Fermi-Liquid Computation of the Phase Diagram of High-T_c Cuprate Superconductors with an Orbital Antiferromagnetic Pseudogap

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A 4-parameter Fermi-liquid calculation of the high-T_c cuprate phase diagram is reported. Simultaneously accounted for are the special doping densities of 5% and 16%, the d-wave functional form of the (orbital antiferromagnetic) pseudogap, the measured T_c, superconducting gap, pseudogap and superfluid density as a function of doping, the particle-hole doping asymmetry and the half-filling spin wave velocity.

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Since its discovery over 25 years ago, cuprate superconductivity has persuasively demonstrated the limits of computability in physics [1–3]. The Hamiltonian of solid matter is known exactly, yet there continues to be no first-principles theoretical control of the quantum mechanics at the energy scales relevant to metallic transport, even with supercomputers. One achieves control, if at all, only by exploiting the universal low-energy properties of quantum phases. The simple equations one obtains then allow predictive computation.

Unfortunately, the cuprates are so anomalous phenomenologically that they have thus far defied categorization as conventional metals or insulators. This has led to speculation that they might involve a new, and as-yet unidentified, parent vacuum. Proposals for such a vacuum include the Mott insulator, the resonating valence bond, the non-Fermi liquid, and the loop-current insulator [4–7].

However, there is a much simpler potential explanation: the zero-temperature phases of the cuprates are conventional, and the strange behaviors are just critical phenomena and glassiness associated with transitions among two or more of these phases [8–10]. This view is supported by the absence of experimental evidence for new states of matter at lowest temperature scales. It is also supported by theory, in that none of the proposed theoretical alternatives to conventional metals and insulators can be (1) written down in a straightforward way at zero temperature or (2) shown to be stabilized by any simple Hamiltonian. There is no mathematical case that any of them actually exist.

The purpose of this Letter is to report the theoretical high-T_c cuprate phase diagram shown in Fig. 1. It is computed using a Fermi-liquid theory with four parameters and standard Hartree-Fock methods [11,12]. It is characterized by interpenetrating spin antiferromagnetic (SDW), d-wave superconducting (DWS), and orbital antiferromagnetic (DDW) order parameters. The latter two cause $d_{x^2-y^2}$ quasiparticle dispersion. The phase diagram matches experiment, including the transition doping densities of 5% and 16% on the p-type side, which are not fit [13]. I identify the "strange-metal" behavior at elevated temperatures near optimal doping as critical scattering from DDW onset, which is physically similar to that of SDW onset [14].

Elementary quantum mechanics requires that the cuprates may be described by adiabatic deformation out of the unperturbed band structure. That is to say, one starts from a fictitious noninteracting electron Hamiltonian $\mathcal{H}_0$ and then slowly turns on the perturbation $\lambda(\mathcal{H}-\mathcal{H}_0)$, where $\mathcal{H}$ is the true Hamiltonian and λ is a parameter that advances from 0 to 1. This evolution is the logical basis of the the Feynman rules, and it requires strict compliance with them [12]. As λ increases, it is perfectly possible for the system to undergo a phase transition to a new state of matter on the way to becoming a superconductor, but one is obligated to say what this state is. More precisely, one must describe it mathematically in terms of conventional particle and hole excitations of the parent band structure. I find no such state.

The Hartree-Fock solution minimizes a variational energy. All three order parameters in Fig. 1 are therefore logical consequences of the equations of motion, not postulates. This is especially important in the case of DDW, which I identify with the pseudogap.

The lack of a clear experimental precedent for DDW has made it controversial ever since a group of us first proposed it over a decade ago [15]. Magnetic Bragg peaks, its most distinctive experimental signature, are inherently difficult to detect by virtue of interference from spin antiferromagnetism, unit cell symmetry, and pseudogap glassiness [16]. There are experimental reports both for and against such magnetism in the literature [17–21]. However, a key prediction of DDW sustained by experiment is the appearance of a reconstructed Fermi surface (in other words, a conventional metallic state) when the superconductivity is crushed with a magnetic field. This has been demonstrated by the experimental observation of quantum oscillations [22,23].

The significant argument for DDW is not phenomenological, however, but theoretical: It is impossible to write down a Hamiltonian that stabilizes DWS that does not also stabilize DDW. The reason is that DDW is a crystal

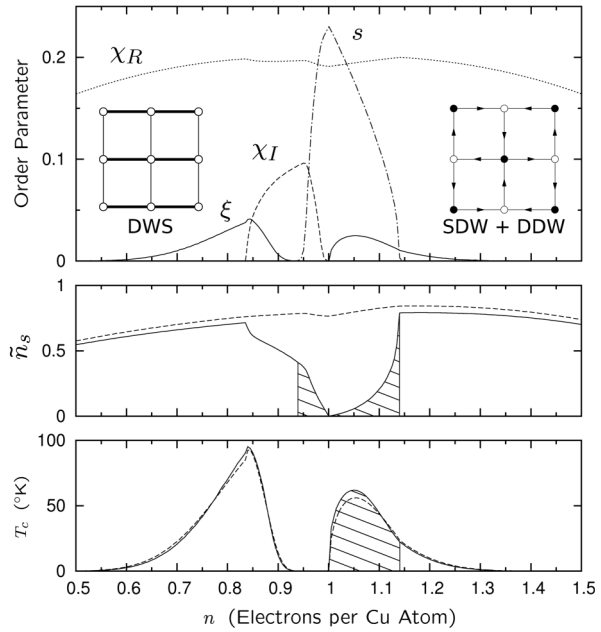

FIG. 1. Top: Zero-temperature order parameters s, χ_I, and ξ as a function of doping computed using $\mathcal{H}_0 + \Delta\mathcal{H}$ with the parameters $V_n = V_t = 0$, $U = 0.76t$, $J = 0.75t$, $V_c = 0.87t$, $t' = 0.1t$, and $t = 0.19$ eV. Insets: Order parameter sign conventions. Middle: Superfluid density in electrons per Cu atom defined by Eq. (6). Dashed curve: Total f-sum rule. Bottom: Superconducting transition temperature T_c. Dashed curve: Maximum superconducting gap $3J|\xi|$ divided by 2.2. The hatching indicates insulation: Superconductivity in this doping range is an artifact of having forced the SDW to be commensurate. Relaxing this condition enables the SDW to form domain walls that trap carriers [29].

of d-wave Cooper pairs. Its relationship to DWS is aptly analogous to the relationship of charge density wave order to s-wave superconductivity in the negative-U Hubbard model [24]. Accordingly, the simplicity of the equations reported in this Letter, their compatibility known principles of solid-state physics, and their ability to reproduce the phase diagram in detail together indicate that the experiments reporting the nonexistence of DDW are either misinterpreted or in error.

I take the fictitious metal Hamiltonian to be

$$\mathcal{H}_0 = -t\sum_{\langle jk\rangle}^{2N}\sum_{\sigma}(c^\dagger_{j\sigma}c_{k\sigma} + c^\dagger_{k\sigma}c_{j\sigma}) + t'\sum_{\langle j\ell\rangle}^{2N}\sum_{\sigma}(c^\dagger_{j\sigma}c_{\ell\sigma} + c^\dagger_{\ell\sigma}c_{j\sigma}), \quad (1)$$

where $\langle jk\rangle$ denotes near-neighbor pairs of N sites on a planar square lattice of length $b = 3.9$ Å and $\langle j\ell\rangle$ denotes the set of second-neighbor pairs. This is a fit to the density functional band structure [25]. It is inaccurate far from the Fermi surface, but the high-energy excitations that it does not describe correctly are not important. Each incremental increase of λ stepping toward $\mathcal{H}$ is described by the perturbation Hamiltonian

$$\begin{aligned}\Delta\mathcal{H} = {} & U\sum_{j}^{N} c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}c_{j\downarrow}c_{j\uparrow} \\ & + \frac{J}{2}\sum_{\langle jk\rangle}^{2N}\sum_{\sigma\sigma'}\left[c^\dagger_{j\sigma}c^\dagger_{k\sigma'}c_{k\sigma}c_{j\sigma'} - \frac{1}{2}c^\dagger_{j\sigma}c^\dagger_{k\sigma'}c_{k\sigma'}c_{j\sigma}\right] \\ & + V_t\sum_{\langle jk\rangle}^{2N}\sum_{\sigma\sigma'}(c^\dagger_{j\sigma}c_{k\sigma} + c^\dagger_{k\sigma}c_{j\sigma})\left(c^\dagger_{j\sigma'}c_{j\sigma'} + c^\dagger_{k\sigma'}c_{k\sigma'} - \frac{1}{2}\right) \\ & + V_n\sum_{\langle jk\rangle}^{2N}\sum_{\sigma\sigma'}c^\dagger_{j\sigma}c^\dagger_{k\sigma'}c_{k\sigma'}c_{j\sigma} \\ & + V_c\sum_{\langle jk\rangle}^{2N}[c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}c_{k\downarrow}c_{k\uparrow} + c^\dagger_{k\uparrow}c^\dagger_{k\downarrow}c_{j\downarrow}c_{j\uparrow}]. \end{aligned} \quad (2)$$

This represents a complete list of the allowed Fermi-liquid parameters. Whether they are purely electronic or mediated by phonons does not matter. Only pairwise interactions are relevant because the perturbation excites a quantum-mechanical gas of quasiparticles that is dilute. Only lattice terms closer than second neighbors are relevant because these exhaust the low angular momentum scattering channels. All terms associated with bonds must also be rotationally invariant about the bond axis and reflection symmetric. All terms must be spin-rotationally invariant and time-reversal symmetric. In principle, Fermi-liquid parameters can depend on doping, but I find they do not.

The number of free parameters is actually only 4. Photoemission measurements find the asymptotic nodal Fermi velocity to be $\hbar v_F = 2.0$ eV Å, for both p-type and n-type doping [26,27]. This requires $V_t = 0$, since the main effect of this parameter is to renormalize t in a doping-dependent way. It also requires $t = 0.19$ eV, a number about half that of the native band structure. The asymmetry parameter $t'/t = 0.1$ is a fit to experiment, although it is also compatible with calculations [28].

The ground state of $\mathcal{H}_0 + \Delta\mathcal{H}$ with the parameters I have chosen is characterized by the expectation values

$$\begin{aligned} &\langle c^\dagger_{j\sigma}c_{k\sigma}\rangle = \chi_R \pm i\chi_I, \qquad \langle c^\dagger_{j\sigma}c_{\ell\sigma}\rangle = \chi'_R, \\ &\langle c^\dagger_{j\uparrow}c^\dagger_{k\downarrow}\rangle = \pm\xi, \quad \langle c^\dagger_{j\sigma}c_{j\sigma}\rangle = \frac{n}{2} \pm (-1)^\sigma s, \end{aligned} \quad (3)$$

with the signs as in Fig. 1. The order parameter ξ describes d-wave superconductivity. The order parameter χ_I describes orbital antiferromagnetism. The order parameter s describes spin antiferromagnetism. To simplify the calculation I have constrained the variational ground state to be periodic in a doubled unit cell. This constraint creates a mild artifact of allowing the system to conduct at all nonzero dopings. If this constraint is relaxed, SDW domain

walls form, trapping carriers and causing the system to insulate everywhere SDW order is developed [29]. The analogous problem with DDW is much less severe because (1) the DDW quasiparticle spectrum is gapless and (2) the DDW symmetry breaking is discrete. χ_R and $\chi_R{}'$ are not order parameters but measures of the ground state kinetic energy. n is the site occupancy. The traditional single-Slater-determinant ansatz gives the variational energy

$$\begin{aligned}\frac{\langle \mathcal{H}_0 + \Delta\mathcal{H}\rangle}{N} &= -8t\chi_R + 8t'\chi_R{}' + \left[\frac{n^2}{4} - s^2\right]U + [2n^2 + 4|\xi|^2 \\ &\quad -4\chi_R^2 - 4\chi_I^2]V_n - [3\chi_R^2 + 3\chi_I^2 + 3|\xi|^2 + 2s^2]J \\ &\quad + [4\chi_R^2 - 4\chi_I^2]V_c. \end{aligned} \tag{4}$$

Minimizing this energy gives the Hartree-Fock Hamiltonian

$$\begin{aligned}\mathcal{H}_{\mathrm{HF}} &= \mathcal{H}_0 - \mu\sum_j^N\sum_\sigma c_{j\sigma}^\dagger c_{j\sigma} + \left(\frac{3}{4}J - V_n\right) \\ &\quad \times \sum_{\langle jk\rangle}^{2N} \pm[\xi^*(c_{j\uparrow}^\dagger c_{k\downarrow}^\dagger + c_{k\uparrow}^\dagger c_{j\downarrow}^\dagger) + \xi(c_{k\downarrow}c_{j\uparrow} + c_{j\downarrow}c_{k\uparrow})] \\ &\quad -\left[t + \left(\frac{3}{4}J + V_n - V_c\right)\chi_R\right]\sum_{\langle jk\rangle}^{2N}\sum_\sigma (c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma}) \\ &\quad + i\left(\frac{3}{4}J + V_n + V_c\right)\chi_I \sum_{\langle jk\rangle}^{2N} \pm \sum_\sigma (c_{j\sigma}^\dagger c_{k\sigma} - c_{k\sigma}^\dagger c_{j\sigma}) \\ &\quad -(U+2J)s\sum_j^N (-1)^j [c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow}], \end{aligned} \tag{5}$$

where μ is the chemical potential. The self-consistency equations for s, ξ, and χ_I are all standard and so need not be reproduced here. I have performed the corresponding integrations over the Brillouin zone numerically.

The parameters I have chosen ($V_n = 0$, $U = 0.76t$, $J = 0.75t$, $V_c = 0.87t$) are fits to experiment. The experimental constraint that the antiferromagnetic spin polarization s be about half the classically allowed value of $s = 1/2$ at half filling fixes the value of $U + 2J \simeq 2.5\tilde{t}$, where $\tilde{t} = t + (0.75J + V_n - V_c)\chi_R$ [30]. The condition that DDW just barely competes with SDW at half filling fixes $0.75J + V_c + V_n \simeq 1.3\tilde{t}$. These two conditions together robustly satisfy the two experimental constraints that the spin order disappear at 5% p-type doping and the maximum T_c occur at 16% doping. They also fix the pseudogap size. The maximum DWS gap then fixes $0.75J - V_n > 0$. The remaining loose parameter, $V_n = 0$, is fixed by the overall phase diagram shape. Attempting to account for the superconductivity with $V_n < 0$ results in destabilizing DDW to DWS at low dopings, an effect incompatible with pseudogap formation. If one chooses $V_n > 0$, the pseudogap problem is solved, but an unphysically large $J > 0$ becomes required to account for the superconductivity. The smallness of V_n also makes sense physically. It is fundamentally a near-neighbor Coulomb interaction that should have been taken care of in the underlying band structure construction.

The $V_c > 0$ required to satisfy these constraints has two important consequences other than destabilizing the superconducting state at half filling: (1) It prevents $U \simeq -2J + (2.5/1.3)[0.75J + V_c + V_n]$ from being negative, and (2) it causes $\tilde{t}/t < 1$. If U were negative, the system would be unstable to s-wave superconductivity. If one had $\tilde{t}/t > 1$, the superfluid density would exceed the total f-sum rule. This would imply that the system was not in its ground state. Thus, $V_c > 0$ is necessary for $J > 0$ to make sense physically.

Figure 2 shows a comparison of the theoretical pseudogap and superconducting gaps with estimates made by Hüfner *et al.* from a variety of experimental sources [31]. The theory is in full agreement with experiment within the fitting error bar of the latter, which is approximately 30%. The presence of two distinct d-wave gaps is consistent with the findings of other researchers [32].

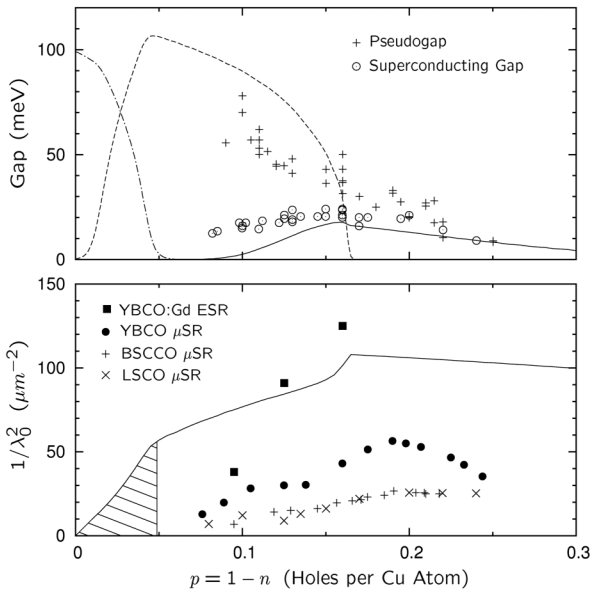

FIG. 2. Top: Maximum spin gap $(U + 2J)s$, maximum bond current gap $(3J + 4V_c)\chi_I$, and maximum superconducting gap $3J\xi$ calculated using the parameters of Fig. 1 compared with estimates of the pseudogap and superconducting gap assembled by Hüfner *et al.* from a variety of sources [31]. Bottom: Calculated London penetration depth compared with μSR measurements on polycrystalline samples reported by Tallon *et al.* (plus, cross, filled circle) and in-plane ESR measurements on oxygen-ordered YBCO:Gd by Pereg-Barnea *et al* (filled square) [33,34]. The hatching is the same as that in Fig. 1 [29].

Also shown is a comparison of the measured London penetration depth λ_0 with the theoretical one I compute assuming an interlayer spacing of $a = 5.8$ Å [33,34]. This comparison is problematic because the experiments do not agree with each other for a variety of reasons, including different averaging of crystal anisotropy and different amounts of disorder degradation. The latter is an allowed effect in a d-wave superconductor. However, the smallest reported value of the in-plane λ_0 is the important number, and it is consistent with a superfluid density $\tilde{n}_s$ that is large. The theoretical value of the latter, defined by

$$\frac{1}{\lambda_0^2} = \frac{4\pi e^2}{\hbar^2 c^2}\left(\frac{t}{a}\right)\tilde{n}_s = 151(\mu\mathrm{m})^{-2}\tilde{n}_s, \tag{6}$$

may be seen in Fig. 1 to be comparable to 1 except when spin and bond antiferromagnetism develop and reconstruct the Fermi surface into pockets. The corresponding Kosterlitz-Thouless temperature $k_B T_{KT} = (\pi/8)t\tilde{n}_s \sim 0.05$ eV is too large for phase fluctuations to affect the superconducting T_c [35,36]. Accordingly, the computation of T_c by conventional BCS gap collapse is appropriate. The T_c computed by this method is shown in Fig. 1.

A standard ladder-sum (RPA) vertex correction of the Hartree-Fock spin susceptibility gives a half-filling spin-wave velocity of $\hbar v_s = 1.0eV\text{-}A$, in full agreement with experiment [37].

My findings point to the oxygen atom in the bond, not Coulomb repulsions on the Cu atom, as the cause of all three phenomena: superconductivity, pseudogap, and antiferromagnetism. While the hopping parameters J and V_c could conceivably be generated by phonons, it is far more reasonable that they should be purely electronic and result from the enormous correlations known to be present in first-row elements. Regardless of whether this is the case, however, adiabatic continuity requires that the cuprates are not the cradle of new states of matter but simply the scene of a titanic struggle among three rather conventional order parameters.

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[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
[2] E. Abrahams and P. W. Anderson, Nature (London) **327**, 363 (1987).
[3] M. R. Norman, Science **332**, 196 (2011).
[4] P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. **78**, 17 (2006); T. Senthil and P. A. Lee, Phys. Rev. Lett. **103**, 076402 (2009).
[5] P. W. Anderson, Science **235**, 1196 (1987); P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, and F. C. Zhang, J. Phys. Condens. Matter **16**, R755 (2004).
[6] T. M. Rice, K.-Y. Yang, and F. C. Zhang, Rep Prog. Phys. **75**, 016502 (2012).
[7] C. M. Varma, Phys. Rev. B **73**, 155113 (2006); Nature (London) **468**, 184 (2010).
[8] C. M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).
[9] S. Sachdev, Rev. Mod. Phys. **75**, 913 (2003); Phys. Status Solidi B **247**, 537 (2010).
[10] S. E. Sebastian, N. Harrison, M. M. Altarawneh, C. H. Mielke, R. Liang, D. A. Bonn, W. N. Hardy, and G. G. Lonzarich, Proc. Natl. Acad. Sci. U.S.A. **107**, 6175 (2010).
[11] D. Pines and P. Noziéres, *Theory of Quantum Liquids: Normal Fermi Liquids* (Perseus, New York, 1989).
[12] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (Dover, New York, 2003).
[13] D. M. Broun, Nat. Phys. **4**, 170 (2008).
[14] D.Bergeron, D. Chowdhury, M. Punk, S. Sachdev, and A.-M. S. Tremblay, Phys. Rev. B **86**, 155123 (2012).
[15] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001); C. Nayak and E. Pivovarov, Phys. Rev. B **66**, 064508 (2002); I. Dimov, P. Goswami, X. Jia, and S. Chakravarty, Phys. Rev. B **78**, 134529 (2008).
[16] K. McElroy, D.-H. Lee, J. E. Hoffman, K. M. Lang, J. Lee, E. W. Hudson, H. Eisaki, S. Uchida, and J. C. Davis, Phys. Rev. Lett. **94**, 197005 (2005).
[17] B. Fauqué, Y. Sidis, V. Hinkov, S. Pailhés, C. T. Lin, X. Chaud, and P. Bourges, Phys. Rev. Lett. **96**, 197001 (2006).
[18] H. A. Mook, Y. Sidis, B. Fauqué, V. Balédent, and P. Bourges, Phys. Rev. B **78**, 020506 (2008); H. A. Mook, P. Dai, S. M. Hayden, A. Hiess, S.-H. Lee, and F. Dogan, Phys. Rev. B **69**, 134509 (2004).
[19] J. E. Sonier, V. Pacradouni, S. A. Sabok-Sayr, W. N. Hardy, D. A. Bonn, R. Liang, and H. A. Mook, Phys. Rev. Lett. **103**, 167002 (2009).
[20] P. Bourges and Y. Sidis, C.R. Phys. **12**, 461 (2011).
[21] S. Strässle, B. Graneli, M. Mali, J. Roos, and H. Keller, Phys. Rev. Lett. **106**, 097003 (2011).
[22] N. Doiron-Leyraud, C. Proust, D. LeBoeuf, J. Levallois, J.-B. Bonnemaison, R. Liang, D. A. Bonn, W. N. Hardy, and L. Taillefer, Nature (London) **447**, 565 (2007); B. Vignolle, D. Vignolles, D. LeBoeuf, S. Lepault, B. Ramshaw, R. Liang, D. A. Bonn, W. N. Hardy, N. Diron-Leyraud, A. Carrington, N. E. Hussey, L. Taillefer, and C. Proust, C.R. Phys. **12**, 446 (2011).
[23] S. Chakravarty, Rep. Prog. Phys. **74**, 022501 (2011).
[24] Y. Nagaoka, Prog. Theor. Phys. **52**, 1716 (1974).
[25] L. F. Mattheiss, Phys. Rev. Lett. **58**, 1028 (1987).
[26] I. M. Vishik, W. S. Lee, R.-H. He, M. Hashimoto, Z. Hussain, T. P. Devereaux, and Z.-X. Shen, New J. Phys. **12**, 105008 (2010).
[27] N. P. Armitage, D. H. Lu, C. Kim, A. Damascelli, K. M. Shen, F. Ronning, D. L. Feng, P. Bogdanov, Z.-X. Shen, Y. Onose, Y. Taguchi, Y. Tokura, P. K. Mang, N. Kaneko, and M. Greven, Phys. Rev. Lett. **87**, 147003 (2001).
[28] E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **87**, 047003 (2001).
[29] H. J. Schulz, Phys. Rev. Lett. **64**, 1445 (1990).
[30] J. Tranquada, in *Handbook of High-Temperature Superconductivity*, edited by J. R. Schrieffer and J. S. Brooks (Springer, New York, 2007), p. 257.
[31] S. Hüfner, M. A. Hossain, A. Damascelli, and G. A. Sawatzky, Rep. Prog. Phys. **71**, 062501 (2008).

[32] B. Valenzuela and E. Bascones, Phys. Rev. Lett. **98**, 227002 (2007).

[33] J. L. Tallon, J. W. Loram, J. R. Cooper, C. Panagopoulos, and C. Bernhard, Phys. Rev. B **68**, 180501 (2003).

[34] T. Pereg-Barnea, P. J. Turner, R. Harris, G. K. Mullins, J. S. Bobowski, M. Raudsepp, R. Liang, D. A. Bonn, and W. N. Hardy, Phys. Rev. B **69**, 184513 (2004).

[35] L. Benfatto, C. Castellani, and T. Giamarchi, Phys. Rev. Lett. **98**, 117008 (2007).

[36] V. J. Emery and S. A. Kivelson, Nature (London) **375**, 434 (1994).

[37] R Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. **86**, 5377 (2001).