\beta}} \int\int_0^\beta d\tau\, d\tau'\, V_{\alpha\beta}(i\tau \mid j\tau')\bar{a}_{\alpha i}(\tau)a_{\beta j}(\tau') \ .$$

We have included a source current j and source vertices $V_{\alpha\beta}(i\tau \mid j\tau')$; functional differentiation with respect to the source j yields correlation functions and generalized susceptibilities. Unless explicitly stated otherwise, we shall henceforth drop the reference energy E_{ref} from all expressions.

At this point, the $a_{\alpha i}(\tau)$ fields may be formally integrated out (the action is a quadratic form in these variables), yielding

$$Z[j] = \int \mathcal{D}[Q, \bar{Q}; \lambda] \exp(-N\mathscr{S}[Q, \bar{Q}; \lambda; j]) . \quad (2.15)$$

We apply the standard procedure of evaluating Eq. (2.15) by the method of steepest descents. Since N is scaled out of the action, this procedure generates an expansion in $1/N$. Nondegenerate saddle points of higher action and endpoint contributions associated with the periodicity $\lambda_i \rightarrow \lambda_i + 2\pi i/\beta$ yield subdominant contributions that are not perturbatively accessible by this expansion.[3] The saddle point of Z is given by the mean-field equations

$$\frac{\delta\mathscr{S}}{\delta Q_{ij}(\tau)} = \frac{\delta\mathscr{S}}{\delta\bar{Q}_{ij}(\tau)} = \frac{\delta\mathscr{S}}{\lambda_i(\tau)} = 0 , \quad (2.16)$$

which defines the mean-field configurations $Q_{ij}^{\mathrm{MF}}(\tau)$ and $\lambda_i^{\mathrm{MF}}(\tau)$. At the saddle point, these fields are in general time independent, spatially uniform, and real. (In the case of the fermionic $S = \frac{1}{2}$ theory, however, the lowest energy mean-field configuration found is the Affleck-Marston configuration, in which the phases of the Q_{ij} fields posses a simple spatial variation.[18]) Since the mean-field free energy is left unaffected by a uniform phase change of the form $Q_{ij} \rightarrow e^{i\phi}Q_{ij}$, Gaussian fluctuations in this phase will lead to infrared divergences in the leading order corrections to the mean-field theory. In one dimension, these zero modes can be eliminated by a time-dependent Read-Newns gauge transformation,[1]

$$Q_{n,n+1} \equiv |Q_{n,n+1}| e^{i\theta_{n,n+1}} ,$$

$$\tilde{\theta}_n \equiv \sum_{k(<n)} \theta_{k,k+1} , \quad (2.17)$$

$$a_{\alpha i} \rightarrow e^{i\tilde{\theta}_i} a_{\alpha i}, \quad \lambda_i \rightarrow \lambda_i + i\frac{\partial\tilde{\theta}_i}{\partial\tau} ,$$

which effectively replaces the Q_{ij} integration by an integration over only the magnitude $|Q_{ij}|$.

The accuracy of the mean-field theory is dictated by the largeness of N; Gaussian intergration of the fluctuations in the Q_{ij} and λ_i fields in Eq. (2.15) yield expressions which are higher order in $1/N$, generating the expansion

$$\frac{1}{N}F = F^{\mathrm{MF}} - F^{(1/N)} + O(N^{-2}) . \quad (2.18)$$

The mean-field free energy F^{MF} is that of a *single flavor* gas of quasiparticles with dispersion $\varepsilon_k(Q, \lambda)$ which is readily obtained from the diagonalization of the quadratic Lagrangian in Eq. (2.14), using the static values of the Bose fields Q and λ. $O(1/N)$ corrections to the mean-field free energy are given by the fluctuations in these fields, which have an RPA form:

$$F^{(1/N)} = (2N\beta)^{-1} \mathrm{Tr}\,\ln D(q) ,$$
$$\quad _q$$
$$D_{rr'}(q) \equiv \left[\frac{\delta^2\mathscr{S}}{\delta r_q \delta r'_{-q}} \right]^{-1} . \quad (2.19)$$

The trace takes over bosonic Matsubara energy-momentum vectors q, and the three boson indices are defined by $r = \mathrm{Re}Q$, $\mathrm{Im}Q$, and λ. (For generality we assume that the phase of Q cannot be eliminated.) Positivity of the matrix D is necessary to ensure stability of the mean-field theory.

The leading order general correlation function $\mathcal{X}$ is given by functionally differentiating the source-dependent free energy, where the source vertices are not necessarily the same for j and j':

$$\mathcal{X} \equiv -\frac{\delta^2 F}{\delta j \delta j'}$$
$$= \mathcal{X}^{\mathrm{MF}} - \frac{1}{\beta}\Lambda^\dagger D\Lambda + \mathcal{X}^{(1/N)} + O(N^{-2}), \quad \Lambda \equiv \frac{\delta^2\mathscr{S}}{\delta j \delta r} . \quad (2.20)$$

$\mathcal{X}^{\mathrm{MF}}$ is the susceptibility of the N-degenerate free gas described by the mean-field theory. In general, however, the correct leading order susceptibility must include the second term in Eq. (2.20) which depends on the functions Λ. In fact, such terms occur at every order in the $1/N$ expansion, and serve to correct the susceptibility in an important way. It is easy to see that this term exactly cancels the mean-field charge susceptibility when j couples to the local charge, say, as

$$V_{\alpha\beta}(i\tau \mid j\tau') = \delta_{ij}\delta_{\alpha\beta}\delta(\tau - \tau')`,$$

while for the spin susceptibility

$$V_{\alpha\beta}(i\tau \mid j\tau') = gS_{\alpha\beta}^z \delta(\tau - \tau') ,$$

Λ vanishes and the mean-field result holds to leading order. (Here, g is the Landé factor.) The last term $\mathcal{X}^{(1/N)}$ is the $1/N$ correction which is given by

$$\mathcal{X}^{(1/N)} = -\frac{\delta^2 F^{(1/N)}[j]}{\delta j \delta j'} . \quad (2.21)$$

Diagrammatically, the terms in Eq. (2.20) are the familiar low-order bubble diagrams with self-energy insertions and vertex corrections. In Fig. 1 we show all the terms contributing to the charge and spin susceptibility, where solid lines represent mean-field Green functions and wiggly lines represent Bose propagators $D_{rr'}$.
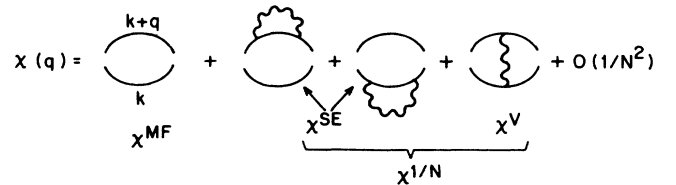

FIG. 1. Diagrammatic representation of the $1/N$ expansion of the spin susceptibility. Solid lines denote mean-field Green functions, while wiggly lines denote boson propagators. $\mathcal{X}^{(1/N)}$ is the $O(1/N)$ correction of Eq. (B11).

III. BOSON LARGE-N THEORY OF THE FERROMAGNET

The ferromagnetic partition function is given by Eqs. (2.2) and (2.13):

$$Z_F = \int \mathcal{D}[b,\bar{b};Q,\bar{Q};\lambda]\exp(-\mathscr{A}_F[b,\bar{b};Q,\bar{Q};\lambda]) \ ,$$

$$\mathscr{A}_F = \int_0^\beta d\tau \left[\frac{1}{2}\sum_{i,\alpha}(\bar{b}_{\alpha i}\dot{b}_{\alpha i} - \dot{\bar{b}}_{\alpha i}b_{\alpha i}) + N\sum_{\langle i,j\rangle}\bar{Q}_{ij}Q_{ij} + \sum_{\substack{\langle i,j\rangle\\\alpha}}(\bar{Q}_{ij}\bar{b}_{\alpha i}b_{\alpha j} + Q_{ij}b_{\alpha i}\bar{b}_{\alpha j}) + \sum_{i,\alpha}\lambda_i(\bar{b}_{\alpha i}b_{\alpha i}-S) \right] \ . \tag{3.1}$$

Making the static assumption

$$Q_{ij}^{\text{MF}}(\tau)=Q, \quad \lambda_i^{\text{MF}}(\tau)=\lambda \ , \tag{3.2}$$

the Schwinger bosons can be integrated out explicitly, resulting in a free energy of

$$F^{\text{MF}} = \frac{1}{2}zQ^2 - S\lambda + \frac{1}{\beta}\int\frac{d^dk}{(2\pi)^d}\ln(1-e^{-\beta\omega_k}) \ , \tag{3.3}$$

where z is the lattice coordination number, d is the number of spatial dimensions, $\mathcal{N}$ is the total number of sites in the lattice, and the integral is performed over the first Brillouin zone. The dispersion ω_k is defined by

$$\mu \equiv \lambda - zQ \ ,$$

$$\varepsilon_k \equiv \frac{1}{z}\sum_\delta (1-e^{ik\cdot\delta}) \ , \tag{3.4}$$

$$\omega_k \equiv \mu + zQ\varepsilon_k \ .$$

The saddle point equations $\delta F/\delta Q = 0$ and $\delta F/\delta \lambda = 0$ are then

$$S = \int\frac{d^dk}{(2\pi)^d}n_k \ , \tag{3.5a}$$

$$Q = S - \int\frac{d^dk}{(2\pi)^d}\varepsilon_k n_k \ , \tag{3.5b}$$

with $n_k = (e^{\beta\omega_k}-1)^{-1}$. Thus, we obtain a free energy per spin of

$$F^{\text{MF}} = -\frac{1}{2}zS^2 + \frac{1}{2}z(Q-S)^2$$

$$-S\mu - \frac{1}{\beta}\int\frac{d^dk}{(2\pi)^d}\ln(1+n_k) \ . \tag{3.6}$$

Upon addition of the reference energy $+\frac{1}{2}zS^2$, and taking $N=2$, the first term gives the classical ferromagnetic ground-state energy per spin, $E_0^{\text{cl}} = -\frac{1}{2}zS^2$. We note that the remaining contribution is precisely *twice* Takahashi's result for $F - E_0^{\text{cl}}$.[22] This factor of 2 is easily seen to be an artifact of the static constraint and is a generic consequence of approximations of this sort. The SU(N) theory is defined in terms of N bosons and 1 constraint (per site). Uniformizing the field λ amounts to ignoring the nonzero wavelength components of the constraint field, enforcing the local restriction $\sum_\alpha b_\alpha^\dagger b_\alpha = NS$ only on average, cf. Eq. (3.5a). Thus, at the mean-field level, the number of independent degrees of freedom is overcounted by a factor $g = N/(N-1)$. This is partially corrected by the $O(1/N)$ contribution $F^{(1/N)}$ arising from integration over the Gaussian fluctuations of the constraint field, as we

shall soon see.

The mean-field equations which determine $Q(T,S)$ and $\mu(T,S)$ are identical to those of Takahashi, and we have independently verified his solutions (details may be found in Ref. 6). From Eq. (3.6), we obtain for the one-dimensional chain

$$(F^{\text{MF}} - E_0^{\text{MF}})_{\text{chain}} = -T\left[\frac{\zeta(\frac{3}{2})}{\sqrt{2\pi}}\left[\frac{T}{2S}\right]^{1/2}\right.$$

$$\left. -\frac{1}{2S}\left[\frac{T}{2S}\right] + O(T^{3/2})\right] \ . \tag{3.7}$$

where $E_0^{\text{MF}} \equiv F^{\text{MF}}$ ($T=0$), which is an expansion in the quantity T/S, assumed here to be small. The calculation of $F^{(1/N)}$ is carried out in Appendix B, where it is found [Eq. (B9)]:

$$F^{(1/N)} = -\frac{1}{N}\frac{\zeta(\frac{3}{2})}{\sqrt{\pi S}}T^{3/2} + O(T^{5/2}) \ . \tag{3.8}$$

Combinging Eqs. (3.7) and (3.8) and setting $N=2$ yields, to $O(1/N)$,

$$(F - E_0^{\text{MF}}) = 2(F^{\text{MF}} - E_0^{\text{MF}} - F^{(1/N)})$$

$$= -\frac{\zeta(\frac{3}{2})}{\sqrt{2\pi}}\left[\frac{T}{2S}\right]^{3/2} + \frac{T^2}{2S^2} + O(T^{5/2}) \ . \tag{3.9}$$

Comparing our expression with that of Takahashi, we see that our coefficient of the $O(T^2)$ term is a factor of 2 too large. The Takahashi result is in remarkable agreement with thermodynamic Bethe ansatz results for $S=\frac{1}{2}$. One unfortunate aspect of Takahashi's variational density matrix is that it is not rotationally invariant, and therefore the longitudinal and transverse susceptibilities in his model will be unequal. Takahashi calculates the static susceptibility

$$\chi = g^2\beta\frac{1}{\mathcal{N}}\sum_{i,j}\langle S_i^z S_j^z\rangle \tag{3.10}$$

by performing a rotational average of $\langle(S_i\cdot\hat{n})(S_j\cdot\hat{n})\rangle$ and finds the corresponding result to be in good agreement with known $S=\frac{1}{2}$ results. That this rotational averaging produces the "correct" result is interesting, although we wish to emphasize that Takahashi's underlying theory is not rotationally invariant. Our model preserves rotational invariance, and we find

$$\chi_{\text{chain}}=\tfrac{1}{2}g^2\int_{-\pi}^{\pi}\frac{dk}{2\pi}n_k(1+n_k)$$

$$=g^2S^4T^{-2}\left[1-\frac{3}{S}\frac{\zeta(\tfrac{3}{2})}{\sqrt{2\pi}}\left[\frac{T}{2S}\right]^{1/2}+O(T)\right]\quad(3.11)$$

which is $\tfrac{3}{2}$ as great as Takahashi's result. For the two-dimensional square lattice, we find

$$(F^{\text{MF}}-E_0^{\text{MF}})_{\text{sq}}=-\tfrac{1}{2}T^2\left[\frac{\zeta(2)}{2\pi S}+\frac{\zeta(3)}{8\pi S}\left[\frac{T}{2S}\right]\right.$$

$$\left.+O(T^2)\right],\quad(3.12)$$

$$\chi_{\text{sq}}=\frac{g^2}{8\pi S}\exp\left[\frac{4\pi S^2}{T}\right]+O(Te^{4\pi S^2/T})\ .$$

The spin-spin correlation function is

$$\langle\mathbf{S}_0\cdot\mathbf{S}_R\rangle=\tfrac{3}{2}|f(\mathbf{R})|^2\ ,$$

$$f(\mathbf{R})\equiv\int\frac{d^dk}{(2\pi)^d}e^{i\mathbf{k}\cdot\mathbf{R}}n_k\ .\quad(3.13)$$

At long distances, one is concerned with the small-k behavior of the occupation function n_k, and we obtain the following asymptotic expressions:

$$\langle\mathbf{S}_0\cdot\mathbf{S}_R\rangle\simeq\tfrac{3}{2}S^2e^{-R/\xi},\quad\xi\simeq S^2/T\quad(d=1)\ ,$$

$$\langle\mathbf{S}_0\cdot\mathbf{S}_R\rangle\simeq\frac{3T^2}{8\pi S^2}\frac{e^{-R/\xi}}{(R/\xi)}\ ,\quad(3.14)$$

$$\xi\simeq\sqrt{S/T}\exp(2\pi S^2/T)\quad(d=2,\text{square})\ .$$

As discussed in Ref. 6, Eq. (3.14) differs only in its prefactor from the Ornstein-Zernike correlation function expected for the two-dimensional *classical* Heisenberg model. However, as in the case of the Kondo lattice, there will be $O(1/N)$ corrections to the prefactor, and the disagreement with σ-model results stressed by Takahashi is likely only an artifact.[23]

IV. FERMION LARGE-N THEORY OF THE $S=\tfrac{1}{2}$ ANTIFERROMAGNET

The fermionic functional integral for the partition function in the $s=\tfrac{1}{2}$ case is given by Eqs. (2.11) and (2.13):

$$Z_{S=1/2}=\int\mathcal{D}[c,\bar{c};Q,\bar{Q};\lambda]\exp(-\mathcal{A}_{S=1/2}[c,\bar{c};Q,\bar{Q};\lambda])\ ,$$

$$\mathcal{A}_{S=1/2}=\int_0^\beta d\tau\left[\tfrac{1}{2}\sum_{i,\alpha}(\bar{c}_{\alpha i}\dot{c}_{\alpha i}-\dot{\bar{c}}_{\alpha i}c_{\alpha i})+N\sum_{\langle i,j\rangle}\bar{Q}_{ij}Q_{ij}+\sum_{\substack{\langle i,j\rangle\\\alpha}}(\bar{Q}_{ij}\bar{c}_{\alpha i}c_{\alpha j}+Q_{ij}\bar{c}_{\alpha j}c_{\alpha i})+\sum_{i,\alpha}\lambda_i(\bar{c}_{\alpha i}c_{\alpha i}-\tfrac{1}{2})\right]\ .\quad(4.1)$$

At the saddle point, the mean-field theory is that of a half-filled tight-binding model,

$$H^{\text{MF}}=\tfrac{1}{2}\mathcal{N}Nz\,|Q|^2-\tfrac{1}{2}\mathcal{N}N\lambda+\lambda\sum_{i,m}c_{im}^\dagger c_{im}$$

$$+|Q|\sum_{\substack{\langle i,j\rangle\\m}}(t_{ij}c_{im}^\dagger c_{jm}+\text{H.c.})\ ,\quad(4.2)$$

where we have assumed spatial uniformity of λ_i and of $|Q_{ij}|$, but not necessarily of the phases $t_{ij}\equiv Q_{ij}/|Q_{ij}|$. [We have also changed notation slightly, letting the flavor index be the magnetic quantum number m, which runs from $-\tfrac{1}{2}(N-1)$ to $+\tfrac{1}{2}(N-1)$.]

A. $d=1$: The linear chain

In one dimension, the phase t_{ij} may be absorbed into the Fermi fields via the Read-Newns transformation of Eq. (2.17). The free energy (per flavor per site) is then given by

$$F^{\text{MF}}=Q^2-\tfrac{1}{2}\lambda-\frac{1}{\beta}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\ln(1+e^{-\beta\omega_k})\ ,\quad(4.3)$$

where $\omega_k=\lambda+2Q\cos k$. The mean-field equations are

$$\lambda=0\ ,$$

$$Q=\frac{1}{\pi}-\int_0^{\pi/2}\frac{dk}{\pi}(\cos k)\operatorname{sech}^2(\beta Q\cos k)\quad(4.4)$$

$$=\frac{1}{\pi}-\frac{\pi}{2}(\ln 2)T^2+\cdots\ .$$

(Using the unimodular decomposition for the $N=2$ model, described in Appendix C, the value of $|Q|$ is fixed at $Q_{\text{um}}=1/\sqrt{2}$. We shall comment on the significance of this later on.) The leading-order values of the specific-heat linear coefficient γ^{MF}, the $T=0$ susceptibility χ_0^{MF}, and spin correlation functions are those of a noninteracting, N-flavored, half-filled cosine band:

$$\gamma^{\text{MF}}=\frac{N\pi}{6Q},\quad\chi_0^{\text{MF}}=\frac{N(N^2-1)g^2\mu^2}{24\pi Q}\ ,$$

$$S^{\text{MF}}(q)=\left[\sum_m m^2\right]\sum_k f_k(1-f_{k+q})$$

$$=\frac{N(N^2-1)}{12}\frac{|q|}{2\pi}\ ,\quad(4.5)$$

$$\langle S_0^z S_n^z\rangle^{\text{MF}}=\int_{-\pi}^{\pi}\frac{dk}{2\pi}e^{-iqn}S(q)$$

$$=\frac{N(N^2-1)}{12}\left[\delta_{n,0}-\frac{(1-e^{i\pi n})}{2n^2}\right]\ ,$$

where $f_k=(e^{\beta\omega_k}+1)^{-1}$ is the Fermi function.

This mean-field theory captures some (but not all) of the essential low-temperature properties of the exactly soluble $N=2$ model. It has been pointed out by Anderson that although strictly speaking this system is not a Fermi liquid (since there is a gap for charge excitations), it might be described as a limit of a Fermi liquid with $F_0^s\to\infty$, where F_0^s is the compressibility Landau parameter. This was motivated by the observation that the

Bethe solution exhibit the Fermi liquid signatures of a linear specific heat,[24] $C \approx 0.7T$, and finite Pauli-like paramagnetism[25] at $T = 0$, $X_0 \approx g^2/\pi^2$. In addition, the gapless des Cloiseaux-Pearson excitations[26] described by $\omega_k = \pi/2 \, | \sin k \, |$ are suggestive of particle-hole excitations about a "pseudo-Fermi-surface" at $k = \pi/2$, termed "spinons" in the RVB theory. Additional support for the validity of this picture is given by the success of the Gutzwiller wave function, which is the image of a half-filled tight-binding Fermi gas under a projection operator which eliminates all configurations with any doubly occupied sites. Numerical and analytical treatments of the Gutzillwer approximation for the strong coupling,[27] half-filled Hubbard model (which maps into the $S = \frac{1}{2}$ Heisenberg antiferromagnet) have reproduced the correct power-law decay of the spin-spin correlations in one dimension. The close analogy between the $1/N$ expansion and the Gutzwiller approximation has been explored in the Kondo lattice[2] and the Hubbard[4] models.

The mean-field theory has therefore the correct temperature dependence of the specific heat and susceptibility. It is interesting to study the discrepancies between the known coefficients and correlations and those obtained from Eq. (4.5) by setting $N = 2$. This comparison gives us a valuable opportunity to study the effects due to higher order corrections that are not calculable. The "Wilson ratio" between X and γ is defined as

$$R = \frac{4\pi^2}{g^2(N^2 - 1)} \frac{X}{\gamma} \tag{4.6}$$

and is unity for the mean-field values, while the exact solution gives $R \simeq 2$. This situation is analogous to that encountered in the $1/N$ expansion of the Kondo problem, where gaussian fluctuations correct R by $1/N$, changing its value from 1 to $\frac{3}{2}$ when $N = 2$. If the expansion is well behaved, R can be expressed as a power series in $1/N$ which presumably adds up to the correct result. Based on intuition garnered in the Kondo problem,[1] a Wilson ratio of 2 is expected in a Fermi liquid with one channel for energy excitations and two for spin excitations.

An important effect of the Gutzwiller projection—one that is not reflected at the mean-field level—is the logarithmic divergence of the structure factor $S(q)$ at the zone edge. Gebhard and Vollhardt[27] have found

$$S^{\text{Gutz.}}(q) = -\frac{1}{4(1 - g^2)} \ln \left[1 - (1 - g^2) \frac{|q|}{\pi} \right] , \tag{4.7}$$

where g is the Gutzwiller correlation parameter. For $g = 0$, Eq. (4.7) agrees remarkably well with numerical results and properly describes the asymptotic power-law decay of $\langle S_0^z S_n^z \rangle \sim e^{i\pi n}/|n|$. By contrast, the mean-field result of $S(q) = |q|/4\pi$, obtained from Eq. (4.7) with $g \to 1$, yields an inverse square decay for the correlation function, cf. Eq. (4.5). The "total-moment" sum rule for $N = 2$,

$$\sum_q S(q) = \frac{1}{3} S(S + 1) = \frac{1}{4} , \tag{4.8}$$

is also not satisfied at the mean-field level, at which the sum is $\frac{1}{8}$. In Appendix B we calculate the first correc-

tions to this sum rule, and adding them to the mean-field result we find

$$\sum_q [S^{\text{MF}}(q) + S^{(1/N)}(q) + O(N^{-2})]$$

$$= \frac{1}{8} \left[1 + \frac{1}{N} + O(N^{-2}) \right] . \tag{4.9}$$

The indication given by this calculation is that the $g = 0$ Gutzwiller projection is approximately enforced by the Gaussian fluctuations of the constraint fields which are represented by an exchange of the propagator $D_{\lambda\lambda}$. As for the Wilson ratio, we note that an extrapolation Eq. (4.9) as a geometric series in $1/N$ yields the correct result of Eq. (4.8). One additional question is that of the actual energy scale of the excitations. Using the mean-field result $Q = 1/\pi$, we find that the $T = 0$ susceptibility is $\pi^2/4 \simeq 2.47$ times higher than the exact result. This is because the exact des Cloiseaux-Pearson bandwidth is a factor $\pi^2/4$ greater than the mean-field value.[28] If, on the other hand, we use the unimodular decomposition of Appendix B (which does *not* yield a $1/N$ expansion), for which $Q_{\text{um}} = 1/\sqrt{2}$, the ratio of bandwidths is $W_{\text{exact}}/W_{\text{um}} = \pi/2\sqrt{2} \simeq 1.11$. The unimodular mean-field theory gives a more accurate result in this case because it circumvents the need to sum over fluctuations in the Q field which introduce corrections to the mean-field theory.

The finite temperature spin-spin correlations at the mean-field level are given by

$$\langle S_0^z S_n^z \rangle \propto n^{-2} \exp(-|n|/\xi), \quad \xi(T) = 2Q/T . \tag{4.10}$$

The finite correlation length is a consequence of the thermal smearing of the Fermi surface.

B. $d = 2$: The square lattice

In one dimension, a position-independent λ_i leads to a stable mean-field solution, i.e., the fluctuation propagator is positive definite. The phase of the bond fields can be absorbed into the fermion fields via a Read-Newns gauge transformation. In two dimensions, on the square lattice, for example, there are two bonds per site and the phase of the bond fields cannot be gauged away. At the saddle point, these phases are time independent, but may not be spatially uniform. These phases resemble Peierls phase factors in tight-binding lattice models in the presence of a magnetic field. One may associate a "flux" to each plaquetter p according to

$$\phi_p \equiv \text{Im} \ln \prod_{\langle i,j \rangle \in p} Q_{ij} , \tag{4.11}$$

where the product is over all bonds bordering the plaquette p. As emphasized by Affleck and Marston (AM),[18] there are many different but gauge-equivalent configurations for the Q_{ij} phases which result in the same set of fluxes $\{\phi_p\}$. One simple configuration discussed by AM is a "flux phase" one in which the phases of all $\hat{y}$-directed bonds are set to 1, while $\hat{x}$-directed bonds are assigned a phase $e^{\mp i\varphi}$ according to whether the "hopping" is from sublattice A to sublattice B or vice versa.[29] The

mean-field Hamiltonian is

$$H^{MF} = 2N\mathcal{N}Q^2 - \tfrac{1}{2}N\mathcal{N}\lambda$$

$$+ \sum_{k,m}{}' (E_k^+ \psi_{km+}^\dagger \psi_{km+} + E_k^- \psi_{km-}^\dagger \psi_{km-}) ,$$

$$E_k^\pm \equiv \lambda \pm Q \mid t_k \mid , \qquad (4.12)$$

$$t_k \equiv 2(\cos k_y + e^{i\varphi}\cos k_x) ,$$

where the prime on the sum denotes that the sum is over the "little zone," which is a square defined by the vertices $k = (0, \pm\pi)$, $(\pm\pi, 0)$, half as large as the original zone. The free energy is

$$F^{MF} = 2Q^2 - \tfrac{1}{2}\lambda$$

$$- \frac{1}{2\beta} \int \frac{d^2k}{(2\pi)^2} [\ln(1 + e^{-\beta E_k^+}) + \ln(1 + e^{-\beta E_k^-})] ,$$

$$(4.13)$$

where the integral is over the entire Brillouin zone. It is easy to prove that the mean-field free energy is minimized for $\varphi = \pi/2$, i.e., the BZA uniform bond phase mean-field theory[17] is unstable toward the flux phase. Mattis[30] has also given arguments for the instability of the former phase. The mean-field equations as $\varphi = \pi/2$ are

$$\lambda = 0 ,$$

$$Q = \frac{2\sqrt{2}}{\pi^2} \int_0^1 dy\, y^2 K[2y(1-y^2)^{1/2}]\tanh(\sqrt{2}\beta Qy) , \qquad (4.14)$$

with $Q\mid_{T=0} \simeq 0.479$. $K(x)$ is the complete elliptic integral of the first kind. The ground-state energy for large N is thus $E_0^{MF} = -2NQ^2 = -0.458N$.

The crucial difference between the two phases lies in the quasiparticle properties. The uniform bond mean-field theory possesses a two-dimensional band structure with logarithmically diverging density of states at the corners of the square Fermi surface defined by $\cos k_x + \cos k_y = 0$. This leads to a specific heat $C \propto -T\ln T$ and a susceptibility $X \propto \ln T$. The correlations develop an algebraic R^{-4} decay at $T = 0$ (see Ap-
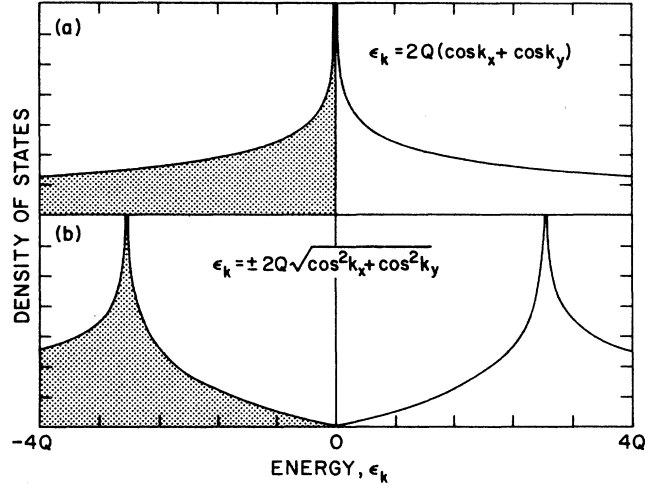

FIG. 2. (a) Density of states for the BZA mean-field theory of the two-dimensional square lattice $S = \tfrac{1}{2}$ antiferromagnet. (b) Density of states in Affleck-Marston flux phase. A comparison demonstrates that the BZA mean-field theory is unstable: Its filled states (shaded) are concentrated at relatively high energies.

pendix D). The flux phase, by contrast, has only four Fermi "points" at $k = (\pm\pi/2, \pm\pi/2)$, where the density of states vanishes linearly. The density of states in the uniform bond phase and the flux phase are plotted in Fig. 2. Therefore, one finds $C \propto T^2$ and $X \propto T$. In addition, the structure factor $S(q)$ is nondivergent as $T \to 0$, reflecting no transition to long-ranged order, with algebraically decaying spin-spin correlations. Experiments[31] on La$_2$CuO$_4$ seem to be inconsistent with this phase since an apparent divergence of the structure factor at the zone edge is seen with decreasing temperature.

V. BOSON LARGE-N THEORY OF THE ANTIFERROMAGNET

The bosonic partition function for the spin-S Heisenberg antiferromagnet is given by Eqs. (2.7) and (2.13):

$$Z_A = \int \mathcal{D}[b,\bar{b};Q,\bar{Q};\lambda]\exp(-\mathcal{A}_A[b,\bar{b};Q,\bar{Q};\lambda])$$

$$\mathcal{A}_A = \int_0^\beta d\tau \left[\tfrac{1}{2}\sum_{i,\alpha}(\bar{b}_{\alpha i}\dot{b}_{\alpha i} - \dot{\bar{b}}_{\alpha i}b_{\alpha i}) + N\sum_{\langle i,j\rangle}\bar{Q}_{ij}Q_{ij} + \sum_{\substack{\langle i,j\rangle \\ \alpha}}(\bar{Q}_{ij}b_{\alpha i}b_{\alpha j} + Q_{ij}\bar{b}_{\alpha i}\bar{b}_{\alpha j}) + \sum_{i,\alpha}\lambda_i(\bar{b}_{\alpha i}b_{\alpha i} - S) \right] . \qquad (5.1)$$

We assume that the bond amplitudes are uniform, and a generalized AM configuration for the phases t_δ (δ is a nearest-neighbor vector).

The mean-field Hamiltonian is then

$$H^{MF} = \tfrac{1}{2}\mathcal{N}NzQ^2 - \mathcal{N}NS\lambda$$

$$+ \tfrac{1}{2}\sum_{k,\alpha}[\lambda(a_{k\alpha}^\dagger a_{k\alpha} + a_{-k\alpha}^\dagger a_{-k\alpha})$$

$$+ zQ(\bar{\gamma}_k a_{k\alpha}a_{-k\alpha} + \gamma_k a_{k\alpha}^\dagger a_{-k\alpha}^\dagger)] , \qquad (5.2)$$

with

$$\gamma_k \equiv \frac{1}{z}\sum_\delta t_\delta e^{-i k\cdot\delta} . \qquad (5.3)$$

H^{MF} is brought to diagonal form by a Bogoliubov transformation, and integrating out the Schwinger bosons gives a mean-field free energy of

$$F^{MF} = \tfrac{1}{2}zQ^2 - \tfrac{1}{2}(2S+1)\lambda$$

$$+ \frac{1}{\beta}\int \frac{d^dk}{(2\pi)^d}\ln(2\sinh\tfrac{1}{2}\beta\omega_k) , \tag{5.4}$$

$$\omega_k = (\lambda^2 - z^2Q^2 \mid \gamma_k \mid^2)^{1/2} .$$

The mean-field equations $\delta F^{MF}/\delta Q = 0$ and $\delta F^{MF}/\delta\lambda = 0$ yield

$$\frac{2S+1}{\lambda} = \int \frac{d^dk}{(2\pi)^d}\omega_k^{-1}\coth\tfrac{1}{2}\beta\omega_k , \tag{5.5a}$$

$$\frac{2}{z} = \int \frac{d^dk}{(2\pi)^d}\omega_k^{-1} \mid \gamma_k \mid^2\coth\tfrac{1}{2}\beta\omega_k , \tag{5.5b}$$

where the integrals are over the first Brillouin zone of the reciprocal lattice.

It proves convenient to rescale our parameters $(\lambda, Q, \beta) \to (\Lambda, \eta, \kappa)$ according to

$$\lambda \equiv \tfrac{1}{2}z\Lambda, \quad \beta \equiv 4\kappa/z ,$$

$$Q \equiv \tfrac{1}{2}\Lambda\eta, \quad \omega_k = \tfrac{1}{2}z\Lambda(1-\eta^2\mid\gamma_k\mid^2)^{1/2} . \tag{5.6}$$

In terms of these rescaled quantities, the free energy and mean-field equations are

$$F^{MF} = \tfrac{1}{8}z\Lambda^2\eta^2 - \tfrac{1}{4}z(2S+1)\Lambda$$

$$+ \frac{z}{4}\kappa^{-1}\int \frac{d^dk}{(2\pi)^d}\ln[2\sinh\kappa\Lambda(1-\eta^2\mid\gamma_k\mid^2)^{1/2}] , \tag{5.7a}$$

$$(2S+1) = \int \frac{d^dk}{(2\pi)^d}(1-\eta^2\mid\gamma_k\mid^2)^{-1/2}$$

$$\times\coth\kappa\Lambda(1-\eta^2\mid\gamma_k\mid^2)^{1/2} , \tag{5.7b}$$

$$\Lambda = \int \frac{d^dk}{(2\pi)^d}\mid\gamma_k\mid^2(1-\eta^2\mid\gamma_k\mid^2)^{-1/2}$$

$$\times\coth\kappa\Lambda(1-\eta^2\mid\gamma_k\mid^2)^{1/2} . \tag{5.7c}$$

A. $d=1$: The linear chain at $T=0$

We first employ the Read-Newns transformation to eliminate the bond phases. At $T=0$, the mean-field equations may be evaluated in terms of known functions:

$$F^{MF}(\Lambda, \eta, 0) = \tfrac{1}{4}\Lambda^2\eta^2 - (S+\tfrac{1}{2})\Lambda + \frac{\Lambda}{\pi}E(\eta) , \tag{5.8a}$$

$$(2S+1) = \frac{2}{\pi}K(\eta) , \tag{5.8b}$$

$$\Lambda\eta^2 = (2S+1) - \frac{2}{\pi}E(\eta) , \tag{5.8c}$$

where $K(\eta)$ and $E(\eta)$ are the complete elliptic integrals of the first and second kind, and $f = F^{MF}/\mathcal{N}$. Since $K(\eta) \geq \pi/2$, the mean-field equations possess a solution for all S. The excitation energy

$$\omega_k = \Lambda(1-\eta^2\cos^2 k)^{1/2}$$

indicates a gap of $\Delta = \Lambda(1-\eta^2)^{1/2}$. For large S, we may use the asymptotic relations

$$K(\eta) = \ln\frac{4}{(1-\eta^2)^{1/2}} + \tfrac{1}{4}(1-\eta^2)$$

$$\times\left[\ln\frac{4}{(1-\eta^2)^{1/2}} - 1\right] + \cdots , \tag{5.9}$$

$$E(\eta) = 1 + \tfrac{1}{2}(1-\eta^2)\left[\ln\frac{4}{(1-\eta^2)^{1/2}} - \frac{1}{2}\right] + \cdots ,$$

which are valid for $\mid 1-\eta\mid \ll 1$, and obtain (to lowest nontrivial order in $1/S$)

$$\eta = 1 - \frac{8}{e^\pi}\exp(-2\pi S) ,$$

$$\Lambda = 2S+1-\frac{2}{\pi} , \tag{5.10}$$

$$F^{MF}\mid_{T=0} = -S^2 - S\left[1-\frac{2}{\pi}\right] - \frac{1}{4}\left[1-\frac{2}{\pi}\right]^2 .$$

Restoring the reference energy $+S^2$ and taking $N=2$, we find for the Heisenberg model a mean-field ground-state energy of

$$E_0^{MF} = -S^2 - 2S\left[1-\frac{2}{\pi}\right] - \frac{1}{2}\left[1-\frac{2}{\pi}\right]^2 .$$

For reference, naive spin-wave theory gives a ground-state energy of

$$E_0^{SWT} = -S^2 - S\left[1-\frac{2}{\pi}\right] ,$$

which is larger in $O(S)$. The spin-spin correlations in our theory decay exponentially at large distances with a correlation length given by

$$\xi = \eta/[8(1-\eta^2)]^{1/2} \sim \exp(\pi S)$$

(this is discussed below). The gap has the asymptotic form $\Delta \sim S\exp(-\pi S)$, which should be compared with the Haldane result $\Delta \sim S^2\exp(-\pi S)$, obtained from the σ-model mapping.[7] It is remarkable that our simple mean-field theory reproduces the asymptotic S dependence of the Haldane gap. All is not well, however, because our mean-field theory is unable to "see" the topological terms responsible for the gaplessness of all half-odd-integer antiferromagnetic chains. Alternatively stated, the Lieb-Schultz-Mattis theorem,[10] which exploits the differing properties of integer and half-odd-integer spins under SU(2) rotations is violated at the mean-field level, since it requires that all half-odd-integer Heisenberg antiferromagnetic chains must have either degenerate ground states or gapless excitations in the thermodynamic limit. We stress that the bosonic mean-field theory is applicable to any model in which the ground state is ordered.

It is a straightforward task to calculate the staggered susceptibility,

$$\tilde{X} = \frac{g^2}{8\pi\Lambda} \left[\frac{E(\eta)}{(1-\eta^2)} - K(\eta) \right] , \qquad (5.11)$$

which behaves asymptotically as $\tilde{X} \sim S^{-1}\exp(2\pi S)$.

B. $d = 2$: The square lattice

We first consider the mean-field theory in which the bond field is real and uniform throughout the lattice, e.g., $Q_{ij} = |Q|$. The bond phases are thus $t_\delta = 1$, in which case

$$\gamma_{\mathbf{k}} = \tfrac{1}{2}(\cos k_x + \cos k_y) ,$$

for which the density of states is

$$n(\gamma) = \int \frac{d^2k}{(2\pi)^2} \delta(\gamma - \gamma_k)$$

$$= \frac{2}{\pi^2}\Theta(1-\gamma^2)K[(1-\gamma^2)^{1/2}] , \qquad (5.12)$$

where $\Theta(x)$ is a step function and $K(x)$ is the complete elliptic integral. The free-energy and mean-field equations are

$$(2S+1) = I_1(\eta^2, \Upsilon) = \frac{4}{\pi^2} \int_0^1 d\gamma \, K[(1-\gamma^2)^{1/2}](1-\eta^2\gamma^2)^{-1/2}\coth\Upsilon(1-\eta^2\gamma^2)^{1/2} , \qquad (5.13a)$$

$$(2S+1) - \Lambda\eta^2 = I_2(\eta^2, \Upsilon) = \frac{4}{\pi^2} \int_0^1 d\gamma \, K[(1-\gamma^2)^{1/2}](1-\eta^2\gamma^2)^{1/2}\coth\Upsilon(1-\eta^2\gamma^2)^{1/2} , \qquad (5.13b)$$

$$F^{\text{MF}}(\Lambda,\eta) = \tfrac{1}{2}\Lambda^2\eta^2 - (2S+1)\Lambda + \frac{\Lambda}{\Upsilon}\frac{4}{\pi^2}\int_0^1 d\gamma \, K[(1-\gamma^2)^{1/2}]\ln[2\sinh\Upsilon(1-\eta^2\gamma^2)^{1/2}] , \qquad (5.13c)$$

with $\Upsilon \equiv \beta\Lambda$. The first of these equations gives $\eta(\Upsilon,S)$. Using this result, the second equation gives $\Lambda(\Upsilon,S)$, and the temperature associated with this solution is then determined by $T = \Lambda/\Upsilon$.

It is easy to see that, unlike the $d = 1$ case, no $T = 0$ solution exists. At $T = 0$, $\Upsilon = \infty$, and the first of the mean-field equations becomes

$$(2S+1) = \frac{4}{\pi^2}\int_0^{\pi/2}dk \, K(\eta\cos k) . \qquad (5.14)$$

Since $K(x)$ is increasing, the right-hand side (rhs) of the above equation is bounded from above by its value at $\eta = 1$, which is

$$4K^2(1/\sqrt{2})/\pi^2 \simeq 1.39 ,$$

which thus rules out any solution with $S \geq 0.2$. We remark that the ground state for $S \geq 1$ on a square lattice has been rigorously shown to display Néel order.[32] The present result suggests that the ground state possesses Néel order for $S = \tfrac{1}{2}$ as well, for a nonsymmetry breaking mean-field solution at $T = 0$ does not exist.

For finite T, the rhs of Eq. (5.13a) is bounded from below by $\coth\Upsilon$, and so no solution exists with

$$\Upsilon < \Upsilon_{\min} = \tfrac{1}{2}\ln(1+S^{-1}) .$$

The following inequalities (which follow from $x^{-1} \leq \coth x \leq 1 + x^{-1}$) will prove useful in our analysis:

$$\frac{2}{\pi}\Upsilon^{-1}K(\eta) \leq I_1(\eta^2,\Upsilon) \leq \frac{2}{\pi}\Upsilon^{-1}K(\eta) + \frac{4}{\pi^2}K^2(1/\sqrt{2}) , \qquad (5.15a)$$

$$\Upsilon^{-1} \leq I_2(\eta^2,\Upsilon) \leq 1 + \Upsilon^{-1} . \qquad (5.15b)$$

When Υ approaches infinity, η^2 tends to one, and for large S the mean-field equations can be solved in asymptotia with the help of Eqs. (5.15a) and (5.15b). We find

$$\Lambda \sim 2S ,$$
$$\eta^2 \sim 1 - 16\exp(-4\pi S^2/T) . \qquad (5.16)$$

When S is not large, the above equations remain qualitatively correct in their temperature dependence, though the numerical values of Λ and the coefficient of $1/T$ in the exponent are different. The most important result here is that there is a temperature-dependent gap which satisfies $\Delta(T) \propto e^{-A/T}$ as $T \to 0$.

In the opposite limit, we write $\Upsilon = \Upsilon_{\min} + d\Upsilon$, $\eta^2 = 0 + d\eta^2$, and thus obtain

$$d\Upsilon/d\eta^2 = -\frac{\partial I_1/\partial\eta^2}{\partial I_1/\partial\Upsilon}$$

$$= \tfrac{1}{8}(\Upsilon_{\min} + \sinh\Upsilon_{\min}\cosh\Upsilon_{\min}) . \qquad (5.17)$$

The equation for Λ then gives $\Lambda = \tfrac{1}{4}\coth\Upsilon_{\min}$, or

$$T_{\max} = \tfrac{1}{4}\Upsilon_{\min}^{-1}\coth\Upsilon_{\min}$$

$$= (S + \tfrac{1}{2})/\ln(1+S^{-1}) . \qquad (5.18)$$

For $S = \tfrac{1}{2}$, $T_{\max} = 1/\ln 3 \simeq 0.91$.

We have found that unlike the case of the fermion large-N theory described in Sec. IV, the *uniform* bond field phase has a lower energy than the corresponding flux phase. For $S = \tfrac{1}{2}$, the $O(N)$ term in the ground-state energy is given by $E_0^{\text{MF}}(\text{Bose}) = -0.671N$, which is lower than the fermionic result $E_0^{\text{MF}}(\text{Fermi}) = -0.458N$ found in Sec. IV. Although this inequality is suggestive, we stress that higher order (in $1/N$) corrections to E_0 have not been evaluated. We plot the mean-field free energy versus temperature for $S = \tfrac{1}{2}$ and $S = 1$ in Fig. 4. If we restore the reference energy of $+\tfrac{1}{2}zS^2$ and restrict ourselves to $N = 2$, then we obtain a mean-field free energy for the SU(2) Heisenberg model of $F^{\text{Heis.}} \equiv 2F^{\text{MF}} + \tfrac{1}{2}zS^2$.

We note that in two dimensions, the gap $\Delta(T)$ satisfies

$T \gg \Delta(T) > 0$ as $T \to 0$. Thus, thermodynamically speaking, at low enough temperatures, the system behaves as if there is no gap, and the free energy behaves as a power law. Although complications in the asymptotic analysis have thus far prevented us from extracting the analytic behavior, numerical differentiation of our results indicates that the specific heat and susceptibility behave as $C_V \sim C_1 T^2$ and $\chi \sim C_2 + C_3 T$ at low temperatures.[33] The correlation length, analyzed below, *does* know about the gap, with $\xi(T) \sim 1/\Delta(T)$.

C. Asymptotic spin-spin correlations

The spin-spin correlation $\langle S_0 \cdot S_R \rangle$ is given by ($R \neq 0$)

$$\langle S_0 \cdot S_R \rangle = \tfrac{3}{2} |f(R)|^2 - \tfrac{3}{2} |g(R)|^2 ,$$

$$f(R) \equiv \tfrac{1}{2} \int \frac{d^d k}{(2\pi)^d} e^{ik \cdot R} \frac{1}{(1-\eta^2 \gamma_k^2)^{1/2}} \coth \tfrac{1}{2}\beta\omega_k , \quad (5.19)$$

$$g(R) \equiv \tfrac{1}{2} \int \frac{d^d k}{(2\pi)^d} e^{ik \cdot R} \frac{\eta\gamma_k}{(1-\eta^2 \gamma_k^2)^{1/2}} \coth \tfrac{1}{2}\beta\omega_k .$$

It is easy to show that $f(R)$ vanishes whenever R is in the odd sublattice and that $g(R)$ vanishes whenever R is in the even sublattice. Thus, the sign of the spin-spin correlation function is always positive on the even sublattice and negative on the odd sublattice, as expected. In one dimension and at $T = 0$, we find

$$\langle S_0 \cdot S_n \rangle \big|_{T=0} \simeq \frac{3}{16\eta^2} e^{-|n|/\xi} , \quad (5.20)$$

with $\xi = \eta/[8(1-\eta^2)]^{1/2}$. In higher dimensions, there is no gap at zero temperature, and the long-distance correlations are dominated by

$$f(R) \simeq \frac{T}{2\Lambda} \int \frac{d^d k}{(2\pi)^d} e^{ik \cdot R} \frac{1}{1-\eta^2 \gamma_k^2} . \quad (5.21)$$

On the square lattice, we obtain

$$\langle S_0 \cdot S_R \rangle \simeq \frac{3}{8\pi} \frac{T^2}{\Lambda^2 \eta^4} \frac{e^{-R/\xi}}{(R/\xi)} , \quad (5.22)$$

again with $\xi = \eta/[8(1-\eta^2)]^{1/2}$. In the limit of large spin S, the results are

$$\xi(0) \simeq \frac{e^{\pi/2}}{16\sqrt{2}} \exp(\pi S), \quad d = 1$$

$$\xi(T) \simeq \frac{W(S)}{8\sqrt{2}} \exp(2\pi S^2/T), \quad d = 2 \quad (5.23)$$

where we have not been able to extract $W(S) \equiv C_1 \exp(C_2 S)$ from our coupled mean-field equations.[34]

In Fig. 3, we plot $T \ln\xi$ vs ξ for the $S = \tfrac{1}{2}$ and $S = 1$ models obtained from numerical solution to our mean-field equations. We find:

$$\xi(T) \big|_{T \to 0} \propto \exp(A/T) , \quad (5.24)$$

with

$$A \simeq 1.16, \quad S = \tfrac{1}{2}$$
$$\qquad\qquad\qquad\qquad (5.25)$$
$$A \simeq 5.46, \quad S = 1$$

As seen from Fig. 3, the quantity $A \equiv T \ln\xi(T)$ is only weakly temperature dependent. Defining the ratio

$$r(S) \equiv A(S)/2\pi S(S+1)$$

of our coefficient of $1/T$ in $\ln\xi$ with the expected σ-model result, we obtain significant renormalization at low values of the spin: $r(\tfrac{1}{2}) \simeq 0.246$ and $r(1) \simeq 0.442$. We stress that these are mean-field results and that $O(1/N)$ corrections due to Gaussian fluctuations will likely further decrease the correlation length, although we have not by any means shown this.
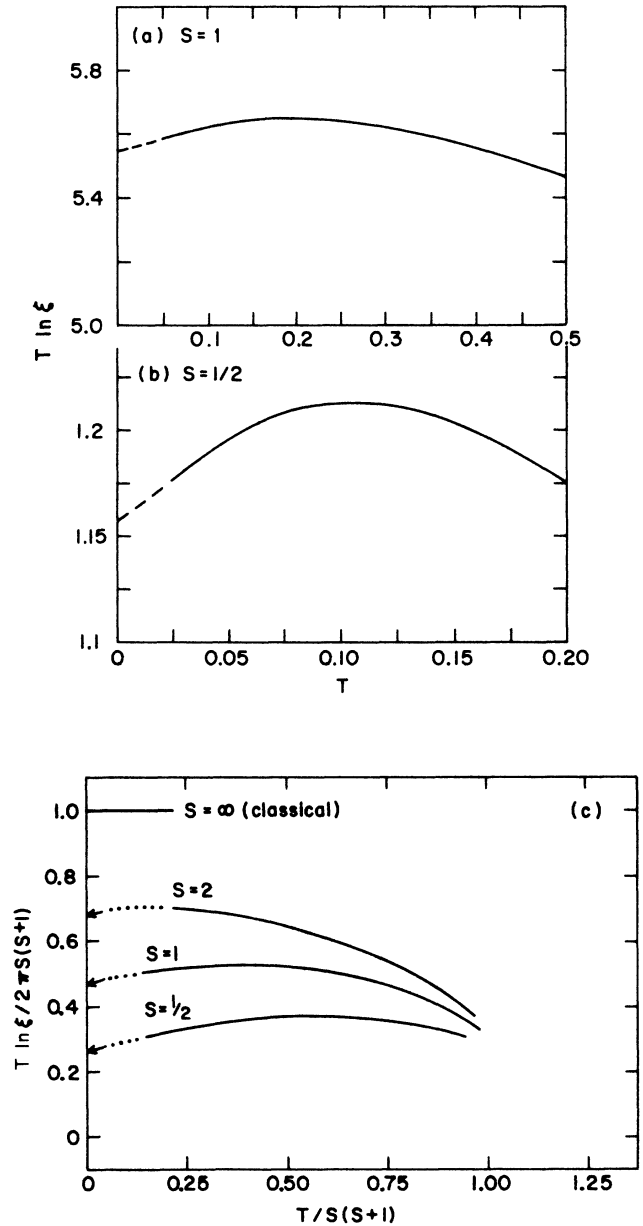

FIG. 3. $T \ln\xi$ vs T for bosonic mean-field theory of square lattice antiferromagnet. (a) $S = \tfrac{1}{2}$; (b) $S = 1$; (c) results scaled by classical expression. Dashed lines indicate extrapolation of numerical results to $T = 0$.

D. $d > 2$: Finite-temperature phase transition

We wish to derive some loose bounds on the region of temperature where our mean-field theory is applicable. For definiteness, we will assume a cubic lattice and uniform ($t_\delta = 1$) phases for the bond field, giving

$$\gamma_{\mathbf{k}} = d^{-1} \sum_{j=1}^{d} \cos k_j$$

and $\kappa = d/2T$ (d is the number of dimensions). From the second of our mean-field equations, Eq. (5.7c), we derive the inequality

$$\frac{1}{2d} \coth \kappa \Lambda \leq \Lambda < (2S + 1) , \qquad (5.26)$$

from which we obtain an upper bound on T:

$$T < \frac{d(2S + 1)}{2 \tanh^{-1}\left[\dfrac{1}{2d(2S + 1)} \right]} \equiv T_+ . \qquad (5.27)$$

As S tends to infinity, we have $T_+ \simeq d^2(2S + 1)^2$.

To derive a lower bound for T, we examine the first of our mean-field equations, Eq. (5.7b), which in conjunction with above results may be massaged to give

$$(2S + 1) < \int \frac{d^d k}{(2\pi)^d} \frac{1}{(1 - \gamma_{\mathbf{k}}^2)^{1/2}} + 4T \int \frac{d^d k}{(2\pi)^d} \frac{1}{(1 - \gamma_{\mathbf{k}}^2)}$$

$$\equiv J_1 + 4J_2 T . \qquad (5.28)$$

For all $d > 2$, the integrals J_1 and J_2 are finite, hence

$$T > \frac{2S + 1 - J_1}{4J_2} \equiv T_- \qquad (5.29)$$

The vanishing of the bandwidth Q at $T \geq T_+$ suggests that the system has entered a local moment phase in which there is no coherence to the spin fluctuations. It seems reasonable that the temperature T_- should be associated with the Néel temperature, since that is also where the correlation length ξ diverges ($\eta \to 1$).

VI. SUMMARY AND CONCLUSIONS

We have generalized the usual SU(2) Heisenberg model to a model with an SU(N) symmetry. The thermodynamics properties and temperature-dependent response functions may then be evaluated using a $1/N$ expansion similar to those formulated for the theory of dilute magnetic alloys and the heavy-fermion problem.[1-3] In the case of the ferromagnet, our saddle point equations are identical to those of Takahashi's constrained spin-wave theory,[5,6] and we obtain the correct temperature dependence of the free energy and susceptibility for the soluble $S = \frac{1}{2}$ chain. For the antiferromagnetic model, our bosonic large-N theory predicts a gap for one-dimensional systems which at the mean-field level tends to zero with increasing values of the spin S as $\Delta_S \propto S \exp(-\pi S)$, in good agreement with the Haldane result $\Delta_S \propto S^2 \exp(-\pi S)$. We note that the bosonic theory is blind to the topological terms responsible for the gaplessness in all half-odd-

integral spin antiferromagnetic chains, and hence violates the Lieb-Schultz-Mattis theorem.[10] The fermionic large-N theory[17,18] for the $S = \frac{1}{2}$ chain does yield a gapless spectrum and a power-law decay of the spin-spin correlations. In two dimensions, the most stable fermionic mean-field theory yet found is the flux phase, which is disordered even at zero temperature. Our bosonic theory predicts a low-temperature correlation length which diverges as $\xi \sim \exp(A/T)$, with $A \simeq 1.16$ for $S = \frac{1}{2}$, and where $A(S \to \infty) \simeq 2\pi S^2$. It also yields a lower mean-field free energy than does the fermionic theory. We have not yet analyzed the temperature dependence of the free energy, although we have provided a plot of our results in Fig. 4 for the cases $S = \frac{1}{2}$ and $S = 1$.

To what extent can one trust the results of the $1/N$ expansion when the physical model lies at $N = 2$? In the case of the ferromagnet, we found that the uniformization of the constraint field λ_i led to a theory with $g = N/(N - 1)$ times as many low-energy excitations as are truly present. At $N = 2$, we therefore found that while the temperature dependence of $F^{MF}(T)$ is correct, the coefficients differ from those of Takahashi by a factor of 2. The $O(1/N)$ corrections to the mean-field theory bring the first of these coefficients in line with the
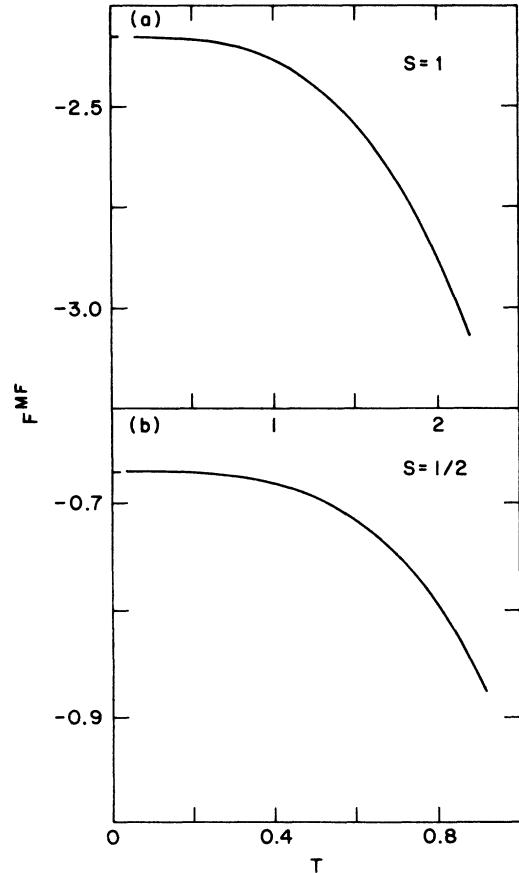

FIG. 4. Free energy per site F^{MF} vs T for the bosonic mean-field theory of the square-lattice antiferromagnet. (a) $S = \frac{1}{2}$; (b) $S = 1$.

Takahashi result; higher-order corrections are in principle calculable, though this is a difficult task. We believe that our mean-field theory is the correct starting point and that the $1/N$ expansion is well behaved. At the very least, we have systematized Takahashi's theory, which we find *ad hoc* as it stands for reasons given in the introduction.

Conventional wisdom has it that if the ground state is *disordered*, subtle topological effects may have profound consequences in the determination of correlations and the excitation spectra. This is true, apparently, in one dimension, where the θ term in the continuum field theory for the Heisenberg antiferromagnet renders the spectrum gapless for S half-odd integral $(\theta = \pi)$, while there is a gap for the integer S $(\theta = 0)$ chains.[7] Concerning the Haldane gap in integer spin antiferromagnetic chains, we obtain $\Delta_{S=1}^{MF} \simeq 0.17$ at the mean-field level, which is almost a factor of 2–3 smaller than current numerical estimates,[13] which give $\Delta_{S=1} \simeq 0.41$. We therefore *overestimate* the $T=0$ correlation length, obtaining $\xi_{S=1}^{MF} \simeq 9.8$, which is to be compared with numerical estimates of $\xi_{S=1} \simeq 5.5$.

There does not exist a unique large-N generalization of the $S = \frac{1}{2}$ Heisenberg model. However, it is our prejudice, based on existing numerical and experimental work,[16,31] that the ground state of the $S = \frac{1}{2}$ Heisenberg antiferromagnet in two dimensions possesses Néel order. Therefore, we suggest that our boson mean-field theory is valid in $d=2$ (for *all* $S > S_c \approx 0.2$), and that the correlation length $\xi_S(T)$ diverges as $\exp(A/T)$. We note that the critical spin S_c is related to the coupling constant and transition temperature of the corresponding *three-dimensional* nonlinear σ model, which is the appropriate continuum theory. Introducing frustration would increase S_c and perhaps allow for a disordered ground state for the $S = \frac{1}{2}$ system.

La_2CuO_4, a sister compound of the high-temperature superconductor $La_{2-x}Sr_xCuO_4$, is believed to behave as an isotropic square lattice $S = \frac{1}{2}$ quantum antiferromagnet above its three-dimensional Néel point 50 K $\lesssim T_N \lesssim 300$ K.[31] Below T_N, a spin-wave velocity of $c \simeq 0.4$ eV Å is measured, implying a coupling $J \simeq 792$ K. At $T=300$ K, we have $T/J \simeq 0.378$, and the mean-field correlation length is $\xi \simeq 35$, in units of the lattice spacing a, a figure which is quite compatible with current experimental estimates. The corresponding σ-model result is

$$\xi \sim \exp[2\pi S(S+1)J/T] = 2.52 \times 10^5 ,$$

which is much too high.

Our $1/N$ formalism allows straightforward calculations of the dynamical susceptibility $\chi(\mathbf{q}, \omega; T)$ which can be compared with results from energy-resolved inelastic neutron-scattering data.[35] This will be presented in a future publication.

Note added. In a recent report,[36] Chakravarty, Halperin, and Nelson (CHN) have investigated the phase diagram of the $(2+1)$-dimensional nonlinear σ model, which is related to the two-dimensional quantum Heisenberg antiferromagnet when the width in the temporal dimension is proportional to the inverse temperature. They obtain exponential temperature dependence of $\xi(T)$ as in

our Eq. (5.24) which agrees in detail with neutron-scattering data. Their value of $A(S)$ is given by $A(S) = 2\pi S^2 Z_\chi Z_c^2$, where $Z_\chi(S)$ and $Z_c(S)$ are known to $O(1/S)$ from spin-wave theory. Plugging in $S = \frac{1}{2}$ and $S=1$ into their expression, one finds $A^{CHN}(\frac{1}{2}) = 0.944$ and $A^{CHN}(1) = 5.30$, which are very close to our mean-field values of Eq. (5.25), $A^{MF}(\frac{1}{2}) = 1.16$ and $A^{MF}(1) = 5.46$.

ACKNOWLEDGMENTS

APPENDIX A: SCHWINGER REPRESENTATION OF THE SPIN ALGEBRA

The algebra of spin is that of the group SU(2):

$$[S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma} S^\gamma , \quad \mathbf{S} \cdot \mathbf{S} = S(S+1) . \tag{A1}$$

Conventional spin-wave theory makes use of the Holstein-Primakoff representation

$$S^+ = h^\dagger[(2S - h^\dagger h)]^{1/2}, \quad S^z = h^\dagger h - S ,$$
$$S^- = [(2S - h^\dagger h)]^{1/2} h, \quad 0 \leq h^\dagger h \leq 2S , \tag{A2}$$

in which each spin is represented by a single Bose oscillator, together with the anholonomic constraint that states in the physical sector must have $0 \leq n_h \leq 2S$. This type of constraint is extremely difficult to handle in a functional integral approach because it defines boundaries in Hilbert space.

In the Schwinger representation, each spin is replaced by two bosons,

$$S^+ = a^\dagger b, \quad S^z = \frac{1}{2}(a^\dagger a - b^\dagger b) ,$$
$$S^- = ab^\dagger, \quad \hat{S} = \frac{1}{2}(a^\dagger a + b^\dagger b) , \tag{A3}$$

together with the holonomic constraint $\hat{S} = \frac{1}{2}(n_a + n_b) = S$. Constraints of this type may be imposed by functional δ functions, and thus this representation lends itself well to the approach we take in the text.

APPENDIX B: GAUSSIAN FLUCTUATIONS AND $O(1/N)$ CORRECTIONS

In this appendix we demonstrate a typical calculation of the $O(1/N)$ corrections to the mean-field theories discussed in the text. We concentrate on two simple one-dimensional cases, those of the bosonic large-N ferromagnet and the fermionic large-N $S = \frac{1}{2}$ antiferromagnet. Since the integrations involved are relatively easy to perform in these cases, this appendix serves as a practical example which highlights the utility of the functional in-

tegral approach.

The Read-Newns transformation of Eq. (2.17) replaces the complex fields Q_{ij} by their absolute values $|Q_{ij}|$. The partition function is given by

$$Z = \int \mathcal{D}[Q^2, \lambda] \exp[-N\mathcal{S}(Q; \lambda; h)] \ , \tag{B1}$$

where h is an external field. The mean-field equations determine the saddle-point values of the temperature-dependent (and field-dependent) constants λ and Q, cf. Eqs. (3.5) and (4.4). One defines the mean-field Green's function

$$G_{\mathbf{k}\mathbf{k'}}^{mm'} \equiv \frac{T}{ik_0 - \omega_k} \delta_{\mathbf{k}\mathbf{k'}} \delta_{mm'}, \quad \omega_k = \lambda + 2Q \cos k \ , \tag{B2}$$

where $\mathbf{k} = (ik_0, k)$ is an energy-momentum vector, and where the Matsubara frequencies ik_0 are $2\pi nT$ for the bosonic model and $(2n+1)\pi T$ for the fermionic model. In addition, in one dimension each bond $Q_{n,n+1}$ may be labeled by a single index, say $n + \frac{1}{2}$, which denotes the midpoint of its terminating sites. The action can now be written as

$$N\mathcal{S} = \pm \mathrm{Tr} \ln G^{-1} \pm \mathrm{Tr} \ln(1 + GR) + N\beta \left[\sum_q Q_q Q_{-q} - \lambda \right] \ , \tag{B3}$$

where the matrix R is defined by

$$R_{\mathbf{k}\mathbf{k'}}^{mm'} \equiv (Q_{\mathbf{k'}-\mathbf{k}} + \lambda_{\mathbf{k'}-\mathbf{k}} + gmh_{\mathbf{k'}-\mathbf{k}}) \delta_{mm'} \ . \tag{B4}$$

[The indices $m = -\frac{1}{2}(N-1), \ldots, \frac{1}{2}(N-1)$ are flavor indices.] The $\pm$ signs in Eq. (B3) apply to the Bose and Fermi case, respectively. Expanding Eq. (B3) to second order in the Bose fields Q and λ (at zero magnetic field h_p) and performing the Gaussian integrals yields the Bose propagator

$$D_{rr'} = \frac{T}{N}(\delta_{r,Q} - \Pi_{rr'})^{-1} \ , \tag{B5}$$

where the index r ranges over Q and λ, and the polarization matrix is explicitly given by

$$\Pi_{rr'}(iq_0, q) = \sum_k \frac{n_k - n_{k+q}}{2Q \cos k - 2Q \cos(k+q) + iq_0} C_{k,q}^r C_{k,q}^{r'} \ , \tag{B6}$$

where n_k is the Bose or Fermi occupation function and the C_{kq}^r are coherence factors:

$$C_{k,q}^Q = 2\cos(k + \tfrac{1}{2}q), \quad C_{k,q}^\lambda = i \ . \tag{B7}$$

For the Bose case, the polarization functions can be expanded at low temperatures using a steepest-descents integration, yielding

$$\Pi = \sum_{n=0}^{\infty} \sum_{\sigma=+,-} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-n\omega_k/T} \frac{C_{k,q}^r C_{k,q}^{r'}}{2Q \cos k - 2Q \cos(k+q) + \sigma i q_0}$$

$$= SC_{0,q}^r C_{0,q}^{r'} \sum_{\sigma=+,-} \frac{1}{2Q(1-\cos q) + \sigma i q_0}[1 + O(T^{1/2})] \ . \tag{B8}$$

Since the coherence terms factor out of Eq. (B8) at low T, there is a cancellation with the off-diagonal term in $\det D$, leaving $\det D = T/N \Pi_{\lambda\lambda} + \cdots$. The trace over Matsubara frequencies can now be accomplished, and we obtain the following correction to the free energy:

$$F^{(1/N)} = +\frac{1}{N\beta} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \ln(e^{2\beta Q \cos k} - 1)$$

$$= +\frac{1}{N} \frac{\zeta(\frac{3}{2})}{\sqrt{\pi S}} T^{3/2} + O(T^{5/2}) \ . \tag{B9}$$

This correction, when added to the mean-field result of Eq. (3.7), brings the coefficient of the $T^{3/2}$ term in line with the result of Takahashi and with the numerical exact result for $S = \frac{1}{2}$. However, no correction to the T^2 term is found at the $O(1/N)$ level. By explicitly including the magnetic field to second order, we find that $F^{(1/N)}$ is independent of h and hence there is no corresponding correction to the static susceptibility.

In the case of the fermionic large-N theory of the $S = \frac{1}{2}$ antiferromagnet, we wish to concentrate on the $O(1/N)$ correction to the total moment sum rule of Eq. (4.8) (equal-time local susceptibility):

$$\chi^{(1/N)}(t = 0^+) = \sum_p S^{(1/N)}(p) = \sum_{i,p_0,p} \chi^{(1/N)}(ip_0, p) \ . \tag{B10}$$

[$S(p)$ is the static structure factor.] $\chi^{(1/N)}$ is determined by the quartic terms in the expansion of the logarithm in Eq. (B3) which have contributions from two Bose fields and two magnetic fields $h_p h_{-p}$. Completing the square the integrating out the Q and λ fields, it can be seen that all the $O(1/N)$ corrections are included in the following integrals:

$$\chi^{SE}(p) = \frac{2}{N} \sum_{\substack{k,q,m \\ r,r'}} m^2 G_{k+p} G_k G_k G_{k+q} C_{k,q}^r C_{k,q}^{r'} D_{rr'}(q) \ ,$$

$$\chi^V(p) = \frac{1}{N} \sum_{\substack{k,q,m \\ r,r'}} m^2 G_{k+p} G_k G_{k+p+q} G_{k+q} \tag{B.11}$$

$$\times C_{k,q}^r C_{k+p,q}^{r'} D_{rr'}(q) \ ,$$

whose diagrams are shown in Fig. 1. (We have adopted the shorthand notation $G_q \equiv G_{qq'}^{mm'}$.) Summing over ip_0, the contribution to the equal-time correlation functions are given by

$$S^{SE}(\mathbf{p}) = g^2 \frac{2}{N} \sum_{\substack{k,q,m \\ r,r'}} m^2 n_{\mathbf{k}+\mathbf{p}} G_k G_k G_{k+q} C^r_{\mathbf{k},\mathbf{q}} C^{r'}_{\mathbf{k},\mathbf{q}} D_{rr'}(q) ,$$

$$S^V(\mathbf{p}) = g^2 \frac{1}{N} \sum_{\substack{k,q,m \\ r,r'}} m^2 \frac{(n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{p}})(n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}+\mathbf{q}+\mathbf{p}})}{(\omega_{\mathbf{k}} - \omega_{\mathbf{k}+\mathbf{p}} + ik_0)(\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}+\mathbf{q}+\mathbf{p}} + ik_0 + iq_0)} C^r_{\mathbf{k},\mathbf{q}} C^{r'}_{\mathbf{k}+\mathbf{p},\mathbf{q}} D_{rr'}(q) .$$

(B12)

By particle-hole symmetry, the off-diagonal propagator matrix elements vanish, i.e., $D_{Q\lambda} = 0$. Using the antisymmetry $\omega_{\mathbf{k}+\pi} = -\omega_{\mathbf{k}}$ ($\lambda = 0$ for the fermionic mean field), it is also possible to show that the $O(1/N)$ corrections to the total moment sum rule all vanish with the exception of the vertex contribution involving $D_{\lambda\lambda}$. This correction is easily found to be

$$\chi^{(1/N)}(t = 0^+) = \frac{1}{N} \chi^{MF}(t = 0^+) . \tag{B13}$$

Since the other contributions to $S(p)$ are antisymmetric in $p \to p + \pi$, the logarithmic divergence at the zone boundary which is missing at the mean-field level is expected to arise from S^V and higher-order terms in the $1/N$ expansion.

APPENDIX C: UNIMODULAR HUBBARD-STRATONOVICH TRANSFORMATION

In the case of the $S = \frac{1}{2}$ Heisenberg antiferromagnet in its physically relevant $N = 2$ fermion incarnation, one can decouple the quartic term in the action by a *unimodular* Hubbard-Stratonovich (HS) transformation, i.e., using a bond field Q_{ij} whose magnitude is fixed to be unity. This result, due to Arovas and Girvin,[37] is derived below.

For $S = \frac{1}{2}$, one can write

$$\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{4} - \frac{1}{2} \mathcal{C}^\dagger_{ij} \mathcal{C}_{ij}$$

$$= \frac{1}{4} - \frac{1}{2} \mathcal{D}^\dagger_{ij} \mathcal{D}_{ij} = -\frac{1}{4} - \frac{1}{2} : \mathcal{D}^\dagger_{ij} \mathcal{D}_{ij} : \tag{C1}$$

with

$$\mathcal{C}_{ij} = (c_{i\uparrow} c_{j\downarrow} + c_{j\uparrow} c_{i\downarrow}) = \mathcal{C}_{ji} ,$$
$$\mathcal{D}_{ij} = (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) , \tag{C2}$$

and where $:\mathcal{X}:$ denotes normal ordering. We shall write everything in terms of the $\mathcal{C}_{ij}$ operators. The Heisenberg Hamiltonian is then

$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$= \frac{1}{8} \mathcal{N} z - \frac{1}{2} \sum_{\langle i,j \rangle} \mathcal{C}^\dagger_{ij} \mathcal{C}_{ij} , \tag{C3}$$

where $\mathcal{N}$ is the number sites and z is the lattice coordination number. Since H is already normal ordered,

$$Z = \int \mathcal{D}[c, \bar{c}; \lambda] \exp(-\mathcal{S}[c, \bar{c}; \lambda]) ,$$

$$\mathcal{S} = \int_0^\beta d\tau \left[\frac{1}{2} \sum_{i,\sigma} (\bar{c}_{i\sigma} \dot{c}_{i\sigma} - \dot{\bar{c}}_{i\sigma} c_{i\sigma}) - \frac{1}{2} \sum_{\langle i,j \rangle} \bar{\mathcal{C}}_{ij} \mathcal{C}_{ij} \right.$$
$$\left. + \sum_i \lambda_i (\bar{c}_{i\uparrow} c_{i\uparrow} + \bar{c}_{i\downarrow} c_{i\downarrow} - 1) \right] , \tag{C4}$$

where the λ_i integration contours run from $-i\infty$ to $+i\infty$. At this point, one can break up the biquadratic $\bar{\mathcal{C}}_{ij} \mathcal{C}_{ij}$ terms with a complex HS bond field, as described in Sec. II of the text. However, the simplicity of the Grassmann algebra allows one to accomplish the same result with a unimodular HS field.

The idea is basically this: The composite field $\mathcal{C}_{ij}$ is bilinear in Grassmann variables and one can check that it satisfies $\mathcal{C}^3_{ij} = 0$. It is then easy to see that by integrating over only the phase angle θ_{ij} with $t \equiv \exp(i\theta)$ the unimodular field, that

$$\int \frac{d\theta}{2\pi} \exp[\frac{1}{2}\alpha(t\bar{\mathcal{C}} + \bar{t}\mathcal{C})] = 1 + \frac{1}{4}\alpha^2 \bar{\mathcal{C}}\mathcal{C} + \frac{1}{64}\alpha^4 (\bar{\mathcal{C}}\mathcal{C})^2$$

$$= \exp(\frac{1}{4}\alpha^2 \bar{\mathcal{C}}\mathcal{C} - \frac{1}{64}\alpha^4 \bar{\mathcal{C}}\bar{\mathcal{C}}\mathcal{C}\mathcal{C}) , \tag{C5}$$

where α is a free parameter, and where we have used the fact that all Grassmann bilinears commute with each other. Setting $\alpha = \sqrt{2}$, one finds that the above integral is given by

$$\int \frac{d\theta}{2\pi} \exp\left[\frac{1}{\sqrt{2}}(t\bar{\mathcal{C}} + \bar{t}\mathcal{C}) \right] = \exp(\frac{1}{2}\bar{\mathcal{C}}\mathcal{C} - \frac{1}{16}\bar{\mathcal{C}}\bar{\mathcal{C}}\mathcal{C}\mathcal{C}) . \tag{C6}$$

Note that the above expression does not exactly reproduce the relevant part of the action in Eq. (2.13) on account of the $\bar{\mathcal{C}}\bar{\mathcal{C}}\mathcal{C}\mathcal{C}$ term. However, we claim that this makes no contribution to the path integral due to the constraint. One way in which we see this is to note that *if* the interaction were not of the form $\frac{1}{4} - \frac{1}{2}\mathcal{C}^\dagger_{ij}\mathcal{C}_{ij}$ but rather

$$\frac{1}{4} - \frac{1}{2}\mathcal{C}^\dagger_{ij}\mathcal{C}_{ij} - \frac{1}{16}\mathcal{C}^\dagger_{ij}\mathcal{C}^\dagger_{ij}\mathcal{C}_{ij}\mathcal{C}_{ij}$$

(which is normal ordered), then the associated term in the action would be exactly that which would be reproduced by the above unimodular HS transformation. The additional eight-point term does commute with the constraint $n_{i\uparrow} + n_{i\downarrow} = 1$, however, it must be zero since the constraint enforces an occupation of one fermion quantum per site. One thus obtains

$$Z = \int \mathcal{D}[c,\overline{c};\lambda;\theta]\exp(-\mathcal{S}[c,\overline{c};\lambda;\theta]) ,$$

$$\text{(C7)}$$

$$\mathcal{S} = \int_0^\beta d\tau \left[\tfrac{1}{2}\sum_{i,\sigma}(\overline{c}_{i\sigma}\dot{c}_{i\sigma} - \dot{\overline{c}}_{i\sigma}c_{i\sigma}) + \sum_i \lambda_i(\overline{c}_{i\uparrow}c_{i\uparrow} + \overline{c}_{i\downarrow}c_{i\downarrow} - 1) + \frac{1}{\sqrt{2}}\sum_{\langle i,j\rangle}[e^{-i\theta_{ij}}(c_{i\uparrow}c_{j\downarrow} + c_{j\uparrow}c_{i\downarrow}) + e^{i\theta_{ij}}(\overline{c}_{i\downarrow}\overline{c}_{j\uparrow} + \overline{c}_{j\downarrow}\overline{c}_{i\uparrow})] \right]$$

for *any* bipartite lattice in an arbitrary number of dimensions. [There is a reference energy per spin of $E_{\text{ref}}/\mathcal{N} = \tfrac{1}{8}z$ not included in Eq. (C7).] In $d = 1$, one can gauge away the HS field via a Read-Newns transformation Eq. (2.17), leaving one with an integral over only the Grassmann variables and the constraint field.

An identical expression may be derived using the $\mathcal{D}_{ij}$ operators, resulting in

$$Z = \int \mathcal{D}[c,\overline{c};\lambda;\theta]\exp(-\mathcal{S}[c,\overline{c};\lambda;\theta]) ,$$

$$\text{(C8)}$$

$$\mathcal{S} = \int_0^\beta d\tau \left[\tfrac{1}{2}\sum_{i,\sigma}(\overline{c}_{i\sigma}\dot{c}_{i\sigma} - \dot{\overline{c}}_{i\sigma}c_{i\sigma}) + \sum_i \lambda_i(\overline{c}_{i\uparrow}c_{i\uparrow} + \overline{c}_{i\downarrow}c_{i\downarrow} - 1) + \frac{1}{\sqrt{2}}\sum_{\langle i,j\rangle}[e^{-i\theta_{ij}}(\overline{c}_{i\uparrow}c_{j\uparrow} + \overline{c}_{i\downarrow}c_{j\downarrow}) + e^{i\theta_{ij}}(\overline{c}_{j\uparrow}c_{i\uparrow} + \overline{c}_{j\downarrow}c_{i\downarrow})] \right] ,$$

where the reference energy per spin is now $E_{\text{ref}}/\mathcal{N} = -\tfrac{1}{8}z$.

APPENDIX D: SPIN-SPIN CORRELATIONS AT $T = 0$ — FERMIONIC THEORY

The fermionic mean-field theories yield gapless spectra and an algebraic decay of the spin-spin correlation function. In this Appendix, we investigate the asymptotic behavior of the correlations in both the BZA phase and the flux phase on the two-dimensional square lattice. In each case, one obtains

$$C(\mathbf{R}) \equiv \langle \mathbf{S}_0 \cdot \mathbf{S}_\mathbf{R} \rangle$$

$$= \tfrac{3}{4}\delta_{\mathbf{R},0} - \tfrac{3}{2}|L(\mathbf{R})|^2 \tag{D1}$$

with

$$L(\mathbf{R}) = \int_\Omega \frac{d^2k}{(2\pi)^2} e^{i\theta_\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} , \tag{D2}$$

where the integral is over the little zone Ω defined by the vertices $(0,\pm\pi)$ and $(\pm\pi,0)$. The coherence angle $\theta_\mathbf{k}$ is 1 in the BZA phase and

$$\exp i\theta_k = \frac{\cos k_y + i\cos k_x}{(\cos^2 k_x + \cos^2 ky)^{1/2}} \tag{D3}$$

in the flux phase.

1. BZA phase

Here, the integral in Eq. (D2) may be done exactly, yielding

$$L(\mathbf{R}) = \tfrac{1}{2} \left[\frac{\sin(\pi/2)R_+}{(\pi/2)R_+} \right]^2 \left[\frac{\sin(\pi/2)R_-}{(\pi/2)R_-} \right]^2 \tag{D4}$$

where $R_\pm \equiv R_x \pm R_y$. Since both R_+ and R_- are even when $\mathbf{R}$ is in sublattice A and odd when $\mathbf{R}$ is in sublattice B, we find that $C(\mathbf{R})$ vanishes for all nonorigin $\mathbf{R}$ in sublattice A. Along the axes $\mathbf{R}\cdot\hat{\mathbf{x}} = 0$ and $\mathbf{R}\cdot\hat{\mathbf{y}} = 0$ the correlations decay as R^{-4}.

The static structure factor, defined by

$$C(\mathbf{k}) \equiv \sum_\mathbf{R} e^{i\mathbf{k}\cdot\mathbf{R}} C(\mathbf{R})$$

$$= \tfrac{3}{2}\int \frac{d^2p}{(2\pi)^2} n_\mathbf{p}(1 - n_{\mathbf{p}+\mathbf{k}}) \tag{D5}$$

is easily shown to be

$$C(\mathbf{k}) = \frac{3}{4}\left[1 + \left| \frac{k_y}{\pi} \right|^2 - \left| 1 - \frac{k_x}{\pi} \right|^2 \right] . \tag{D6}$$

Note that $C(\mathbf{k}=0) = 0$, i.e., the ground state is a singlet. As emphasized in the text, the total-moment sum rule is violated, and we obtain

$$\int \frac{d^2k}{(2\pi)^2} C(\mathbf{k}) = \tfrac{3}{8} \tag{D7}$$

at the mean-field level, rather than the correct value of $S(S+1) = \tfrac{3}{4}$. Note also the nonanalyticity of $C(\mathbf{k})$ at the zone edges.

2. Flux phase

The nontrivial coherence angle in Eq. (D3) makes an exact evaluation of $L(\mathbf{R})$ difficult. However, we can extract the leading asymptotic behavior of the integral in Eq. (D2) using the saddle point approximation:

$$\nabla_\mathbf{k}\theta_\mathbf{k}\Big|_{\mathbf{k}=\mathbf{K}} = \mathbf{R} ,$$

$$L(\mathbf{R}) \sim -\frac{1}{4\pi}\frac{1}{\sqrt{\det A}}e^{i\theta_\mathbf{K}}e^{-i\mathbf{K}\cdot\mathbf{R}} , \tag{D8}$$

$$A_{ab} \equiv (\partial^2\theta_k/\partial k_a\partial k_b)\big|_{\mathbf{k}=\mathbf{K}} .$$

As R gets larger, the solutions are confined to small regions about the four Fermi points $(\pm\pi/2,\pm\pi/2)$. By translating the region of the little zone in the lower-left quadrant by (π,π) and translating the region of the little zone in the lower-right quadrant by $(-\pi,\pi)$, we find that there are really only two saddle points to consider. In the vicinity of $\mathbf{K}_0 \equiv (\pi/2,\pi/2)$, we write $\mathbf{k} \equiv \mathbf{K}_0 + \mathbf{q}$, with q small, yielding

$$e^{i\theta_k} = -\frac{q_y + iq_x}{(q_x^2 + q_y^2)^{1/2}} \,,$$

$$\nabla_k \theta_k = \left[\frac{q_y}{q^2}, -\frac{q_x}{q^2}\right] \,, \qquad\qquad (D9)$$

$$\mathbf{K} = \mathbf{K}_0 + \frac{\hat{\mathbf{z}} \times \mathbf{R}}{R^2} \,,$$

from which one easily obtains $\det A = R^4$. Summing over the two saddle points at $(\pm\pi/2, \pi/2)$, we obtain

$$|L(\mathbf{R})|^2 \sim \frac{1}{4\pi^2} R^{-4} p(\mathbf{R}) \,, \qquad\qquad (D10)$$

with $p(\mathbf{R}) = 0$ if $R_x + R_y$ is even (i.e., if $\mathbf{R}$ is in sublattice A), $p(\mathbf{R}) = R_y^2/R^2$ if R_x is even and R_y is odd, and $p(\mathbf{R}) = R_x^2/R^2$ if R_y is even and R_x is odd.

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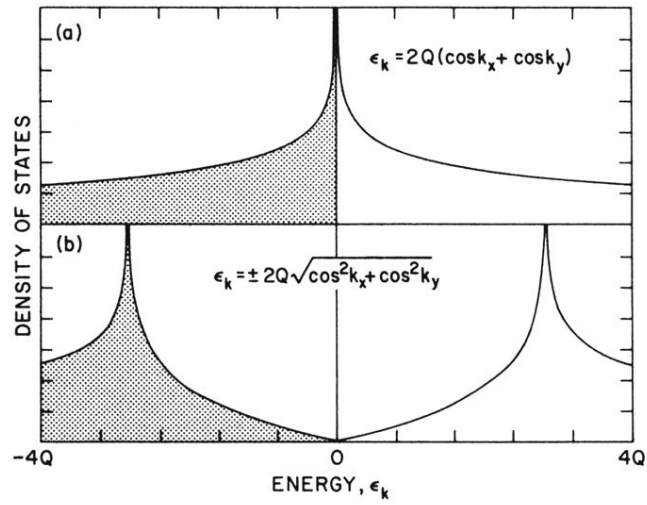
FIG. 2. (a) Density of states for the BZA mean-field theory of the two-dimensional square lattice $S = \frac{1}{2}$ antiferromagnet. (b) Density of states in Affleck-Marston flux phase. A comparison demonstrates that the BZA mean-field theory is unstable: Its filled states (shaded) are concentrated at relatively high energies.