

Phase diagrams in the SO(5) quantum rotor theory of high- T_c superconductivity

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Using the spherical approach for the three-dimensional quantum rotor we have studied the thermodynamic properties of Zhang's SO(5) quantum rotor theory. We have performed a non-mean-field treatment of the lattice version of the nonlinear quantum σ model and discussed possible scenarios for temperature-doping phase diagrams. The model considered can contain large SO(5) anisotropy parameters (like spin, charge, and so-called " π " susceptibilities which regulate the strength of the quantum fluctuations). It is found that the topology of the temperature-chemical-potential (T - μ) phase diagrams assumes different forms depending on the strength of the quantum fluctuations. In the SO(5)-symmetric kinetic energy model we established the condition for the existence of the quantum critical point separating antiferromagnetic and superconducting states at zero temperature. In the intermediate quantum fluctuation regime there is a first-order transition between the antiferromagnetic and superconducting phases. For the class of models with an asymmetric kinetic energy parts we found no evidence for the existence of the intermediate mixed so-called "spin bag" phase in the T - μ phase diagram.

I. INTRODUCTION

The unified theory of antiferromagnetism (AF) and superconductivity (SC) proposed for the high- T_c cuprates by Zhang¹ and based on the SO(5) symmetry between AF and SC states offers a unified description of the global phase diagram of this class of materials. The AF phase is described by a three-dimensional order parameter (the staggered magnetization), while a spin-singlet d -wave SC phase is described by a complex order parameter (with two real components). The idea of the SO(5) theory is to group these five components into an object called "superspin" and to introduce a well-defined rotation operator, which can transform AF into SC and vice versa. This SO(5) symmetry contains as subgroups the SO(3) symmetry of spin rotations (which is spontaneously broken in the AF phase) and the electromagnetic SO(2) invariance (whose breaking defines the SC phase). In Zhang's theory both ordered phases arise once SO(5) is spontaneously broken and the competition between antiferromagnetism and superconductivity is related to the direction of the "superspin" in the five-dimensional space. The low-energy dynamics of the system is determined in terms of Goldstone bosons and their interactions specified by the SO(5) symmetry. The kinetic energy of the system is that of a SO(5) rigid rotor and the system is described by a SO(5) nonlinear quantum σ model (NLQ σ M). The SO(5) quantum rotor model offers a Landau-Ginzburg-like (LG-like) theory for the high- T_c problem. However, it goes much beyond traditional LG theory, since it captures dynamics.

While the SO(5) symmetry was originally proposed in the context of an effective field-theory description of the high- T_c superconductors, its prediction can also be tested within microscopic models.²⁻⁷ For example, numerical evidence for an approximate SO(5) symmetry of the Hubbard model came from the exact diagonalization of small-sized clusters.⁸ Ultimately one should compare the prediction from SO(5) theory with experimentally observed phase diagrams. While the

global features of the phase diagram deduced from SO(5) theory based on a mean-field-type treatment¹ agree reasonably with the general topology of the observed phase diagram of high- T_c superconductors, systematic thermodynamic studies of the SO(5) theory are called for. Very recently the temperature vs chemical-potential phase diagrams of an SO(5) model for high- T_c cuprates were calculated by Monte Carlo simulations.^{9,10} A bicritical point was found, where the AF and SC transition lines merge into a first-order line. However, quantum fluctuations, which may reduce the bicritical point, were not included in this calculation. When quantum fluctuations are gradually increased ordering in some phases might be destroyed. In order to include quantum effects properly one has to treat the kinetic and potential energies on an equal footing. Very recently a quantum vector spin model based on the spinor representation of the SO(5) group, in which the SO(5) symmetry is weakly broken into $U(1) \times SO(3)$, was proposed as a model for systems with strong correlations between superconductivity and antiferromagnetism.¹¹

Because the superspin vector in the SO(5) theory is affected by thermal *and* quantum fluctuations, the effect on the competition between them is highly nontrivial. Therefore, investigation of the SO(5) theory, which takes into account both of them in the rotation of superspins between AF and SC subspaces, is of paramount importance. This issue is also of great interest from the general viewpoint of the theory of quantum phase transitions and related critical phenomena. Of special interest is the possibility of the SO(5)-symmetric quantum critical point to account for the non-Fermi-liquid normal-state properties, d -wave superconductivity, and strong doping dependence of the superconducting critical temperature.^{12,13}

It is the goal of the present paper to explore the possible scenarios for the phase diagrams within the SO(5) theory by focusing on the role of thermal and quantum effects. A systematic formulation of the quantum problem is complicated

by two factors: (1) the problem has a dynamical nature from the outset, and (2) the role of thermal and quantum fluctuations precludes the implementation of mean-field-type approaches. Therefore, it is essential to find a way of systematic parametrization of quantum and thermal effects. To this end we introduce in the present paper a mapping of the quantum SO(5) Hamiltonian onto the lattice version of the NLQ σ M and subsequently onto the spherical quantum rotor model (SQRM) in three-dimensional (3D) space which offers the remarkable opportunity of being exactly solvable.

The outline of the remainder of the paper is as follows. In Sec. II we begin by setting up the quantum Hamiltonian and the corresponding Euclidean Lagrangian. In Sec. III the classical approximation yielding the effective energy is employed to reveal the structure of the ground state as a function of doping. Subsequently, in Sec. IV we introduce a non-mean-field treatment of the lattice version of the NLQ σ M in a form of a spherical approach for 3D quantum rotors and discuss possible scenarios for temperature-doping phase diagrams. Finally, in Sec. V we summarize the conclusions to be drawn from our work. Some supplementary material regarding the construction of the effective quantum Lagrangian and SQRM approach appears in the Appendixes.

II. QUANTUM HAMILTONIAN AND THE EFFECTIVE LAGRANGIAN

We have considered the low-energy Hamiltonian proposed by Zhang on a discrete lattice (the lattice quantum nonlinear σ model¹):

$$H = \frac{1}{2} \sum_i \sum_{\mu < \nu} (\chi_{\mu\nu})^{-1} L_i^{\mu\nu} L_i^{\nu\mu} - V(\mathbf{n}) - 2\mu \sum_i L_i^{15} - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}), \quad (1)$$

where $i = 1, \dots, N$ (N is the number of lattice sites). The fundamental quantity in the SO(5) theory is the locally defined five-component superspin vector $\mathbf{n}_i = (n_1, n_2, n_3, n_4, n_5)_i$ describing the local antiferromagnetic $\mathbf{n}_{AF,i} = (n_2, n_3, n_4)_i$ and superconducting $\mathbf{n}_{SC,i} = (n_1, n_5)_i$ parameters, respectively. In Zhang's formulation these are treated as mutually commuting coordinates and their dynamics is given by their conjugate momenta:

$$p_{\mu i} = i \frac{\partial}{\partial n_{\mu i}}, \quad [n_{\mu}, p_{\nu}] = i \delta_{\mu\nu}. \quad (2)$$

The kinetic energy of the system is simply that of a SO(5) rigid rotor ($\mathbf{n}_i^2 = 1$, $\mathbf{p}_i \cdot \mathbf{n}_i = 0$; see Ref. 14) and is given by the first part of Eq. (1). Here

$$L_i^{\mu\nu} = n_{\mu i} p_{\nu i} - n_{\nu i} p_{\mu i} \quad (3)$$

are the generators of SO(5) algebra and L_i^{15} is a charge operator, whose expectation value yields the doping concentration (μ is the chemical potential measured from the half-filling). The parameters $\chi_{\mu\nu}$ measure the kinetic energy of the rotors (moment of inertia). They describe the charge ($\chi_{15} \equiv \chi_c$), spin ($\chi_{23} = \chi_{24} = \chi_{34} \equiv \chi_s$), and so-called ‘‘ π ’’ susceptibilities ($\chi_{1(2,3,4)} = \chi_{(2,3,4)5} \equiv \chi_\pi$). Furthermore, the corresponding stiffness in the charge (J_{ij}^{SC}) and spin (J_{ij}^{AF}) channel has also been introduced. This quantum nonlinear σ model can be derived from a microscopic SO(5)-symmetric model.¹⁵ Then, the superspin coordinates (\mathbf{n}_i , \mathbf{p}_i) are microscopically constructed using lattice (hard-core) bosons¹⁶ and $J_{ij}^{AF(SC)}$ terms stand for their hopping and spontaneous creation (destruction). In the presence of SO(5) symmetry breaking, a quadratic term of the form

$$V(\mathbf{n}_i) = \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2) \quad (4)$$

is also allowed. The anisotropy constant g selects either the ‘‘easy plane’’ in the SC space (n_1, n_5), or an ‘‘easy sphere’’ in the AF space (n_2, n_3, n_4), depending on the sign of g . At half-filling ($\mu = 0$) $g > 0$ is chosen so that the superspin prefers the AF state.

We express the partition function $Z = \text{Tr} e^{-H/k_B T}$ using the functional integral in the Matsubara ‘‘imaginary time’’ τ formulation ($0 \leq \tau \leq 1/k_B T \equiv \beta$, with T being the temperature). We obtain

$$Z = \int \prod_i [D\mathbf{n}_i] \int \prod_i \left[\frac{D\mathbf{p}_i}{2\pi} \right] \delta(1 - \mathbf{n}_i^2) \delta(\mathbf{n}_i \cdot \mathbf{p}_i) \times \exp \left(- \int_0^\beta d\tau \mathcal{L}[\mathbf{p}, \mathbf{n}] \right), \quad (5)$$

with the Euclidean Lagrangian

$$\mathcal{L}[\mathbf{p}, \mathbf{n}] = i\mathbf{p}(\tau) \cdot \frac{d}{d\tau} \mathbf{n}(\tau) + H(\mathbf{n}, \mathbf{p}). \quad (6)$$

We note that the path integral in Eq. (5) is Gaussian in momenta \mathbf{p}_i . Due to the rigid nature of the quantum rotors, one must be careful and integrate only over the transverse components to \mathbf{n}_i with fixed length. This can be implemented by the introduction of a second δ function to maintain the local constraint $\mathbf{p}_i \cdot \mathbf{n}_i = 0$ and $\mathbf{n}_i^2 = 1$. Performing the path integration over the momenta (see Appendix A) we obtain

$$Z = \int \prod_i [D\mathbf{n}_i] \delta(1 - \mathbf{n}_i^2) \exp \left(- \int_0^\beta d\tau \mathcal{L}[\mathbf{n}] \right), \quad (7)$$

where

$$\begin{aligned}
\mathcal{L} = & \frac{1}{2} \sum_i \left[\frac{1}{\mathbf{n}_{SC,i}^2} \left(\chi_\pi - \frac{1}{\chi_c^{-1} \mathbf{n}_{SC,i}^2 + \chi_\pi^{-1} \mathbf{n}_{AF,i}^2} \right) \left(\frac{1}{2} \frac{\partial \mathbf{n}_{SC,i}^2}{\partial \tau} \right)^2 + \frac{1}{\chi_c^{-1} \mathbf{n}_{SC,i}^2 + \chi_\pi^{-1} \mathbf{n}_{AF,i}^2} \left(\frac{\partial \mathbf{n}_{SC,i}}{\partial \tau} \right)^2 \right] \\
& + \frac{1}{2} \sum_i \left[\frac{1}{\mathbf{n}_{AF,i}^2} \left(\chi_\pi - \frac{1}{\chi_\pi^{-1} \mathbf{n}_{SC,i}^2 + \chi_s^{-1} \mathbf{n}_{AF,i}^2} \right) \left(\frac{1}{2} \frac{\partial \mathbf{n}_{AF,i}^2}{\partial \tau} \right)^2 + \frac{1}{\chi_\pi^{-1} \mathbf{n}_{SC,i}^2 + \chi_s^{-1} \mathbf{n}_{AF,i}^2} \left(\frac{\partial \mathbf{n}_{AF,i}}{\partial \tau} \right)^2 \right] \\
& - \frac{1}{2} \sum_i \frac{1}{\chi_c^{-1} \mathbf{n}_{SC,i}^2 + \chi_\pi^{-1} \mathbf{n}_{AF,i}^2} \left[4\mu^2 (n_{1i}^2 + n_{5i}^2) + 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) \right] \\
& - \sum_{i<j} J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} - \sum_{i<j} J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j} - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2)
\end{aligned} \tag{8}$$

is the effective Lagrangian written in terms of superspin vectors.

III. EFFECTIVE CLASSICAL POTENTIAL AND STATIC SOLUTIONS

The classical path extremizing the path integral [see Eqs. (7) and (8)] is the static solutions. For the static and uniform solutions [$\mathbf{n}_i(\tau) \equiv \mathbf{n}_i$], the only nonvanishing contribution to the kinetic energy is the chemical potential term, which gives us the effective potential energy per superspin,

$$E(\theta, \mu) \equiv \frac{1}{\beta N} \int_0^\beta d\tau \mathcal{L}[\mathbf{n}_i(\tau) \equiv \mathbf{n}], \tag{9}$$

in the form¹⁷

$$E(\theta, \mu) = - \frac{2\mu^2 (n_{1i}^2 + n_{5i}^2)}{\chi_\pi^{-1} \mathbf{n}_{AF}^2 + \chi_c^{-1} \mathbf{n}_{i,SC}^2} - \frac{g}{2} (n_{2i}^2 + n_{3i}^2 + n_{4i}^2). \tag{10}$$

Without loss of generality one can choose the superspin vector $\mathbf{n} = (\sin \theta, \cos \theta, 0, 0, 0)$ which tilts between SC and AF states according to the angular parameter θ (for $\theta=0$ the superspin lies on the AF sphere, for $\theta=\pi/2$ in the SC plane). Then the energy (10) reads

$$E(\theta, \mu) = - \frac{2\mu^2 \sin^2 \theta}{\chi_\pi^{-1} \cos^2 \theta + \chi_c^{-1} \sin^2 \theta} - \frac{g}{2} \cos^2 \theta. \tag{11}$$

Depending on the relative magnitude of the parameters (χ_π, χ_c) the following cases are in order.

A. Symmetric case ($\chi_c = \chi_\pi = \chi$)

The effective potential energy (11) reduces to

$$E(\theta, \mu) = -2\mu^2 \chi \sin^2 \theta - \frac{g}{2} \cos^2 \theta. \tag{12}$$

The energy reaches its local extrema

$$\frac{\partial E(\theta, \mu)}{\partial \theta} = \cos \theta \sin \theta [-4\chi\mu^2 + g] = 0 \tag{13}$$

for

$$\theta = 0; \quad \theta = \frac{\pi}{2} \text{ or } \mu = \sqrt{\frac{g}{4\chi}}. \tag{14}$$

Inspection of the second derivative

$$\frac{\partial^2 E(\theta, \mu)}{\partial \theta^2} = (g - 4\chi\mu^2) \cos 2\theta \tag{15}$$

leads us to the conclusion that the minima of the energy exist for

$$\begin{aligned}
\theta = 0, \quad \text{when } \mu < \sqrt{\frac{g}{4\chi}}, \\
\theta = \pi/2, \quad \text{when } \mu > \sqrt{\frac{g}{4\chi}}.
\end{aligned} \tag{16}$$

Consequently, at $\mu = \sqrt{g/(4\chi)}$ there is a superspin ‘‘flop’’ between the angles $\theta=0$ and $\theta=\pi/2$; i.e., there is a first-order transition between AF and SC states. This happens at the chemical potential given by

$$E(0, \mu_c) = E\left(\frac{\pi}{2}, \mu_c\right) \Rightarrow \mu_c = \sqrt{\frac{g}{4\chi}}. \tag{17}$$

The corresponding doping concentration x for AF and SC phases is given by

in the AF state,

$$x_{AF}(\mu) = -\frac{1}{2} \frac{\partial E(0, \mu)}{\partial \mu} = 0 \quad \text{for } \mu < \sqrt{\frac{g}{4\chi}},$$

in the SC state,

$$\begin{aligned}
x_{SC}(\mu) &= -\frac{1}{2} \frac{\partial E(\pi/2, \mu)}{\partial \mu} \\
&= 2\chi\mu \quad \text{for } \mu > \sqrt{\frac{g}{4\chi}}.
\end{aligned} \tag{18}$$

That is, at the transition point there is a discontinuity in x , which jumps from $x_{AF}(\mu_c) = 0$ to $x_{SC}(\mu_c) = \sqrt{g\chi}$ [see Fig. 1(a)].

B. Asymmetric case ($\chi_c \neq \chi_\pi$)

The extremum condition for the classical effective potential is

$$\frac{\partial E(\theta, \mu)}{\partial \theta} = \cos \theta \sin \theta \left[\frac{4\mu^2 \sin^2 \theta (\chi_c^{-1} - \chi_\pi^{-1})}{(\chi_\pi^{-1} \cos^2 \theta + \chi_c^{-1} \sin^2 \theta)^2} + g - \frac{4\mu^2}{\chi_\pi^{-1} \cos^2 \theta + \chi_c^{-1} \sin^2 \theta} \right] = 0, \quad (19)$$

which gives

$$\theta = 0; \quad \theta = \frac{\pi}{2}; \quad \sin \theta = \sqrt{\frac{\chi_c - 2\chi_c \mu \sqrt{\chi_\pi/g}}{\chi_c - \chi_\pi}}. \quad (20)$$

From the second-derivative analysis

$$\frac{\partial^2 E(\theta, \mu)}{\partial \theta^2} = g \cos 2\theta - \frac{8\chi_c^2 \chi_\pi \mu^2 [2(\chi_c + \chi_\pi) \cos 2\theta + (\chi_c - \chi_\pi)(3 - \cos 4\theta)]}{[\chi_c + \chi_\pi + (\chi_c - \chi_\pi) \cos 2\theta]^3}, \quad (21)$$

we find that the minima of the energy exist for

$$\begin{aligned} \theta = 0 \quad \text{when} \quad \mu < \mu_c^{AF} &\equiv \sqrt{\frac{g}{4\chi_\pi}}, \\ \theta = \pi/2 \quad \text{when} \quad \mu > \mu_c^{SC} &\equiv \sqrt{\frac{\chi_\pi}{\chi_c}} \sqrt{\frac{g}{4\chi_c}}, \\ \sin \theta = \sqrt{\frac{\chi_c - 2\chi_c \mu \sqrt{\chi_\pi/g}}{\chi_c - \chi_\pi}} &\quad \text{when} \quad \chi_\pi > \chi_c. \end{aligned} \quad (22)$$

As a result, for $\chi_\pi < \chi_c$ there is the superspin ‘‘flop’’ between the angles $\theta = 0$ and $\theta = \pi/2$, similarly as in the symmetric case. In analogy, the first-order transition point can be obtained from the condition of the energy equality:

$$E(0, \mu_c) = E\left(\frac{\pi}{2}, \mu_c\right) \Rightarrow \mu_c = \sqrt{\frac{g}{4\chi_c}}. \quad (23)$$

However, we notice that for the chemical potential regime $\mu_c^{SC} < \mu < \mu_c^{AF}$ the energy has two local minima corresponding to $\theta = 0$ and $\theta = \pi/2$ states. Although the transition point is at μ_c , for $\mu_c < \mu < \mu_c^{AF}$ there is a metastable AF state and for $\mu_c^{SC} < \mu < \mu_c$ a metastable SC state [see Fig. 1(b)]. The charge concentration in the corresponding phases is given by

$$\begin{aligned} \text{in the AF state,} \quad x_{AF}(\mu) &= -\frac{1}{2} \frac{\partial E(0, \mu)}{\partial \mu} \\ &= 0 \quad \text{for} \quad \mu < \sqrt{\frac{g}{4\chi_\pi}}, \\ \text{in the SC state,} \quad x_{SC}(\mu) &= -\frac{1}{2} \frac{\partial E(\pi/2, \mu)}{\partial \mu} \\ &= 2\chi_c \mu \quad \text{for} \quad \mu > \frac{\chi_\pi}{\chi_c} \sqrt{\frac{g}{4\chi_\pi}}. \end{aligned} \quad (24)$$

For $\chi_\pi > \chi_c$ a mixed phase (M) exists for

$$0 < \theta_M = \arcsin\left(\sqrt{\frac{\chi_c - 2\chi_c \mu \sqrt{\chi_\pi/g}}{\chi_c - \chi_\pi}}\right) < \pi/2, \quad (25)$$

the energy of which is

$$E(\theta_M, \mu) = \frac{g\chi_\pi - 4\chi_c \sqrt{g\chi_\pi} + 4\chi_c \chi_\pi \mu^2}{2(\chi_c - \chi_\pi)}. \quad (26)$$

The transition points between AF (SC) and M states are, respectively,

$$\begin{aligned} \text{AF} \Leftrightarrow M: \quad E(\theta_M, \mu_{c1}) &= E(0, \mu_{c1}) \Rightarrow \mu_{c1} = \sqrt{\frac{g}{4\chi_\pi}} = \mu_c^{AF}, \\ \text{SC} \Leftrightarrow M: \quad E(\theta_M, \mu_{c2}) &= E\left(\frac{\pi}{2}, \mu_{c2}\right) \\ &\Rightarrow \mu_{c2} = \frac{\chi_\pi}{\chi_c} \sqrt{\frac{g}{4\chi_\pi}} = \mu_c^{SC}. \end{aligned} \quad (27)$$

The charge concentration for the mixed phase is given by

$$x_M(\mu) = -\frac{1}{2} \frac{\partial E(\theta_M, \mu)}{\partial \mu} = \frac{\sqrt{g\chi_\pi} \chi_c + 2\chi_c \chi_\pi \mu}{\chi_\pi - \chi_c}. \quad (28)$$

At the transition points (μ_c^{AF} and μ_c^{SC}) there are discontinuities in x , which jumps at μ_c^{AF} from $x_{AF}(\mu_c^{AF}) = 0$ to

$$x_M(\mu_c^{AF}) = \frac{2\sqrt{g\chi_\pi} \chi_c}{\chi_\pi - \chi_c} \quad (29)$$

and at μ_c^{SC} from

$$x_M(\mu_c^{SC}) = \frac{\sqrt{g\chi_\pi} (\chi_c + \chi_\pi)}{\chi_\pi - \chi_c} \quad (30)$$

to $x_{SC}(\mu_c^{SC}) = \sqrt{g\chi_\pi}$ [see Fig. 1(c)].

Before attempting to construct the global phase diagram from SO(5) theory, we must remember that the discussion above is based merely on the classical approximation by assuming that quantum effects are negligible. On the other hand, quantum fluctuations may have a strong effect on the long-range order. In the limit when the kinetic energy domi-

nates, the first term of the Eq. (1) can be no longer treated as a perturbation. In the following section we address the issue of quantum effects by establishing a theoretical framework for treating interacting quantum rotors.

IV. SPHERICAL QUANTUM ROTOR MODEL

A. Models with a SO(5)-symmetric kinetic part

If $\chi_c = \chi_s = \chi_\pi = \chi$, then the kinetic part of the energy is symmetric and the Lagrangian simplifies to the form

$$\begin{aligned} \mathcal{L}[\mathbf{n}] = & \sum_i \frac{\chi}{2} \left[\left(\frac{\partial \mathbf{n}_i}{\partial \tau} \right)^2 - 4\mu^2 (n_{1i}^2 + n_{5i}^2) \right. \\ & + 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) \left. - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2) \right. \\ & \left. - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}) \right]. \end{aligned} \quad (31)$$

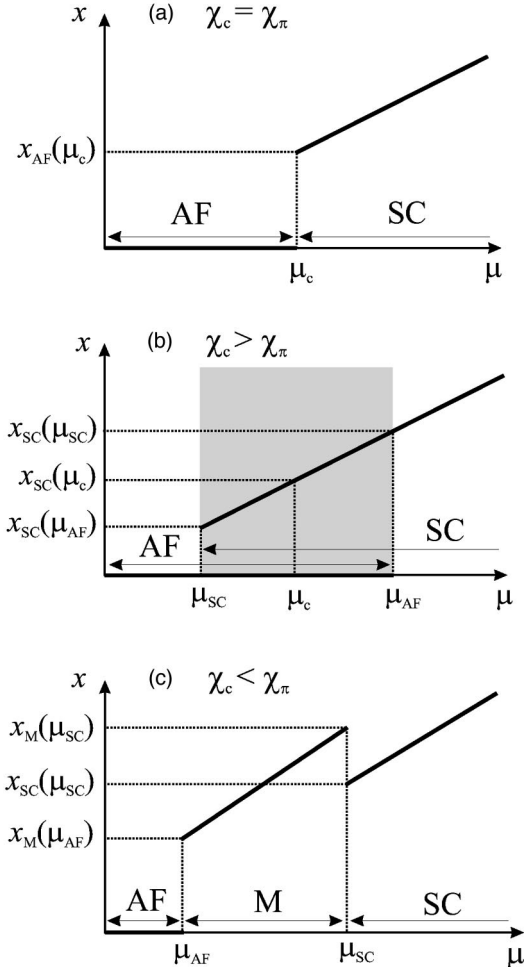


FIG. 1. Doping concentration vs chemical potential dependence from the classical effective energy. Shown are (a) the symmetric case $\chi_c = \chi_\pi$ with first-order phase transition, (b) the asymmetric case $\chi_c > \chi_\pi$ with first-order phase transition, and (c) the asymmetric case $\chi_c < \chi_\pi$ with mixed region.

From the definition of the superspin variables \mathbf{n}_i the rigid constraint $\mathbf{n}_i^2 = 1$ implies that a weaker conditions also applies, namely,

$$\sum_{i=1}^N \mathbf{n}_i^2 = N. \quad (32)$$

The main idea of our approach is to attempt to generate an effective partition function, which incorporates the constrained nature of the original variables. This leads us to the formulation of the problem in terms of the spherical model¹⁸ by implementing the constraint (32). The name of the model comes from the observation that in Eq. (32) the allowed states are all points on the surface of a hypersphere (in dimension $d = 5N$) of radius \sqrt{N} . The model defined by Eq. (32) is in fact a hybrid of the genuine spherical model and five-component vector model. Therefore, with the replacement

$$\prod_i \delta(1 - \mathbf{n}_i^2) \rightarrow \delta\left(N - \sum_i \mathbf{n}_i^2\right), \quad (33)$$

the global constraint in Eq. (5) may be implemented by using the functional analog of the Dirac δ function:

$$\begin{aligned} \delta\left(N - \sum_i \mathbf{n}_i^2\right) = & \int_{c-i\infty}^{c+i\infty} \left[\frac{d\lambda}{2\pi i} \right] \\ & \times \exp\left[\int_0^\beta d\tau \lambda(\tau) \left(N - \sum_i \mathbf{n}_i^2(\tau) \right) \right], \end{aligned} \quad (34)$$

where $\mathbf{n}_i(\tau)$ are c -number fields which satisfy the quantum periodic boundary condition $\mathbf{n}_i(\beta) = \mathbf{n}_i(0)$ and are taken as *continuous* variables, i.e., $-\infty < \mathbf{n}_i(\tau) < \infty$, but constrained [on average, due to Eq. (32)] to have unit length. This introduces the Lagrange multiplier $\lambda(\tau)$, adding an additional quadratic term (in \mathbf{n}_i fields) to the Lagrangian (8). We obtain

$$Z = \int \frac{d\lambda}{2\pi i} e^{-N\phi(\lambda)}, \quad (35)$$

where the function $\phi(\lambda)$ is defined as

$$\begin{aligned} \phi(\lambda) = & - \int_0^\beta d\tau \lambda(\tau) - \frac{1}{N} \ln \int \prod_i [D\mathbf{n}_i] \\ & \times \exp\left[- \sum_i \int_0^\beta d\tau (\mathbf{n}_i^2 \lambda(\tau) - \mathcal{L}[\mathbf{n}]) \right]. \end{aligned} \quad (36)$$

In the thermodynamic limit $N \rightarrow \infty$ the method of steepest descents is exact and the saddle point $\lambda(\tau) = \lambda(0)$ will satisfy the condition

$$\left. \frac{\delta\phi(\lambda)}{\delta\lambda(\tau)} \right|_{\lambda=\lambda_0} = 0. \quad (37)$$

Therefore, we finally arrive at the following expression for the free energy per superspin $f = -(\beta N)^{-1} \ln Z$:

$$f = -\lambda_0 - \frac{1}{\beta N} \ln \int \prod_i [D\mathbf{n}_i] \times \exp \left[- \sum_i \int_0^\beta d\tau (\lambda_0 \mathbf{n}_i^2 - \mathcal{L}[\mathbf{n}]) \right]. \quad (38)$$

This expression is ready for evaluation of the free energy of the system after performing the remaining functional integration over the superspin variables \mathbf{n}_i . In the next sections we shall deal with various SO(5) models resulting from different choices of parameters in the Hamiltonian (1).

Substituting the Lagrangian from Eq. (31), the free energy is equal to

$$f = -\lambda - \frac{1}{\beta N} \ln \int \prod_i [D\mathbf{n}_i] \exp \left(- \int_0^\beta d\tau \left\{ -\lambda \sum_i \mathbf{n}_i^2(\tau) + \sum_i \chi \left[\left(\frac{\partial \mathbf{n}_i}{\partial \tau} \right)^2 - 4\mu^2 (n_{1i}^2 + n_{5i}^2) - 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) \right] - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}) - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2) \right\} \right). \quad (39)$$

Note that the integrations over the superspin variables are now Gaussian and the corresponding quadratic form can be diagonalized. We introduce the Fourier transform fields $\mathbf{n}(\mathbf{k}, \omega_l)$:

$$\mathbf{n}_i(\tau) = \frac{1}{\beta N} \sum_{\mathbf{k}} \sum_{l=-\infty}^{\infty} \mathbf{n}_i(\mathbf{k}, \omega_l) e^{-i(\omega_l \tau - \mathbf{k} \cdot \mathbf{r}_i)}$$

$$J(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{R}_i} J(\mathbf{R}_i) e^{-i\mathbf{R}_i \cdot \mathbf{k}}, \quad (40)$$

with $\omega_l = 2\pi l/\beta$ ($l = 0, \pm 1, \pm 2, \dots$) being the (Bose) Matsubara frequencies and $J^{AF(SC)}(\mathbf{R}_i) = J^{AF(SC)}(|\mathbf{r}_i - \mathbf{r}_j|) \equiv J_{ij}^{AF(SC)}$. We finally obtain for the free energy

$$f = \frac{3}{\beta N} \sum_l \sum_{\mathbf{k}} \ln [2\lambda_0 - J^{AF}(\mathbf{k}) - g + \chi \omega_l^2] + \frac{1}{\beta N} \sum_l \sum_{\mathbf{k}} \ln [2\lambda_0 - J^{SC}(\mathbf{k}) + \chi(\omega_l + 2i\mu)^2] + \frac{1}{\beta N} \sum_l \sum_{\mathbf{k}} [2\lambda_0 - J^{SC}(\mathbf{k}) + \chi(\omega_l - 2i\mu)^2] - \lambda_0. \quad (41)$$

In the presence of a uniform order parameter field $\mathbf{h} = (h_1, h_2, h_3, h_4, h_5)$, which adds a term $\mathbf{h} \cdot \Sigma_i \mathbf{n}_i$ to the Hamiltonian (1), the saddle-point equation (37) and the free energy (41) are modified (see Appendix B). Then the ‘‘magnetization’’ $\mathbf{m} = (m_1, m_2, m_3, m_4, m_5) = -\nabla_{\mathbf{h}} f$ singles out the corresponding AF [$\mathbf{m}_{AF} \equiv (m_1, m_5)$] and/or SC [$\mathbf{m}_{SC} = (m_2, m_3, m_4)$] state.

Criticality conditions and phase diagrams

The critical lines for the AF and SC states in the spherical model are obtained by setting corresponding ‘‘magnetizations’’ to zero ($\mathbf{m}_{AF} = 0$ for AF and $\mathbf{m}_{SC} = 0$ for SC). Alternatively we may define the critical lines using order parameter susceptibilities given by the following correlation functions:

$$G_{ij}^{AF}(\tau) = \langle \mathbf{n}_{AF,i}(\tau) \cdot \mathbf{n}_{AF,j}(0) \rangle,$$

$$G_{ij}^{SC}(\tau) = \langle \mathbf{n}_{SC,i}(\tau) \cdot \mathbf{n}_{SC,j}(0) \rangle, \quad (42)$$

where the average $\langle \dots \rangle$ is defined as

$$\langle \dots \rangle = \frac{1}{Z} \int \prod_i [D\mathbf{n}_i] \int \prod_i \left[\frac{D\mathbf{p}_i}{2\pi} \right] \times \delta \left(N - \sum_i \mathbf{n}_i^2 \right) \delta(\mathbf{n}_i \cdot \mathbf{p}_i) \dots \exp \left(- \int_0^\beta d\tau \mathcal{L}[\mathbf{p}, \mathbf{n}] \right). \quad (43)$$

Using the Lagrangian from Eq. (31) we obtain for the Fourier-transformed quantities

$$G_{AF}(\mathbf{k}, \omega_l) = \frac{3}{2\lambda - J^{AF}(\mathbf{k}) + \chi \omega_l^2 - g},$$

$$G_{SC}(\mathbf{k}, \omega_l) = \frac{1}{2\lambda - J^{SC}(\mathbf{k}) + \chi(\omega_l + 2i\mu)^2} + \frac{1}{2\lambda - J^{SC}(\mathbf{k}) + \chi(\omega_l - 2i\mu)^2}. \quad (44)$$

At criticality corresponding susceptibilities becomes infinite:

$$G_{AF}^{-1}(\mathbf{k} = \mathbf{0}, \omega_l = 0) = 0,$$

$$G_{SC}^{-1}(\mathbf{k} = \mathbf{0}, \omega_l = 0) = 0, \quad (45)$$

which allows one to find Lagrange multipliers as

$$\lambda_0^{AF} = \frac{1}{2} J^{AF}(\mathbf{k}=\mathbf{0}) + \frac{g}{2}, \quad J \equiv J^{SC} \quad \text{and} \quad \kappa = \frac{J^{AF}}{J^{SC}} \Rightarrow J^{AF} \equiv \frac{J^{AF}}{J^{SC}} J = \kappa J, \quad (49)$$

$$\lambda_0^{SC} = \frac{1}{2} J^{SC}(\mathbf{k}=\mathbf{0}) + 2\chi\mu^2. \quad (46)$$

Furthermore, it is convenient to introduce the density of states defined as

$$\rho(z) = \frac{1}{N} \sum_{\mathbf{k}} \delta[z - \varepsilon(\mathbf{k})], \quad (47)$$

where $\varepsilon(\mathbf{k}) = \cos k_x + \cos k_y + \cos k_z$ is the structure factor for the simple cubic lattice in three dimensions.¹⁹ Explicitly,

$$\rho(z) = \frac{1}{\pi^3} \int_{\max(-1, -2-z)}^{\min(1, 2-z)} du \frac{1}{\sqrt{1-u^2}} \times \mathbf{K} \left[\sqrt{1 - \left(\frac{z+u}{2} \right)^2} \right] \Theta(3-|z|), \quad (48)$$

where $\mathbf{K}(x)$ is an elliptic integral of the first kind.²⁰ Introducing

the free energy (41) can be written then

$$f(\lambda_0, \mu) = -\lambda_0 + \frac{2}{\beta} \int_{-\infty}^{\infty} dz \rho(z) \times \ln \left\{ \left[2 \sinh \left(\frac{\beta}{2} \sqrt{\frac{2\lambda_0 - \kappa J z - g}{\chi}} \right) \right]^3 \times 2 \sinh \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda_0 - J z}{\chi}} + 2\mu \right) \right] \times 2 \sinh \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda_0 - J z}{\chi}} - 2\mu \right) \right] \right\}. \quad (50)$$

Using the saddle-point condition and the appropriate Lagrange multipliers (λ_0^{AF} , λ_0^{SC}) we obtain equations for the second-order transition critical lines separating AF (SC) and quantum-disordered (QD) phases:

$$\text{QD} \Leftrightarrow \text{AF}: \quad 1 = \int_{-\infty}^{\infty} \rho(z) dz \left\{ 3 \frac{\coth \left(\frac{\beta}{2} \sqrt{\frac{3\kappa J - \kappa J z}{\chi}} \right)}{\sqrt{\chi(3\kappa J - \kappa J z)}} + 2 \frac{\coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3\kappa J - J z + g}{\chi}} + 2\mu \right) \right] + \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3\kappa J - J z + g}{\chi}} - 2\mu \right) \right]}{2\sqrt{\chi(3\kappa J - J z + g)}} \right\};$$

$$\text{QD} \Leftrightarrow \text{SC}: \quad 1 = \int_{-\infty}^{\infty} \rho(z) dz \left\{ 3 \frac{\coth \left(\frac{\beta}{2} \sqrt{\frac{3J - \kappa J z - g + 4\chi\mu^2}{\chi}} \right)}{\sqrt{\chi(3J - \kappa J z - g + 4\chi\mu^2)}} + 2 \frac{\coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3J - J z + 4\chi\mu^2}{\chi}} + 2\mu \right) \right] + \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3J - J z + 4\chi\mu^2}{\chi}} - 2\mu \right) \right]}{2\sqrt{\chi(3J - J z + 4\chi\mu^2)}} \right\}. \quad (51)$$

The self-consistent equations (51) determine the external phase boundaries $T_c(\mu)$ between AF (SC) and QD phases. The above expressions give the dependence of the physical quantities in terms of the chemical potential μ . From Eq. (50) it follows that the free energy of the AF phase, $f(\lambda_0^{AF}, \mu)$, assumes real values for $\mu \leq \mu_{\text{crit}}$, whereas the free energy of the SC phase, $f(\lambda_0^{SC}, \mu)$, assumes real values for $\mu \geq \mu_{\text{crit}}$. Moreover,

$$f(\lambda_0^{AF}, \mu_c) = f(\lambda_0^{SC}, \mu_c), \quad (52)$$

which is just a condition for the first-order phase transition between AF and SC phases at $\mu = \mu_c$ [see Figs. 2 and 3(a)]. As a consequence, there is no intermediate mixed region on the T - μ phase diagram, where AF and SC states can coexist in contrast to the findings in Sec. III based on the quasiclassical approximation. Therefore, it appears that the scenario

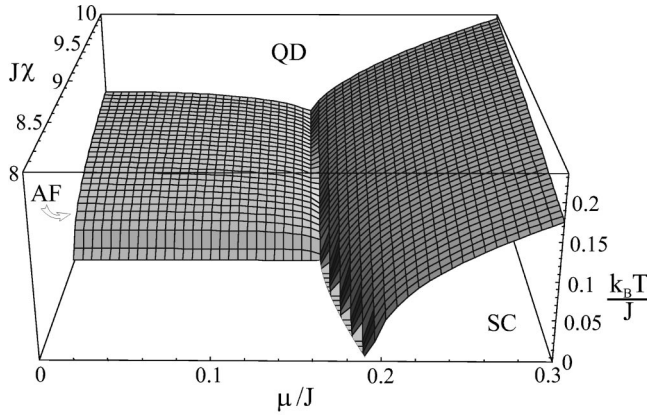


FIG. 2. $k_B T/J$ - μ/J - $J\chi$ phase diagram for the SO(5)-symmetric kinetic energy part model.

depicted in Fig. 1(b) in Zhang's paper,¹ where there are two second-order phase transitions with an intermediate "spin-bag" phase and tetracritical point, is ruled out. The dependence of parameter interplay on system ordering can be also found from investigation of the zero-temperature ground state of the system (see Figs. 4 and 5). Depending on the kinetic energy parameter χ (which regulates the strength of the quantum fluctuations) we can identify the following scenarios for the possible phase diagrams.

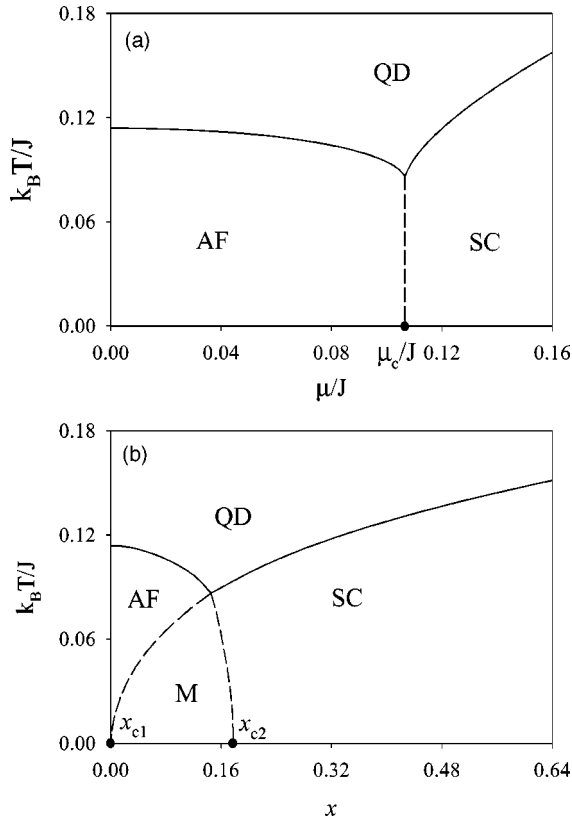


FIG. 3. Phase diagram for the SO(5)-symmetric kinetic energy part model ($g/J=0.5$, $J\chi=10$, and $\kappa=1$). Plotted is the critical temperature vs (a) chemical potential μ/J and (b) charge doping x . (a) The AF and SC phases are separated by the first-order transition line, and (b) the first-order transition line spreads, forming a mixed (M) region with constant chemical-potential value.

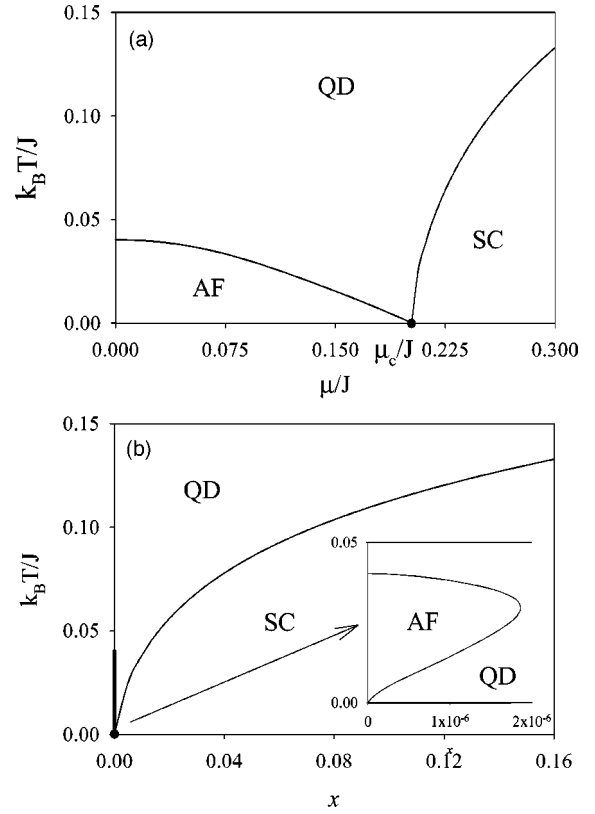


FIG. 4. Zero-temperature phase diagram for the SO(5)-symmetric kinetic energy part model: parameter χJ vs chemical potential μ/J for different values of g/J parameter.

(i) There is a first-order phase transition that can be described as a superspin flop transition ($\chi < \chi_{\text{crit}}$) at the critical line,

$$\mu_c = \sqrt{\frac{g + 3J(\kappa - 1)}{4\chi}}, \quad (53)$$

where $J\chi_{\text{crit}} = \gamma^2$ with

$$\gamma = \int_{-\infty}^{\infty} dz \rho(z) \left(\frac{3}{\sqrt{3\kappa - \kappa z}} + \frac{2}{\sqrt{3\kappa - \kappa z + g}} \right). \quad (54)$$

Here the second-order critical lines merge at the (μ_c, T_c) bicritical point [see Fig. 3(a)].

(ii) Increasing the strength of quantum fluctuations (the value of the χ parameter), we arrive at the phase diagram with $\chi = \chi_{\text{crit}}$, where there is a single second-order phase transition at the quantum critical point ($T=0, \mu_c$) [see Fig. 6(a)].

(iii) For $\chi > \chi_{\text{crit}}$ we arrive finally at the scenario depicted at the Fig. 7(a), where there are two second-order quantum phase transitions with an intermediate quantum-disordered phase.

However, it would be more useful if phase diagrams were expressed in terms of the physically measured quantity—the

doping (or charge concentration) x . The charge concentration $x = \langle L_{15} \rangle \equiv -\frac{1}{2} \partial f / \partial \mu$ can be deduced from the free energy (50). We obtain explicitly

$$x = \left\{ \begin{array}{l} \int_{-\infty}^{\infty} \rho(z) dz \left\{ \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3\kappa J - J_z + g}{\chi}} - 2\mu \right) \right] - \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3\kappa J - J_z + g}{\chi}} + 2\mu \right) \right] \right\} \equiv x_{AF}, \\ \frac{1}{2} \int_{-\infty}^{\infty} \rho(z) dz \left\{ 4\chi\mu - \left(\frac{4\mu}{\sqrt{3J - J_z + 4\chi\mu^2}} - 2 \right) \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3J - J_z + 4\chi\mu^2}{\chi}} - 2\mu \right) \right] \right. \\ \left. - \left(\frac{4\mu}{\sqrt{3J - J_z + 4\chi\mu^2}} + 2 \right) \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{3J - J_z + 4\chi\mu^2}{\chi}} + 2\mu \right) \right] \right. \\ \left. - \frac{12\mu \coth \left(\frac{\beta}{2} \sqrt{\frac{3J - \kappa J_z - g + 4\chi\mu^2}{\chi}} \right)}{\sqrt{3J - \kappa J_z - g + 4\chi\mu^2}} \right\} \equiv x_{SC}, \\ \int_{-\infty}^{\infty} \rho(z) dz \left\{ \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda_0 - J_z + g}{\chi}} - 2\mu \right) \right] - \coth \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda_0 - J_z + g}{\chi}} + 2\mu \right) \right] \right\} \equiv x_{QD}, \end{array} \right. \quad (55)$$

where x_{AF} , x_{SC} , and x_{QD} describe the charge density within the AF, SC, and QD phases, respectively, and λ_0 is determined by the self-consistent equation (37). In the zero-temperature limit, the charge densities are

$$x_{AF} = 0 \text{ for } \mu < \mu_c = \sqrt{\frac{g + 3J(\kappa - 1)}{4\chi}},$$

$$x_{SC} = 2\chi\mu_c \mathbf{m}_{SC}^2 \text{ for } \mu \geq \mu_c = \sqrt{\frac{g + 3J(\kappa - 1)}{4\chi}}, \quad (56)$$

where \mathbf{m}_{SC}^2 is the superconducting order parameter (see the next subsection and Appendix B) nonvanishing within the ordered phases. Therefore at zero temperature and for $\mu < \mu_c$ the charge density vanishes, for $\mu > \mu_c$ it is finite, and a discontinuous jump of the density is proportional to the superconducting order parameter. By raising the temperature the discontinuous jump diminishes and vanishes at the bicritical point on the T - μ phase diagram, where AF and SC critical lines merge (see Fig. 8). As a consequence, if the phase diagram is plotted with the charge density rather as a μ variable, the phase diagram will contain a mixed region with the coexistence of two phases with a constant chemical potential pinned at $\mu = \mu_c$ [see Fig. 3(b)]. This implies an infinite compressibility (which defined as $dx/d\mu$). This behavior can be explained by a two-phase mixture with different densities at the first-order phase transition. In this case the system globally phase separates into two different spatial regions with different charge densities, but the same free energy. As a result, the added charges only change the pro-

portion of the mixture of the two phases, but not the free energy (and therefore, $d\mu/dx = 0$).²¹ With increasing the strength of quantum fluctuations (i.e., by raising the χ parameter), the mixed region on the T - x phase diagram diminishes and disappears for $\chi \geq \chi_{\text{crit}}$ [see Figs. 3(b) and 6(b)]. In this case the AF phase on the T - x phase diagram is profoundly suppressed with a characteristic reentrant feature [see Figs. 7(b) and 7(c)].

B. Models with broken SO(5) symmetry of the kinetic energy part

When $\chi_c \neq \chi_\pi \neq \chi_s$, the Lagrangian (8) no longer has quadratic form in the \mathbf{n}_i variables. Therefore it is not possible to evaluate the free energy of the spherical model exactly. Hence, a further approximation is necessary. We replace $\mathbf{n}_{AF,i}^2$ and $\mathbf{n}_{SC,i}^2$ by their *average* values $\langle \mathbf{n}_{AF,i}^2 \rangle$ and $\langle \mathbf{n}_{SC,i}^2 \rangle$, according to

$$\mathbf{n}_{SC,i}^2(\tau) \rightarrow \langle \mathbf{n}_{SC,i}^2 \rangle,$$

$$\mathbf{n}_{AF,i}^2(\tau) \rightarrow \langle \mathbf{n}_{AF,i}^2 \rangle. \quad (57)$$

Using Eq. (42) we observe that

$$\langle \mathbf{n}_{AF(SC),i}^2(\tau) \rangle = G_{ij}^{AF(SC)}(\tau=0^+) \quad (58)$$

is independent of ‘‘imaginary time.’’ As a consequence the two quartic (in \mathbf{n}_i field) terms in the Lagrangian vanish:

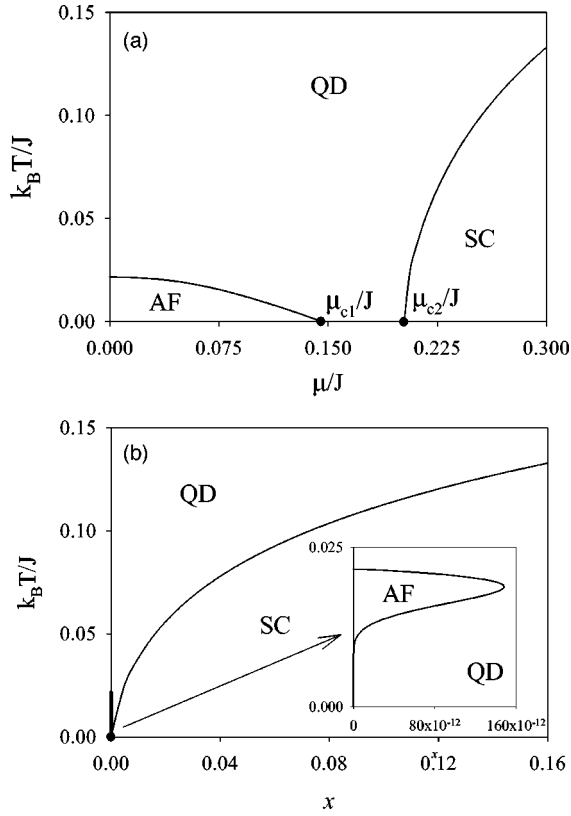


FIG. 5. Zero-temperature phase diagram for the SO(5)-symmetric kinetic energy part model: parameter g/J vs chemical potential μ/J . Solid lines correspond to AF and SC phases for $\chi J = 7$, dashed line for $\chi J = 8$. Ordered regions exist above (below) the corresponding lines.

$$\left(\frac{1}{2} \frac{\partial \mathbf{n}_{SC,i}^2}{\partial \tau} \right)^2 \Big|_{\mathbf{n}_{SC,i}^2 \rightarrow \langle \mathbf{n}_{SC,i}^2 \rangle} \Rightarrow \left(\frac{1}{2} \frac{\partial \langle \mathbf{n}_{SC,i}^2 \rangle}{\partial \tau} \right)^2 = 0,$$

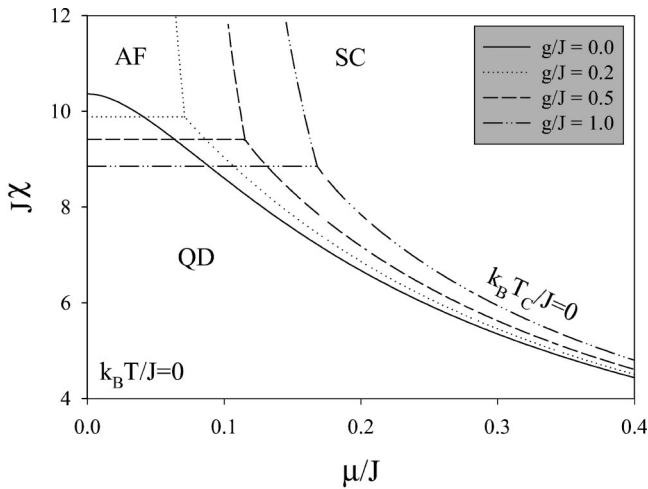


FIG. 6. Phase diagram for the SO(5)-symmetric kinetic energy part model ($g/J = -26.5$, $J\chi = 3.054725$, and $\kappa = 10$). Plotted is the critical temperature vs (a) chemical potential μ/J and (b) charge doping x . Here, two second-order phase transition lines meet at the quantum critical point x_c ($T=0$).

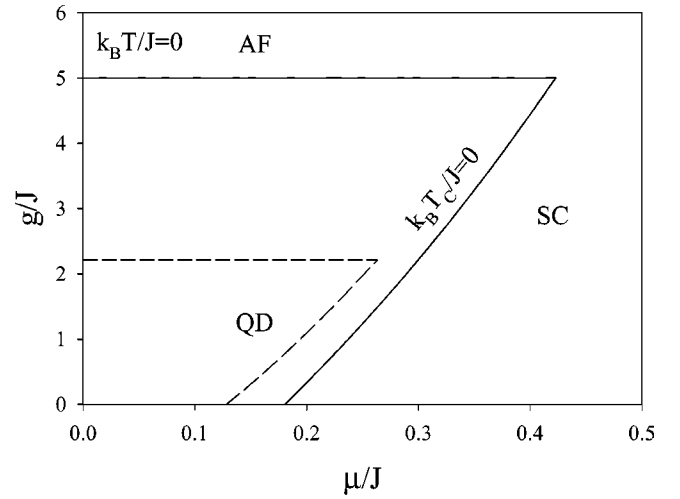


FIG. 7. Phase diagram for the SO(5)-symmetric kinetic energy part model ($g/J = -26.5$, $J\chi = 3.05465$, and $\kappa = 10$). Plotted is the critical temperature vs (a) chemical potential μ/J and (b) charge doping x . Here, the ordered AF and SC phases are separated by a nonordered intermediate region.

$$\left(\frac{1}{2} \frac{\partial \mathbf{n}_{AF,i}^2}{\partial \tau} \right)^2 \Big|_{\mathbf{n}_{AF,i}^2 \rightarrow \langle \mathbf{n}_{AF,i}^2 \rangle} \Rightarrow \left(\frac{1}{2} \frac{\partial \langle \mathbf{n}_{AF,i}^2 \rangle}{\partial \tau} \right)^2 = 0. \quad (59)$$

Therefore the Lagrangian simplifies to the form

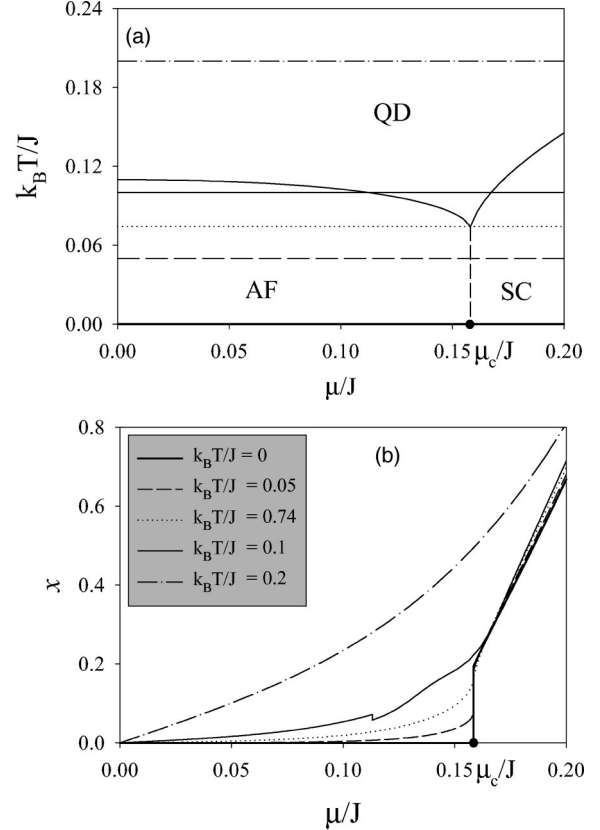


FIG. 8. (a) Generic phase diagram with AF and SC regions separated by the first-order transition line with five chosen constant-temperature lines. (b) Doping charge density x vs chemical potential μ/J for the temperatures from the plot (a).

$$\begin{aligned} \mathcal{L} = & \frac{1}{2} \sum_i \left[\chi_{SC,i} \left(\frac{\partial \mathbf{n}_{SC,i}}{\partial \tau} \right)^2 + \chi_{AF,i} \left(\frac{\partial \mathbf{n}_{AF,i}}{\partial \tau} \right)^2 \right] \\ & - \frac{1}{2} \sum_i \chi_{SC,i} \left[4\mu^2 (n_{1i}^2 + n_{5i}^2) \right. \\ & \left. + 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) + g \sum_j (n_{2i}^2 + n_{3i}^2 + n_{4i}^2) \right] \\ & + \frac{1}{2} \sum_{i,j} (J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j} + J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j}), \quad (60) \end{aligned}$$

which is now quadratic in \mathbf{n}_i fields, allowing one to perform Gaussian integrations (7) over \mathbf{n}_i variables exactly.

Here,

$$\begin{aligned} \chi_{AF,i}(\lambda_0) &= \frac{1}{\chi_\pi^{-1} + (\chi_s^{-1} - \chi_\pi^{-1}) \langle \mathbf{n}_{AF,i}^2 \rangle}, \\ \chi_{SC,i}(\lambda_0) &= \frac{1}{\chi_\pi^{-1} + (\chi_c^{-1} - \chi_\pi^{-1}) \langle \mathbf{n}_{SC,i}^2 \rangle}, \quad (61) \end{aligned}$$

with

$$\begin{aligned} \langle \mathbf{n}_{AF}^2 \rangle &= 3 \int_{-\infty}^{\infty} \rho(z) dz \frac{\coth \left[\frac{\beta}{2} \sqrt{\chi_{AF}^{-1}} (2\lambda_0 - \kappa J z - g) \right]}{\sqrt{\chi_{AF} (2\lambda_0 - \kappa J z - g)}}, \\ \langle \mathbf{n}_{SC}^2 \rangle &= 2 \int_{-\infty}^{\infty} \rho(z) dz \frac{\coth \left\{ \frac{\beta}{2} [\sqrt{\chi_{SC}^{-1}} (2\lambda_0 - J z) + 2\mu] \right\} + \coth \left\{ \frac{\beta}{2} [\sqrt{\chi_{SC}^{-1}} (2\lambda_0 - J z) - 2\mu] \right\}}{2\sqrt{\chi_{SC} (2\lambda_0 - J z)}}. \quad (62) \end{aligned}$$

In this case the order parameter susceptibilities take the form

$$\begin{aligned} G_{AF}(\mathbf{k}, \omega_l) &= \frac{3}{2\lambda - J^{AF}(\mathbf{k}) + \chi_{AF} \omega_l^2 - g}, \\ G_{SC}(\mathbf{k}, \omega_l) &= \frac{1}{2\lambda - J^{SC}(\mathbf{k}) + \chi_{SC} (\omega_l + 2i\mu)^2} + \frac{1}{2\lambda - J^{SC}(\mathbf{k}) + \chi_{SC} (\omega_l - 2i\mu)^2}, \quad (63) \end{aligned}$$

and from the criticality condition

$$G_{AF}^{-1}(\mathbf{k}=\mathbf{0}, \omega_l=0) = 0, \quad G_{SC}^{-1}(\mathbf{k}=\mathbf{0}, \omega_l=0) = 0, \quad (64)$$

one can obtain the corresponding Lagrange multiplier for AF and SC phases, respectively:

$$\lambda_0^{AF} = \frac{1}{2} J^{AF}(\mathbf{k}=\mathbf{0}) + \frac{g}{2}, \quad \lambda_0^{SC} = \frac{1}{2} J^{SC}(\mathbf{k}=\mathbf{0}) + 2\chi_{SC} \mu^2. \quad (65)$$

The saddle point condition (37) can be put in a very simple form (see Appendix B):

$$\langle \mathbf{n}_{AF,i}^2 \rangle + \langle \mathbf{n}_{SC,i}^2 \rangle = 1 - \mathbf{m}_{AF}^2 - \mathbf{m}_{SC}^2. \quad (66)$$

The second-order transition critical lines, separating ordered (AF or SC) and QD high-temperature regions, can be obtained using the appropriate Lagrange multiplier (AF or SC) and putting the superspin ‘‘magnetization’’ $\mathbf{m}^2 = \mathbf{m}_{AF}^2 + \mathbf{m}_{SC}^2$ equal to zero. For the disordered to AF (SC) transition we obtain

$$\text{QD} \Leftrightarrow \text{AF: } \langle \mathbf{n}_{AF,i}^2 \rangle |_{\lambda_0 = \lambda_0^{AF}} + \langle \mathbf{n}_{SC,i}^2 \rangle |_{\lambda_0 = \lambda_0^{AF}} = 1; \quad \text{QD} \Leftrightarrow \text{SC: } \langle \mathbf{n}_{AF,i}^2 \rangle |_{\lambda_0 = \lambda_0^{SC}} + \langle \mathbf{n}_{SC,i}^2 \rangle |_{\lambda_0 = \lambda_0^{SC}} = 1, \quad (67)$$

explicitly

$$\begin{aligned}
\text{QD} \Leftrightarrow \text{AF}: \quad 1 &= \int_{-\infty}^{\infty} \rho(z) dz \left\{ 3 \frac{\coth\left(\frac{\beta}{2} \sqrt{\frac{3\kappa J - \kappa J z}{\chi_{AF}^a}}\right)}{\sqrt{\chi_{AF}^a(3\kappa J - \kappa J z)}} \right. \\
&\quad \left. + 2 \frac{\coth\left[\frac{\beta}{2} \left(\sqrt{\frac{3\kappa J - Jz + g}{\chi_{SC}^a}} + 2\mu\right)\right] + \coth\left[\frac{\beta}{2} \left(\sqrt{\frac{3\kappa J - Jz + g}{\chi_{SC}^a}} - 2\mu\right)\right]}{2\sqrt{\chi_{SC}^a(3\kappa J - Jz + g)}} \right\}; \\
\text{QD} \Leftrightarrow \text{SC}: \quad 1 &= \int_{-\infty}^{\infty} \rho(z) dz \left\{ 3 \frac{\coth\left(\frac{\beta}{2} \sqrt{\frac{3J - \kappa J z - g + 4\chi_{SC}^s \mu^2}{\chi_{AF}^s}}\right)}{\sqrt{\chi_{AF}^s(3J - \kappa J z - g + 4\chi_{SC}^s \mu^2)}} \right. \\
&\quad \left. + 2 \frac{\coth\left[\frac{\beta}{2} \left(\sqrt{\frac{3J - Jz + 4\chi_{SC}^s \mu^2}{\chi_{SC}^s}} + 2\mu\right)\right] + \coth\left[\frac{\beta}{2} \left(\sqrt{\frac{3J - Jz + 4\chi_{SC}^s \mu^2}{\chi_{SC}^s}} - 2\mu\right)\right]}{2\sqrt{\chi_{SC}^s(3J - Jz + 4\chi_{SC}^s \mu^2)}} \right\}, \quad (68)
\end{aligned}$$

where

$$\chi_{AF(SC)}^{a(s)} \equiv \chi_{AF(SC)}(\lambda_0^{AF(SC)}). \quad (69)$$

The set of self-consistent equations (68) with Eqs. (61) and (62) determines the external phase boundaries $T_c(\mu)$ between AF (SC) and QD phases. The internal critical phase boundaries can be obtained in a similar fashion. On the AF (SC) $\Leftrightarrow M$ phase $\mathbf{m}_{SC(AF)}$ is nonzero. For the SC $\Leftrightarrow M$ transition $\mathbf{m}_{AF} = 0$ and $\lambda_0 = \lambda_0^{AF}$. From Eq. (66) the equation for the critical line reads

$$[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{AF}} = 1 - \mathbf{m}_{SC}^2. \quad (70)$$

On the other hand, the equation for the order parameter \mathbf{m}_{SC} (within the AF state) follows from the equation of state (66) with $\lambda_0 = \lambda_0^{SC}$:

$$[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{SC}} = 1 - \mathbf{m}_{SC}^2. \quad (71)$$

Both equations can be combined to give

$$[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{AF}} = [\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{SC}}. \quad (72)$$

Similarly, for the AF $\Leftrightarrow M$ transition $\mathbf{m}_{SC} = 0$ and $\lambda_0 = \lambda_0^{SC}$. Correspondingly, we obtain

$$[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{SC}} = 1 - \mathbf{m}_{AF}^2. \quad (73)$$

The order parameter \mathbf{m}_{AF} is, in turn, defined by the equation for the AF state:

$$[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{AF}} = 1 - \mathbf{m}_{AF}^2. \quad (74)$$

Equating the right-hand side (RHS) of the Eqs. (73) and (74) we obtain

$$[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{AF}} = [\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{SC}}. \quad (75)$$

Subsequently, comparing the Eqs. (72) and (75) we can deduce

$$\begin{aligned}
[\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{AF}} &= [\langle \mathbf{n}_{AF}^2 \rangle + \langle \mathbf{n}_{SC}^2 \rangle]_{\lambda_0 = \lambda_0^{SC}} \Rightarrow \mathbf{m}_{AF}^2 \\
&= \mathbf{m}_{SC}^2 \Rightarrow \lambda_0^{AF} = \lambda_0^{SC}. \quad (76)
\end{aligned}$$

From the equality of the Lagrange multipliers we obtain the equation for the critical line:

$$\mu^2 = \frac{g + 3J(\kappa - 1)}{4} [\chi_{\pi}^{-1} + (\chi_c^{-1} - \chi_{\pi}^{-1}) \langle \mathbf{n}_{SC}^2 \rangle]. \quad (77)$$

This equation turns out to be the equation for a *single* line. From the inspection of the free energy we have $\lambda_0^{AF} = \lambda_0^{SC} \Rightarrow f(\lambda_0^{AF}) = f(\lambda_0^{SC})$, implying that the critical line (77) refers to the first-order transition line. It is easy to see that for the $\chi_{\pi} = \chi_c = \chi$, Eq. (77) simplifies to

$$\mu = \sqrt{\frac{g + 3J(\kappa - 1)}{4\chi}}, \quad (78)$$

as in the case of the model with a SO(5)-symmetric kinetic energy part [see Eq. (53)]. Similarly as in the case from the previous subsection we found no evidence for the T - μ phase diagram with four critical lines merging at the tetracritical point [phase diagram in Fig. 1(b) from Ref. 1].

By varying the kinetic energy parameters χ_{π} , χ_c , and χ_s we arrive basically at the same type of phase diagrams as in the symmetric case described at the previous subsection. However, the line of the first-order superspin-flop phase transition on the T - μ phase diagram will not be in general exactly vertical for the case of different susceptibilities χ_{π} , χ_c , and χ_s . The first-order superspin flop will occur at the $\mu(T)$ line described by

$$\mu = \sqrt{\frac{g + 3J(\kappa - 1)}{4\chi_{SC}(T)}}. \quad (79)$$

Furthermore, the corresponding condition for the quantum critical point ($T=0, \mu_{\text{crit}}$) now reads

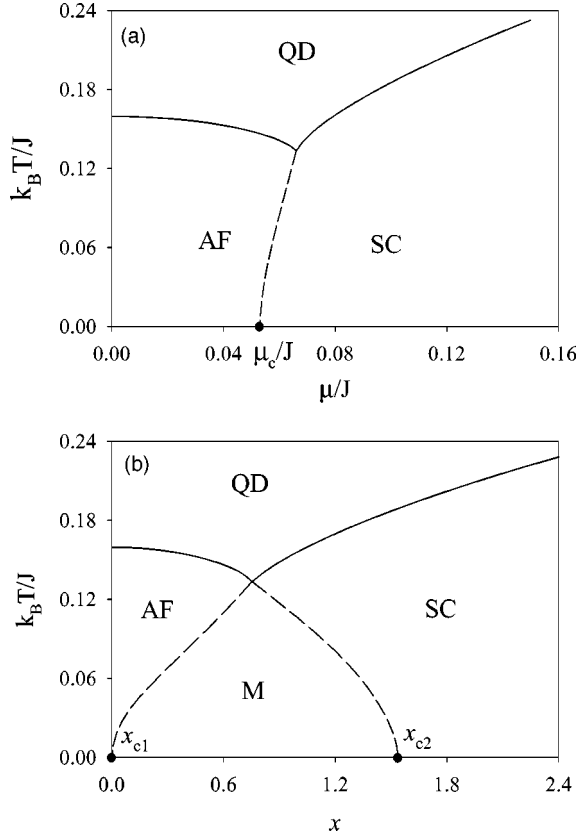


FIG. 9. Phase diagram for the SO(5)-nonsymmetric kinetic energy part model ($g/J=0.5$, $J\chi_\pi=100$, $J\chi_s=8$, $J\chi_c=12$, and $\kappa=1$). Plotted is the critical temperature vs (a) chemical potential μ/J and (b) charge doping x . (a) The AF and SC phases are separated by the first-order transition line, and (b) the first-order transition line spreads, forming a mixed (M) region with constant chemical-potential value.

$$\mu_{\text{crit}} = \sqrt{\frac{g+3J(\kappa-1)}{4\chi_{SC}}} \Big|_{\lambda_0=\lambda_0^{AF}=\lambda_0^{SC}} \quad (80)$$

[see Figs. 9(a) and 10(a)].

Similarly we can obtain the phase diagram as a function of doping concentration x and temperature. Here the charge density is given by

$$x = \langle L_{15} \rangle = \begin{cases} -\frac{1}{2} \frac{df(\lambda_0^{AF})}{d\mu} \equiv x_{AF}, \\ -\frac{1}{2} \frac{df(\lambda_0^{SC})}{d\mu} \equiv x_{SC}, \\ -\frac{1}{2} \frac{df(\lambda^{QD})}{d\mu} \equiv x_{QD}, \end{cases} \quad (81)$$

and the T - x phase diagrams with mixed regions are presented in Figs. 9(b) and 10b.

V. SUMMARY AND CONCLUSIONS

In the present paper we have studied the thermodynamic properties of the SO(5) quantum rotor theory which accounts for both thermal and quantum effects in the rotation of superspins between SC and AF subspaces. We have performed

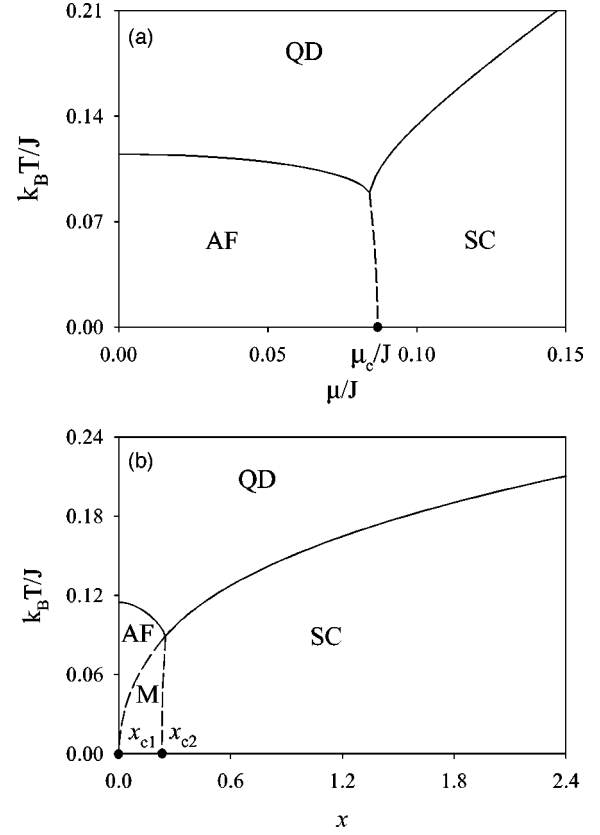


FIG. 10. Phase diagram for the SO(5)-nonsymmetric kinetic energy part model ($g/J=0.5$, $J\chi_\pi=12$, $J\chi_s=8$, $J\chi_c=1000$, and $\kappa=1$). Plotted is the critical temperature vs (a) chemical potential μ/J and (b) charge doping x . (a) The AF and SC phases are separated by the first-order transition line, and (b) the first-order transition line spreads, forming a mixed (M) region with constant chemical-potential value.

a non-mean-field treatment of the lattice version of the NLQ σ M using the spherical approach for 3D quantum rotors and discussed possible scenarios for temperature-doping phase diagrams. The model considered can contain large SO(5) anisotropy parameters (spin, charge, and so-called “ π ” susceptibilities which regulate the strength of the quantum fluctuations). We found out that the topology of the temperature-chemical-potential phase diagrams assumes different forms depending on the strength of the quantum fluctuations. In the SO(5) symmetric kinetic energy model we established the condition for the existence of the quantum critical point, where the AF state goes to the SC state through the second-order phase transition. For strong quantum fluctuations the region between AF and SC phases becomes quantum disordered and both transitions (from the quantum-disordered phase to AF and SC) are of second order, respectively. In the intermediate quantum regime there is a first-order superspin-flop transition (where the direction of the superspin changes abruptly). Finally, for the general class of models with symmetric and asymmetric kinetic energy parts we found no evidence for the existence of a phase diagram, where four second-order lines merge at the tetracritical point (T_{tc}, μ_{tc}) and two of them enclose an intermediate “spin-bag” phase [phase diagram from the Fig. 1(b) from Zhang’s paper¹]. This is in contrast to the quasiclassical approach where this scenario appears to be possible. There-

fore, we conclude that quantum fluctuations are responsible for the destruction of the “spin-bag” phase on the T - μ phase diagram. However, a phase separation region will occur on the *temperature-charge concentration* T - x phase diagram for intermediate quantum fluctuations. In this region the long-range Coulomb interaction can lead presumably to the formation of a stripe order with alternating AF and SC phases. To compare theoretical predictions with experiments it is important to establish precisely the high- T_c phase diagrams in the AF-SC transition regime. Unfortunately, this is complicated by the fact that charge doping is the experimentally tunable parameter. Nevertheless, there is experimental evidence that in the vicinity of the AF-SC transition region the high- T_c superconductors exhibit an increased sensitivity to disorder and inhomogeneity. Presumably, in order to understand the precise nature of the intermediate AF-SC regime it is important to include other perturbing effects such

as the above-mentioned long-range Coulomb interaction²² to study how spatially inhomogeneous states can emerge. Finally, it would be very important to see whether there will be a *dynamical* restoration of the SO(5) symmetry at the quantum (bi)critical point even when the model defined at the short length scales is not exactly SO(5) invariant (i.e., with different susceptibilities along different directions). A quantum version of the Polyakov-Migdal low-temperature expansion for the NL σ M combined with a renormalization group treatment around lower critical dimensionality²³ would be instrumental to address these issues.

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APPENDIX A: CONSTRUCTION OF THE EFFECTIVE LAGRANGIAN

1. SO(5)-symmetric kinetic energy part

The kinetic energy of the system is simply that of a SO(5) rigid rotor given by

$$\begin{aligned} \frac{1}{2\chi} \sum_i \sum_{\mu < \nu} L_i^{\mu\nu} L_i^{\nu\mu} &= -\frac{1}{2\chi} \sum_i \sum_{\mu < \nu} \left(n_{i\mu} \frac{\partial}{\partial n_{i\nu}} - n_{i\nu} \frac{\partial}{\partial n_{i\mu}} \right) \left(n_{i\mu} \frac{\partial}{\partial n_{i\nu}} - n_{i\nu} \frac{\partial}{\partial n_{i\mu}} \right) \\ &= \frac{1}{2\chi} \sum_i \sum_{\mu, \nu} (n_{i\mu}^2 p_{i\nu}^2 - n_{i\mu} n_{i\nu} p_{i\mu} p_{i\nu}) = \frac{1}{2\chi} \sum_i \left[\sum_{\nu} n_{i\mu}^2 \sum_{\mu} p_{i\mu}^2 - \left(\sum_{\mu} n_{i\mu} p_{i\mu} \right)^2 \right] \\ &= \frac{1}{2\chi} \sum_i [\mathbf{n}_i^2 \mathbf{p}_i^2 - (\mathbf{n}_i \cdot \mathbf{p}_i)^2]. \end{aligned} \quad (\text{A1})$$

Therefore, the partition function is

$$\begin{aligned} Z &= \int \prod_i [D\mathbf{n}_i] \int \prod_i \left[\frac{D\mathbf{p}_i}{2\pi} \right] \delta(1 - \mathbf{n}_i^2) \delta(\mathbf{n}_i \cdot \mathbf{p}_i) \exp \left(- \int_0^\beta d\tau \mathcal{L}[\mathbf{p}, \mathbf{n}] \right) \\ &= \exp \left(- \int_0^\beta d\tau \left[\sum_i \left[i\mathbf{p}_i \cdot \frac{\partial \mathbf{n}_i}{\partial \tau} + \frac{1}{2\chi} \mathbf{n}_i^2 \mathbf{p}_i^2 - \frac{1}{2\chi} (\mathbf{n}_i \cdot \mathbf{p}_i)^2 \right] - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}) - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2) \right. \right. \\ &\quad \left. \left. - 2\mu \sum_i L_i^{15} \right] \right). \end{aligned} \quad (\text{A2})$$

The integral over momenta reads then

$$I = \int \prod_{\mu} \left[\frac{Dp_{\mu}}{2\pi} \right] \delta(\mathbf{n} \cdot \mathbf{p}) \exp \left\{ - \int_0^\beta d\tau \left[\sum_{\mu} i p_{\mu} \frac{\partial n_{\mu}}{\partial \tau} + \frac{1}{2\chi} \mathbf{n}^2 \mathbf{p}^2 - \frac{(\mathbf{n} \cdot \mathbf{p})^2}{2\chi} - 2\mu (n_1 p_5 - n_5 p_1) \right] \right\}. \quad (\text{A3})$$

Due to the constraint on integrating over the momenta (given by the δ function), one must be careful and integrate only over momenta perpendicular to superspins \mathbf{n}_i . We can split the momentum \mathbf{p} into longitudinal \mathbf{p}_{\parallel} and transverse momenta \mathbf{p}_{\perp} , which obey the condition $\mathbf{p}_{\perp} \cdot \mathbf{n} = 0$:

$$\mathbf{p} = \mathbf{p}_{\perp} + \mathbf{p}_{\parallel},$$

$$p_a^{\perp} = -\frac{1}{\mathbf{n}^2} \sum_b L_{ab} n_b = p_a - \frac{n_a (\mathbf{n} \cdot \mathbf{p})}{\mathbf{n}^2}. \quad (\text{A4})$$

Therefore, for an arbitrary functional $F[\mathbf{p}_{\perp}, \mathbf{n}\mathbf{p}]$ we have the identity

$$\int d\mathbf{p} \delta(\mathbf{n} \cdot \mathbf{p}) F[\mathbf{p}_\perp, \mathbf{n} \cdot \mathbf{p}] = \int d\mathbf{p}_\perp F[\mathbf{p}_\perp, 0]. \quad (\text{A5})$$

As a consequence of Eq. (A3), the integral I reads

$$\begin{aligned} I &= \int \prod_\mu \left[\frac{Dp_{\mu\perp}}{2\pi} \right] \exp \left\{ - \int_0^\beta d\tau \left[\sum_\mu ip_{\mu\perp} \frac{\partial n_\mu}{\partial \tau} + \frac{1}{2\chi} \mathbf{p}_\perp^2 - 2\mu(n_1 p_{5\perp} - n_5 p_{1\perp}) \right] \right\} \\ &= \exp \left\{ - \frac{\chi}{2} \int_0^\beta d\tau \left[\left(\frac{\partial \mathbf{n}}{\partial \tau} \right)^2 - 4\mu^2(n_1^2 + n_5^2) - 4i\mu \left(\frac{\partial n_1}{\partial \tau} n_5 - n_1 \frac{\partial n_5}{\partial \tau} \right) \right] \right\}. \end{aligned} \quad (\text{A6})$$

This leaves us with a Lagrangian of the form

$$\begin{aligned} \mathcal{L} &= \sum_i \frac{\chi}{2} \left[\left(\frac{\partial \mathbf{n}_i}{\partial \tau} \right)^2 - 4\mu^2(n_{1i}^2 + n_{5i}^2) - 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) \right] - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}) \\ &\quad - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2). \end{aligned} \quad (\text{A7})$$

2. SO(5)-asymmetric kinetic energy part

In this case the first term in the Hamiltonian (1) is

$$S = \sum_i \sum_{\mu < \nu} (\chi_{\mu\nu})^{-1} L_i^{\mu\nu} L_i^{\nu\mu} = \frac{1}{2} \sum_i \sum_{\mu, \nu} p_{i\mu} A_{\mu\nu} p_{i\nu}, \quad (\text{A8})$$

where the matrix $A_{\mu\nu}$ is given by

$$A_{\mu\nu} = \delta_{\mu\nu} \sum_\varepsilon n_{i\varepsilon}^2 (\chi_{\varepsilon\nu})^{-1} - n_{i\mu} (\chi_{\mu\nu})^{-1} n_{i\nu}. \quad (\text{A9})$$

Analogous to Eq. (A3), the integral over momenta reads

$$I = \int \left[\frac{D\mathbf{p}_i}{2\pi} \right] \delta(\mathbf{n}_i \cdot \mathbf{p}_i) \exp \left\{ - \int_0^\beta d\tau \left[i\mathbf{p}_i \cdot \frac{\partial \mathbf{n}_i}{\partial \tau} + \frac{1}{2} \mathbf{p}_i^T \cdot \mathbf{A} \mathbf{p}_i \right] \right\}. \quad (\text{A10})$$

Due to the constraint $\mathbf{n}_i \cdot \mathbf{p}_i = 0$, one has to integrate over the momenta, which are transverse to \mathbf{n}_i . For a given direction of the vector \mathbf{n}_i we choose a new basis $\{\boldsymbol{\eta}_a, a=1, \dots, 5\}$ which obeys the following conditions:

$$\boldsymbol{\eta}_a \cdot \boldsymbol{\eta}_b = \delta_{ab}, \quad \sum_a \eta_{\mu a} \eta_{\nu a} = \delta_{\mu\nu}, \quad \boldsymbol{\eta}_a \cdot \mathbf{n} = \delta_{1a}. \quad (\text{A11})$$

That is, the basis is orthonormal and complete and its first basis vector $\boldsymbol{\eta}_1$ is parallel to \mathbf{n} . This is always possible, since the last condition in Eq. (A11) leaves the freedom to perform SO(4) rotation on the transverse basis. In the new basis the momentum vector \mathbf{p}' can be written as

$$\mathbf{p}' = \sum_a p'_a \boldsymbol{\eta}_a, \quad (\text{A12})$$

where $p'_a = \boldsymbol{\eta}_a \cdot \mathbf{p}$. As a result the parallel \mathbf{p}'_{\parallel} and perpendicular \mathbf{p}'_{\perp} (to \mathbf{n}) momenta are given by

$$\mathbf{p}'_{\parallel} = p_1 \boldsymbol{\eta}_1, \quad \mathbf{p}'_{\perp} = \sum_{a=2}^5 p_a \boldsymbol{\eta}_a. \quad (\text{A13})$$

Using the completeness relation [Eq. (A11)] we can invert the relation (A12) and write original momentum components in term of new ones:

$$p_v = \sum_a p'_a \eta_{va} \equiv \sum_a p'_a [\hat{\boldsymbol{\eta}}]_{va}. \tag{A14}$$

Explicitly, in terms of the components of the unit vector \mathbf{n} ,

$$\hat{\boldsymbol{\eta}} = [[\hat{\boldsymbol{\eta}}_{||}], [\hat{\boldsymbol{\eta}}_{\perp}]], \hat{\boldsymbol{\eta}}_{||} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \end{bmatrix}, \hat{\boldsymbol{\eta}}_{\perp} = \begin{bmatrix} n_1 \sqrt{\frac{n_2^2 + n_3^2 + n_4^2}{n_1^2 + n_5^2}} & -n_5 \frac{1}{\sqrt{n_1^2 + n_5^2}} & 0 & 0 \\ -n_2 \sqrt{\frac{n_1^2 + n_5^2}{n_2^2 + n_3^2 + n_4^2}} & 0 & -n_4 \frac{1}{\sqrt{n_2^2 + n_4^2}} & \frac{-n_2 n_3}{\sqrt{n_2^2 + n_4^2} \sqrt{n_2^2 + n_3^2 + n_4^2}} \\ -n_3 \sqrt{\frac{n_1^2 + n_5^2}{n_2^2 + n_3^2 + n_4^2}} & 0 & 0 & \frac{\sqrt{n_2^2 + n_4^2}}{\sqrt{n_2^2 + n_3^2 + n_4^2}} \\ -n_4 \sqrt{\frac{n_1^2 + n_5^2}{n_2^2 + n_3^2 + n_4^2}} & 0 & n_2 \frac{1}{\sqrt{n_2^2 + n_4^2}} & \frac{-n_3 n_4}{\sqrt{n_2^2 + n_4^2} \sqrt{n_2^2 + n_3^2 + n_4^2}} \\ n_5 \sqrt{\frac{n_2^2 + n_3^2 + n_4^2}{n_1^2 + n_5^2}} & n_1 \frac{1}{\sqrt{n_1^2 + n_5^2}} & 0 & 0 \end{bmatrix}. \tag{A15}$$

As a consequence, the constrained functional integration of a functional $F[\mathbf{p}, \mathbf{n}]$ becomes

$$\int [D\mathbf{p}] \delta(\mathbf{n} \cdot \mathbf{p}) F[\mathbf{p}, \mathbf{n}] = \int [D\mathbf{p}'_{\perp}] F[\mathbf{p}'_{\perp}, \mathbf{p}'_{||} = 0, \mathbf{n}]. \tag{A16}$$

The Gaussian integral (A10) can be now written as

$$I = \int [D\mathbf{p}_{\perp}] \exp \left[- \int_0^{\beta} d\tau \left(i \mathbf{p}_{\perp}^T \cdot \hat{\boldsymbol{\eta}}_{\perp}^T \mathbf{c} + \frac{1}{2} \mathbf{p}_{\perp}^T \cdot \hat{\boldsymbol{\eta}}_{\perp}^T \mathbf{A} \hat{\boldsymbol{\eta}}_{\perp} \mathbf{p}_{\perp} \right) \right] = \exp \left\{ \frac{1}{2} \int_0^{\beta} d\tau \mathbf{c}^T \cdot [\hat{\boldsymbol{\eta}}_{\perp} (\hat{\boldsymbol{\eta}}_{\perp}^T \mathbf{A} \hat{\boldsymbol{\eta}}_{\perp})^{-1} \hat{\boldsymbol{\eta}}_{\perp}^T] \mathbf{c} \right\}, \tag{A17}$$

where

$$\mathbf{c}_i = \begin{bmatrix} i \frac{\partial n_{i1}}{\partial \tau} - 2\mu n_{i5} \\ i \frac{\partial n_{i2}}{\partial \tau} \\ i \frac{\partial n_{i3}}{\partial \tau} \\ i \frac{\partial n_{i4}}{\partial \tau} \\ i \frac{\partial n_{i5}}{\partial \tau} + 2\mu n_{i1} \end{bmatrix}. \tag{A18}$$

The matrix appearing in the exponent of the RHS of Eq. (A17) reads

$$\begin{aligned} [\hat{\boldsymbol{\eta}}_{\perp} (\hat{\boldsymbol{\eta}}_{\perp}^T \mathbf{A} \hat{\boldsymbol{\eta}}_{\perp})^{-1} \hat{\boldsymbol{\eta}}_{\perp}^T]_{\mu\nu} &= -\chi_{\pi} n_{\mu} n_{\nu} + (\delta_{\mu 1} + \delta_{\mu 5})(\delta_{\nu 1} + \delta_{\nu 5}) \frac{n_{\mu} n_{\nu}}{\mathbf{n}_{SC}^2} \left(\chi_{\pi} - \frac{1}{\chi_c^{-1} \mathbf{n}_{SC}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF}^2} \right) \\ &+ (\delta_{\mu 1} \delta_{\nu 1} + \delta_{\mu 5} \delta_{\nu 5}) \frac{1}{\chi_c^{-1} \mathbf{n}_{SC}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF}^2} + (\delta_{\mu 2} + \delta_{\mu 3} + \delta_{\mu 4})(\delta_{\nu 2} + \delta_{\nu 3} + \delta_{\nu 4}) \frac{n_{\mu} n_{\nu}}{\mathbf{n}_{AF}^2} \\ &\times \left(\chi_{\pi} - \frac{1}{\chi_{\pi}^{-1} \mathbf{n}_{SC}^2 + \chi_s^{-1} \mathbf{n}_{AF}^2} \right) + (\delta_{\mu 2} \delta_{\nu 2} + \delta_{\mu 3} \delta_{\nu 3} + \delta_{\mu 4} \delta_{\nu 4}) \frac{1}{\chi_{\pi}^{-1} \mathbf{n}_{SC}^2 + \chi_s^{-1} \mathbf{n}_{AF}^2}. \end{aligned} \tag{A19}$$

Performing the summation over the components of vector \mathbf{c}_i [see Eq. (A18)], we find

$$\begin{aligned}
\mathbf{c}^T \cdot [\hat{\boldsymbol{\eta}}_{\perp} (\hat{\boldsymbol{\eta}}_{\perp}^T \mathbf{A} \hat{\boldsymbol{\eta}}_{\perp})^{-1} \hat{\boldsymbol{\eta}}_{\perp}^T] \mathbf{c} &\equiv \sum_{\mu, \nu} c_{\mu}^T [\hat{\boldsymbol{\eta}}_{\perp} (\hat{\boldsymbol{\eta}}_{\perp}^T \mathbf{A} \hat{\boldsymbol{\eta}}_{\perp})^{-1} \hat{\boldsymbol{\eta}}_{\perp}^T]_{\mu \nu} c_{\nu} \\
&\equiv -\frac{1}{\mathbf{n}_{SC}^2} \left(\chi_{\pi} - \frac{1}{\chi_c^{-1} \mathbf{n}_{SC}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF}^2} \right) \left(\frac{1}{2} \frac{\partial \mathbf{n}_{SC}^2}{\partial \tau} \right)^2 - \frac{1}{\chi_c^{-1} \mathbf{n}_{SC}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF}^2} \left(\frac{\partial \mathbf{n}_{SC}}{\partial \tau} \right)^2 - \frac{1}{\mathbf{n}_{AF}^2} \left(\chi_{\pi} - \frac{1}{\chi_{\pi}^{-1} \mathbf{n}_{SC}^2 + \chi_s^{-1} \mathbf{n}_{AF}^2} \right) \left(\frac{1}{2} \frac{\partial \mathbf{n}_{AF}^2}{\partial \tau} \right)^2 \\
&\quad - \frac{1}{\chi_{\pi}^{-1} \mathbf{n}_{SC}^2 + \chi_s^{-1} \mathbf{n}_{AF}^2} \left(\frac{\partial \mathbf{n}_{AF}}{\partial \tau} \right)^2 + \frac{1}{2} \sum_i \frac{1}{\chi_c^{-1} \mathbf{n}_{SC}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF}^2} \left[4\mu^2 (n_{1i}^2 + n_{5i}^2) - 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) \right].
\end{aligned} \tag{A20}$$

Finally, the Lagrangian takes the form

$$\begin{aligned}
\mathcal{L} &= \frac{1}{2} \sum_i \left[\frac{1}{\mathbf{n}_{SC,i}^2} \left(\chi_{\pi} - \frac{1}{\chi_c^{-1} \mathbf{n}_{SC,i}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF,i}^2} \right) \left(\frac{1}{2} \frac{\partial \mathbf{n}_{SC,i}^2}{\partial \tau} \right)^2 + \frac{1}{\chi_c^{-1} \mathbf{n}_{SC,i}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF,i}^2} \left(\frac{\partial \mathbf{n}_{SC,i}}{\partial \tau} \right)^2 \right] \\
&\quad + \frac{1}{2} \sum_i \left[\frac{1}{\mathbf{n}_{AF,i}^2} \left(\chi_{\pi} - \frac{1}{\chi_{\pi}^{-1} \mathbf{n}_{SC,i}^2 + \chi_s^{-1} \mathbf{n}_{AF,i}^2} \right) \left(\frac{1}{2} \frac{\partial \mathbf{n}_{AF,i}^2}{\partial \tau} \right)^2 + \frac{1}{\chi_{\pi}^{-1} \mathbf{n}_{SC,i}^2 + \chi_s^{-1} \mathbf{n}_{AF,i}^2} \left(\frac{\partial \mathbf{n}_{AF,i}}{\partial \tau} \right)^2 \right] \\
&\quad - \frac{1}{2} \sum_i \frac{1}{\chi_c^{-1} \mathbf{n}_{SC,i}^2 + \chi_{\pi}^{-1} \mathbf{n}_{AF}^2} \left[4\mu^2 (n_{1i}^2 + n_{5i}^2) + 4i\mu \left(\frac{\partial n_{1i}}{\partial \tau} n_{5i} - n_{1i} \frac{\partial n_{5i}}{\partial \tau} \right) \right] - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}) \\
&\quad - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2).
\end{aligned} \tag{A21}$$

It is easy to see that for the symmetric model ($\chi_c = \chi_{\pi} = \chi_s = \chi$) the Lagrangian (A21) reduces to Eq. (A7).

APPENDIX B: ORDER PARAMETER IN THE SPHERICAL QUANTUM ROTOR MODEL

Introducing a uniform order parameter field \mathbf{h} in the Hamiltonian,

$$H = \frac{1}{2} \sum_i \sum_{\mu < \nu} (\chi_{\mu\nu})^{-1} L_i^{\mu\nu} L_i^{\mu\nu} - \sum_{i < j} (J_{ij}^{AF} \mathbf{n}_{AF,i} \cdot \mathbf{n}_{AF,j} + J_{ij}^{SC} \mathbf{n}_{SC,i} \cdot \mathbf{n}_{SC,j}) - \frac{g}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2) - 2\mu \sum_i L_i^{15} - \sum_i \mathbf{h} \cdot \mathbf{n}_i \tag{B1}$$

the free energy can be written as follows:

$$\begin{aligned}
f(\lambda_0, \mu) &= -\lambda_0 + \frac{2}{\beta} \int_{-\infty}^{\infty} dz \rho(z) \ln \left\{ \left[2 \sinh \left(\frac{\beta}{2} \sqrt{\frac{2\lambda - \kappa J z - g}{\chi_{AF}}} \right) \right]^3 2 \sinh \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda - Jz}{\chi_{SC}}} + 2\mu \right) \right] \right\} \\
&\quad \times 2 \sinh \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda - Jz}{\chi_{SC}}} - 2\mu \right) \right] \left\{ \right\} - \left[\frac{\mathbf{h}_{AF}^2}{8\lambda_0 - 4\kappa J - 2g} + \frac{\mathbf{h}_{SC}^2}{8\lambda_0 - 4J - 8\chi\mu^2} \right].
\end{aligned} \tag{B2}$$

The superspin ‘‘magnetization’’ \mathbf{m} is defined as

$$\mathbf{m} = -\nabla_{\mathbf{h}} f = (m_1, m_2, m_3, m_4, m_5). \tag{B3}$$

We can introduce also order parameters which refer to AF and SC states, respectively, in the form

$$\mathbf{m}_{AF} = -\nabla_{\mathbf{h}_{AF}} f = (m_2, m_3, m_4), \quad \mathbf{m}_{SC} = -\nabla_{\mathbf{h}_{SC}} f = (m_1, m_5), \tag{B4}$$

where $\mathbf{h}_{AF} = (h_2, h_3, h_4)$ and $\mathbf{h}_{SC} = (h_1, h_5)$. Using Eq. (B2) for the free energy, we obtained

$$\mathbf{m} = \frac{2\mathbf{h}_{AF}}{8\lambda_0 - 4\kappa J - 2g} + \frac{2\mathbf{h}_{SC}}{8\lambda_0 - 4J - 8\chi\mu^2} = \mathbf{m}_{AF} + \mathbf{m}_{SC}. \tag{B5}$$

Applying the saddle-point condition, one obtains

$$1 - \mathbf{m}^2 = \int_{-\infty}^{\infty} \rho(z) dz \left[3 \frac{\coth\left(\frac{\beta}{2} \sqrt{\frac{2\lambda_0 - \kappa Jz - g}{\chi_{AF}}}\right)}{\sqrt{\chi_{AF}(2\lambda_0 - \kappa Jz - g)}} + 2 \frac{\coth\left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda_0 - Jz}{\chi_{SC}}} + 2\mu\right)\right] + \coth\left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda_0 - Jz}{\chi_{SC}}} - 2\mu\right)\right]}{2\sqrt{\chi_{SC}(2\lambda_0 - Jz)}} \right] \quad (\text{B6})$$

and find the equation for the order parameter in the spherical model:

$$1 - \langle \mathbf{n}^2 \rangle = \mathbf{m}^2,$$

$$1 - \langle \mathbf{n}_{AF}^2 \rangle - \langle \mathbf{n}_{SC}^2 \rangle = \mathbf{m}_{AF}^2 + \mathbf{m}_{SC}^2. \quad (\text{B7})$$

In the nonordered phase the average superspin length is constant, and in ordered 1 is decreased by the presence of a nonzero order parameter.

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- ¹S. C. Zhang, *Science* **275**, 1089 (1997).
²C. Henley, *Phys. Rev. Lett.* **80**, 3590 (1998).
³S. Rabello, H. Kohno, E. Demler, and S. C. Zhang, *Phys. Rev. Lett.* **80**, 3586 (1998).
⁴C. Burgess, J. Cline, R. MacKenzie, and R. Ray, *Phys. Rev. B* **57**, 8549 (1998).
⁵D. Scalapino, S. C. Zhang, and W. Hanke, *Phys. Rev. B* **58**, 443 (1998).
⁶R. Eder *et al.*, *Phys. Rev. B* **59**, 561 (1999).
⁷E. Arrigoni and W. Hanke, *Phys. Rev. Lett.* **82**, 2115 (1999).
⁸S. Meixner, W. Hanke, E. Demler, and S. C. Zhang, *Phys. Rev. Lett.* **79**, 4902 (1997).
⁹X. Hu, T. Koyama, and M. Tachiki, *Phys. Rev. Lett.* **82**, 2568 (1999).
¹⁰X. Hu, cond-mat/9906237 (unpublished).
¹¹T. Koyama, *J. Phys. Soc. Jpn.* **66**, 4051 (1997).
¹²C. Castellani, C. Di Castro, and M. Grilli, *J. Phys. Chem. Solids* **59**, 1694 (1998).
¹³C. Castellani, C. Di Castro, and M. Grilli, *Physica C* **282-287**, 260 (1997).
¹⁴The NL σ M Hamiltonian [Eq. (1)] describes the system of interacting *quantum* rigid rotors with *fixed* length. However, by coarse graining the Hamiltonian with order parameter variables which couple to the original ‘‘microscopic’’ superspin components (e.g., by using the Hubbard-Stratonovich formula) one can derive the effective *classical* Ginzburg-Landau (GL) free energy functional written in terms of powers of order parameters. These order parameter fields are, in turn, of an *unrestricted* nature, allowing a conventional GL mean-field-type approach [see, e.g., S. Alama *et al.*, *Phys. Rev. B* **60**, 6901 (1999)].
¹⁵C. Henley, *Phys. Rev. Lett.* **80**, 3590 (1998); S. Rabello, H. Kohno, E. Demler, and S. C. Zhang, *Phys. Rev. Lett.* **80**, 3586 (1998); C. Burgess, J. Cline, R. MacKenzie, and R. Ray, *Phys. Rev. B* **57**, 8549 (1998).
¹⁶S. C. Zhang, J. P. Hu, E. Arrigoni, W. Hanke, and A. Auerbach, *Phys. Rev. B* **60**, 13 070 (1999).
¹⁷This expression agrees with the analogous formula [Eq. (13)] given by F. J. Wegner, *Eur. Phys. J. B* **14**, 11 (2000), but disagrees with Eq. (20) of Zhang’s paper (see Ref. 1). If $\chi_c \neq \chi_\pi$, then the effective potentials are different (actually, in the first-order in $\chi_c - \chi_\pi$ there is still agreement). Nevertheless, many of Zhang’s conclusions will continue to hold. As pointed out by Wegner this discrepancy comes from the fact that in Zhang’s Lagrangian [see Eq. (18) in Zhang’s paper] the only allowed rotations are in the plane spanned by n_μ and $\partial_\tau n_\mu - i \sum_\nu B_{\mu\nu} n_\nu$, whereas it does not permit a rotation around a second perpendicular plain (which exists in five dimensions) as it should. For the derivation of formula (10) the proper integration in the Lagrangian over the transverse momenta (to maintain the constraint $\mathbf{p} \cdot \mathbf{n} = 0$) is the key for the effective interaction (10).
¹⁸T. H. Berlin and M. Kac, *Phys. Rev.* **86**, 821 (1952); H. E. Stanley, *ibid.* **176**, 718 (1968); G. S. Joyce, *ibid.* **146**, 349 (1966); in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic, New York, 1972), Vol. 2, p. 375.
¹⁹Using a spherical approach one is not restricted to a particular lattice structure. Other choices of physical interest are possible; for example, one can realistically accommodate the *c*-axis anisotropy by assuming $J(\mathbf{k}) = J[\cos(k_x) + \cos(k_y)] + J_z \cos(k_z)$ with $J_z \ll J$. In that case one expects a suppression of the critical temperature of the AF and SC orderings as compared to the isotropic case. For a strictly two-dimensional system ($J_z = 0$) there will be no long-range order for $T \neq 0$ (i.e., the spherical model complies with the Mermin-Wagner theorem).
²⁰*Handbook of Mathematical Functions*, edited by M. Abramovitz and I. Stegun (Dover, New York, 1970).
²¹However, the situation of global phase separation will not occur in systems with a long-range Coulomb interaction (not considered in the present paper). This interaction could presumably induce a stripe order of alternating AF and SC phases.
²²M. Veillette, Ya. B. Bazaliy, A. J. Berlinsky, and C. Kallin, *Phys. Rev. Lett.* **83**, 2413 (1999).
²³R. A. Pelcovits and D. R. Nelson, *Phys. Lett.* **57A**, 23 (1976).