Second-order phase transitions in a frustrated two-dimensional Heisenberg antiferromagnet

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The frustrated two-dimensional Heisenberg antiferromagnet on a square lattice is considered by the method of two-time temperature spin Green's functions in the approximation of spherically symmetric spin correlations. Unlike other theories, this approach does not require assumptions about a two-sublattice form of the ground state. As the frustration parameter $p=J_2/(J_1+J_2)$ increases at $T=0$ two continuous transitions occur in the system, between the following three states: a phase I with long-range order of the form $(-1)^{n_x+n_y}$ (the analog of the Néel phase), a spin-liquid phase without long-range order, and a phase II with long-range order of the form $(-1)^{n_x}+(-1)^{n_y}$ (the analog of the "stripe" phase), where n_x, n_y are the integer labels of the sites of the square lattice. The first transition occurs at $p\approx 0.1$ and is accompanied by the appearance of a gap in the spin-excitation spectrum at the points $\mathbf{q}_{\mathrm{I}}=(\pm\pi,\pm\pi)$, and the second occurs at $p\approx 0.62$, when the gap closes at the points $\mathbf{q}_{\mathrm{II}}=(\pm\pi,0)$ and $(0,\pm\pi)$. The values found for the spin correlation functions agree qualitatively with known numerical results in the entire range $0<p<1$ of the parameter p. The approach used is compared in detail with other theories. © *1994 American Institute of Physics.*

1. INTRODUCTION

In connection with the well known problem of the long-range order in the theory of quantum spin systems considerable attention has been paid to the two-dimensional antiferromagnetic Heisenberg model on a square lattice in the quantum limit with spin value $S=1/2$. In the real world this is a good model for the CuO_2 planes that are responsible for the superconductivity in high-temperature superconductors.

The antiferromagnetic exchange interaction between the spins of first-nearest-neighbor Cu^{2+} ions in a given CuO_2 plane are extremely large [greater than 1000 K for La_2CuO_4 (Ref. 1)] and considerably greater than the interplanar exchange. The interplanar exchange is primarily responsible for the onset of the long-range order that is observed in the dielectric phase of the CuO_2 planes [for La_2CuO_4 the characteristic Néel temperature is $T_N\sim 300$ K (Ref. 2)]. However, in the case of comparatively light doping of the system by holes (the holes form $2p_{x,y}$ orbitals on the oxygen sites) the antiferromagnetic long-range order disappears over the whole range of temperatures. It is customary to assume that the doping leads to antiferromagnetic interaction between second-nearest neighbors in the Cu^{2+} subsystem in a given plane, i.e., to frustration.[3] In view of this, intensive studies are currently being made of the frustrated two-dimensional Heisenberg model, described by the Hamiltonian

$$H=\frac{1}{2}\left(J_1\sum_{\mathbf{i},\mathbf{g}} S_{\mathbf{i}}S_{\mathbf{i}+\mathbf{g}}+J_2\sum_{\mathbf{i},\mathbf{d}} S_{\mathbf{i}}S_{\mathbf{i}+\mathbf{d}}\right), \tag{1}$$

where $J_1, J_2>0$ are the antiferromagnetic interactions between first-nearest neighbors ($\mathbf{g}=\pm\mathbf{g}_x\ \pm\mathbf{g}_y$) and between second-nearest neighbors ($\mathbf{d}=\pm\mathbf{g}_x\pm\mathbf{g}_y$) on a square lattice (see Fig. 1a). For convenience, J_1 and J_2 can be expressed in terms of the frustration parameter p:

$$J_1=(1-p)J,\quad J_2=pJ,\quad 0\leqslant p\leqslant 1,\quad J>0. \tag{2}$$

The frustration parameter p can be regarded as the analog of the number x of holes per copper atom. An estimate based on the single-band Hubbard model with realistic values $U/t\sim 5$ leads, e.g., to a value of $p\sim 0.26$ for $x=0.1$. We note that in the case of $La_{2-x}Sr_xCuO_4$ the spin system of the CuO_2 plane loses its long-range order for $x>0.02$.

In the case of the model without frustration the Mermin–Wagner theorem[4] asserts the absence of spontaneous magnetization at finite temperatures (i.e., the absence of long-range order), but does not rule it out at $T=0$ (see the review in Ref. 5).

In the classical approximation ($S\gg 1$) the frustrated model (1) has at $p=1/3$ a first-order transition between two ordered phases. Phase I ($p<1/3$) is characterized by order vector $\mathbf{q}_{\mathrm{I}}=(\pi,\pi)$ and corresponds to the Néel state (Fig. 1a). Phase II (Fig. 1b) is realized for $p>1/3$ and corresponds to the so-called "stripe" state [order vector $\mathbf{q}_{\mathrm{II}}=(\pi,0)$ or $(0,\pi)$]. The spin correlation functions in these phases have the form

$$C_{\mathbf{r}}^{\mathrm{I}}\propto(-1)^{n_x+n_y}, \tag{3.1}$$

$$C_{\mathbf{r}}^{\mathrm{II}}\propto(-1)^{n_x}\ \text{or}\ (-1)^{n_y}, \tag{3.2}$$

$$C_{\mathbf{r}}=\sum_{\alpha} C_{\mathbf{r}}^{\alpha},\quad C_{\mathbf{r}}^{\alpha}=\langle S_{\mathbf{i}}^{\alpha}S_{\mathbf{i}+\mathbf{r}}^{\alpha}\rangle,$$

$$\alpha=x,y,z\quad \mathbf{r}=n_x\mathbf{g}_x+n_y\mathbf{g}_y,$$

where n_x and n_y are integers. We note that in the case $p=1$ ($J_1=0$) the spin system takes the form of two superimposed noninteracting Néel lattices (Fig. 1b), for each of which a situation analogous to the case for phase I at $p=0$ is realized.

In the quantum limit $S=1/2$ at $T=0$ we may regard it as established that the system possesses long-range order of

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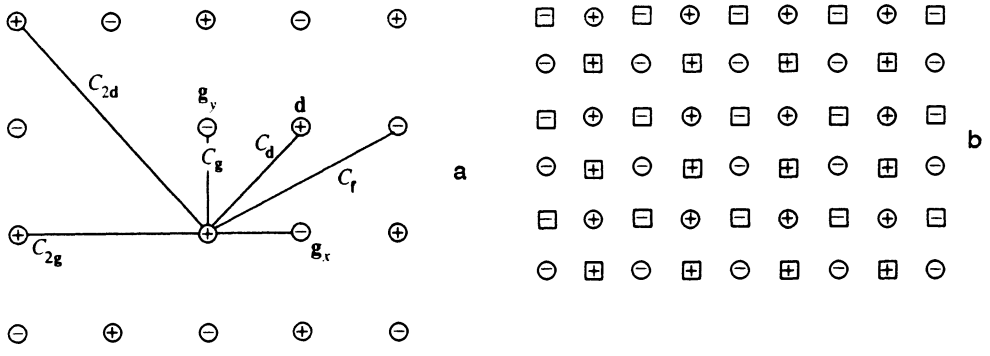

FIG. 1. Classical states of the spin system: (a) the Néel phase I (the corresponding correlation functions C_r are indicated); (b) the "stripe" phase II, with two mutually penetrating square sublattices, represented by circles and squares.

type I and type II in the limiting cases at $p=0$ and $p=1$ (Ref. 5). In this paper we are interested in the properties of the system and the phase transition between these states in the parameter p.

We shall discuss the results given by different approaches for the frustrated model with the Hamiltonian (1).

In Refs. 6–8 this model was considered in terms of the theory of linear spin waves. For $p<1/3$ in this approach the operators of the spin-wave excitations are constructed relative to the Néel state, and for $p>1/3$ they are constructed relative to the stripe state. From the theory of linear spin waves it follows that for $p<p_{1L}=0.274$ the phase I with sublattice magnetization $m_{1L} \propto (-1)^{n_x+n_y}$ is realized, while for $p>p_{2L}=1/3$ the phase II with $m_{2L} \propto (-1)^{n_x}$ is realized. At the points p_{1L} and p_{2L} the corresponding sublattice magnetizations m_{1L} and m_{2L} vanish. On this basis it was postulated in Ref. 6 that in the interval $p_{1L}<p<p_{2L}$ the system loses its long-range order and goes over into a spin-liquid state. However, the theory of linear spin waves does not permit one to describe the state of the system at $T=0$ for this range of values of p. In the framework of this theory, for any value of p, it is also not possible to consider the case of nonzero temperatures (because of the well known divergence for m with $T\neq 0$ in the two-dimensional case). We note that in Ref. 7 correlation functions C_r for both phases were found with allowance for biquadratic terms in the Dyson–Maleev transformation.[9] Values of C_r over the whole range of p, obtained by numerical calculations on finite blocks of up to 20 spins, are also given in Ref. 7.

In Ref. 10 the frustrated model was studied on the phase-I side in the framework of the theory of linear spin waves with the additional condition that the sublattice magnetization be equal to zero (a detailed account of a sublattice-symmetric theory of linear spin waves can be found in Refs. 11 and 12). In the case $T=0$ it was shown that for $p<p_{1L}$ the spin-wave spectrum $\omega(\mathbf{q})$ is gapless at $\mathbf{q}=0$, i.e., there exists long-range order determined by Bose condensation of the spin waves with $\mathbf{q}=0$. Here and below, by Bose condensation we understand the anomalous (as $T\to 0$) contribution to the expression for the spin correlators from a small region of wave-vector values in the neighborhoods of the points $\mathbf{q}_i$ at which $\omega(\mathbf{q}_i)=0$. For $p>p_{1L}$ a gap appears in the spin-wave spectrum. This implies that the system loses its long-range order and goes over into a spin-liquid state, in which the spin excitations have nonzero mass. The sublattice-symmetric theory of linear spin waves permits generalization to the case $T\neq 0$. However, for $p>0.275$ the correlation functions C_r found on the basis of this theory over short distances differ strongly from the corresponding values of C_r from numerical calculations of finite blocks.[10]

The theory of modified spin waves,[11,13,14] which takes into account terms proportional to S^0 in the Dyson–Maleev or Holstein–Primakoff transformations, leads to different results. In Refs. 15–17 it was shown that phase I possesses long-range order in the interval $0<p<p_{1M}$ ($p_{1M}=0.38$), while phase II possesses long-range order for $p_{2M}<p<1$ ($p_{2M}=0.35$). Here, the average spin $\langle \mathbf{S}_i \rangle$ per site is zero, while long-range order corresponds to a nonzero effective spin m, defined in terms of the spin correlation functions at large distances by $m^2 = |C_{\mathbf{r}\to\infty}|$. In phases I and II, $C_{\mathbf{r}\to\infty}$ has a form analogous to (3). Thus, in the theory of modified spin waves the long-range order is preserved for all values of p, and in the region $p_{2M}<p<p_{1M}$ a transition should occur between two phases with different long-range order. We emphasize that in the theory of modified spin waves, as in the theory of linear spin waves, the spin-excitation operators in the different phases are constructed relative to different classical states. As a consequence, in the framework of these theories the transition in the parameter p between phases I and II should be a first-order transition.

The approaches listed above are not spherically symmetric, in the sense that there is no spherical symmetry of the spin correlation functions in them, i.e., $C_{\mathbf{r}}^z \neq C_{\mathbf{r}}^x = C_{\mathbf{r}}^y$. In Ref. 18 the model (1) was studied in terms of a spherically symmetric theory based on a mean-field approximation for Schwinger bosons.[19] For $S=1/2$ the results are the same as in the theory of modified spin waves. It is easy to see that in the approach of Ref. 19 the way in which the mean field is introduced for the two phases can only yield a first-order transition, analogously to the theory of modified spin waves. We note also that at nonzero temperatures both theories lead to a nonphysical first-order phase transition at values of $T\sim J$ (Refs. 20, 21).

The possibility of a first-order transition from a state with long-range order to a spin-liquid state at the comparatively small value $p\approx 0.2$ was pointed out in Refs. 3 and 22. There a variational approach was used, and for the spherically symmetric ground state of the spin-liquid phase a state of the resonance-valence-bond type was constructed. A second-order transition from the state with long-range order to the spin-liquid state at $p\approx 0.2$ was obtained assuming

spherically symmetric spin correlation functions in Ref. 23, in which the spin excitations were considered on the basis of four-spin blocks covering an infinite lattice. However, a detailed analysis turns out to be complicated in the region $p>1/3$, when inversion of the energy levels of a block sets in.

Finally, we also mention a number of theoretical approaches that predict the absence of long-range order in a certain interval near $p=1/3$. These are the numerous papers on exact diagonalization on finite systems,[7,8,24] the renormalization-group method combined with the mean-field approximation for Schwinger bosons[25] (this approach gives a transition from the state with long-range order to the spin-liquid state at $p\approx 0.13$), a self-consistent spin-wave approach on the basis of the dimer classical state,[26] and, finally, analysis based on the technique of the $1/N$-expansion.[27] As can be seen, different analytical approaches give contradictory results for the frustrated model.

In the present paper the model is investigated in the approximation of spherically symmetric spin correlations for two-time temperature retarded spin Green's functions.[28,29] Unlike most of the analytical approaches mentioned above, this treatment makes it possible to describe both the two phases with long-range order and the intermediate spin-liquid phase over the whole range of p in a single approximation.

In Sec. 2 we obtain the equations of motion for the Green's functions, which make it possible to express the spin-excitation spectrum $\omega(\mathbf{q})$ and the correlation functions. Closed expressions for the Green's functions, and a self-consistent system of equations for the correlation functions C_r, are found by a decoupling procedure with effective allowance for vertex corrections.[28] In Sec. 3 we give the results of solving the self-consistent system of equations at $T=0$ in the entire range of the frustration parameter p, namely, the value of the effective spin m, the energy of the ground state, the magnitude of the gap in the spin-excitation spectrum at the points $\mathbf{q}_{\mathrm{I}}=(\pi,\pi)$ and $\mathbf{q}_{\mathrm{II}}=(\pi,0)$, and the correlation functions $C_{\mathbf{r}}$ for the first five nearest neighbors. It is found that as the frustration increases a continuous transition occurs in the system, from a phase with long-range order (the analog of phase I) to a spin-liquid phase, and then to a phase with long-range order (the analog of phase II). Also in Sec. 3, we calculate the temperature dependence of the static uniform susceptibility $\chi(T)$. Section 4 is devoted to a brief discussion of the results.

2. SELF-CONSISTENT EQUATIONS ASSUMING SPHERICALLY SYMMETRIC SPIN CORRELATIONS

To determine the spin correlation functions we shall consider the two-time retarded Green's functions (and their Fourier transforms with respect to time) for the spin operators:

$$G_{\mathbf{ij}}^{\sigma}(\omega)=\langle S_{\mathbf{i}}^{\sigma}|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle=-i\int_0^{\infty}dt e^{i\omega t}\langle[S_{\mathbf{i}}^{\sigma}(t)S_{\mathbf{j}}^{\tilde{\sigma}}]\rangle, \tag{4}$$

$\sigma=t, \quad \tilde{\sigma}=-\sigma.$

For the operators S^{σ} we introduce the site correlation functions $C_{\mathbf{r}}^{\sigma}$, and also the spatial Fourier transforms of these functions and of the Green's functions $G_{\mathbf{ij}}^{\sigma}(\omega)$:

$$C_{\mathbf{r}}^{\sigma}=\langle S_{\mathbf{i}}^{\sigma}S_{\mathbf{i}+\mathbf{r}}^{\sigma}\rangle=N^{-1}\sum_{\mathbf{q}} e^{-i\mathbf{qr}}C_{\mathbf{q}}^{\sigma}; \quad G^{\sigma}(\mathbf{q},\omega)$$

$$=\sum_{\mathbf{r}} e^{i\mathbf{qr}}G_{\mathbf{i},\mathbf{i}+\mathbf{r}}^{\sigma}(\omega). \tag{5}$$

The functions $C_{\mathbf{q}}^{\sigma}$ and $G^{\sigma}(\mathbf{q},\omega)$ are connected by the relation

$$C_{\mathbf{q}}^{\sigma}=-\frac{1}{\pi}\int d\omega[1+n(\omega)]|m\{G^{\sigma}(\mathbf{q},\omega+i\varepsilon)\}, \tag{6}$$

where $n(\omega)=[\exp(\omega/T)-1]^{-1}$.

The first-order and second-order equations of motion for the Green's functions $G_{\mathbf{ij}}^{\sigma}(\omega)$ have the form

$$\omega G_{\mathbf{ij}}^{\sigma}(\omega)=2\sigma\delta_{\mathbf{ij}}\langle S_{\mathbf{i}}^{2}\rangle+\sigma\sum_{\mathbf{r}_1=\mathbf{q}_1,\mathbf{d}_1}J_{\mathbf{r}_1}\{\langle S_{\mathbf{i}}^{z}S_{\mathbf{i}+\mathbf{r}_1}|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle$$

$$-\langle S_{\mathbf{i}+\mathbf{r}_1}^{2}S_{\mathbf{i}}^{\sigma}|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle\}, \tag{7.1}$$

$$\omega\sigma\{\langle S_{\mathbf{i}}^{z}S_{\mathbf{i}+\mathbf{r}_1}^{\sigma}|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle-\langle S_{\mathbf{i}+\mathbf{r}_1}^{z}S_{\mathbf{i}}^{\sigma}|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle\}=(2\langle S_{\mathbf{i}}^{z}S_{\mathbf{j}}^{z}\rangle$$

$$+\langle S_{\mathbf{i}}^{\sigma}S_{\mathbf{j}}^{\tilde{\sigma}}\rangle)\delta_{\mathbf{i}+\mathbf{r}_1,\mathbf{j}}-(2\langle S_{\mathbf{i}+\mathbf{r}_1}^{z}S_{\mathbf{j}}^{z}\rangle+\langle S_{\mathbf{i}+\mathbf{r}_1}^{\sigma}S_{\mathbf{j}}^{\tilde{\sigma}}\rangle)\delta_{\mathbf{ij}}$$

$$+\tfrac{1}{2}J_{\mathbf{r}_1}(G_{\mathbf{ij}}^{\sigma}(\omega)-G_{\mathbf{i}+\mathbf{r}_1,\mathbf{j}}^{\sigma}(\omega))$$

$$+\frac{1}{2}\sum_{\substack{\mathbf{r}_2=\mathbf{g}_2,\mathbf{d}_2\\ \mathbf{r}_2\neq\mathbf{r}_1}}J_{\mathbf{r}_2}\Bigg\{\sum_{\sigma_1=\sigma,\tilde{\sigma}}(\sigma_1\sigma)(\langle S_{\mathbf{i}}^{\sigma_1}S_{\mathbf{i}+\mathbf{r}_2}^{\tilde{\sigma}_1}S_{\mathbf{i}+\mathbf{r}_1}^{\sigma}$$

$$-S_{\mathbf{i}+\mathbf{r}_1}^{\sigma_1}S_{\mathbf{i}+\mathbf{r}_1-\mathbf{r}_2}^{\tilde{\sigma}_1}S_{\mathbf{i}}^{\sigma}|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle)+\langle 2S_{\mathbf{i}}^{z}(S_{\mathbf{i}+\mathbf{r}_1}^{z}S_{\mathbf{i}+\mathbf{r}_1-\mathbf{r}_2}^{\sigma}$$

$$-S_{\mathbf{i}+\mathbf{r}_1-\mathbf{r}_2}^{z}S_{\mathbf{i}+\mathbf{r}_1}^{\sigma})|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle-\langle 2S_{\mathbf{i}+\mathbf{r}_1}^{z}(S_{\mathbf{i}}^{z}S_{\mathbf{i}+\mathbf{r}_2}^{\sigma}$$

$$-S_{\mathbf{i}+\mathbf{r}_2}^{z}S_{\mathbf{i}}^{\sigma})|S_{\mathbf{j}}^{\tilde{\sigma}}\rangle\Bigg\}, \tag{7.2}$$

where $J_g=J_1$ and $J_d=J_2$.

For the Green's functions that arise in the right-hand side of (7.2) we use a decoupling procedure analogous to that performed in Ref. 28. This decoupling has the following features.

First, it preserves the local correlation on a single site. This is expressed in the fact that for the Green's functions the decoupling is performed only when the three site spin operators in the left part of the bracket pertain to different sites.

Second, when identifying averages of the form $\langle S_{\mathbf{i}}^{z}S_{\mathbf{i}+\mathbf{r}}^{z}\rangle$ and $\langle S_{\mathbf{i}}^{\sigma}S_{\mathbf{i}+\mathbf{r}}^{\tilde{\sigma}}\rangle$ ($\mathbf{r}\neq 0$) we introduce extra factors α_1, α_2, and α_3 that have the meaning of vertex corrections. The factor α_1 is introduced if the sites $\mathbf{i}$ and $\mathbf{i}+\mathbf{r}$ are nearest neighbors, i.e., $r=g$; α_2 is introduced if $\mathbf{r}$ corresponds to a third-, fourth-, or fifth-nearest neighbor ($\mathbf{r}>\mathbf{d}$); $\alpha_3=(1-p)\alpha_2+p\alpha_1$ is used in the intermediate case when $r=d$.

We shall explain how our method of taking vertex corrections into account makes it possible to pass correctly from the limiting case $p=0$ to the limiting case $p=1$. As noted above, for $p=1$ we have two noninteracting superposed antiferromagnetic sublattices, each of which is physically equivalent to the complete lattice for $p=0$. We shall show

that our decoupling scheme satisfies this equivalence. For the case $p=0$ (i.e., in the absence of frustration) we take the very simple scheme that was discussed in detail in Ref. 28: If correlation functions with operators on nearest neighbors arise in the decoupling, we introduce α_1, while for more distant neighbors we introduce α_2. For $p=0$ we have $\alpha_3=\alpha_2$, and our scheme coincides with that adopted above. For $p=1$ we have $\alpha_3=\alpha_1$, and it is easily verified that for each of the sublattices our scheme goes over exactly into the scheme of Ref. 28. In particular, it leads to the result that the effective spins m found below for $p=0$ and $p=1$ coincide.

Furthermore, by virtue of the assumption that the correlation functions are spherically symmetric, we assume

$$C_{\mathbf{r}}=3\langle S_{\mathbf{i}}^z S_{\mathbf{i}+\mathbf{r}}^z\rangle=\tfrac{3}{2}\langle S_{\mathbf{i}}^\sigma S_{\mathbf{i}+\mathbf{r}}^{\tilde\sigma}\rangle=\langle S_{\mathbf{i}}S_{\mathbf{i}+\mathbf{r}}\rangle, \tag{8}$$

and also $\langle S_{\mathbf{i}}^z\rangle = 0$.

Then, after the decoupling, Eq. (7.2) takes the following form:

$$\begin{aligned}\sigma\omega[\langle S_{\mathbf{i}}^z S_{\mathbf{i}+\mathbf{r}_1}^\sigma|S_{\mathbf{j}}^{-\sigma}\rangle-\langle S_{\mathbf{i}+\mathbf{r}_1}^z S_{\mathbf{i}}^\sigma|S_{\mathbf{j}}^{-\sigma}\rangle]=\tfrac{2}{3}\Bigg\{&2C_{\mathbf{r}_1}(\delta_{\mathbf{i}+\mathbf{r}_1\mathbf{j}}\\ &-\delta_{\mathbf{i},\mathbf{j}})+(J_{\mathbf{r}_1}(\alpha_2 C_{2\mathbf{r}_1}+2\alpha_{\mathbf{r}_1}C_{\mathbf{r}_{1x}+\mathbf{r}_{1y}}+1/2)\\ &+2\tilde J_{\mathbf{r}_1}(\alpha_1 C_{\mathbf{g}}+\alpha_2 C_{\mathbf{f}}))(G_{\mathbf{ij}}^\sigma-G_{\mathbf{i}+\mathbf{r}_1,\mathbf{j}}^\sigma)\\ &+\tilde\alpha_{r_1}C_{\mathbf{r}_1}\Bigg(\sum_{\substack{\mathbf{r}_2=\mathbf{g}_2,\mathbf{d}_2\\ \mathbf{r}_2\neq\mathbf{r}_1}}(G_{\mathbf{i}+\mathbf{r}_1-\mathbf{r}_2,\mathbf{j}}^\sigma-\mathbf{G}_{\mathbf{i}+\mathbf{r}_2,\mathbf{j}}^\sigma)\Bigg)\Bigg\},\end{aligned} \tag{9}$$

where

$$J_g=J_1,\quad J_d=J_2,\quad \tilde J_g=J_2,\quad \tilde J_d=J_1,\quad \alpha_g=\alpha_3,$$
$$\alpha_d=\alpha_2,\quad \tilde\alpha_g=\alpha_1,\quad \tilde\alpha_d=\alpha_2.$$

An expression for the Green's function $G^\sigma(\mathbf{q},\omega)$ can be obtained by going over to Fourier components in Eqs. (7) and (9). As a result, we have

$$\begin{aligned}G^\sigma(\mathbf{q},\omega)=&-(16/3)(J_1(1-\gamma_{\mathbf{g}})C_{\mathbf{g}}+J_2\\ &\times(1-\gamma_{\mathbf{d}})C_{\mathbf{d}})(\omega^2-\omega^2(\mathbf{q}))^{-1},\end{aligned} \tag{10}$$

where the excitation spectrum $\omega(q)$ has the form

$$\begin{aligned}\omega^2(\mathbf{q})=&\tfrac{8}{3}((1-\gamma_{\mathbf{g}})A_1+(1-\gamma_{\mathbf{g}}^2)A_2+(1-\gamma_{\mathbf{d}})A_3\\ &+(1-\gamma_{\mathbf{d}}^2)A_4+\gamma_{\mathbf{g}}(1-\gamma_{\mathbf{d}})A_5),\\ A_1=&J_1^2(\alpha_2 C_{2g}+2\alpha_3 C_d+\tfrac{3}{4}+3\alpha_1 C_g)+2J_1J_2\\ &\times(\alpha_2 C_{\mathbf{g}+\mathbf{d}}-\alpha_1 C_{\mathbf{g}}),\\ A_2=&-4J_1^2\alpha_1 C_g,\quad A_3=2J_1J_2(3\alpha_1 C_{\mathbf{g}}+\alpha_2 C_{\mathbf{f}})\\ &+J_2^2(\alpha_2(C_{2\mathbf{d}}+2C_{2\mathbf{g}})+\tfrac{3}{4}+3\alpha_3 C_{\mathbf{d}}),\\ A_4=&-4J_2^2\alpha_3 C_{\mathbf{d}},\quad A_5=-4J_1J_2(\alpha_1 C_{\mathbf{g}}+\alpha_3 C_{\mathbf{d}}),\\ \gamma_{\mathbf{d}}=&\cos(q_x g)\cos(q_y g),\quad \gamma_{\mathbf{g}}=\tfrac{1}{2}(\cos(q_x g)+\cos(q_y g)).\end{aligned} \tag{11}$$

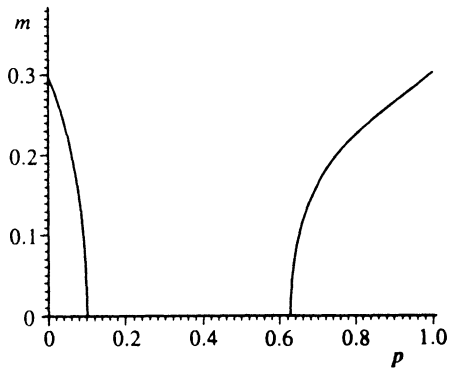

FIG. 2. Dependence of the effective spin m on the frustration parameter p.

Using the expression (10) for the Green's functions, and also Eqs. (5) and (6), we can obtain a self-consistent system of equations for the five correlation functions $C_{\mathbf{g}}$, $C_{\mathbf{d}}$, $C_{2\mathbf{g}}$, $C_{\mathbf{f}}$, and $C_{2\mathbf{d}}$ in terms of which the spectrum (11) is determined:

$$\begin{aligned}C_{\mathbf{r}}=&N^{-1}\sum_{\mathbf{q}}F(\mathbf{q})\omega(\mathbf{q})^{-1}e^{-i\mathbf{q}\mathbf{r}}[n(\omega(\mathbf{q}))+1/2],\\ F(\mathbf{q})=&(-8)(J_1(1-\gamma_{g\mathbf{q}})C_g+J_2(1-\gamma_{d\mathbf{q}})C_d).\end{aligned} \tag{12}$$

The sum rule $C_0=\langle \mathbf{S_i}\mathbf{S_i}\rangle=3/4$ gives an additional condition for the determination of α_1. Thus, putting α_2 aside, we have six self-consistent equations for the six unknowns $C_{\mathbf{r}}$ ($\mathbf{r}=\mathbf{g}$, $\mathbf{d}$, $2\mathbf{g}$, $\mathbf{f}$, $2\mathbf{d}$) and $\alpha_1(\mathbf{f}=2\mathbf{g}_x+\mathbf{g}_y)$.

The last unknown—the decoupling parameter α_2—is found from the following condition: In the absence of frustration at $T=0$ it is well known that the effective spin has the value $m\approx 0.3$, and we require that the quantity m calculated for $p=0$ and $T=0$ coincide with this value. In the problem without frustrations a phenomenological choice of this type for the parameter α_2 was used in Ref. 28. Also in Ref. 28 it was noted that as T increases the vertex corrections tend to unity, and for $T\neq 0$ it was suggested that one fix the value of the parameter

$$r_\alpha=(\alpha_1-1)/(\alpha_2-1)=\text{const}, \tag{13.1}$$

obtained from the additional condition

$$m(r_\alpha, T=0, p=0)=0.3. \tag{13.2}$$

Analogously, for arbitrary frustrations and temperatures, we also determine α_2 from the condition (13.1): The parameter r_α remains equal to the value given by Eq. (13.2). This scheme for the determination of α_2 not only satisfies the requirement that the vertex corrections become equal to unity with increase of T, but also permits us to obtain at $T=0$ the correct values of m in the two limiting cases $p=0$ and $p=1$.

3. PHASE TRANSITIONS AT $T=0$ AND PROPERTIES OF A SYSTEM WITH FRUSTRATION

At $T=0$, depending on the value of the frustration parameter p, for the self-consistent system of equations (12) two types of solutions are possible. The first type corre-

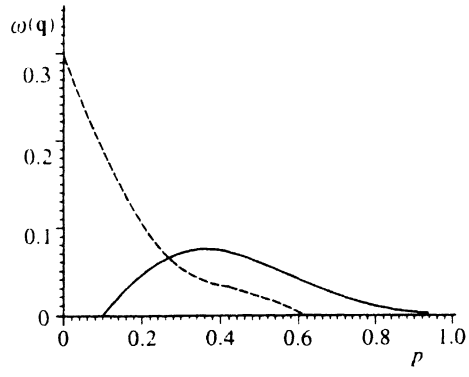

FIG. 3. Spectrum $\omega(\mathbf{q})$ at the Bose-condensation points, as a function of the frustration parameter p: The solid curve shows $\omega[\mathbf{q}=(\pi,\pi)]$, and the dashed curve shows $\omega[\mathbf{q}=(0,\pi)]$.

sponds to the case when the spectrum contains no gap at $\mathbf{q}\neq 0$. The second type of solution corresponds to $\omega(\mathbf{q})>0$ for all $\mathbf{q}\neq 0$.

A solution of the first type occurs in two intervals of values of the frustration. For $p<p_1$ ($p_1=0.1$) the spectrum is found to be gapless at the point $\mathbf{q}_{\mathrm{I}}$, while for $p>p_2$ ($p_2=0.62$) it is found to be gapless at the point $\mathbf{q}_{\mathrm{II}}$. In these cases, in Eqs. (12) we can separate out the condensate part $m^2_{\mathbf{q}_0}$ corresponding to Bose condensation on the corresponding antiferromagnetic vector $\mathbf{q}_0$, equal to $\mathbf{q}_{\mathrm{I}}$ or $\mathbf{q}_{\mathrm{II}}$:

$$C_{\mathbf{r}}=\frac{1}{2N}\sum_{\mathbf{q}} F(\mathbf{q})\omega(\mathbf{q})^{-1}e^{-i\mathbf{q}\mathbf{r}}+e^{-i\mathbf{q}_0\mathbf{r}}m^2_{\mathbf{q}0}. \qquad (14)$$

The new unknown $m^2_{\mathbf{q}_0}$ is determined from the equation $\omega(\mathbf{q}_0)=0$. From the expression (11) for $\omega^2(\mathbf{q})$ we can see that $\omega^2(\mathbf{q}_{\mathrm{I}})$ is proportional to A_1, and $\omega^2(\mathbf{q}_{\mathrm{II}})$ is proportional to the sum of the first three terms in the right-hand side of Eq. (11). A nonzero value of $m_{\mathbf{q}_0}$ is the effective spin, since

$$C^{\mathrm{I}}_{r\to\infty}=m^2_{\mathbf{q}0}(-1)^{n_x+n_y}, \quad p<p_1 \qquad (15.1)$$

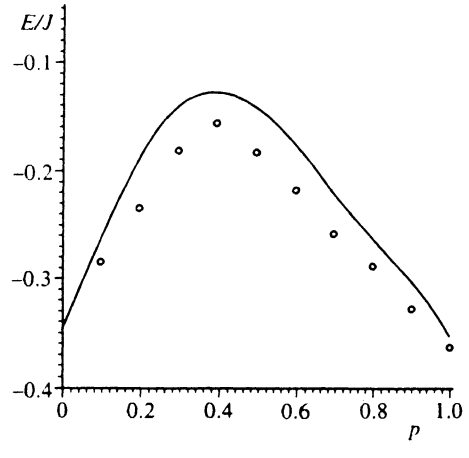

FIG. 4. Energy per bond (E/J) as a function of the frustration parameter p, and results from a calculation in Ref. 7 on blocks of 20 spins.

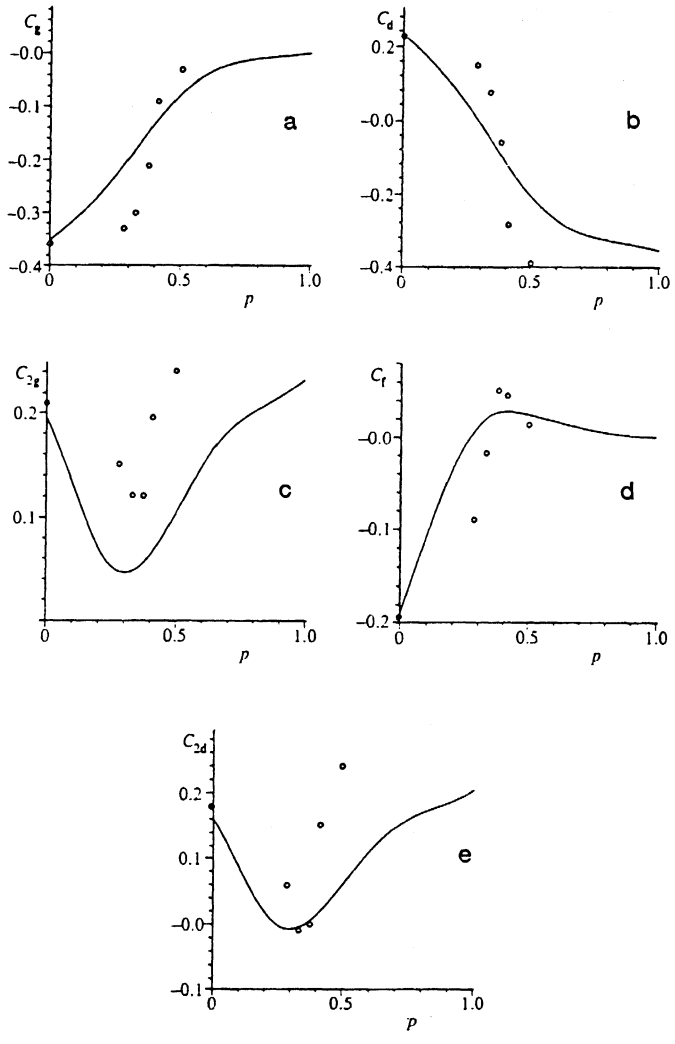

FIG. 5. Correlation functions $C_{\mathbf{r}}$ as functions of the frustration parameter p. The points are the results from a calculation in Ref. 24 on blocks of 20 spins: (a) $C_{\mathbf{g}}$; (b) $C_{\mathbf{d}}$; (c) $C_{2\mathbf{g}}$; (d) $C_{\mathbf{f}}$; (e) $C_{2\mathbf{d}}$.

$$C^{\mathrm{II}}_{r\to\infty}=(1/2)m^2_{\mathbf{q}0}((-1)^{n_x}+(-1)^{n_y}), \quad p>p_2. \qquad (15.2)$$

Thus, in two different intervals of values of the frustration parameter we are describing two different states with long-range order, analogous to the Néel phase I and stripe phase II. We draw attention to the fact that the long-range order (15.2) in the phase II preserves the square symmetry, in contrast to the approaches mentioned in the Introduction, which lead to long-range order of the form (3.2). In addition, unlike the theories of modified spin waves and the mean-field approximation for Schwinger bosons, in our approach Bose condensation at $\mathbf{q}=0$ is absent. The dependence of the effective spin on the frustration parameter is presented in Fig. 2.

Solutions of the second type, when $\omega(\mathbf{q})>0$ holds for all $\mathbf{q}\neq 0$, are found in the interval $p_1<p<p_2$. In this region of values of p the effective spin is equal to zero, the correlation functions fall off exponentially at large distances, and the system is in the spin-liquid state.

We shall explain how the system of equations (12), (13.1) is solved for $T=0$. In the cases $p=0$ and $p=1$ this

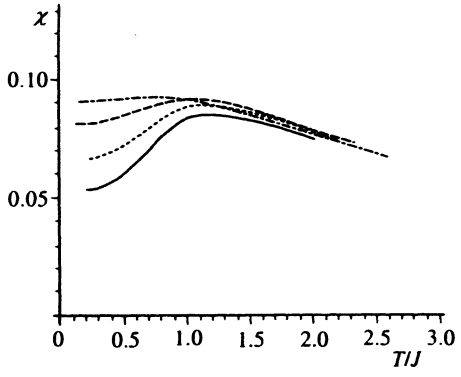

FIG. 6. Temperature dependence of the uniform static susceptibility $\chi(T)$ for different values of the frustration parameter: $p=0$ (the solid curve), $p=0.09$ (the dotted curve), $p=0.16$ (the dashed curve), and $p=0.23$ (the dashed-dotted curve).

system [with allowance for (14)] is solved analytically. The values obtained for the spin correlation functions, r_α, and α_1 are used as the starting point for a numerical iterative method of solution of the system of equations for $p\neq 0$ and $p\neq 1$. After each step in p we first solve the truncated self-consistent system (12), (13.1) for α_1, the correlator $C_{\mathbf{g}}$, and also m or the gap in the spectrum (11) (in the case when a solution with a gap arises). Here we first use the values obtained for the long-range correlators $C_{\mathbf{d}}$, $C_{2\mathbf{g}}$, $C_{\mathbf{f}}$, and $C_{2\mathbf{d}}$ in the previous step in p. The resulting self-consistent values of α_1, $C_{\mathbf{g}}$, and m (or the gap) are used to find new values of the long-range correlators, and with the latter we again implement self-consistency for the truncated system. This procedure leads to rapid convergence of the results.

In Fig. 3 we show the dependences of the gaps $\omega(\mathbf{q}_{\mathrm{I}})$ and $\omega(\mathbf{q}_{\mathrm{II}})$ on the frustration, which determine the properties of the system. At $p=p_1$ a gap opens up at the point $\mathbf{q}_{\mathrm{I}}$. With further increase of p the gap $\omega(\mathbf{q}_{\mathrm{I}})$ remains nonzero, but behaves nonmonotonically. The gap $\omega(\mathbf{q}_{\mathrm{II}})$ decreases monotonically with increase of p, and vanishes at the point p_2. At the points p_1 and p_2 a continuous transition is realized between a phase with long-range order and the spin-liquid phase.

The energy per site and the first five correlation functions are presented as functions of p in Figs. 4 and 5. There too, for comparison, we give results of calculations on finite blocks[24,7] of up to 20 sites. As can be seen, our results agree qualitatively with the results of exact diagonalization on finite systems. It is difficult to speak of quantitative agreement, especially for $p>1/3$. This is because, as p increases, the system approaches two noninteracting square sublattices. For example, a block of 16 sites decomposes into two noninteracting blocks of 8 sites. Consequently, in calculations on finite lattices the correlators are calculated in different approximations for small and large p. In particular, this leads to the result that relations of the form $C_{\mathbf{d}}(p=1)=C_{\mathbf{g}}(p=0)$ are not fulfilled. Our results, however, satisfy this condition.

In the case of finite temperatures ($T\neq 0$), for all values of the frustration parameter p, in the spectrum $\omega(\mathbf{q})$ there is a nonzero gap everywhere except $\mathbf{q}=0$. Solving the system of equations (12) makes it possible to determine the uniform static susceptibility $\chi(T,p)$. The latter is the Green's function $G^{\sigma}(\mathbf{q},\omega)$ at $\mathbf{q}=0$ and $\omega=0$.

Figure 6 shows the temperature dependences $\chi(T)$ for values of the frustration parameter p that correspond to the ordered phase I and the spin liquid. It can be seen that for small p the susceptibility $\chi(T)$ has a broad maximum at $T\sim J$. With increase of the frustration this maximum is shifted in the direction of lower T. We shall regard the frustration parameter p as the analog of the doping x for $La_{2-x}Sr_xCuO_4$. It can then be seen that the dependence $\chi(p,T)$ in Fig. 6 coincides qualitatively with the experimental dependence $\chi(x,T)$ in Ref. 30.

4. CONCLUSION

In conclusion we shall formulate the principal results and note the essential difference between our method and previous treatments.

Using Green functions and approximations of spherically symmetric spin correlations we have succeeded in describing within the framework of a single theory two phases with different long-range order and the spin-liquid phase separating them, and also the continuous transitions between them in the frustration parameter. For small values $p<0.1$ the system is in a state with long-range order, analogous to the Néel state, and the spin-excitation spectrum is gapless at the point $\mathbf{q}_{\mathrm{I}}=(\pm\pi,\pm\pi)$, at which Bose condensation of the spin waves occurs. At $p_1=0.1$ a gap opens up at the point $\mathbf{q}_{\mathrm{I}}$, the system loses its long-range order, and the ground state is the spin-liquid state. With increase of p the gap at the points $\mathbf{q}_{\mathrm{II}}=(\pm\pi,0)$, $(0,\pm\pi)$ decreases, and vanishes at $p_2=0.62$. For $p>0.62$ Bose condensation occurs at the point $\mathbf{q}_{\mathrm{II}}$, and the system is in a state with long-range order, analogous to the stripe phase but without loss of the square symmetry. At the points p_1 and p_2 second-order transitions occur in the system between the phases described above. We draw attention to the fact that the parameter value $p=0.1$ for the first transition between a phase with long-range order and the spin-liquid phase differs greatly from the results obtained by other approaches (0.274 in Refs. 6 and 10, 0.2 in Refs. 22 and 23, and 0.38 in Refs. 15–17). A close value $p=0.13$ was obtained in Ref. 25.

Finally, we note that the temperature dependence obtained in this work for the static uniform susceptibility $\chi(T,p)$ for different frustrations p agrees qualitatively with $\chi(T,x)$ for high-temperature superconductors (x is the parameter specifying the doping of the CuO_2 plane by holes), if we assume that the frustration is the analog of the doping. At the same time, the temperature behavior found for $\chi(T)$ for the spin-liquid state ($p>0.1$) differs fundamentally from the results of the theory based on the mean-field approximation for Schwinger bosons,[18] in which, in the spin-liquid state, $\chi(T)\to 0$ as $T\to 0$. The reason for the discrepancy could be the fact that, in contrast to our approach, in this theory (and in the others listed in the Introduction), the spin-excitation spectrum is found to be symmetric with respect to the boundaries of the magnetic Brillouin zone both in the Néel phase and in the stripe phase. The point $\mathbf{q}_0=(0,0)$ is identical to the

corresponding Bose-condensation points $\mathbf{q}_{\mathrm{I}}$ and $\mathbf{q}_{\mathrm{II}}$ in these phases. Therefore, in the mean-field approximation for Schwinger bosons, when long-range order is lost as $T\to 0$ a gap simultaneously opens up at the points $\mathbf{q}_{\mathrm{I}}$ and $\mathbf{q}_{0}$, and, as a consequence, $\chi(T)\propto(1/T)\exp(-\Delta/T)\to 0$ as $T\to 0$ $[\Delta=\omega(\mathbf{q}_{0})]$.

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