Scaling near the Quantum-Critical Point in the SO(5) Theory of the High-T_c Superconductivity

T. K. Kopeć and T. A. Zaleski
Institute for Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wrocław, Poland
(Received 9 January 2001; published 13 August 2001)

We study the quantum-critical point scenario within the unified theory of superconductivity and antiferromagnetism based on the SO(5) symmetry. Closed-form expression for the quantum-critical scaling function for the dynamic spin susceptibility is obtained from the lattice SO(5) quantum nonlinear σ-model in three dimensions, revealing that in the quantum-critical region the frequency scale for spin excitations is simply set by the absolute temperature. Implications for the non-Fermi liquid behavior of the normal-state resistivity due to spin fluctuations in the quantum-critical region are also presented.

DOI: 10.1103/PhysRevLett.87.097002 PACS numbers: 74.20.Mn, 74.25.Dw, 75.10.Jm

The principal idea behind the universality at phase transitions—that the physics at the transition point is ruled only by interaction at macroscopic length scales—leads to critical behavior, where classical thermal fluctuations govern the phase transition scenario. However, there is an ample class of systems for which quantum effects dominate the phase transition, resulting in a critical point accessible by tuning the relevant variable other than the temperature [1]. Recently, there have been a number of detailed dynamic scattering measurements on superconducting cuprates [2] showing that the overall frequency ω scale of the spin excitation spectrum is given simply by the absolute temperature k_BT. Interestingly, this ω/k_BT scaling is consistent with an existence of the nearby *quantum critical point* (QCP). The possibility of a quantum critical behavior governing the physical properties of the superconducting cuprates has attracted great attention in recent years motivated by the fact that quantum criticality affords the way of a controlled study of the non-Fermi liquid behavior [3].

Proximity of the magnetism and superconductivity (and competition between these phases) is one of the most important hallmarks in the physics of high-T_c superconductors. In a recent theoretical framework, antiferromagnetic (AF) and superconducting (SC) order parameters form a five-dimensional supervector $\mathbf{n}$, and the SO(5) rotation turns AF into SC states and vice versa [4]. With increasing quantum fluctuations, ordering in some phases can be suppressed opening the possibility to a QCP where the AF state goes into the SC state through direct second-order phase transition [5]. In this paper we characterize the quantum critical behavior which develops in the vicinity of this special point. Our purpose is twofold: First, our quantitative study substantiates the (sometimes vague) QCP scenario by putting it into a specific theoretical framework. Second, it may also provide a useful diagnostic tool for testing the SO(5) theory in the critical region by comparing the quantitative predictions (e.g., for scaling functions) with the outcome of the relevant experiments [6].

We begin by writing down the SO(5) Hamiltonian for a simple cubic (s.c.) three-dimensional (3D) lattice:

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

where $i = 1,\ldots,N$ (N is the number of lattice sites). The locally defined five-component superspin vector $\mathbf{n}_i = (n_1,n_2,n_3,n_4,n_5)_i$ describes AF $(n_2,n_3,n_4)_i$ and SC $(n_1,n_5)_i$ degrees of freedom. In the Zhang formulation [4], these are treated as mutually commuting coordinates and their dynamics is given by their conjugate momenta: $p_{\mu i} = i\partial/\partial n_{\mu i}$ and $[n_\mu, p_\nu] = i\delta_{\mu\nu}$. Here, $L_i^{\mu\nu} = n_{\mu i}p_{\nu i} - n_{\nu i}p_{\mu i}$ are the generators of SO(5) algebra and L_i^{15} is a charge operator coupled to the chemical-potential μ (measured from the half filling). The parameter u in turn regulates the quantum fluctuation effects by controlling the kinetic energy of rotors (u is simply the moment of inertia of the rigid rotor). Furthermore, J_{ij} ($\equiv J$ for nearest neighbors and 0 otherwise) corresponds to the stiffness in the charge and spin channel [7]. In the presence of SO(5) symmetry breaking, a quadratic term of the form $V(\mathbf{n}_i) = \frac{g}{2}\sum_i(n_{2i}^2 + n_{3i}^2 + n_{4i}^2)$ is also allowed. The anisotropy constant g selects either the "easy plane" in the SC space, or an "easy sphere" in the AF space, depending on the sign of g.

Given H, one can simply perform a Legendre transformation to obtain the corresponding Euclidean Lagrangian in the Matsubara "imaginary time" τ formulation ($0 \leq \tau \leq 1/k_BT \equiv \beta$):

$$\mathcal{L}[\mathbf{p},n] = i\mathbf{p}(\tau)\cdot\frac{d}{d\tau}\mathbf{n}(\tau) + H(\mathbf{n},\mathbf{p})\,. \tag{2}$$

The partition function $Z = \mathrm{Tr}e^{-H/k_BT}$ of the system is then given by

$$Z = \int\prod_i[D\mathbf{n}_i]\int\prod_i\left[\frac{D\mathbf{p}_i}{2\pi}\right] \times \delta(1-\mathbf{n}_i^2)\delta(\mathbf{n}_i\cdot\mathbf{p}_i)e^{-\int_0^\beta d\tau\mathcal{L}[\mathbf{p},\mathbf{n}]}. \tag{3}$$

Because of the rigid nature of the quantum rotors, one must be cautious and integrate only over the momenta transverse to the supervector ($\mathbf{p}_i\cdot\mathbf{n}_i = 0$) with fixed length ($\mathbf{n}_i^2 = 1$). To this end, we cast the problem in terms of the exactly soluble *quantum spherical model* [8] by taking the superspin components as *continuous* variables, i.e., $-\infty < \mathbf{n}_i(\tau) < \infty$, but constrained (on average) to have unit length. The spherical closure relation amounts then to the replacement: $\prod_i \delta(1 - \mathbf{n}_i^2) \to \delta(N - \sum_i \mathbf{n}_i^2)$. The convenient way to enforce the spherical constraint is to use the functional analog of the Dirac-δ-function representation $\delta(x) = \int_{-\infty}^{+\infty}(d\lambda/2\pi)e^{i\lambda x}$ which introduces the Lagrange multiplier $\lambda(\tau)$ [8]. In the thermodynamic limit $N \to \infty$, the method of steepest descents becomes exact and at the saddle point $\lambda(\tau) \equiv \lambda_0$ will satisfy

$$1 = \frac{1}{\beta N}\sum_{\mathbf{k},\omega_\ell}[2G_s(\mathbf{k},\omega_\ell) + 3G_a(\mathbf{k},\omega_\ell)], \tag{4}$$

where $G_a(\mathbf{k},\omega_\ell) = 1/[2\lambda_0 - J(\mathbf{k}) + u\omega_\ell^2 - g]$ and $G_s(\mathbf{k},\omega_\ell) = 1/[2\lambda_0 - J(\mathbf{k}) + u(\omega_\ell + 2i\mu)^2]$ are the (order parameter) susceptibilities in the AF and SC sector, respectively. The summation in Eq. (4) is performed over all wave vector components $\mathbf{k}$ ($-\pi p/Na \le k_\alpha \le \pi p/Na$, where $\alpha = x, y, z$; p are integers $0 \le p \le N-1$ and a is the lattice spacing). Furthermore, $\omega_\ell = 2\pi\ell/\beta$ ($\ell = 0, \pm1, \pm2, \ldots$) are the (Bose) Matsubara frequencies arising from the restriction to periodic functions along the imaginary time direction. Finally, $J(\mathbf{k}) = J\varepsilon(\mathbf{k})$, where $\varepsilon(\mathbf{k}) = \cos(ak_x) + \cos(ak_y) + \cos(ak_z)$ is the structure factor for the s.c. lattice in 3D.

At the critical lines for the AF and SC phases, the Lagrange multiplier λ assumes values at which corresponding uniform and static order parameter susceptibilities diverge: $G_a^{-1}(\mathbf{k}=0,\omega_\ell=0) = 0$ and $G_s^{-1}(\mathbf{k}=0,\omega_\ell=0) = 0$, which yields $\lambda_0^a = (3J+g)/2$ for AF and $\lambda_0^s = (3J + 4\mu^2 u)/2$ for the SC state, respectively. On examining of the saddle point equation (4), one finds that $g > 0$ favors the AF state whereas the $\mu > 0$ term prefers the SC state. For $\lambda_0^a = \lambda_0^s$ (which happens for $\mu_c = \sqrt{g/4u}$) both AF and SC transition lines merge at the bicritical point at $(T_{\rm bc}, \mu_c)$. However, for sufficiently small parameter u, quantum fluctuations will drive T_{bc} to zero giving rise to a *quantum critical point* (see Fig. 1). An especially interesting regime appears in the vicinity of the QCP where k_BT is significantly larger than any energy scale which measures deviations of the

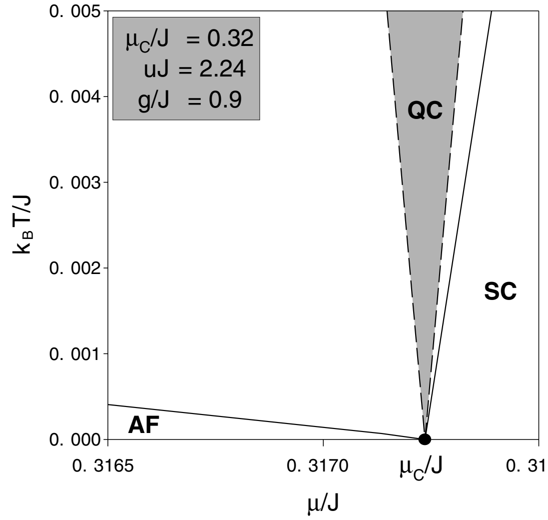

FIG. 1. $T - \mu$ phase diagram for parameters indicated in the inset. The QCP is at $T = 0$, $\mu = \mu_c$ with the critical exponents $z = 2$ and $\nu = 1/2$. Solid lines demarcate ordered SC and AF phases. Broken lines defined by $|\mu - \mu_c|^{\nu z} = (8u\mu_c)^{-1}k_BT$ mark the boundary of the QC region (shaded area).

coupling constants from their zero-temperature critical values. In this so-called *quantum critical* (QC) region [9], the system feels the finite value of the temperature before becoming sensitive to the deviations of μ from μ_c (i.e., the leading behavior of the system will be described at all scales by the $T = 0$ critical point and its universal response to a finite temperature). To quantify this observation, we introduce the deviation of λ from the QCP value $\delta_\lambda = \lambda - \lambda_0$ [which plays the role of the critical "mass" vanishing at QCP; note that δ_λ is related to the correlation length $\xi = \hbar c/2\delta_\lambda$ which diverges as $\xi \sim (\mu - \mu_c)^{-\nu}$]. At finite temperatures, the deviations from $T = 0$ behavior are distinguished by the scale set by the thermal coherence length $\xi_T \sim T^{-1/z}$ (where z is the dynamic critical exponent). The QC region is then defined by the inequality $\xi_T < \xi$.

To extract the universal information in the QC region, we evaluate in the saddle point equation (4) the momentum integration and subsequent frequency summations using the Poisson formula. We find

$$1 = 3\int_{-\infty}^{+\infty} d\kappa \frac{\rho(\kappa)}{\sqrt{4u(2\delta_\lambda + 3J - J\kappa)}} + 2\int_{-\infty}^{+\infty} d\kappa \frac{\rho(\kappa)}{\sqrt{4u(2\delta_\lambda + 4u\mu^2 + 3J - J\kappa)}} + \frac{1}{\beta J}\sum_{\ell=1}^{\infty}\left[\frac{3}{\pi}\sqrt{\frac{\delta_\lambda}{J}}\frac{1}{\ell}K_1\left(2\ell\beta\sqrt{\frac{\delta_\lambda}{2u}}\right) + \frac{2}{\pi}\sqrt{\frac{\delta_\lambda}{J} + \frac{2u\mu^2}{J}}K_1\left(2\ell\beta\sqrt{\frac{\delta_\lambda}{2u} + \mu^2}\right)\frac{\cosh(2\beta\mu\ell)}{\ell}\right]. \tag{5}$$

Here, $K_1(x)$ stands for the modified Bessel function [10] and $\rho(\kappa) = (1/N)\sum_{\mathbf{k}}\delta[\kappa - \varepsilon(\mathbf{k})]$ is the density of states for the 3D s.c. lattice:

$$\rho(\kappa) = \frac{1}{\pi^3}\int_{\max(-1,-2-\kappa)}^{\min(1,2-\kappa)} \frac{dw}{\sqrt{1-w^2}} \times \mathbf{K}\left[\sqrt{1 - \left(\frac{\kappa + w}{2}\right)^2}\right]\Theta(3 - |\kappa|), \tag{6}$$

where $\mathbf{K}(x)$ and $\Theta(x)$ are the elliptic integral of the first kind [10] and the unit step function, respectively. Utilizing the asymptotic form $K_1(x) \sim 1/x + O(x)$ for small x and the relation $\sum_{\ell=1}^{\infty}\ell^{-2} = \pi^2/6$, we evaluate from Eq. (5) the leading temperature dependence of δ_λ near QCP:

$$\delta_\lambda = \frac{\pi\sqrt{2}\,u}{C_1(g_c/J)}(k_BT)^2\Omega^2\left(\frac{\mu}{k_BT}\right), \tag{7}$$

where

$$\Omega(y) = \sqrt{1 + \frac{4y}{\pi^2}\sum_{\ell=1}^{\infty}\frac{\cosh(2y\ell)}{\ell}K_1(2y\ell)},$$
$$C_1(y) = \int_{-\infty}^{+\infty} d\kappa\,\rho(\kappa)\left[\frac{3}{(3-\kappa)^{3/2}} + \frac{2}{(y+3-\kappa)^{3/2}}\right]. \tag{8}$$

With the result for δ_λ at hand, we now turn to analysis of the measurable magnetic correlation functions in the quantum-critical region. The magnetic scattering cross section for neutrons which is proportional to the dynamic structure factor $S(\mathbf{Q},\omega)$ is directly related to the spin-spin correlation function $\langle \mathbf{S}_0(0)\cdot\mathbf{S}_j(t)\rangle$ [11]:

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\, e^{i\omega t}\sum_{\mathbf{r}_j} e^{i\mathbf{Q}\cdot\mathbf{r_j}}\langle \mathbf{S}_0(0)\cdot\mathbf{S}_j(t)\rangle$$
$$= \frac{1}{\pi}[1+n(\omega)]\chi''(\mathbf{Q},\omega), \tag{9}$$

where $\chi''(\mathbf{Q},\omega)$ is the imaginary part of the dynamic susceptibility and $n(\omega) = [1+\exp(-\omega/k_BT)]^{-1}$ is the Bose function. An integration of the spectral function $\chi''(\mathbf{Q},\omega)$ over wave vectors $\mathbf{Q}$ yields the integrated (local) spin susceptibility $\chi''(\omega) = \int d^3\mathbf{Q}\chi''(\mathbf{Q},\omega)$—an important quantity for verification of the ω/k_BT scaling in the QC region. To establish the connection with our SO(5) calculations, we consider the "imaginary-time" spin-spin correlation function $\mathcal{G}_{ij}(\tau-\tau') = \langle \mathbf{S}_i(\tau)\cdot\mathbf{S}_j(\tau')\rangle$, where $\langle\ldots\rangle$ denotes the ensemble averaging with the Hamiltonian (1). Utilizing the relation between spin operators and SO(5) Lie algebra generators [4] we can write

$$\mathcal{G}_{ij}(\tau-\tau') = \langle L_i^{43}(\tau)L_j^{43}(\tau')\rangle + \langle L_i^{42}(\tau)L_j^{42}(\tau')\rangle + \langle L_i^{32}(\tau)L_j^{32}(\tau')\rangle. \tag{10}$$

The averages over the product of angular momentum operators can be conveniently performed using functional differentiation by adding to the Lagrangian (2) sources which couple linearly to $L^{\mu\nu}$. As a result, we obtain the following in the momentum-frequency representation for the propagator (10):

$$\mathcal{G}(\mathbf{Q},\omega_\ell) = \frac{4u}{\beta N}\sum_{\mathbf{q},\nu_n} G_a(\mathbf{q},\nu_n)[1+u(\omega_\ell-2\nu_n)^2 \times G_a(\mathbf{Q}-\mathbf{q},\omega_\ell-\nu_n)]. \tag{11}$$

Subsequent summation over the internal Matsubara frequencies gives

$$\mathcal{G}(\mathbf{Q},\omega_\ell) = -\frac{4}{N}\sum_{\mathbf{q}}\Bigg\{\left[\frac{(\mathcal{A}_{\mathbf{Q-q}}+i\omega_\ell/2)^2}{\mathcal{A}_{\mathbf{q}}^2-(\mathcal{A}_{\mathbf{Q-q}}+i\omega_\ell)^2}-\frac{1}{4}\right]\times\frac{\coth\left(\frac{\beta\mathcal{A}_{\mathbf{Q-q}}}{2}\right)}{\mathcal{A}_{\mathbf{Q-q}}} + \left[\frac{(\mathcal{A}_{\mathbf{q}}-i\omega_\ell/2)^2}{\mathcal{A}_{\mathbf{Q-q}}^2-(\mathcal{A}_{\mathbf{q}}-i\omega_\ell)^2}-\frac{1}{4}\right]\times\frac{\coth\left(\frac{\beta\mathcal{A}_{\mathbf{q}}}{2}\right)}{\mathcal{A}_{\mathbf{q}}} + \text{c.c.}\Bigg\}, \tag{12}$$

where $\mathcal{A}_{\mathbf{q}} = \sqrt{[2\delta_\lambda - J(\mathbf{q}) + 3J]/u}$. To proceed, we perform now the analytic continuation of $\mathcal{G}(\mathbf{Q},\omega_\ell)$ to *real* frequences $i\omega_n \to \omega + i0^+$ (where 0^+ stands for the positive infinitesimal). After integration over external momenta, we obtain, finally, the imaginary part of the local *dynamic* susceptibility $\chi''(\omega)$ in the scaling form:

$$\chi''(\omega) = \chi''\left(\frac{\omega}{k_BT},\frac{\mu}{k_BT},\frac{\Delta}{k_BT}\right) \equiv \frac{1}{k_BT}\Phi_\chi\left[\frac{\frac{\omega}{k_BT}}{\Omega_c(\frac{\mu}{k_BT})},\frac{\frac{\Delta}{k_BT}}{\Omega_c(\frac{\mu}{k_BT})},\Omega_c\left(\frac{\mu}{k_BT}\right)\right], \tag{13}$$

where $\Delta = \sqrt{J/u}$, $\Omega_c(y) = \pi^{1/2}2^{1/4}C_1^{-1/2}(g_c/J)\Omega(y)$, and

$$\Phi_\chi(y_1,y_2,y_3) = \frac{\pi}{y_3y_2^2}\int_{-\infty}^{+\infty} d\zeta\,\rho(\zeta)\rho\left\{\zeta - \frac{y_1}{y_2^2}\left[y_1 - 2\sqrt{2+(3-\zeta)y_2^2}\right]\right\}\frac{[y_1+2\sqrt{2+(3-\zeta)y_2^2}]^2}{\sqrt{2+(3-\zeta)y_2^2}} \times\left\{\coth\left[\frac{y_3}{2}\sqrt{2+(3-\zeta)y_2^2}\right] - \coth\left[\frac{y_3}{2}\sqrt{2+(3-\zeta)y_2^2}+\frac{y_1y_3}{2}\right]\right\} \tag{14}$$

is the universal scaling function. Our results for $\chi''(\omega)$ are summarized in Fig. 2. The appearance of the temperature as the relevant energy scale for spin dynamics may be very significant because of its possible relation to the normal state characteristics of superconducting cuprates.

Moriya, Takahashi, and Ueda [12] have calculated the contribution to the electrical resistivity from quasiparticle-spin fluctuation scattering. Monien *et al.* [13] have combined the formula of Moriya *et al.* with the results of the NMR phenomenology; the knowledge of the dynamic spin susceptibility allows one to calculate the spin fluctuation scattering contribution to the dc resistivity from

$$R(T) \sim \frac{1}{k_BT}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty} d\omega\,\frac{\omega e^{\omega/k_BT}}{(e^{\omega/k_BT}-1)^2}\chi''(\mathbf{q},\omega). \tag{15}$$

Accordingly, the calculated closed-form formula for the spin susceptibility $\chi''(\omega)$ may serve as input for calculations of transport properties near the QCP. Using Eqs. (13) and (14), we argue that the contribution to the electrical resistivity R/R_0 due spin fluctuations should scale similar to

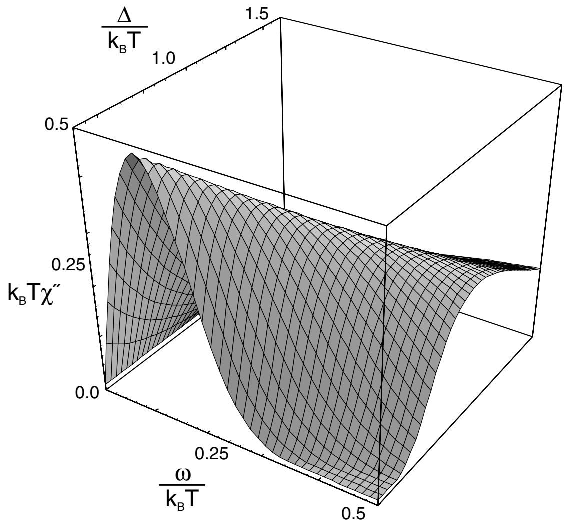

FIG. 2. Plot of the imaginary part of the dynamic spin susceptibility $k_BT\chi''(\frac{\omega}{k_BT}, \frac{\mu}{k_BT}, \frac{\Delta}{k_BT})$ as a function of ω/k_BT and Δ/k_BT (for fixed scaling variable $\mu/k_BT = 0$).

$$\frac{R}{R_0} = \int_0^\infty dy \, \frac{2ye^y}{(e^y - 1)^2} \times \Phi_\chi\left[\frac{y}{\Omega_c(\frac{\mu}{k_BT})}, \frac{\frac{\Delta}{k_BT}}{\Omega_c(\frac{\mu}{k_BT})}, \Omega_c\left(\frac{\mu}{k_BT}\right)\right]. \quad (16)$$

In Fig. 3 we plotted the normal-state resistivity $R(T)/R_0$ for several values of the parameter Δ that controls the quantum fluctuations. For increasing Δ, one observes that the temperature dependence of the resistivity becomes linear in T—a hallmark example of anomalous properties in cuprate materials.

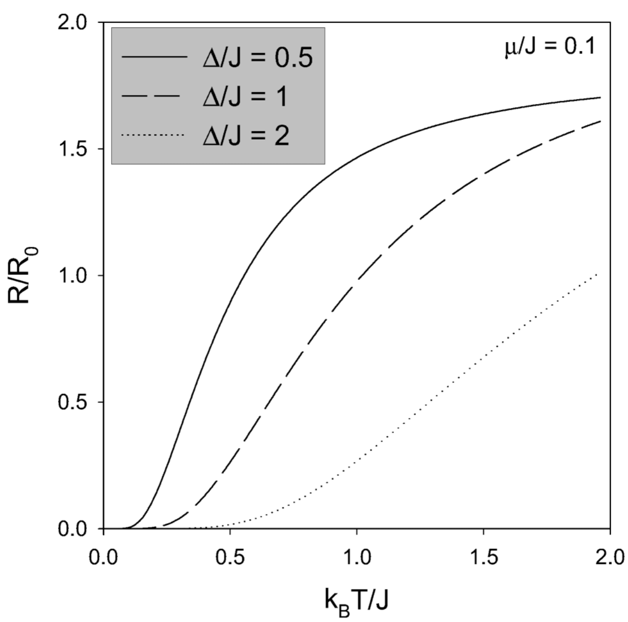

FIG. 3. Temperature dependence of the resistivity R/R_0 due to spin fluctuations in the QC region for several values of the parameter Δ (for fixed μ). The parameter values are indicated in the inset.

In conclusion, we have performed a quantitative study of the quantum-critical point scenario within the concept of the SO(5) group based theory of superconductivity and antiferromagnetism for high-T_c materials. The physical properties governed by the proximity to the AF/SC quantum-critical point account for the universal scaling for the finite temperature behavior. The general prerequisite of a given QCP scenario is that it *must* involve the concept of a broken symmetry. Several questions related to this issue arise in applying other alternative QCP based theories (such as charge instability near optimum doping; see, e.g., [14]) to cuprates: What are the relevant phases with order and associated broken symmetries? Some possibilities that address these problems are being currently debated [15]; however, further theoretical work on quantum-critical dynamics in cuprate materials is clearly called for.

[1] S. L. Sondhi, S. M. Girvin, J. P. Carini, and D. Shahar, Rev. Mod. Phys. **69**, 315 (1997).
[2] B. Keimer, R. J. Birgeneau, A. Cassanho, Y. Endoh, R. W. Erwin, M. A. Kastner, and G. Shirane, Phys. Rev. Lett. **67**, 1930 (1991); B. Keimer, N. Belk, R. J. Birgeneau, A. Cassanho, C. Y. Chen, M. Greven, M. A. Kastner, A. Aharony, Y. Endoh, R. W. Erwin, and G. Shirane, Phys. Rev. B **46**, 14 034 (1992); G. Aeppli, T. E. Mason, S. M. Hayden, H. A. Mook, and J. Kulda, Science **278**, 1432 (1997).
[3] S. Sachdev and J. Ye, Phys. Rev. Lett. **69**, 2411 (1992); A. Sokol and D. Pines, Phys. Rev. Lett. **71**, 2813 (1993); C. M. Varma, Phys. Rev. Lett. **75**, 898 (1995); C. Castellani, C. Di Castro, and M. Grilli, Phys. Rev. Lett. **75**, 4650 (1995).
[4] S. C. Zhang, Science **275**, 1089 (1997).
[5] This would correspond to the scenario depicted in Fig. 1C of the Zhang paper (see Ref. [4]).
[6] For a recent account on how to experimentally measure the number 5 of the SO(5) theory, see J.-P. Hu and S. C. Zhang, Physica (Amsterdam) **341C–348C**, 93 (2000).
[7] 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 $J_z \ll J$.
[8] T. Zaleski and T. K. Kopeć, Phys. Rev. B **62**, 9059 (2000).
[9] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989).
[10] M. Abramovitz and I. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970).
[11] W. Marshall and R. D. Lowde, Rep. Prog. Phys. **31**, 705 (1968).
[12] T. Moriya, Y. Takahashi, and K. Ueda, J. Phys. Soc. Jpn. **59**, 2905 (1990).
[13] H. Monien, P. Monthoux, and D. Pines, Phys. Rev. B **43**, 275 (1991).
[14] C. di Castro, L. Benefatto, S. Caprara, C. Castellani, and M. Grilli, Physica (Amsterdam) **341C**, 1715 (2000).
[15] C. M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).