Indications of Spin-Charge Separation in the Two-Dimensional t-J Model

W. O. Putikka
National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306

R. L. Glenister and R. R. P. Singh
Department of Physics, University of California, Davis, California 95616

Hirokazu Tsunetsugu
Theoretische Physik, Eidgenössische Technische Hochschule, 8093 Zürich, Switzerland
and Interdisziplinäres Projektzentrum für Supercomputing, Eidgenössische Technische Hochschule-Zentrum, 8092 Zürich, Switzerland

(Received 21 September 1993)

We have calculated the high temperature expansion for the density correlation function $N(\mathbf{q})$ of the two-dimensional t-J model. On extrapolation by Padé approximants to low temperatures we find that $N(\mathbf{q})$ has $2\mathbf{k}_F^{\mathrm{SF}}$ as a characteristic wave vector. Previous studies have shown that $n_\mathbf{k}$ has a steplike feature at $\mathbf{k}_F$ and $S(\mathbf{q})$ has $2\mathbf{k}_F$ as a characteristic wave vector. Here $\mathbf{k}_F$ and $\mathbf{k}_F^{\mathrm{SF}}$ are the Fermi wave vectors of the nearest-neighbor square lattice tight-binding and spinless fermion models, respectively. By comparison to known results for one dimension this suggests spin-charge separation in the two-dimensional t-J model.

PACS numbers: 74.20.Mn, 74.72.–h

The study of strongly correlated electrons in two dimensions (2D) is currently one of the most interesting and controversial topics in condensed matter physics, particularly with regard to high temperature superconductivity (HTSC) [1]. Anderson [2] has put forward the idea that the ground state of strongly correlated electron systems in 2D is a Luttinger liquid analogous to the case in one dimension. In 1D, a Luttinger liquid has spin and charge degrees of freedom with different velocities and wave vectors, behaving at low energies as independent elementary excitations, a situation which has become known as spin-charge separation [2].

Determining whether or not spin-charge separation can also occur in 2D has proven quite difficult. We have used high temperature expansions for equal time correlation functions (ETCF) of the 2D t-J model [3] to investigate this possibility. This combines previously calculated series for the momentum distribution function [4] and the spin correlation function [5] with a newly calculated series for the density correlation function. We find two distinct characteristic wave vectors for the spin and charge degrees of freedom, $2\mathbf{k}_F$ and $2\mathbf{k}_F^{\mathrm{SF}}$ defined below. This shows that the spin and charge degrees of freedom have different distributions in the Brillouin zone and may provide an indication for spin-charge separation in this model.

We consider the 2D t-J model on a square lattice, where the Hamiltonian is

$$\mathcal{H}_{tJ} = -t \sum_{<ij>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.}) + J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

with the constraint of no double occupancy. The constraint represents the strong correlations between the electrons and is difficult to treat by conventional many-body techniques.

We have studied three ETCF of this model using the high temperature series expansion method. These are the single spin momentum distribution function, $n_\mathbf{k}$, and the equal time spin and density correlation functions, $S(\mathbf{q})$ and $N(\mathbf{q})$, defined by the relations

$$n_\mathbf{k} = \sum_\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \langle c_{0\sigma}^\dagger c_{\mathbf{r}\sigma} \rangle,$$
$$S(\mathbf{q}) = \sum_\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \langle S_0^z S_\mathbf{r}^z \rangle,$$
$$N(\mathbf{q}) = \sum_\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \langle \Delta n_0 \Delta n_\mathbf{r} \rangle, \quad (2)$$

where the angular brackets refer to thermal averaging in the grand canonical ensemble, $S_\mathbf{r}^z = \frac{1}{2}\sum_{\alpha\beta} c_{\mathbf{r}\alpha}^\dagger \sigma_{\alpha\beta}^z c_{\mathbf{r}\beta}$ and $\Delta n_\mathbf{r} = \sum_\sigma c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma} - n$. Here n is the average density of electrons. The expansions are calculated for $n_\mathbf{k}$ [4] to eighth order and $S(\mathbf{q})$ [5] and $N(\mathbf{q})$, to tenth order in the reciprocal temperature T^{-1}, first at fixed fugacity, and then by a change of variables at fixed n. The series are extrapolated at fixed n by Padé approximants to determine the low T properties.

The form of the ETCF for tight-binding (TB) (noninteracting, spin-half electrons with nearest-neighbor hopping on a square lattice) and spinless fermions (SF) (physically, SF are fully spin-polarized TB electrons, freezing out the spin degrees of freedom and doubling the number of occupied $\mathbf{k}$ states) in 2D are helpful in understanding the t-J model results presented below. They are given by

$$N(\mathbf{q}) = n - g \int \frac{d\mathbf{k}}{(2\pi)^2} n_\mathbf{k} n_{\mathbf{k}+\mathbf{q}}, \quad (3)$$

where $g = 2$ for TB or $g = 1$ for SF, and $4S(\mathbf{q}) = N(\mathbf{q})$ for TB. From the form of this equation we can see that

0031-9007/94/73(1)/170(4)$06.00

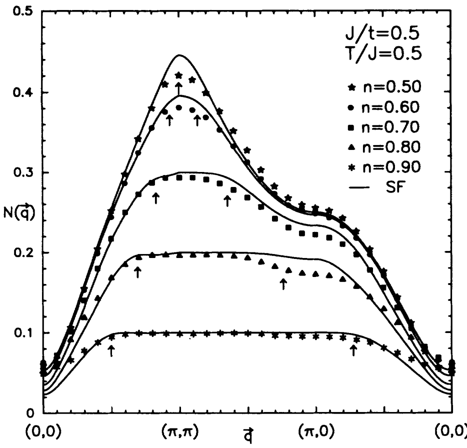

FIG. 1. Plot of $N(\mathbf{q})$ at $T/J = 0.5$ and $J/t = 0.5$ along the irreducible wedge for a range of n. The data points are the t-J model and the solid lines are spinless fermions for the same temperature. The small vertical arrows are the $T = 0$ locations of nesting vectors for spinless fermions.

at $T = 0$ and $n \leq 1$ the ETCF will saturate at n when $n_{\mathbf{k}}$ and $n_{\mathbf{k+q}}$ no longer overlap [note that for SF with $n > 0.5$, $N(\mathbf{q})$ saturates at $1 - n$ when the hole Fermi surfaces no longer overlap]. The Kohn anomaly [6] at $2\mathbf{k}_F$ or $2\mathbf{k}_F^{\mathrm{SF}}$ is due to the existence of a sharp Fermi surface.

In Fig. 1 we compare $N(\mathbf{q})$ of the 2D t-J model to $N(\mathbf{q})$ of SF at the same density for $T/J = 0.5$, $J/t = 0.5$, and a range of n. The similarities are remarkable throughout the Brillouin zone, with the differences near the Γ point due to the t-J model having a larger compressibility than SF. To focus the discussion below we now limit ourselves to two sets of parameters outside of the phase separated [7] or ferromagnetic [8] regions of the 2D t-J model. We fix $J/t = 0.5$ and consider $n = 0.75$ and $n = 0.20$. The results for $n_{\mathbf{k}}$, $S(\mathbf{q})$, and $N(\mathbf{q})$ along $q_{\Gamma M} = (0,0) \rightarrow (\pi,\pi)$ are shown in Fig. 2. We see that $n_{\mathbf{k}} \approx 1/2$ at $k_{F\Gamma M}$, the Fermi momentum of the TB model at the same density [4,9] and $S(\mathbf{q})$ is enhanced over its TB value and either flattens out or has a peak [5] at $q \approx 2k_{F\Gamma M}$. However, the most anomalous curves are for $N(\mathbf{q})$. They are suppressed from their TB values and flatten out at $q \approx 2k_{F\Gamma M}^{\mathrm{SF}}$, the Fermi momentum of SF at the same density. We observe no feature at $\mathbf{q} = 2\mathbf{k}_F$, though $N(\mathbf{q})$ flattens out more gradually for $n = 0.20$ than for $n = 0.75$.

For comparison, we recall the behaviors of n_k, $S(q)$, and $N(q)$ for the $U/t \rightarrow \infty$ Hubbard model ($J/t \rightarrow 0$ t-J model) in 1D. From the work of Ogata and Shiba [10] we know that n_k has a power law singularity at k_F with $n_{k_F} = 1/2$. Also $S(q)$ has a peak at $2k_F$ and $N(q)$ has $2k_F^{\mathrm{SF}} = 4k_F$ as a characteristic wave vector. For arbitrary U/t, $N(q)$ also has a feature at $2k_F$ due to a mixture of spin and charge excitations, but the $2k_F^{\mathrm{SF}}$ feature is due to charge alone [11] and shows that the charge degrees of freedom truly reside at k_F^{SF}. In addition to the singularity at k_F, n_k has a singularity at $3k_F$, but with a very small step size.

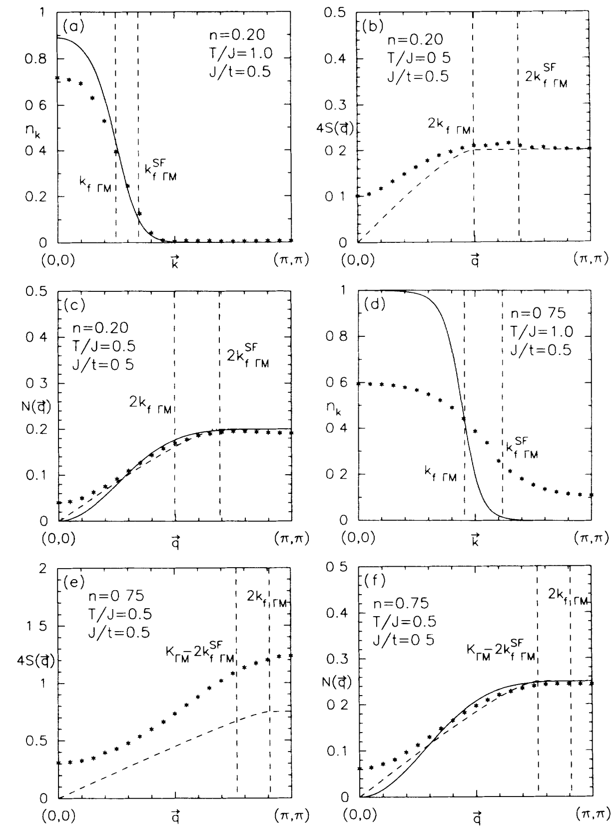

FIG. 2. Plots along the diagonal $\Gamma \rightarrow M$ at $n = 0.20$. (a) Single spin momentum distribution function. Data points, t-J model; solid line, tight-binding model at $T/J = 1.0$. (b) Spin correlation function. Data points, t-J model; dashed line, $T = 0$ tight-binding model. (c) Density correlation function. Data points, t-J model; solid line, $T = 0$ flux phase mean field approximation for hard core bosons; dashed line, $T = 0$ spinless fermions; and dotted line, $T = 0$ tight-binding model. The vertical dashed lines indicate the important wave vectors along this line in the Brillouin zone for tight-binding electrons and spinless fermions: nesting wave vectors $2k_{F\Gamma M}$ and $2k_{F\Gamma M}^{\mathrm{SF}}$, or Fermi wave vectors $k_{F\Gamma M}$ and $k_{F\Gamma M}^{\mathrm{SF}}$. (d)–(f) Same as (a)–(c) with $n = 0.75$. $K_{\Gamma M} = (2\pi, 2\pi)$ is a reciprocal lattice vector.

Our calculated 2D ETCF show behaviors very similar to their counterparts in 1D. The characteristic wave vectors for $S(\mathbf{q})$ and $N(\mathbf{q})$ are $2\mathbf{k}_F$ and $2\mathbf{k}_F^{\mathrm{SF}}$, respectively, which we believe implies low energy spin degrees of freedom near $\mathbf{k}_F$ and low energy charge degrees of freedom near $\mathbf{k}_F^{\mathrm{SF}}$. Note that in 2D $\mathbf{k}_F$ and $\mathbf{k}_F^{\mathrm{SF}}$ are *incommensurate* wave vectors; the charge degrees of freedom do not occur at a harmonic of $\mathbf{k}_F$, but at an independent wave vector. In Fig. 3 we show $\mathbf{k}_F$ and $\mathbf{k}_F^{\mathrm{SF}}$ for the whole Brillouin zone at $n = 0.75$ with representative nesting wave vectors. For weak coupling calculations of the 2D Hubbard model [12] and Gutzwiller projected free electrons [13] the picture is quite different. In these cases while $S(\mathbf{q})$ is enhanced and $N(\mathbf{q})$ is suppressed, they both have $2\mathbf{k}_F$ as a characteristic wave vector which is not what we

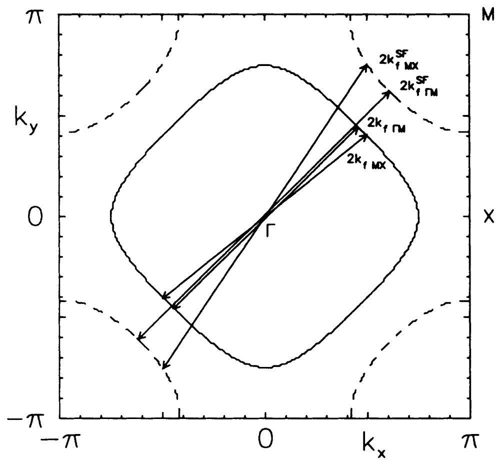

FIG. 3. Fermi wave vectors for $n = 0.75$. Solid curve, tight-binding electrons; dashed curve, spinless fermions. The arrows are representative nesting wave vectors along ΓM and MX.

find for the 2D t-J model. The behavior of $n_{\mathbf{k}}$ is also similar to 1D. The step in $n_{\mathbf{k}}$ at $n = 0.20$ is comparable in size and shape to the TB model at the same T, but at $n = 0.75$ the step is much weaker and too smeared out to be explained by thermal broadening alone [4]. We have not seen any evidence for a singularity at $3\mathbf{k}_F$ in 2D. This could be due to the relatively high temperature $T/J = 1.0$ in our calculation or possibly the angular averaging in 2D which is not present in 1D.

A limitation of our calculation is that it is restricted to high temperatures so that the features at different wave vectors are rounded. Thus we cannot observe nonanalytic behavior, which would be a definitive signal of two characteristic wave vectors for the t-J model. In this sense our results may not reflect asymptotic long wavelength properties, but perhaps effective behavior at an intermediate length scale. This question cannot be resolved within our current numerical calculation.

In 1D the statistics of the excitations play no role, but in 2D they are important. Our data give no direct evidence on the statistics of the excitations in 2D, but we can formulate a hypothesis as to what they might be [2,14]. If we think of a single electron as being composed of an elementary spin degree of freedom and an elementary charge degree of freedom, we would expect one of them to be fermionic and the other bosonic to give a fermionic electron [15]. Since $n_{\mathbf{k}}$ shows a step at $\mathbf{k}_F$ and $S(\mathbf{q})$ has $2\mathbf{k}_F$ as a characteristic wave vector, we assign the spin degrees of freedom as fermionic and the charge degrees of freedom as bosonic, but note that the charge degrees of freedom are not free bosons, but hard core bosons (HCB) to enforce the constraint of no double occupancy. This can be seen in Fig. 1 for $n = 0.5$ where the data points near (π, π) are already more rounded than SF at $T/J = 0.5$. Further evidence for this point of view can be gained from the work of Long and Zotos [16] and Sorella, Parola, and Tosatti [17].

We have also estimated the behavior of the HCB $N(\mathbf{q})$ by a flux phase mean field calculation. In 2D, HCB on a square lattice with nearest-neighbor hopping can be exactly mapped into SF by attaching a quantum of magnetic flux ϕ_0 to each particle [18]. If density fluctuations are not large, we can replace the attached flux tubes by a uniform magnetic field, $B_0 = n\phi_0$, which will couple to the orbital motion of the particles. This corresponds to a SF model with a site dependent phase (the uniform flux phase). Using this flux phase mean field approximation we have calculated $N(\mathbf{q})$, with the results at $T = 0$ shown in Fig. 2. The global features show a rounded flattening out of $N(\mathbf{q})$ at $2\mathbf{k}_F^{\mathrm{SF}}$ and general agreement with SF and the t-J model. For small $\mathbf{q}$ the approximation we are using gives $N(\mathbf{q}) \propto q^2$, but by general hydrodynamic arguments we know that for $T = 0$ if the system has a finite, nonzero compressibility the $q \to 0$ limit should be linear. The quadratic dependence is due to the "Fermi energy" of the flux phase sitting in an energy gap [19]. Therefore the q^2 dependence is an artifact due to our mean field approximation and should become linear after including fluctuations, which we will discuss in a future paper.

More information on the interactions between the spin and charge degrees of freedom could be obtained by considering the 2D t-J model with a nonzero spin polarization. If the spin and charge are coupled we would expect both $S(\mathbf{q})$ and $N(\mathbf{q})$ to change. However, if the spin and charge degrees of freedom are truly separate, the characteristic $\mathbf{q}$ vector of $N(\mathbf{q})$ should not be affected by a nonzero spin polarization [20] but $S(\mathbf{q})$ would now have transverse and longitudinal components with features at wave vectors that depend on the number of up and down spins. This has been observed by Ogata, Sugiyama, and Shiba [21] for the 1D $U \to \infty$ Hubbard model.

Having elementary degrees of freedom at $\mathbf{k}_F$ and $\mathbf{k}_F^{\mathrm{SF}}$ should have experimental consequences for the copper oxide planes in HTSC. Neutron scattering experiments [22] on $La_{2-x}Sr_xCuO_4$ show four incommensurate peaks centered around (π, π) that move with doping. This can be understood in terms of the nesting properties of the weak coupling Fermi surface [23] where our results also put the spin degrees of freedom. The energy integrated weight of angle resolved photoemission is a direct measure of $n_{\mathbf{k}}$ and photoemission has also been interpreted as supporting a large Fermi surface [24]. But the transport measurements [25] are not so easy to understand in this picture.

Reconciling experiments which show a large electronlike contour in $\mathbf{k}$ space with a density of n carriers, with transport measurements, which show a much smaller hole density of $1 - n$ carriers, is one of the most puzzling problems of the copper oxides [25]. Our results for the 2D t-J model show one way this might occur [2,26]. One expects the transport experiments to couple most strongly to charge. For $1 - n \ll 1$, the charge degrees of freedom at $\mathbf{k}_F^{\mathrm{SF}}$ have a small *holelike* locus in momentum space centered around (π, π) as shown in Fig. 3. With this the transport measurements are satisfied. At the same time the spin degrees of freedom give a large, weak coupling Fermi surface also shown in Fig. 3, which is seen in neutron scattering and photoemission experiments. We wish to emphasize that experiments which could probe $N(\mathbf{q})$ directly may prove to be very interesting for HTSC materials.

In conclusion, we have studied the equal time correlation functions of the 2D t-J model by high temperature series expansion methods. We find that the spin and charge ETCF exhibit signatures of two different wave vectors: the characteristic wave vector for the spins being $\mathbf{k}_F$ and that for charge $\mathbf{k}_F^{\mathrm{SF}}$, the Fermi wave vectors for TB and SF, respectively. In comparison with the results for 1D this suggests spin-charge separation in this strongly correlated 2D model.

W.O.P. was supported by NSF Grant No. DMR-9222682 and by the National High Magnetic Field Laboratory at Florida State University. R.L.G. and R.R.P.S. were supported by NSF Grant No. DMR-9318537. H.T. was supported by the Swiss National Science Foundation Grant No. NFP-304030-032833. The authors thank T. M. Rice for many useful conversations and a critical reading of the manuscript. The authors also thank N. E. Bonesteel, H. Fukuyama, M. Ogata, N. P. Ong, D. J. Scalapino, and G. Zimanyi for many useful discussions. W.O.P. and R.R.P.S. thank the C.M.S. group at Los Alamos for hospitality while this manuscript was being completed. Part of the computations were done on a Cray YMP at Cray Research, Inc.

Note added.—After completion of this work we received a preprint by Chen and Lee [27] which arrives at results similar to ours.

[1] For a recent review see T. M. Rice, in *High Temperature Superconductivity*, Proceedings of the Thirty-Ninth Scottish Universities Summer School in Physics, edited by D. P. Tunstall and W. Barford (Adam Hilger, Bristol, 1992).

[2] P. W. Anderson, Science **235**, 1196 (1987); **256**, 1526 (1992); **258**, 672 (1992); in *Frontiers and Borderlines in Many-Particle Physics*, International School of Physics "Enrico Fermi," Course CIV, edited by R. A. Broglia and J. R. Schrieffer (North-Holland, Amsterdam, 1987); Phys. Scr. **T27**, 60 (1989); Phys. Rev. Lett. **64**, 1839 (1990); **65**, 2306 (1990); **66**, 3226 (1988); **67**, 2092 (1991); **67**, 3844 (1991); **71**, 1220 (1993); Phys. Rep. **184**, 195 (1989); Phys. Rev. B **42**, 2624 (1990); J. Phys. Chem. Solids **52**, 1313 (1991); Prog. Theor. Phys. Suppl. **107**, 41 (1992); (to be published); G. Baskaran, Z. Zou and P. W. Anderson, Solid State Commun. **63**, 973 (1987); P. W. Anderson and Z. Zou, Phys. Rev. Lett. **60**, 132 (1988); P. W. Anderson and Y. Ren, in *High Temperature Superconductivity*, edited by K. S. Bedell *et al.* (Addison-Wesley, Redwood City, CA, 1990); (to be published); M. Ogata and P. W. Anderson, Phys. Rev. Lett. **70**, 3087 (1993).

[3] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[4] R. R. P. Singh and R. L. Glenister, Phys. Rev. B **46**, 14 313 (1992).

[5] R. R. P. Singh and R. L. Glenister, Phys. Rev. B **46**, 11 871 (1992).

[6] W. Kohn, Phys. Rev. Lett. **2**, 393 (1959).

[7] W. O. Putikka, M. U. Luchini, and T. M. Rice, Phys. Rev. Lett. **68**, 538 (1992); V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1991).

[8] W. O. Putikka, M. U. Luchini, and M. Ogata, Phys. Rev. Lett. **69**, 2288 (1992).

[9] W. Stephan and P. Horsch, Phys. Rev. Lett. **66**, 2258 (1991).

[10] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990).

[11] H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10 553 (1990); N. Kawakami and S.-K. Yang, Phys. Rev. Lett. **65**, 2039 (1990).

[12] D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch, Phys. Rev. B **34**, 8190 (1986); **35**, 6694 (1987); N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. B **47**, 2742 (1993); D. J. Scalapino (private communication).

[13] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **59**, 3669 (1990).

[14] S. A. Kivelson, D. S. Rokhsar, and J. P. Sethna, Phys. Rev. B **35**, 8865 (1987).

[15] We do not consider the possibility of anyons, which cannot be ruled out.

[16] M. W. Long and X. Zotos, Phys. Rev. B **48**, 317 (1993).

[17] S. Sorella, A. Parola, and E. Tosatti, in *Strongly Correlated Electron Systems II*, edited by G. Baskaran *et al.* (World Scientific, Singapore, 1991).

[18] E. Fradkin, Phys. Rev. Lett. **63**, 322 (1989); Y. R. Wang, Phys. Rev. B **43**, 3786 (1991).

[19] D. Hofstadter, Phys. Rev. B **14**, 2239 (1976); Y. Hasegawa, P. Lederer, T. M. Rice, and P. B. Wiegmann, Phys. Rev. Lett. **63**, 907 (1989).

[20] The feature for $N(\mathbf{q})$ at $2\mathbf{k}_F^{\mathrm{SF}}$ will sharpen up at low T as the spin polarization saturates due to the system going over to interacting spinless fermions with a sharp Fermi surface at $T = 0$. But the characteristic wave vector $2\mathbf{k}_F^{\mathrm{SF}}$ should not change.

[21] M. Ogata, T. Sugiyama, and H. Shiba, Phys. Rev. B **43**, 8401 (1991); see also J. M. P. Carmelo, P. Horsch, D. K. Campbell, and A. H. Castro Neto, Phys. Rev. B **48**, 4200 (1993).

[22] T. E. Mason, G. Aeppli, and H. A. Mook, Phys. Rev. Lett. **68**, 1414 (1992).

[23] P. B. Littlewood, J. Zaanen, G. Aeppli, and H. Monien, Phys. Rev. B **48**, 487 (1993); Q. Si, Y. Zha, K. Levin, and J. P. Lu, Phys. Rev. B **47**, 9055 (1993).

[24] C. G. Olson *et al.*, Phys. Rev. B **42**, 381 (1990).

[25] For experimental reviews see *High Temperature Superconductivity*, edited by K. S. Bedell *et al.* (Addison-Wesley, Redwood City, CA, 1990); *Physical Properties of High Temperature Superconductors*, edited by D. M. Ginsberg (World Scientific, Singapore, 1989–1992), Vols. 1–3.

[26] H. Fukuyama and Y. Hasegawa, Physica (Amsterdam) **148B**, 204 (1987); H. Fukuyama, in *Superconducting Materials,* edited by S. Nakajima and H. Fukuyama (Japanese Journal of Applied Physics, Tokyo, 1988), p. 205.

[27] Y. C. Chen and T. K. Lee, Z. Phys. B (to be published).