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Thermodynamic properties of the $SO(5)$ model of high- T_c superconductivity

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Abstract

In this paper we present calculations of thermodynamic functions within Zhang's $SO(5)$ quantum rotor theory of high- T_c superconductivity. Using the spherical approach for three-dimensional quantum rotors we derive explicit analytical formulae for entropy and specific heat related to the lattice version of the $SO(5)$ nonlinear quantum sigma model. We present the temperature dependence of these quantities for various settings of relevant control parameters (quantum fluctuations and chemical potential). We find our results in overall qualitative agreement with basic thermodynamics of high- T_c cuprates.

1. Introduction

A theory unifying antiferromagnetism (AF) and superconductivity (SC) to describe the global phase diagram of high- T_c superconductors was recently proposed by Zhang [1]. In this approach, based on symmetry principles, a three-dimensional order parameter (the staggered magnetization) describing the AF phase and a complex order parameter (with two real components), describing a spin singlet d-wave SC phase, are grouped in a five-component vector called a 'superspin'. The $SO(3)$ symmetry of spin rotations (which is spontaneously broken in the AF phase) and the electro-magnetic $SO(2)$ invariance (whose breaking defines the SC phase) along with well defined AF to SC and vice versa rotation operators form $SO(5)$ symmetry. In the Zhang theory both ordered phases arise once $SO(5)$ is spontaneously broken and the competition between AF and SC 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 the 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 an $SO(5)$ nonlinear quantum σ model (NLQ σ M). The $SO(5)$ quantum rotor model offers a Landau–Ginzburg–(LG)-like approach for the high- T_c problem. However, it goes far beyond the 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 approximate $SO(5)$ symmetry of the Hubbard model emerged from exact diagonalization of small clusters [8]. The global features of the phase diagram deduced from $SO(5)$ theory based on a spherical quantum rotor [9] agree qualitatively with the general topology of the observed phase diagram of high- T_c superconductors. The quantitative investigation of the quantum critical point scenario within the concept of the $SO(5)$ group, for example the scaling of the contribution to the electrical resistivity due to spin fluctuations, showed a linear resistivity dependence on temperature for increasing quantum fluctuation—this being a hallmark example of anomalous properties in cuprate materials [10]. The systematic studies of magnetic properties of the $SO(5)$ theory showed that the theory yields a qualitative scenario for the evolution of magnetic behaviour, which is consistent with experiments [11]. It qualitatively explains the results of experimental measurements (notably the nuclear magnetic resonance (NMR) relaxation rates) with correct predictions of behaviour of uniform spin susceptibility at high temperatures. Also the energy dependence of the momentum-integrated dynamic spin susceptibility shows features which are in qualitative agreement with experimental findings.

Thermal fluctuations are pronounced in the high- T_c superconductors for a number of reasons. The carrier density is rather small, the anisotropy is large and the critical temperature is high. It turns out that deviations from the mean-field behaviour are present in the specific heat C at the SC transition temperature T_c . In the mean-field BCS theory, a second-order transition with a jump in specific heat at T_c takes place. In contrast, in most high- T_c superconductors thermal fluctuations seem to restore common behaviour.

The aim of this paper is to study quantitatively basic thermodynamic functions resulting from the $SO(5)$ theory, thereby substantiating this theoretical framework. Our study may also provide a useful diagnostic tool for testing the basic principles of $SO(5)$ theory by comparing the quantitative predictions (e.g. specific heat) with the outcome of the relevant experiments.

The outline of the remainder of the paper is as follows. In section 2 we begin by setting up the quantum $SO(5)$ Hamiltonian and the corresponding Lagrangian. In section 3 we find closed forms of various thermodynamic functions. We calculate free energy, entropy and specific heat. Finally, in section 4 we summarize the conclusions to be drawn from our work.

2. The Hamiltonian and the effective Lagrangian

We consider the low-energy Hamiltonian of superspins placed in the nodes of a discrete three-dimensional simple cubic (3DSC) lattice,

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

Indices i and j number lattice sites running from 1 to N —the total number of sites, while $\mu, \nu = 1, \dots, 5$ denote superspin $\mathbf{n}_i = (n_1, n_2, n_3, n_4, n_5)_i$ components ($\mathbf{n}_{AF,i} = (n_2, n_3, n_4)_i$ refers to AF and $\mathbf{n}_{SC,i} = (n_1, n_5)_i$ SC order, respectively). The superspin components are mutually commuting (according to Zhang's formulation) and their values are restricted by the rigidity constraint $\mathbf{n}_i^2 = 1$.

The first part of the equation (1) is the kinetic energy of the system (being simply that of a $SO(5)$ rigid rotor), where

$$L_i^{\mu\nu} = n_{\mu i} p_{\nu i} - n_{\nu i} p_{\mu i} \quad (2)$$

are generators of Lie $SO(5)$ algebra (expressed by total charge L_i^{15} , spin and so-called ‘ π ’ operators), $p_{\mu i}$ are momenta conjugated to respective superspin components,

$$\begin{aligned} p_{\mu i} &= i \frac{\partial}{\partial n_{\mu i}}, \\ [n_{\mu}, p_{\nu}] &= i \delta_{\mu\nu}, \end{aligned} \quad (3)$$

and parameter u measures the kinetic energy of the rotors (an analogue of moment of inertia).

The second part of the Hamiltonian is the inter-superspin interaction energy with J being the stiffness in the charge and spin channel. In the 3DSC lattice, J is nonvanishing for the nearest neighbours and its Fourier transform

$$J_q = \frac{1}{N} \sum_{\mathbf{R}_i} J(\mathbf{R}_i) e^{-i\mathbf{R}_i \cdot \mathbf{q}} \quad (4)$$

is simply

$$J_q/J = \cos q_x + \cos q_y + \cos q_z. \quad (5)$$

For convenience, we shall further introduce the density of states

$$\rho(\xi) = \frac{1}{N} \sum_{\mathbf{q}} \delta(\xi - J_{\mathbf{q}}/J), \quad (6)$$

which for the 3DSC¹ lattice reads

$$\rho(\xi) = \frac{1}{\pi^3} \int_{\max(-1, -2-\xi)}^{\min(1, 2-\xi)} \frac{dy}{\sqrt{1-y^2}} \mathbf{K} \left[\sqrt{1 - \left(\frac{\xi+y}{2} \right)^2} \right] \Theta(3 - |\xi|), \quad (7)$$

where $\mathbf{K}(x)$ is the elliptic integral of the first kind and $\Theta(x)$ is the step function [12].

The last two parts of the equation (1) provide symmetry $SO(5)$ breaking terms. In the result of their interplay, the system favours 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). The first of the two terms is defined as

$$V(n_i) = \frac{w}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2), \quad (8)$$

with the anisotropy constant w , of which positive value favours the AF state. The second term contains a charge operator L_i^{15} , whose expectation value yields the doping concentration and the chemical potential μ (measured from half-filling), whose positive values favour the SC state.

The partition function $Z = \text{Tr} e^{-H/k_B T}$ is expressed using the functional integral in the Matsubara ‘imaginary time’ τ formulation [9] ($0 \leq \tau \leq 1/k_B T \equiv \beta$, with T being the temperature). We obtain

$$\begin{aligned} Z &= \int \prod_i [Dn_i] \int \prod_i \left[\frac{Dp_i}{2\pi} \right] \delta(1 - n_i^2) \delta(\mathbf{n}_i \cdot \mathbf{p}_i) \\ &\quad \times \exp \left\{ - \int_0^\beta d\tau \left[i\mathbf{p}(\tau) \cdot \frac{d}{d\tau} \mathbf{n}(\tau) + H(\mathbf{n}, \mathbf{p}) \right] \right\} \\ &= \int \prod_i [Dn_i] \delta(1 - n_i^2) \exp \left\{ - \int_0^\beta d\tau \mathcal{L}(\mathbf{n}) \right\}, \end{aligned} \quad (9)$$

¹ Our approach is not restricted to the three-dimensional cubic lattice and can be easily accommodated to virtually any other lattice (by using the proper density of states function).

with \mathcal{L} being the Lagrangian:

$$\mathcal{L}(\mathbf{n}) = \frac{1}{2} \sum_i \left[u \left(\frac{\partial \mathbf{n}_{SC}}{\partial \tau} \right)^2 + u \left(\frac{\partial \mathbf{n}_{AF}}{\partial \tau} \right)^2 - 4u\mu^2 n_{SC}^2 + 4iu\mu \left(\frac{\partial n_1}{\partial \tau} n_5 - \frac{\partial n_5}{\partial \tau} n_1 \right) \right] - \sum_{i < j} J_{ij} \mathbf{n}_i \cdot \mathbf{n}_j - \frac{w}{2} \sum_i (n_{2i}^2 + n_{3i}^2 + n_{4i}^2). \quad (10)$$

The problem can be solved *exactly* in terms of the spherical model [13]. To accommodate this we notice that the superspin rigidity constraint ($n_i^2 = 1$) implies that a weaker condition also holds, namely

$$\sum_{i=1}^N \mathbf{n}_i^2 = N. \quad (11)$$

Therefore, the superspin components $\mathbf{n}_i(\tau)$ must be treated as *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 equation (11)) to have unit length.

This introduces the Lagrange multiplier $\lambda(\tau)$ adding an additional quadratic term (in \mathbf{n}_i fields) to the Lagrangian (10). The Fourier transform $\mathbf{n}(\mathbf{k}, \omega_\ell)$ of the superspin components

$$\mathbf{n}_i(\tau) = \frac{1}{\beta N} \sum_{\mathbf{k}} \sum_{\ell=-\infty}^{\infty} \mathbf{n}(\mathbf{k}, \omega_\ell) e^{-i(\omega_\ell \tau - \mathbf{k} \cdot \mathbf{r}_i)} \quad (12)$$

introduces the Matsubara (Bose) frequencies $\omega_\ell = 2\pi\ell/\beta$ ($\ell = 0, \pm 1, \pm 2, \dots$).

Using the equation (9), the partition function can be written in the form

$$Z = \int \frac{d\lambda}{2\pi i} e^{-N\phi(\lambda)}, \quad (13)$$

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

$$\phi(\lambda) = - \int_0^\beta d\tau \lambda(\tau) - \frac{1}{N} \ln \int \prod_i [D\mathbf{n}_i] \exp \left[- \sum_i \int_0^\beta d\tau (n_i^2 \lambda(\tau) - \mathcal{L}[\mathbf{n}]) \right]. \quad (14)$$

The exact value of the partition function can be found in the thermodynamic limit ($N \rightarrow \infty$), when the method of steepest descents is exact and the saddle point $\lambda(\tau) = \lambda_0$ satisfies the condition

$$\left. \frac{\delta \phi(\lambda)}{\delta \lambda(\tau)} \right|_{\lambda=\lambda_0} = 0. \quad (15)$$

At criticality, corresponding order parameter susceptibilities become infinite and corresponding Lagrange multipliers are

$$\begin{aligned} \lambda_0^{AF} &= \frac{1}{2} J_{k=0} + \frac{w}{2}, \\ \lambda_0^{SC} &= \frac{1}{2} J_{k=0} + 2\chi\mu^2, \end{aligned} \quad (16)$$

for AF and SC critical lines, respectively. Furthermore, using the spherical condition (11) and the values (16), we finally arrive at the expression for the critical lines separating AF, SC and QD (quantum disordered) states (for more specific description of these calculations see [9, 11]).

3. Thermodynamic functions

3.1. Free energy

The free energy is defined as $f = -(\beta N)^{-1} \ln Z = (\beta)^{-1} \phi(\lambda_0)$. Using the formula (14), we obtain

$$f = -\lambda + \frac{3}{2\beta N} \sum_{k,\ell} \ln[2\lambda - J_k + u\omega_\ell^2 - w] + \frac{1}{2\beta N} \sum_{k,\ell} \ln[2\lambda - J_k + u(\omega_\ell + 2i\mu)^2] + \frac{1}{2\beta N} \sum_{k,\ell} \ln[2\lambda - J_k + u(\omega_\ell - 2i\mu)^2]. \quad (17)$$

After performing the summation over Matsubara's frequencies, we obtain the free energy:

$$f = -\lambda + \frac{1}{\beta} \int_{-\infty}^{\infty} \rho(\xi) d\xi \left\{ 3 \ln 2 \sinh \left(\frac{\beta}{2} \sqrt{\frac{2\lambda - J\xi - w}{u}} \right) + \ln 2 \sinh \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda - J\xi}{u}} - 2\mu \right) \right] + \ln 2 \sinh \left[\frac{\beta}{2} \left(\sqrt{\frac{2\lambda - J\xi}{u}} + 2\mu \right) \right] \right\}. \quad (18)$$

3.2. Entropy

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

$$S(\beta) = \frac{k_B}{2} \int_{-\infty}^{\infty} \rho(\xi) d\xi \left\{ 3 \left[\beta A(\xi) \coth \frac{\beta}{2} A(\xi) - 2 \ln 2 \sinh \frac{\beta}{2} A(\xi) \right] + \left[\beta B_-(\xi) \coth \frac{\beta}{2} B_-(\xi) - 2 \ln 2 \sinh \frac{\beta}{2} B_-(\xi) \right] + \left[\beta B_+(\xi) \coth \frac{\beta}{2} B_+(\xi) - 2 \ln 2 \sinh \frac{\beta}{2} B_+(\xi) \right] \right\}, \quad (19)$$

where

$$A(\xi) = \sqrt{\frac{2\lambda - J\xi - w}{u}}, \quad B_-(\xi) = \sqrt{\frac{2\lambda - J\xi}{u}} - 2\mu, \quad B_+(\xi) = \sqrt{\frac{2\lambda - J\xi}{u}} + 2\mu. \quad (20)$$

The dependence of the entropy on temperature and chemical potential is shown in figure 1. Starting from $T = 0$, the entropy increases in any ordered phase (AF or SC) until reaching T_c (or T_N). The further increase is slower, but saturation in higher temperatures is not observed. The absolute value of the entropy is lower for higher quantum fluctuation (see, figure 2). We find obtained results in qualitative agreement with experimentally measured properties of high- T_c superconductors (e.g. for the Bi2212 compound, see [14]).

3.3. Specific heat

The specific heat at constant volume is defined

$$C = -k_B \beta^2 \frac{\partial^2}{\partial \beta^2} (\beta f) = -k_B \beta^2 \left\{ 2 \frac{\partial f}{\partial \beta} + \beta \frac{\partial^2 f}{\partial \beta^2} + \beta \frac{d\lambda}{d\beta} \left[\frac{\partial^2 f}{\partial \lambda^2} \frac{d\lambda}{d\beta} + 2 \frac{\partial^2 f}{\partial \lambda \partial \beta} \right] \right\}. \quad (21)$$

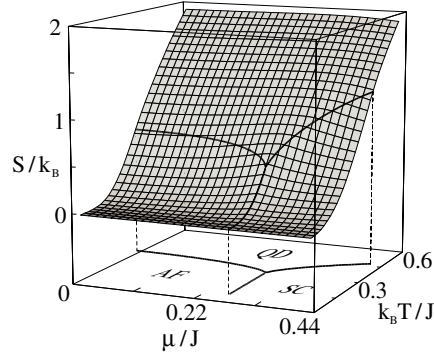


Figure 1. Plot of the entropy S versus chemical potential μ/J and temperature $k_B T/J$ for fixed $uJ = 3$ and $w/J = 1$. Solid curves indicate the projection of the μ - T phase diagram. (This figure is in colour only in the electronic version)

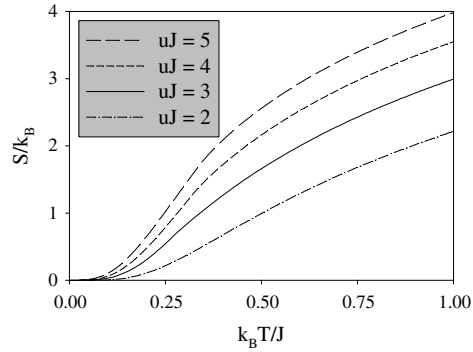


Figure 2. Plot of the entropy S versus temperature $k_B T/J$ for $w/J = 1$, $\mu/J = 0.2$ and different values of uJ , as indicated in the inset.

The derivative $d\lambda/d\beta$ can be found from the saddle-point condition (15):

$$\left. \frac{\partial f[\lambda(\beta), \beta]}{\partial \lambda} \right|_{\lambda=\lambda_0} = 0. \quad (22)$$

Explicitly, we obtain

$$\frac{d\lambda}{d\beta} = -\frac{\partial^2 f / \partial \lambda \partial \beta}{\partial^2 f / \partial \lambda^2}. \quad (23)$$

The specific heat

$$C = -k_B \beta^2 \left[2 \frac{\partial f}{\partial \beta} + \beta \frac{\partial^2 f}{\partial \beta^2} + \beta \frac{d\lambda}{d\beta} \frac{\partial^2 f}{\partial \lambda \partial \beta} \right]. \quad (24)$$

Using the formula (18) we obtain

$$C = \frac{k_B \beta^2}{4} \int_{-\infty}^{\infty} \rho(\xi) d\xi \left\{ 3A^2(\xi) \sinh^{-2} \frac{\beta}{2} A(\xi) + B_-^2(\xi) \sinh^{-2} \frac{\beta}{2} B_-(\xi) + B_+^2(\xi) \sinh^{-2} \frac{\beta}{2} B_+(\xi) \right\} + \frac{k_B \beta^3}{4u} \frac{d\lambda}{d\beta} \int_{-\infty}^{\infty} \rho(\xi) d\xi$$

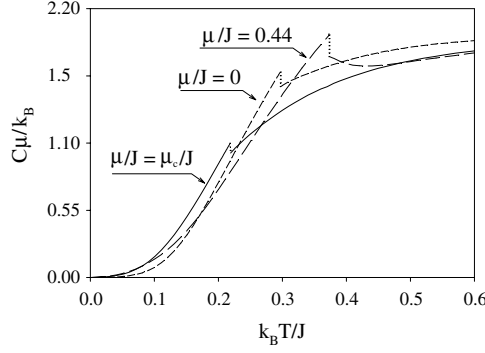


Figure 3. Specific heat versus temperature $k_B T/J$ for $w/J = 1$, $uJ = 3$ and various values of chemical potential, as indicated in the figure.

$$\times \left\{ 3 \sinh^{-2} \frac{\beta}{2} A(\xi) + \frac{B_-(\xi)}{C(\xi)} \sinh^{-2} \frac{\beta}{2} B_-(\xi) + \frac{B_+(\xi)}{C(\xi)} \sinh^{-2} \frac{\beta}{2} B_+(\xi) \right\}, \quad (25)$$

where $A(\xi)$, $B_-(\xi)$ and $B_+(\xi)$ are defined by formula (20),

$$C(\xi) = \sqrt{\frac{2\lambda - J_k}{u}}, \quad (26)$$

and

$$\begin{aligned} \frac{d\lambda}{d\beta} = & -\frac{u}{2} \int_{-\infty}^{+\infty} \rho(\xi) d\xi \left\{ 3 \sinh^{-2} \frac{\beta}{2} A(\xi) + \frac{B_-(\xi)}{C(\xi)} \sinh^{-2} \frac{\beta}{2} B_-(\xi) \right. \\ & \left. + \frac{B_+(\xi)}{C(\xi)} \sinh^{-2} \frac{\beta}{2} B_+(\xi) \right\} / \int_{-\infty}^{+\infty} \rho(\xi) d\xi \left\{ \frac{\beta}{2A^2(\xi)} \sinh^{-2} \frac{\beta}{2} A(\xi) \right. \\ & \left. + \frac{\coth \frac{\beta}{2} A(\xi)}{A^3(\xi)} + \frac{\beta}{2C^2(\xi)} \sinh^{-2} \frac{\beta}{2} B_-(\xi) \right. \\ & \left. + \frac{\coth \frac{\beta}{2} B_-(\xi)}{C^3(\xi)} + \frac{\beta}{2C^2(\xi)} \sinh^{-2} \frac{\beta}{2} B_+(\xi) + \frac{\coth \frac{\beta}{2} B_+(\xi)}{C^3(\xi)} \right\}. \quad (27) \end{aligned}$$

The temperature dependence of the specific heat is presented in figure 3. The low-temperature behaviour of $C(T)$ may be approximated by $C(T) \sim T^3$ for $\mu/J = 0$ and $C(T) \sim T^{2.5}$ for $\mu/J = 0.44$. For higher temperatures (but still below the transition temperature) the linear behaviour of the specific heat is observed. Reaching the critical temperature (T_c or T_N), the specific heat experiences a finite jump (implying the value $\alpha = 0$ for the critical exponent of the specific heat). For higher temperatures, saturation is observed.

4. Summary and final remarks

In conclusion, we have calculated the entropy and specific heat dependence on temperature and various other parameters using the unified theory of AF and SC proposed for the high- T_c cuprates by Zhang and based on the $SO(5)$ symmetry between AF and SC states. The theory yields a qualitative scenario for the evolution of thermodynamic function behaviour, which is consistent with experiments. Most experimental work on the specific heat in the high- T_c superconductors has concentrated on the yttrium compound Y-123 [15–17]. Optimally doped Y-123 does not show a jump in the specific heat, but a λ -peak at T_c . However, the shape for

overdoped Y-123 is intermediate between a BCS step and a λ -type transition. Furthermore, optimally doped Bi-2212 shows a symmetric anomaly (intermediate between a λ -peak and finite jump). Experimentally, the specific heat is not very sensitive to the critical exponent α and one can ascertain that $|\alpha| \ll 1$ for Y-123 compounds. However, the result of the present work ($\alpha = 0$) agrees with the critical behaviour of the 3D-XY model. Finally, checking the validity of basic principles of the $SO(5)$ theory, by comparing parameters discussed here with relevant ones obtained from calculations on microscopic models of high- T_c superconductors, is still called for.

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