Magnetic correlation functions in SO(5) theory of high-T_c superconductivity

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In this paper we present analytical calculations of a variety of magnetic correlation functions within Zhang's SO(5) quantum rotor theory of high-T_c superconductivity. Using the spherical approach for three-dimensional quantum rotors we derived explicit analytical formulas for variety of dynamic spin susceptibilities related to the lattice version of the SO(5) nonlinear quantum-sigma model . We show in detail the frequency dependence of these quantities for various settings of relevant control parameters (like temperature, quantum fluctuations) in normal and superconducting state. We found the results in overall qualitative agreement with basic phenomenology of high-T_c cuprates.

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I. INTRODUCTION

Over a last decade neutron-scattering experiments have provided a considerable insight in understanding of high-T_c superconductors. Neutron measurements have shown the persistence of antiferromagnetic (AF) correlations over the whole metallic state of cuprates demonstrating the strong electronic correlations existing in these compounds. It is now well known that all the cuprates show the same generic behavior. Depending on charge doping they can show up as antiferromagnets or *d*-wave superconductors (SC) and the intimate connection between these two orders is believed to be fundamental to the underlying superconducting effects. In undoped cuprates, the magnetic interactions between the electrons force an antiferromagnetic arrangement of their spins. These interactions must change when electrons start to move around, with the pairing of charge carriers being a consequence. As a result, magnetic interactions must play an important role in every theory of high-T_c superconductivity. The precise nature of antiferromagnetic correlations and how they influence electronic properties are the most puzzling aspects of high-T_c cuprate superconductors.

It is now widely accepted that studying dynamical spin susceptibility of high-temperature superconducting cuprates may be instrumental for the understanding of their many unusual properties. Among these issues, the existence of resonance peaks in the superconducting state and its suppression in the normal state are the most intriguing. A great deal of theoretical studies have been made to understand the structure of measured dynamical spin susceptibility in both normal and superconducting states. A phenomenological antiferromagnetic Fermi-liquid theory has been developed.[1] Furthermore, quantum Monte Carlo simulations of a two-dimensional Hubbard model have been performed.[2] In other works calculations of susceptibilities using random-phase approximation have been carried out.[3–7]

Recently Zhang proposed a theory for high-T_c cuprates, which uses SO(5) symmetry to unify antiferromagnetism and superconductivity, offering uniform description of the global phase diagram of this class of materials.[8] In that approach a three-dimensional order parameter describing the AF phase (the staggered magnetization) is combined with a complex order parameter of a spin singlet *d*-wave SC phase creating a five-component vector called "superspin." The main idea of SO(5) theory is to introduce well-defined rotation operators, which can transform AF into SC and vice versa. Aside from them, the SO(5) symmetry group contains as subgroups SO(3) symmetry of spin rotations (which is spontaneously broken in the AF phase) and the electromagnetic SO(2) invariance (whose breaking defines SC phase). 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. In Zhang's theory, 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 an SO(5) rigid rotor and the system is described by an SO(5) nonlinear quantum σ model (NLQσM). The SO(5) quantum rotor model offers a Landau-Ginzburg-like (LG) for the high-T_c problem. However, it goes much beyond the traditional LG theory, since it captures the 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.[9–14] For example, numerical evidence for approximate SO(5) symmetry of the Hubbard model came out from exact diagonalization of small-sized clusters.[15] Moreover the SO(5) symmetry requires that collective charge excitations at half-filling must have the same mass as the collective spin-wave excitations. This requirement is clearly violated in a Mott insulating system, where all charge excitations (measured with respect to a particle-hole symmetric point) have a large energy gap, while the spin-wave excitations are massless. To address this issue Zhang *et al.*[16] constructed a low-energy effective theory [the so-called projected, pSO(5) model], where the Mott-Hubbard gap is taken into account by means of a Gutzwiller projection, which eliminates double-occupied states. It has been shown that despite the symmetry-breaking effects of the projection, static correlation functions remain exactly SO(5) symmetric, while dynamic breaking of SO(5) symmetry becomes important when quantum fluctuations are taken into account. Ultimately one should be able to compare the prediction from the SO(5) theory with experimentally observed features of high-T_c superconductors. While the global features of the phase diagram deduced from SO(5) theory based on spherical quantum rotors[17] agree qualitatively with the general topology of the observed phase diagram of high-T_c superconductors, a systematic study of magnetic properties of the SO(5) theory are called for.

The purpose of the present paper is twofold: firstly, we want to study quantitatively the variety of magnetic correlation functions resulting from the SO(5) theory, thereby substantiating this theoretical framework. Secondly, 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., magnetic correlation functions) with the outcome of the relevant experiments.

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 Lagrangian. In Sec. III we introduce the intersite spin-spin correlation function in terms of SO(5) algebra generators. We calculate static magnetic susceptibility and, subsequently, dynamic magnetic responses. Finally, in Sec. IV we summarize the conclusions to be drawn from our work.

II. HAMILTONIAN AND THE EFFECTIVE LAGRANGIAN

We start from the low-energy Hamiltonian proposed by Zhang on a discrete three-dimensional simple-cubic (3DSC) lattice,[8]

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

where i, $j=1,\ldots,N$ label lattice sites (N is the number of lattice sites) and μ, $\nu=1,\ldots,5$ mark the superspin components $\mathbf{n}_i=(n_1,n_2,n_3,n_4,n_5)_i$, where $\mathbf{n}_{AF,i}=(n_2,n_3,n_4)_i$ refers to antiferromagnetic and $\mathbf{n}_{SC,i}=(n_1,n_5)_i$ superconducting order parameters, respectively. In Zhang's formulation these are treated as mutually commuting coordinates and their dynamics is given by their conjugate momenta,

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

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

The kinetic energy of the system, given by the first part of Eq. (1), is simply that of an SO(5) rigid rotor ($\mathbf{n}_i^2=1$, $\mathbf{p}_i\cdot\mathbf{n}_i=0$, see Ref. 18). Here,

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

are the generators of the SO(5) algebra and L_i^{15} corresponds to a charge operator Q, whose expectation value yields the charge concentration (μ is the chemical potential measured from the half-filling). The remaining $L^{\mu\nu}$ operators are expressed via total spin $\mathbf{S}=(S_x,S_y,S_z)$ and so-called "π" [$\pi=(\pi_x,\pi_y,\pi_z)$] operators as follows:

$$L=\begin{bmatrix}0&&&&\\ \pi_x^\dagger+\pi_x&0&&&\\ \pi_y^\dagger+\pi_y&-S_z&0&&\\ \pi_z^\dagger+\pi_z&S_y&-S_x&0&\\ Q&-i(\pi_x^\dagger-\pi_x)&-i(\pi_y^\dagger-\pi_y)&-i(\pi_z^\dagger-\pi_z)&0\end{bmatrix}. \qquad (4)$$

Parameter u measures the kinetic energy of the rotors (an analog of moment of inertia). Furthermore, J is the stiffness in the charge and spin channel, nonvanishing for nearest neighbors of the 3DSC lattice. In the presence of SO(5) symmetry breaking, a quadratic term of the form

$$V(\mathbf{n}_i)=\frac{w}{2}\sum_i(n_{2i}^2+n_{3i}^2+n_{4i}^2) \qquad (5)$$

is also allowed. The anisotropy constant w 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 w.[19]

To proceed, we express the partition function $Z=\mathrm{Tr}e^{-H/k_BT}$ using the functional integral in the Matsubara "imaginary-time" τ formulation ($0\leq\tau\leq 1/k_BT\equiv\beta$, with T being the temperature). Performing the path integration over momenta we obtain[17]

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

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

$$\mathcal{L}(\mathbf{n})=\frac{1}{2}\sum_i\left[u\left(\frac{\partial \mathbf{n}_{SC}}{\partial\tau}\right)^2+u\left(\frac{\partial \mathbf{n}_{AF}}{\partial\tau}\right)^2-4u\mu^2\mathbf{n}_{SC}^2+4iu\mu\left(\frac{\partial n_1}{\partial\tau}n_5-\frac{\partial n_5}{\partial\tau}n_1\right)\right]-\sum_{i<j}J_{ij}\mathbf{n}_i\cdot\mathbf{n}_j-\frac{w}{2}\sum_i(n_{2i}^2+n_{3i}^2+n_{4i}^2). \quad (7)$$

The definition of the superspin variables $\mathbf{n}_i$ and the rigid constraint $\mathbf{n}_i^2=1$ imply that a weaker condition also holds, namely,

$$\sum_{i=1}^{N}\mathbf{n}_i^2=N. \quad (8)$$

Utilizing Eq. (8), the problem can be formulated then, in terms of the *exactly* solvable spherical model.[20] Therefore, with the replacement

$$\prod_i \delta(1-\mathbf{n}_i^2)\rightarrow\delta\left(N-\sum_i \mathbf{n}_i^2\right), \quad (9)$$

the global constraint in Eq. (6) may be implemented by using the functional analog of the Dirac-delta function,

$$\delta\left(N-\sum_i \mathbf{n}_i^2\right)=\int_{c-i\infty}^{c+i\infty}\left[\frac{d\lambda}{2\pi i}\right]\times\exp\left[\int_0^\beta d\tau\lambda(\tau)\left(N-\sum_i \mathbf{n}_i^2(\tau)\right)\right], \quad (10)$$

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. (8)] to have unit length. This introduces the Lagrange multiplier $\lambda(\tau)$ adding an additional quadratic term (in $\mathbf{n}_i$ fields) to the Lagrangian (7). Introducing the Fourier transform of the fields $\mathbf{n}(\mathbf{k},\omega_m)$ and interaction J_{ij},

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

$$J_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{R}_i}J(\mathbf{R}_i)e^{-i\mathbf{R}_i\cdot\mathbf{k}}, \quad (11)$$

where $\omega_m=2\pi m/\beta$ $(l=0,\pm1,\pm2,\dots)$ being the (Bose) Matsubara frequencies and $J(\mathbf{R}_i)=J(|\mathbf{r}_i-\mathbf{r}_j|)\equiv J_{ij}$. The Lagrangian with an additional quadratic λ term then reads

$$\mathcal{L}+\lambda\sum_i \mathbf{n}_i^2=\frac{1}{\beta N}\sum_{\mathbf{k},m}\sum_{\alpha,\beta}n_\alpha(\mathbf{k},\omega_m)\times[\mathbf{g}_0^{-1}]_{\alpha\beta}(\mathbf{k},\omega_m)n_\beta^*(\mathbf{k},\omega_m), \quad (12)$$

where

$$\mathbf{g}_0(\mathbf{k},\omega_m)=\begin{bmatrix}\mathrm{Re}\,A_1(\mathbf{k},\omega_m) & 0 & 0 & 0 & \mathrm{Im}\,A_1(\mathbf{k},\omega_m)\\ 0 & A_2(\mathbf{k},\omega_m) & 0 & 0 & 0\\ 0 & 0 & A_2(\mathbf{k},\omega_m) & 0 & 0\\ 0 & 0 & 0 & A_2(\mathbf{k},\omega_m) & 0\\ \mathrm{Im}\,A_1(\mathbf{k},\omega_m) & 0 & 0 & 0 & \mathrm{Re}\,A_1(\mathbf{k},\omega_m)\end{bmatrix}, \quad (13)$$

with $A_1(\mathbf{k},\omega_m)$ and $A_2(\mathbf{k},\omega_m)$ defined as follows:

$$A_1(\mathbf{k},\omega_m)=\frac{1}{2\lambda-J_{\mathbf{k}}+u(\omega_m+2i\mu)^2},$$
$$A_2(\mathbf{k},\omega_m)=\frac{1}{2\lambda-J_{\mathbf{k}}+u\omega_m^2-w}. \quad (14)$$

As a consequence of Eq. (6), the partition function can be written in the form

$$Z=\int\frac{d\lambda}{2\pi i}e^{-N\phi(\lambda)}, \quad (15)$$

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

$$\phi(\lambda)=-\int_0^\beta d\tau\lambda(\tau)-\frac{1}{N}\ln\int\prod_i[D\mathbf{n}_i]\times\exp\left[-\sum_i\int_0^\beta d\tau(\mathbf{n}_i^2\lambda(\tau)-\mathcal{L}[\mathbf{n}])\right]. \quad (16)$$

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

$$\left.\frac{\delta\phi(\lambda)}{\delta\lambda(\tau)}\right|_{\lambda=\lambda_0}=0. \quad (17)$$

At criticality, corresponding order-parameter susceptibilities become infinite. Specifically, for the SC state,

$$\frac{1}{g_0^{11}(\mathbf{k}=\mathbf{0},\omega_m=0)}=0 \tag{18}$$

and for the AF state,

$$\frac{1}{g_0^{22}(\mathbf{k}=\mathbf{0},\omega_m=0)}=0. \tag{19}$$

Therefore, the corresponding Lagrange multipliers are

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

$$\lambda_0^{SC}=\frac{1}{2}J_{\mathbf{k}=0}+2\chi\mu^2 \tag{20}$$

for AF and SC critical lines, respectively. Furthermore, using the spherical condition

$$1=\frac{1}{\beta N}\sum_{\mathbf{q},m}\sum_{\alpha} g_0^{\alpha\alpha}(\mathbf{k},\omega_m) \tag{21}$$

and the values (20), we finally arrive at the following expression for the critical lines to AF and SC states. Explicitly

$$1=\int_{-\infty}^{\infty}\rho(\xi)d\xi\left[3\frac{\coth\left(\frac{\beta}{2}\sqrt{\frac{2\lambda_0^X-J\xi-w}{u}}\right)}{\sqrt{u(2\lambda_0^X-J\xi-w)}}+2\frac{\coth\left[\frac{\beta}{2}\left(\sqrt{\frac{2\lambda_0^X-J\xi}{u}}+2\mu\right)\right]+\coth\left[\frac{\beta}{2}\left(\sqrt{\frac{2\lambda_0^X-J\xi}{u}}-2\mu\right)\right]}{2\sqrt{u(2\lambda_0^X-J\xi)}}\right], \tag{22}$$

where $X=AF$ and $X=SC$ for antiferromagnetic and superconducting states, respectively. Furthermore, in Eq. (22) we have introduced for convenience the density of states (DOS) for the 3DSC (Ref. 21) defined as

$$\rho(\xi)=\frac{1}{N}\sum_{\mathbf{q}}\delta(\xi-J_{\mathbf{q}}/J), \tag{23}$$

where

$$J_{\mathbf{q}}/J=\cos q_x+\cos q_y+\cos q_z. \tag{24}$$

Explicitly, the DOS function reads

$$\rho(\xi)=\frac{1}{\pi^3}\int_{\max(-1,-2-\xi)}^{\min(1,2-\xi)}dy\frac{1}{\sqrt{1-y^2}}\times\mathbf{K}\left[\sqrt{1-\left(\frac{\xi+y}{2}\right)^2}\right]\Theta(3-|\xi|), \tag{25}$$

where $\mathbf{K}(x)$ is the elliptic integral of the first kind and $\Theta(x)$ is the step function.[22]

III. MAGNETIC CORRELATION FUNCTIONS

The method of choice for the investigation of magnetic-ordering phenomena in cuprates and the spin dynamics is magnetic neutron scattering. Among various experimental tools neutron experiments are unique, in the sense that they allow the determination of the full frequency, momentum, and temperature dependence of the spin structure function (for simplicity we consider an isotropic magnetic system),

$$\mathcal{S}(\mathbf{q},\omega)=\frac{1}{6\pi}\int_{-\infty}^{+\infty}dte^{-i\omega t}\sum_{\mathbf{R}_i}e^{i\mathbf{q}\cdot\mathbf{R}_i}\langle\mathbf{S}_i(t)\cdot\mathbf{S}_0(0)\rangle. \tag{26}$$

The neutron-scattering cross section therefore allows one to determine the structure of the spin order as well as spin dynamics. In the SO(5) theory there is an SO(3) spin symmetry acting on the subspace defined by the vector $\mathbf{n}_{AF}$ with spin operator $\mathbf{S}=(S_x,S_y,S_z)$ being a generator of rotation. In order to identify the correspondence between spin components and SO(5)-symmetry-group generators, we may write, using Eq. (4), the spin-spin correlation function in the "imaginary-time" Matsubara formalism,

$$\begin{aligned}G_{ij}(\tau-\tau')&=\langle\mathbf{S}_i(\tau)\cdot\mathbf{S}_j(\tau')\rangle=\langle S_{x,i}(\tau)S_{x,j}(\tau')\rangle\\&\quad+\langle S_{y,i}(\tau)S_{y,j}(\tau')\rangle+\langle S_{z,i}(\tau)S_{z,j}(\tau')\rangle\\&=\langle L_{43,i}(\tau)L_{43,j}(\tau')\rangle+\langle L_{42,i}(\tau)L_{42,j}(\tau')\rangle\\&\quad+\langle L_{32,i}(\tau)L_{32,j}(\tau')\rangle\\&=3\langle L_{43,i}(\tau)L_{43,j}(\tau')\rangle,\end{aligned} \tag{27}$$

where $\langle\cdots\rangle$ denotes the ensemble average according to

$$\langle\cdots\rangle=\frac{\int\prod_i[D\mathbf{n}_i]\delta\left(N-\sum_i\mathbf{n}_i^2\right)\ldots e^{-\int_0^\beta d\tau\mathcal{L}(\mathbf{n})}}{\int\prod_i[D\mathbf{n}_i]\delta\left(N-\sum_i\mathbf{n}_i^2\right)e^{-\int_0^\beta d\tau\mathcal{L}(\mathbf{n})}}. \tag{28}$$

It is convenient to write the Fourier transform of the function (27),

$$\begin{aligned}G(\mathbf{k},\omega_m)&=\sum_{\mathbf{r}_i}\int_0^\beta d\tau\langle\mathbf{S}_{\mathbf{r}_i}(\tau)\cdot\mathbf{S}_{\mathbf{0}}(0)\rangle e^{i(\omega_m\tau-\mathbf{k}\mathbf{r}_i)}\\&=3\sum_{\mathbf{r}_i}\int_0^\beta d\tau\langle L_{\mathbf{r}_i}^{\alpha\beta}(\tau)L_{\mathbf{0}}^{\alpha\beta}(0)\rangle e^{i(\omega_m\tau-\mathbf{k}\mathbf{r}_i)}.\end{aligned} \tag{29}$$

Furthermore, by expressing the SO(5) generators $L^{\alpha\beta}(\tau)$ by superspin-vector components [cf. Eq. (3)] we obtain

$$\langle L_i^{\alpha\beta}(\tau)L_j^{\alpha'\beta'}(\tau')\rangle=\frac{1}{(\beta N)^4}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{m,m',n}\Bigg\{(2\chi\beta N)\exp\{-i[(\omega_m+\omega_{m'})\tau-(\mathbf{k}+\mathbf{k}')\mathbf{r}_i+(\tau-\tau')\omega_n+(\mathbf{r}_i-\mathbf{r}_j)\mathbf{q}]\}$$
$$\times(\langle n_{\alpha\mathbf{k}m}n_{\alpha\mathbf{k}'m'}\rangle+\langle n_{\beta\mathbf{k}m}n_{\beta\mathbf{k}'m'}\rangle)+\sum_{\mathbf{q}',n}\exp\{-i[(\omega_m+\omega_n)\tau+(\omega_{m'}+\omega_{n'})\tau'-(\mathbf{k}+\mathbf{q})\mathbf{r}_i$$
$$-(\mathbf{k}'+\mathbf{q}')\mathbf{r}_j]\}[4\chi^2(\omega_m-\omega_n)(\omega_{m'}-\omega_{n'})\langle n_{\alpha\mathbf{k}m}n_{\alpha\mathbf{k}'m'}n_{\beta\mathbf{q}n}n_{\beta\mathbf{q}'n'}\rangle]\Bigg\} \tag{30}$$

The remaining four-point expectation values of the superspin components can be conveniently calculated using the following Wick-type formula [which can be deduced from the Eq. (12)], namely,

$$\langle n_{\alpha\mathbf{k}_1m_1}n_{\beta\mathbf{k}_2m_2}\rangle=\left(\frac{\partial}{\partial b_{\alpha\mathbf{k}_1m_1}}\frac{\partial}{\partial b_{\beta\mathbf{k}_2m_2}}\exp\left\{\beta N\sum_{\mathbf{k},\alpha,\beta,m}b_{\alpha\mathbf{k}m}[\mathbf{g}_0^{-1}(\mathbf{k},\omega_m)]_{\alpha\beta}b^*_{\beta\mathbf{k}m}\right\}\right)_{\mathbf{b}=0}$$
$$=\beta N g_0^{\alpha\beta}(\mathbf{k}_1,\omega_{m_1})\delta_{\mathbf{k}_1,-\mathbf{k}_2}\delta_{m_1,-m_2} \tag{31}$$

with the result

$$\langle n_{\alpha\mathbf{k}m}n_{\alpha'\mathbf{k}'m'}n_{\beta\mathbf{q}n}n_{\beta'\mathbf{q}'n'}\rangle=\langle n_{\alpha\mathbf{k}m}n_{\alpha'\mathbf{k}'m'}\rangle\langle n_{\beta\mathbf{q}n}n_{\beta'\mathbf{q}'n'}\rangle+\langle n_{\alpha\mathbf{k}m}n_{\beta\mathbf{q}n}\rangle\langle n_{\alpha'\mathbf{k}'m'}n_{\beta'\mathbf{q}'n'}\rangle+\langle n_{\alpha\mathbf{k}m}n_{\beta'\mathbf{q}'n'}\rangle\langle n_{\alpha'\mathbf{k}'m'}n_{\beta\mathbf{q}n}\rangle$$
$$=(\beta N)^2 g_0^{\alpha\alpha'}(\mathbf{k},\omega_m)g_0^{\beta\beta'}(\mathbf{q},\omega_n)\delta_{\mathbf{k},-\mathbf{k}'}\delta_{\mathbf{q},-\mathbf{q}'}\delta_{n,-n'}\delta_{m,-m'}$$
$$+(\beta N)^2 g_0^{\alpha\beta}(\mathbf{k},\omega_m)g_0^{\alpha'\beta'}(\mathbf{k}',m')\delta_{\mathbf{k},-\mathbf{q}}\delta_{\mathbf{k}',-\mathbf{q}'}\delta_{m,-n}\delta_{m',-n'}$$
$$+(\beta N)^2 g_0^{\alpha\beta'}(\mathbf{k},\omega_m)g_0^{\alpha'\beta}(\mathbf{k}',m')\delta_{\mathbf{k},-\mathbf{q}'}\delta_{\mathbf{k}',-\mathbf{q}}\delta_{m,-n'}\delta_{m',-n}. \tag{32}$$

Explicitly, for the spin-spin correlation function, we obtain

$$G(\mathbf{k},\omega_m)=3[\mathcal{G}'+\mathcal{G}(\mathbf{k},\omega_m)], \tag{33}$$

where

$$\mathcal{G}'=\frac{2u}{\beta N}\sum_{\mathbf{q},n}[g_0^{44}(\mathbf{q},\omega_n)+g_0^{33}(\mathbf{q},\omega_n)]=\frac{8u}{\beta N}\sum_{\mathbf{q},n}\frac{1}{2\lambda-J_{\mathbf{q}}+u\omega_n^2-w}=\frac{4u}{N}\sum_{\mathbf{q}}\frac{\coth\left(\frac{\beta}{2}\sqrt{\frac{2\lambda-J_{\mathbf{q}}-w}{u}}\right)}{\sqrt{u(2\lambda-J_{\mathbf{q}}-w)}},$$
$$\mathcal{G}(\mathbf{k},\nu_m)=-\frac{4u^2}{\beta N}\sum_{\mathbf{q},n}(\nu_m-2\omega_n)^2[g_0^{44}(\mathbf{k}-\mathbf{q},\nu_m-\omega_n)g_0^{33}(\mathbf{q},\omega_n)-g_0^{43}(\mathbf{k}-\mathbf{q},\nu_m-\omega_n)g_0^{43}(\mathbf{q},\omega_n)]$$
$$=-\frac{4u^2}{\beta N}\sum_{\mathbf{q},n}\frac{(\nu_m-2\omega_n)^2}{[2\lambda-J_{\mathbf{k}-\mathbf{q}}-w+u(\nu_m-\omega_n)^2][2\lambda-J_{\mathbf{q}}-w+u\omega_n^2]} \tag{34}$$

is the generic formula for the spin-spin correlation function in the "imaginary-time" Matsubara formalism, from which a variety of magnetic correlators can be deduced by specifying the wave-vector and frequency dependence.

A. Static susceptibility

While the neutron-scattering experiments provide functional dependencies of dynamical susceptibilities on frequency and momentum, it is the advantage of neutron-experiment methods (i.e., NMR) to give local specific information. For example, the uniform susceptibility is given by

$$\chi_s\equiv G(\mathbf{k}=0,\omega_m=0) \tag{35}$$

and related to the Knight shift $K_s=A\chi_s(T)$, where A is the corresponding hyperfine coupling. Using formula (34) we immediately obtain

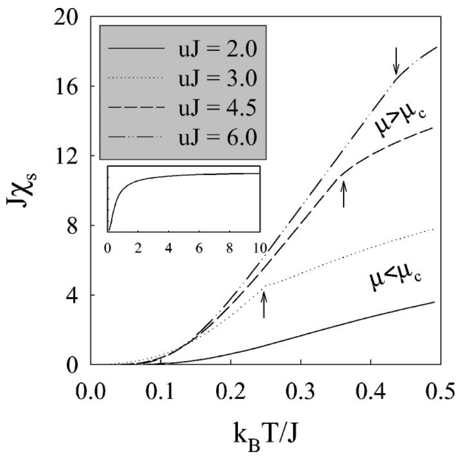

FIG. 1. Static spin susceptibility $J\chi_s$ vs temperature k_BT/J for $\mu/J=0.26$ and several values of uJ as indicated in the inset of the figure. Arrows indicate the onset of the superconducting or antiferromagnetic transition temperatures (the chemical potential indicates, whether the transition is on AF or SC side). The small inlay shows $J\chi_s-T$ dependence (for $uJ=2.0$) on larger temperature scale.

$$\chi_s=\frac{12}{N}\sum_{\mathbf{q}}\sqrt{u}\frac{\coth\left(\frac{\beta}{2}\sqrt{\frac{2\,\delta\lambda+(3J-J_{\mathbf{q}})}{u}}\right)}{\sqrt{2\,\delta\lambda+(3J-J_{\mathbf{q}})}}-\frac{12u^2}{\beta N}\sum_{\mathbf{q},n}\frac{4\omega_n^2}{[2\,\delta\lambda+(3J-J_{\mathbf{q}})+u\,\omega_n^2]^2}$$
$$=\frac{6\beta}{N}\sum_{\mathbf{q}}\left[\coth^2\left(\frac{\beta}{2}\sqrt{\frac{2\,\delta\lambda+(3J-J_{\mathbf{q}})}{u}}\right)-1\right]$$
$$=6\beta\int d\xi\rho(\xi)\left[\coth^2\left(\frac{\beta}{2}\sqrt{\frac{\delta\lambda}{u}}\sqrt{2+\frac{J}{\delta\lambda}\{3-\xi\}}\right)-1\right], \tag{36}$$

where $\delta\lambda=\lambda-\lambda_0^{AF}$. The temperature dependence of χ_s is shown in Fig. 1, while temperature-doping dependence across the phase diagram is shown in Fig. 2. We find that the temperature dependence of $\chi_s(T)$ resembles that of the magnetic susceptibility of copper oxide describing qualitatively the decreasing of $K_s(T)$ with lowering of the temperature.

Specifically, the theory predicts saturation of $\chi_s(T)$ above critical temperature in accordance with experimental findings. The temperature dependence of $\chi_s(T)$ extrapolates to zero at zero temperature. This feature may be viewed as the signature of the opening of a spin excitation gap at low temperatures [noteworthy, $\chi_s(T)$ in doped YBCO indeed extrapolates to zero at zero temperature, however underdoped LaBaCuO compounds apparently extrapolate to a finite zero-temperature value].

B. Dynamic spin susceptibility

Knowledge of the *dynamic* spin-spin correlation function is becoming a crucial topic for the description of the physical

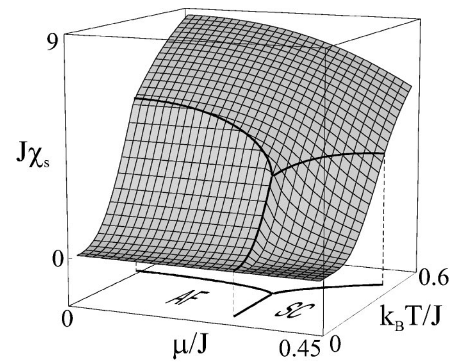

FIG. 2. Plot of the static spin susceptibility $J\chi_s$ vs chemical potential μ/J and temperature k_BT/J for fixed $uJ=3$ and $w/J=1$. Solid lines indicate the projection of the $\mu-T$ phase diagram.

properties of the high-T_c cuprates. Calculations of the dynamical spin susceptibility allow one to test the applicability of the SO(5) theory for magnetic correlation in cuprates. In particular, it is interesting to verify whether the quantum rotor SO(5) Hamiltonian provides the minimal model, which consists of essential physics of cuprate superconductors. To answer this question, analytical closed-form results are needed for dynamic spin responses, which are so far available mainly from numerical calculations on small clusters.

Performing the summation over Matsubara's frequency in Eq. (34) results in

$$G(\mathbf{k},\omega_m)=\frac{12u}{N}\sum_{\mathbf{q}}\frac{\coth\left(\frac{\beta}{2}\sqrt{\frac{2\lambda-J_{\mathbf{q}}-w}{u}}\right)}{\sqrt{u(2\lambda-J_{\mathbf{q}}-w)}}+\frac{12}{N}\sum_{\mathbf{q}}\left\{\frac{\left(\Omega_{\mathbf{k-q}}+\frac{i}{2}\nu_m\right)^2\coth\left(\frac{\beta}{2}\Omega_{\mathbf{k-q}}\right)}{\Omega_{\mathbf{k-q}}[\Omega_{\mathbf{q}}^2-(\Omega_{\mathbf{k-q}}+i\nu_m)^2]}+\frac{\left(\Omega_{\mathbf{q}}+\frac{i}{2}\nu_m\right)^2\coth\left(\frac{\beta}{2}\Omega_{\mathbf{q}}\right)}{\Omega_{\mathbf{q}}[\Omega_{\mathbf{k-q}}^2-(\Omega_{\mathbf{q}}+i\nu_m)^2]}+\text{c.c.}\right\}, \tag{37}$$

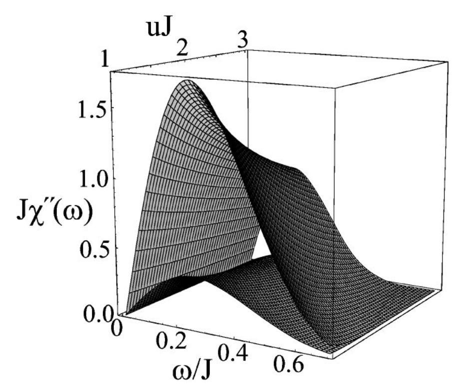

FIG. 3. Local dynamic spin susceptibility $J\chi''(\omega)$ (imaginary part) vs frequency ω/J and quantum fluctuation parameter uJ. Lower surface for $k_BT/J=0.4$, upper for $k_BT/J=1$, respectively.

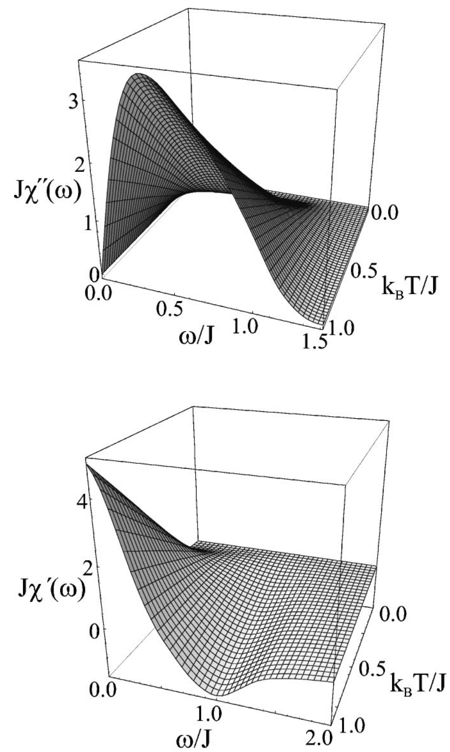

FIG. 4. Imaginary $[J\chi''(\omega)$, upper panel$]$ and real part $[J\chi'(\omega)$, lower panel$]$ of the local dynamic spin susceptibility as a function of the frequency ω/J and temperature k_BT/J for $uJ=3$.

where, for the sake of simplicity, we have introduced the notation

$$\Omega_{\mathbf{q}}=\sqrt{\frac{2\lambda-J_{\mathbf{q}}-w}{u}}. \tag{38}$$

Of special interest is the imaginary part of the dynamic correlation function, which can be obtained from the Eq. (37) by performing the analytic continuation from Matsubara's frequency to real frequency $(i\nu_m\to\omega+i\varepsilon)$ with the help of the identity

$$\lim_{\varepsilon\to 0^+}\frac{1}{x\pm i\varepsilon}=P\left(\frac{1}{x}\right)\mp i\pi\delta(x). \tag{39}$$

The imaginary part of the correlation function $\chi''(\mathbf{k},\omega)=\mathrm{Im}\,G(\mathbf{k},\omega)$, then reads

$$\chi''(\mathbf{k},\omega)=\frac{\pi}{2N}\sum_{\mathbf{q}}\frac{\coth\left[\frac{\beta}{2}\Omega_{\mathbf{k}-\mathbf{q}}\right]-\coth\left[\frac{\beta}{2}\Omega_{\mathbf{q}}\right]}{\Omega_{\mathbf{q}}\Omega_{\mathbf{k}-\mathbf{q}}}\{[2\Omega_{\mathbf{k}-\mathbf{q}}+\omega][2\Omega_{\mathbf{q}}-\omega]\delta(\Omega_{\mathbf{q}}-\Omega_{\mathbf{k}-\mathbf{q}}-\omega)-[2\Omega_{\mathbf{q}}+\omega]\times[2\Omega_{\mathbf{k}-\mathbf{q}}-\omega]\delta(\Omega_{\mathbf{q}}-\Omega_{\mathbf{k}-\mathbf{q}}+\omega)\}+\frac{\pi}{2N}\sum_{\mathbf{q}}\frac{\coth\left[\frac{\beta}{2}\Omega_{\mathbf{k}-\mathbf{q}}\right]+\coth\left[\frac{\beta}{2}\Omega_{\mathbf{q}}\right]}{\Omega_{\mathbf{q}}\Omega_{\mathbf{k}-\mathbf{q}}}\times\{[2\Omega_{\mathbf{k}-\mathbf{q}}+\omega][2\Omega_{\mathbf{q}}+\omega]\delta(\Omega_{\mathbf{q}}+\Omega_{\mathbf{k}-\mathbf{q}}+\omega)-[2\Omega_{\mathbf{k}-\mathbf{q}}-\omega][2\Omega_{\mathbf{q}}-\omega]\delta(\Omega_{\mathbf{q}}+\Omega_{\mathbf{k}-\mathbf{q}}-\omega)\}. \tag{40}$$

1. Local spin susceptibility

To facilitate the comparison with other theoretical approaches, it is convenient to perform the $\mathbf{k}$ integration of the spin susceptibility over the first Brillouin zone to obtain the momentum-integrated (local) dynamic spin susceptibility,

$$\chi(\omega)=\int\frac{d^3\mathbf{k}}{(2\pi)^3}G(\mathbf{k},\omega). \tag{41}$$

Performing the integration over the momenta we obtain explicitly the imaginary part $\chi''(\omega)=\mathrm{Im}\,\chi(\omega)$,

$$\chi''(\omega)=3\pi\frac{\sqrt{u\delta\lambda}}{J}\int_{-\infty}^{\infty}d\xi\rho(\xi)\rho\left[\xi-\frac{\sqrt{u\delta\lambda}}{J}\omega\left(\sqrt{\frac{u}{\delta\lambda}}\omega+2\sqrt{2+\frac{J}{\delta\lambda}(3-\xi)}\right)\right]\times\frac{\left(2\sqrt{2+\frac{J}{\delta\lambda}(3-\xi)}+\sqrt{\frac{u}{\delta\lambda}}\omega\right)^2}{\sqrt{2+\frac{J}{\delta\lambda}(3-\xi)}}\left\{\coth\left(\frac{1}{2}\beta\sqrt{\frac{\delta\lambda}{u}}\sqrt{2+\frac{J}{\delta\lambda}(3-\xi)}\right)-\coth\left[\frac{1}{2}\beta\sqrt{\frac{\delta\lambda}{u}}\left(\sqrt{2+\frac{J}{\delta\lambda}(3-\xi)}+\sqrt{\frac{u}{\delta\lambda}}\omega\right)\right]\right\}. \tag{42}$$

The corresponding real part can be deduced from Kramers-Krönig relation

$$\chi'(\omega)=\mathrm{Re}\,\chi(\omega)=\frac{2}{\pi}\mathcal{P}\int_0^\infty d\omega'\frac{\omega'\chi''(\omega')}{\omega'^2-\omega^2}, \tag{43}$$

where $\mathcal{P}$ is the principal value of the integral. Frequency dependence of the real and imaginary part of the dynamic spin susceptibility (as a function of various control parameters) is presented in Figs. 3 and 4. In particular, the imaginary part of the momentum-integrated dynamic spin susceptibility exhibits a linear behavior at low energy and then passes to the broad maximum and decays at higher energies, in agreement with experimental findings.

The local spin susceptibility allows one to find the NMR relaxation rate

$$\frac{1}{T_1}=\lim_{\omega\to 0}\frac{\chi''(\omega)}{\beta\omega}. \tag{44}$$

From Eq. (42) we obtain explicitly

$$\frac{1}{T_1}=6\pi\frac{\sqrt{\chi}}{J}\int dY\rho^2(Y)\sqrt{2\delta\lambda+J(3-Y)}\times\left\{\coth^2\left[\frac{\beta}{2}\sqrt{\frac{2\delta\lambda+J(3-Y)}{\chi}}\right]-1\right\}. \tag{45}$$

Temperature dependence of $(T_1T)^{-1}$ is presented in Fig. 5. We find this in qualitative agreement with experimentally observed NMR relaxation rates for underdoped YBCO.[23]

2. Antiferromagnetic susceptibility

Another example of interest is the antiferromagnetic dynamic spin susceptibility defined by Eq. (40) by specifying the antiferromagnetic wave vector $\mathbf{k}\equiv\mathbf{Q}=(\pi,\pi,\pi)$. The imaginary part of the antiferromagnetic spin susceptibility is given by $\chi''_{AF}(\omega)\equiv\mathrm{Im}[G(\mathbf{k}=\mathbf{Q},\omega)]$, explicitly,

$$\chi''_{AF}(\omega)=4\pi\frac{u}{J}\rho\left(\frac{u}{2J}\omega\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}\right)\left\{\Theta\left(\sqrt{2\frac{2\delta\lambda+3J}{u}}-\omega\right)\right.$$
$$\times\frac{\coth\left(\frac{\beta}{4}\left|\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}+\omega^2\right|\right)-\coth\left(\frac{\beta}{4}\left|\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}-\omega^2\right|\right)}{\left|\omega+\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}\right|+\left|\omega-\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}\right|}\left(4\frac{2\delta\lambda+3J}{u}-\omega^2\right)$$
$$-\Theta\left(\omega-\sqrt{2\frac{2\delta\lambda+3J}{u}}\right)\Theta\left(2\sqrt{\frac{2\delta\lambda+3J}{u}}-\omega\right)$$
$$\left.\times\frac{\coth\left(\frac{\beta}{4}\left|\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}+\omega^2\right|\right)+\coth\left(\frac{\beta}{4}\left|\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}-\omega^2\right|\right)}{\left|\omega+\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}\right|-\left|\omega-\sqrt{4\frac{2\delta\lambda+3J}{u}-\omega^2}\right|}\left(4\frac{2\delta\lambda+3J}{u}-\omega^2\right)\right\}. \tag{46}$$

Frequency dependence of real and imaginary part of χ''_{AF} for various temperatures is depicted in Fig. 6.

IV. SUMMARY AND FINAL REMARKS

In conclusion, we have calculated the momentum and energy dependence of the real and imaginary part of dynamical spin susceptibility using the unified theory of antiferromagnetism and superconductivity proposed for the high-T_c cuprates by Zhang, and based on the SO(5) symmetry between antiferromagnetic and superconducting states. The theory of magnetic correlation in high-T_c cuprates based on SO(5) theory yields a qualitative scenario for the evolution of magnetic behavior, which is consistent with experiments. It qualitatively explains the results of experimental measurements [notably the nuclear magnetic resonance (NMR) relaxation rates] with correct predictions of behavior of $\chi_s(T)$ in high temperatures. Also the energy dependence of the momentum-integrated dynamical spin susceptibility shows features that are in qualitative agreement with experimental findings. Another important problem is to determine the pre-

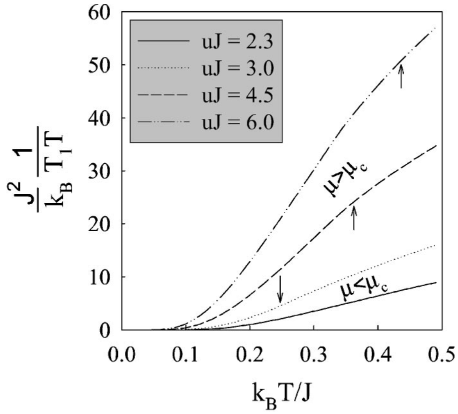

FIG. 5. Plot of the NMR relaxation rate $1/(T_1T)$ vs temperature k_BT/J for $\mu/J=0.2$ and several values of uJ as indicated in the inset of the figure. Arrows indicate the onset of the superconducting or antiferromagnetic transition temperatures (the chemical potential indicates whether the transition is on AF or SC side).

cise role of anisotropy (which can be easily incorporated in our approach) and bilayer coupling (present in YBCO compound), which might be crucial, for example, to the scenario of spin-gap formation.[24] Closing, we note that the SO(5) theory predicts also an existence of the resonant mode in the superconducting state. It would be interesting to follow this mode by studying the so-called "π-π" response functions. It is desirable also to study dynamical properties of the projected SO(5) theory,[16] where quantum fluctuations may lead to a breaking of the pSO(5) symmetry. However, as far as magnetic correlations are concerned, we expect that projection should not introduce important changes in magnetic correlation functions because the implementation of the Gutzwiller constraint affects the superconducting sector of the SO(5) theory. We hope to address this issue in future work. Further studies of microscopic models of high-T_c cuprates should help to clarify whether the experimentally observed evolution of physical parameters of the model discussed here is similar to that obtained in microscopic calculations, thereby allowing to check the validity of basic principles of the SO(5) theory.

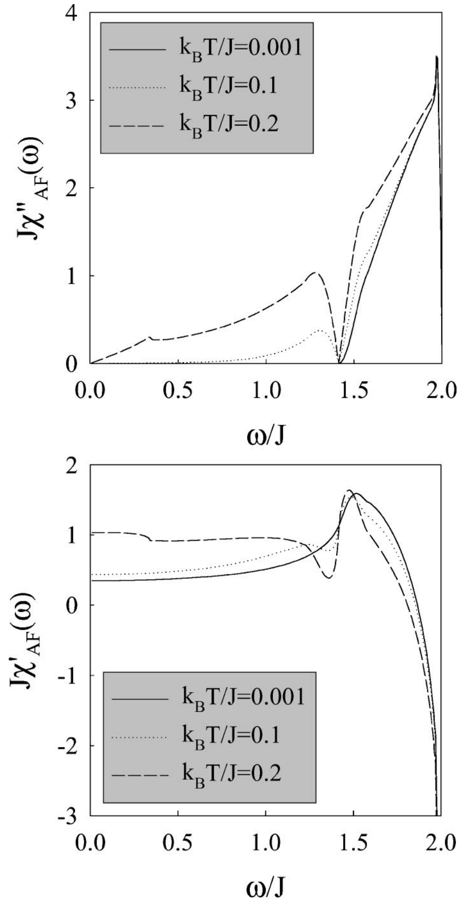

FIG. 6. Imaginary $[J\chi''_{AF}(\omega)$, upper panel] and real part $[J\chi'_{AF}(\omega)$, lower panel] of the local dynamic antiferromagnetic spin susceptibility vs frequency ω/J for different values of temperature k_BT/J as shown in the insets of the figures.

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