SO(5) superconductor in a Zeeman magnetic field: Phase diagram and thermodynamic properties

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In this paper we present calculations of the SO(5) quantum rotor theory of high-T_c superconductivity in a Zeeman magnetic field. We use the spherical approach for five-component quantum rotors in a three-dimensional lattice to obtain formulas for the critical lines, free energy, entropy, specific heat, and present temperature dependences of these quantities for different values of the magnetic field. Our results are in qualitative agreement with relevant experiments on high-T_c cuprates.

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I. INTRODUCTION

The SO(5) theory of high-T_c superconductivity, unifying antiferromagnetism and superconductivity, was proposed to combine SO(3) antiferromagnetic (AF) staggered magnetization with superconducting (SC) two-component U(1) real paring field into a new order parameter.[1] The smallest symmetry group meeting this requirements is the SO(5) group. It contains the SO(3) group of spin rotation and the U(1) gauge group of ''charge rotation'' as subgroups along with additional, the so-called ''π'' operators rotating the AF to SC state and vice versa. In the SO(5) theory ordered phases arise once SO(5) symmetry is spontaneously broken: with SO(3) symmetry breaking the AF phase arises, while for U(1) symmetry breaking the SC phase appears. Consequently, AF and SC order parameters are grouped into five component vectors called ''superspin,'' the direction of which is related to the competition between AF and SC states and the kinetic energy of the system is that of a SO(5) quantum rigid rotor. The low-energy dynamics is determined in terms of the Goldstone modes and their interactions specified by the SO(5) symmetry.

Although, the SO(5) theory was originally proposed in the context of an effective quantum nonlinear σ model (NLQσM) description of the SO(5) rotor model, its predictions were tested also within microscopic models.[2–7] Calculations based on the NLQσM showed that the features of the phase diagram deduced from the SO(5) theory agree qualitatively with the global topology of the observed phase diagrams of high-T_c superconductors.[8] Magnetic correlation functions within the SO(5) theory were investigated, showing that the theory predicts a scenario for the evolution of magnetic behavior, which is qualitatively consistent with experiments.[9] Furthermore, the study of the quantum critical point scenario within the concept of the SO(5) group showed that the scaling of the contribution to the electrical resistivity due to spin fluctuations displayed a linear resistivity dependence on temperature for increasing quantum fluctuations, which is a hallmark example of anomalous properties of cuprate materials.[10] Finally, thermodynamic properties of the SO(5) model were studied, where entropy and specific heat were calculated and compared with experimental findings.[11]

Many experimentally observed properties of high-T_c cuprates show a strong dependence on the magnetic field, e.g., entropy, specific heat, magnetic susceptibility, electrical resistivity, etc. Therefore, a proper theory of high-T_c superconductors must be able to explain the magnetic properties of these materials. Since the SO(5) model in the presence of a finite chemical potential and a finite Zeeman magnetic field has exact SU(2)$\times$U(1) symmetry, the Zeeman magnetic field can be introduced, and the SO(5) theory can be tested in any doping level.[12]

The aim of this paper is to study influence of the Zeeman magnetic field within the SO(5) theory. The results obtained (e.g., specific heat) can be then (qualitatively) compared with the relevant experiments and test the basic principles of the SO(5) theory.

The outline of the reminder of the paper is as follows. In Sec. II we introduce the quantum SO(5) Hamiltonian in the Zeeman magnetic field and find the corresponding Lagrangian of the NLQσM. In Sec. III we establish the phase diagram of the system in an applied magnetic field. Section IV is devoted to the study of magnetic dependence of various thermodynamic functions: free energy, entropy, and the specific heat. Finally, in Sec. V we summarize the conclusions to be drawn from our work.

II. HAMILTONIAN AND THE EFFECTIVE LAGRANGIAN

We start from the low-energy Hamiltonian of superspins $\mathbf{n}_i$ placed in the discrete three-dimensional (3D) SC (3DSC) lattice in the Zeeman magnetic field B along the y axis. The sites are numbered by indices i and j running from 1 to N—the total number of sites. The superspin components, labeled by μ and $\nu=1,\ldots,5$, refer to AF $[\mathbf{n}_i^{AF}=(n_2,n_3,n_4)_i]$ and SC $[\mathbf{n}_i^{SC}=(n_1,n_5)_i]$ order parameters, respectively. The superspin components are mutually commuting variables[1] and their values are restricted by the rigid rotator constraint $\mathbf{n}_i^2=1$. The SO(5) Hamiltonian

$$H=\frac{1}{2u}\sum_i\sum_{\mu<\nu}L_i^{\mu\nu}L_i^{\mu\nu}-\sum_{i<j}J_{ij}\mathbf{n}_i\cdot\mathbf{n}_j-V(\mathbf{n}_i)$$
$$-B\sum_i L_i^{24}-2\mu\sum_i L_i^{15} \tag{1}$$

consists of three parts: the kinetic energy of the rotors (where u is an analog of the moment of inertia), intersite interaction energy (with J_{ij} being the stiffness in the charge and spin channel), and SO(5) symmetry breaking part (including the

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Zeeman magnetic field acting in the AF sector). The quantities $L_i^{\mu\nu}=n_{\mu i}p_{\nu i}-n_{\nu i}p_{\mu i}$ are generators of the Lie SO(5) algebra (related to the total charge, spin, and so-called "π" operators[1]) and $p_{\mu i}$ are linear momenta given by

$$p_{\mu i}=i\frac{\partial}{\partial n_{\mu i}},$$

$$[n_\mu,p_\nu]=i\delta_{\mu\nu}. \tag{2}$$

Furthermore, we assume that $J_{ij}\equiv J(\mathbf{R}_i-\mathbf{R}_j)$ is nonvanishing for the nearest neighbors and its Fourier transform

$$J_{\mathbf{q}}=\frac{1}{N}\sum_{\mathbf{R}_i} J(\mathbf{R}_i)e^{-i\mathbf{R}_i\cdot\mathbf{q}} \tag{3}$$

is simply $J_{\mathbf{q}}=J\epsilon(\mathbf{k})$, where

$$\epsilon_{\mathbf{q}}=\cos q_x+\cos q_y+\cos q_z \tag{4}$$

is the structure factor for the 3D SC lattice.[13]

The last three parts of the Hamiltonian provide SO(5) symmetry breaking terms. In the result of their interplay, the system favors 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). Two of the three terms influence directly the AF order parameter:

$$V(\mathbf{n}_i)-B\sum_i L_i^{24}=\frac{w}{2}\sum_i (n_{2i}^2+n_{3i}^2+n_{4i}^2)-B\sum_i L_i^{24}, \tag{5}$$

where w is the anisotropy constant, B is the Zeeman magnetic field, and L_i^{24} is the y component of the spin vector. Positive values of w and B favor the AF state. The remaining term acts on the SC sector and contains the total charge operator L_i^{15}, whose expectation value yields the doping concentration and the chemical potential μ (measured from half-filling), the positive value of which favors the SC state.

We express the partition function $Z=\mathrm{Tr}\,e^{-\beta H}$ using the functional integral in the Matsubara "imaginary time" τ formulation[8] ($0\leqslant\tau\leqslant 1/k_BT\equiv\beta$, with T being the temperature). Explicitly,

$$\begin{aligned}Z&=\int\prod_i [D\mathbf{n}_i]\int\prod_i\left[\frac{D\mathbf{p}_i}{2\pi}\right]\delta(1-\mathbf{n}_i^2)\,\delta(\mathbf{n}_i\cdot\mathbf{p}_i)\\&\quad\times\exp\left\{-\int_0^\beta d\tau\left[i\mathbf{p}(\tau)\cdot\frac{d}{d\tau}\mathbf{n}(\tau)+H(\mathbf{n},\mathbf{p})\right]\right\}\\&=\int\prod_i [D\mathbf{n}_i]\,\delta(1-\mathbf{n}_i^2)\exp\left(-\int_0^\beta d\tau\mathcal{L}(\mathbf{n})\right),\end{aligned} \tag{6}$$

with $\mathcal{L}$ being the Lagrangian:

$$\begin{aligned}\mathcal{L}(\mathbf{n})=\frac{1}{2}\Bigg[&\sum_i u\left(\frac{\partial\mathbf{n}_{SC}}{\partial\tau}\right)^2+u\left(\frac{\partial\mathbf{n}_{AF}}{\partial\tau}\right)^2-4u\mu^2\mathbf{n}_{SC}^2\\&+4iu\mu\left(\frac{\partial n_1}{\partial\tau}n_5-\frac{\partial n_5}{\partial\tau}n_1\right)-uB^2(n_2^2+n_4^2)\\&+2iuB\left(\frac{\partial n_2}{\partial\tau}n_4-\frac{\partial n_4}{\partial\tau}n_2\right)-\sum J_{ij}\mathbf{n}_i\cdot\mathbf{n}_j\\&-w\sum_i (n_{2i}^2+n_{3i}^2+n_{4i}^2)\Bigg].\end{aligned} \tag{7}$$

The problem can be solved exactly in terms of the spherical model.[14] We note that the superspin rigidity constraint ($\mathbf{n}_i^2=1$) implies that a weaker condition also holds, namely,

$$\frac{1}{N}\sum_{i=1}^N \mathbf{n}_i^2=1. \tag{8}$$

Therefore, the superspin components $\mathbf{n}_i(\tau)$ satisfying the quantum periodic boundary condition $\mathbf{n}_i(\beta)=\mathbf{n}_i(0)$ will be treated as *continuous* variables, i.e., $-\infty<\mathbf{n}_i(\tau)<\infty$, but constrained on average [due to Eq. (8)]. The constraint can be implemented using the Dirac δ function $\delta(x)=\int_{-\infty}^{+\infty}[d\lambda/2\pi]e^{i\lambda x}$, which introduces the Lagrange multiplier $\lambda(\tau)$ adding an additional quadratic term (in $\mathbf{n}_i$ fields) to the Lagrangian (7). Consequently, the partition function reads

$$Z=\int\left[\frac{d\lambda}{2\pi i}\right]e^{-N\phi(\lambda)}, \tag{9}$$

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

$$\begin{aligned}\phi(\lambda)=&-\int_0^\beta d\tau\lambda(\tau)-\frac{1}{N}\ln\int\prod_i [D\mathbf{n}_i]\\&\times\exp\left[-\sum_i\int_0^\beta d\tau(\mathbf{n}_i^2\lambda(\tau)-\mathcal{L}[\mathbf{n}])\right].\end{aligned} \tag{10}$$

In the thermodynamic limit ($N\to\infty$), the method of steepest descent is exact and the saddle point $\lambda(\tau)=\lambda_0$ satisfies the condition

$$\frac{\delta\phi(\lambda)}{\delta\lambda(\tau)}\Big|_{\lambda=\lambda_0}=0. \tag{11}$$

At the antiferromagnetic and superconducting phase transition boundaries the corresponding order susceptibilities become infinite (see Ref. 8), which implies for the Lagrange multipliers

$$\lambda_0^{AF}=\frac{1}{2}J_{\mathbf{k}=0}+\frac{w}{2}+\frac{uB^2}{2},$$

$$\lambda_0^{SC}=\frac{1}{2}J_{\mathbf{k}=0}+2u\mu^2, \tag{12}$$

for the AF and SC critical lines, respectively.

III. PHASE DIAGRAM

Providing the spherical condition (8) with values of the Lagrange multipliers (12) one can finally arrive at the expression for the critical lines separating AF (or SC) and QD (quantum disordered) states:

$$1=\frac{1}{2u}\int_{-\infty}^{\infty}\rho(\xi)d\xi\left\{\frac{\cosh\left[\frac{\beta}{2}A(\xi)\right]}{A(\xi)}+\frac{\cosh\left[\frac{\beta}{2}D_{-}(\xi)\right]}{A(\xi)}+\frac{\cosh\left[\frac{\beta}{2}D_{+}(\xi)\right]}{A(\xi)}+\frac{\cosh\left[\frac{\beta}{2}B_{-}(\xi)\right]}{C(\xi)}+\frac{\cosh\left[\frac{\beta}{2}B_{+}(\xi)\right]}{C(\xi)}\right\}, \tag{13}$$

where

$$A(\xi)=\sqrt{\frac{2\lambda_0-J\xi-w}{u}},\quad C(\xi)=\sqrt{\frac{2\lambda_0-J\xi}{u}},$$

$$B_{-}(\xi)=\sqrt{\frac{2\lambda_0-J\xi}{u}}-2\mu,\quad D_{-}(\xi)=\sqrt{\frac{2\lambda_0-J\xi-w}{u}}-B,$$

$$B_{+}(\xi)=\sqrt{\frac{2\lambda_0-J\xi}{u}}+2\mu,\quad D_{+}(\xi)=\sqrt{\frac{2\lambda_0-J\xi-w}{u}}+B, \tag{14}$$

and $\lambda_0=\lambda_0^{AF}$ (λ_0^{SC}) for the AF (SC) line. For convenience, in order to perform momentum integration over the 3D Brillouin zone, we have introduced the density of states

$$\rho(\xi)=\frac{1}{N}\sum_{\mathbf{q}}\delta[\xi-\epsilon(\mathbf{q})] \tag{15}$$

(for the explicit formula, see Ref. 8).

Regions of AF and SC phases are separated by the first-order transition line (for $\mu=\mu_c$) given by the condition of equality of free energies of both states, which reads

$$\lambda_0^{SC}=\lambda_0^{AF}\Rightarrow\mu_c^2=\frac{w}{4u}+\frac{B^2}{4}. \tag{16}$$

It is instructive to present the phase diagram as a function of a physically measured quantity—the charge concentration x instead of the chemical potential. In the SO(5) theory, the charge concentration can be deduced from the free energy:

$$x=\langle L^{15}\rangle=-\frac{1}{2}\frac{df}{d\mu}=-\frac{1}{2\beta}\frac{d\phi(\lambda_0)}{d\mu}. \tag{17}$$

The temperature-charge concentration phase diagram is depicted in Fig. 1. Here, the AF to SC transition line splits into a region of constant chemical potential, where AF and SC states coexist (mixed region M). 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 in two different spatial regions with different charge densities, but the same free energy. As a result, the added charges only change the proportion of the mixture of the two phases, but not the free energy, which implies infinite compressibility (defined as $dx/d\mu$).

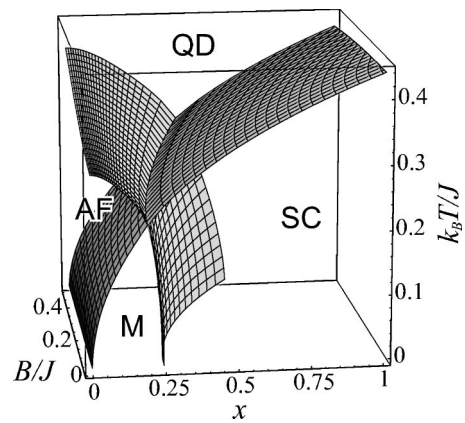

FIG. 1. T-x-B phase diagram for $uJ=3$ and $w/J=1$.

IV. THERMODYNAMIC FUNCTIONS

A. Free energy

The free energy is defined as $f=-(\beta N)^{-1}\ln Z=(\beta)^{-1}\phi(\lambda_0)$. Using the formula (10), it can be explicitly written

$$f=-\lambda+F_1(A)+F_1(B_-)+F_1(B_+)+F_1(D_-)+F_1(D_+), \tag{18}$$

where the function

$$F_1(\Xi)=\frac{1}{\beta}\int_{-\infty}^{\infty}\rho(\xi)d\xi\ln\left\{2\sinh\left[\frac{\beta}{2}\Xi(\xi)\right]\right\} \tag{19}$$

and $A(\xi)$, $B_-(\xi)$, $B_+(\xi)$, $D_-(\xi)$, and $D_+(\xi)$ are defined by formulas (14).

B. Entropy

The entropy is defined as $S=k_B\beta^2\partial f/\partial\beta$. Using the formula (18) we obtain

$$S(\beta)=F_2(A)+F_2(B_-)+F_2(B_+)+F_2(D_-)+F_2(D_+), \tag{20}$$

where the function

$$F_2(\Xi)=\frac{k_B}{2}\int_{-\infty}^{\infty}\rho(\xi)d\xi\left(\beta\Xi(\xi)\coth\left[\frac{\beta}{2}\Xi(\xi)\right]-2\ln\left\{2\sinh\left[\frac{\beta}{2}\Xi(\xi)\right]\right\}\right). \tag{21}$$

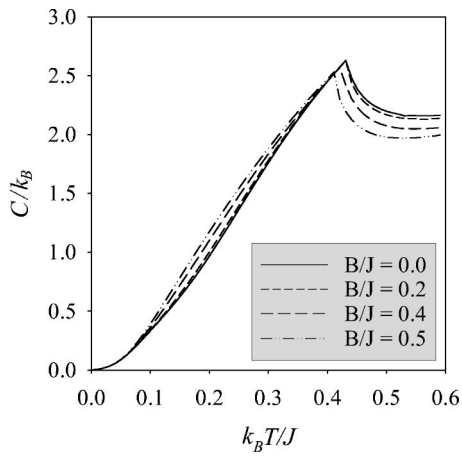

FIG. 2. Temperature dependence of the specific heat for various magnetic fields, for $uJ=3$ and $w/J=1$.

C. Specific heat

The specific heat at constant volume is defined as

$$C=-k_B\beta^2\frac{\partial^2}{\partial\beta^2}(\beta f)=-k_B\beta^2 \times\left\{2\frac{\partial f}{\partial\beta}+\beta\frac{\partial^2 f}{\partial\beta^2}+\beta\frac{d\lambda}{d\beta}\left[\frac{\partial^2 f}{\partial\lambda^2}\frac{d\lambda}{d\beta}+2\frac{\partial^2 f}{\partial\lambda\,\partial\beta}\right]\right\}. \tag{22}$$

The temperature dependence of the specific heat in various magnetic field is depicted in Fig. 2. For low temperatures $C(T)$ is independent of B and can be approximated by $C(T)\sim T^3$. For higher temperatures the dependence becomes roughly linear with higher values of $C(T)$ for higher magnetic fields. The critical temperature is depressed for higher fields, which is in agreement with experimental findings. Only the size of the finite jump occurring at the critical point seems to be independent of B (for Y-123 the jump of the specific heat in the critical temperature is absent because of flux lattice melting; see Refs. 15 and 16). Consequently, the Zeeman magnetic field does not influence the value of the critical exponent $\alpha=0$. In high temperatures the $C(T)$ dependence saturates.

V. FINAL REMARKS

In conclusion, we have considered the influence of the Zeeman magnetic field in the SO(5) theory of high-T_c superconductivity proposed by Zhang. Experimentally, in high-T_c cuprates the Zeeman magnetic field can be realized by applying a magnetic field parallel to the *ab* planes. Using the nonlinear quantum σ model and the spherical approximation we have found explicit expressions for the critical lines and various thermodynamic functions (free energy, entropy, and specific heat). The results obtained are in qualitative agreement with experimentally observed features of high-T_c cuprates. The maximum of the specific heat is depressed and shifted towards lower temperature in higher magnetic fields. However, it should be stressed that the case of the Zeeman field considered in the present paper neglects the orbital effects, which are important in high-T_c cuprates, when the magnetic field is applied perpendicularly to the *ab* planes.

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