Quantum Corrals, Eigenmodes, and Quantum Mirages in *s*-Wave Superconductors

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We study the electronic structure of magnetic and nonmagnetic quantum corrals embedded in two-dimensional *s*-wave superconductors. We demonstrate that a quantum mirage of an impurity bound state is projected from the occupied into the empty focus of a nonmagnetic quantum corral via the excitation of the corral's eigenmodes. We show that quantum corrals provide a new tool for manipulating the interaction between magnetic impurities by exciting oscillations in the corral's impurity potential. Finally, we discuss the form of eigenmodes in magnetic quantum corrals.

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The interaction of nanoscale impurity structures with fermionic quantum many-body systems has led to the observation of a large number of novel physical phenomena [1–5] over the past few years. In superconducting (SC) systems, quantum interference of electronic waves that are scattered by a small number of impurities can lead to the splitting of impurity states, as observed in the one-dimensional chains of the high-temperature superconductor $YBa_2Cu_3O_{6+x}$ [3], and discussed theoretically for these chains [6] as well as two-dimensional $d_{x^2-y^2}$-wave [7] and *s*-wave superconductors (SSC) [8,9]. In more complex impurity structures, such as quantum corrals, the existence of discrete eigenmodes can be employed for the creation of *quantum mirages*. This effect was beautifully demonstrated by Manoharan *et al.* [1] who used the Kondo resonance of a magnetic impurity located in the focus of an elliptical quantum corral as the "electronic candle" whose quantum image was projected into the empty focus. A theoretical explanation of this phenomenon was provided in a series of articles [10].

Of particular interest is the possibility that nanoscale impurity structures can provide insight into the nature of complex electronic systems. In general, one expects that the presence of strong electronic correlations or that of a broken symmetry state in the host system affects the eigenmode's spatial pattern and provides novel electronic candles whose spectroscopic signatures in the density of states (DOS) can be projected. As a first step in the exploration of this idea, we study in this Letter quantum corrals that are embedded in a 2D *s*-wave superconductor whose nontrivial electronic correlations arise from particle-hole mixing. We consider a variety of quantum corrals consisting of nonmagnetic or magnetic impurities with constant or oscillating scattering potentials. Magnetic impurities that are placed inside the corral induce bound states whose spectroscopic signatures are peaks in the DOS. We utilize these peaks as the electronic candle to investigate the corral's and the host system's electronic properties. We demonstrate that, by placing a magnetic impurity in one of the corral's foci, a quantum image of its bound state peaks is projected into the empty focus via the excitation of the corral's eigenmodes. We illustrate that the spatial pattern of eigenmodes can be changed by exciting oscillations in the corral's impurity potential. This provides a new tool for manipulating the interaction between magnetic impurities located in the foci of the corral, a topic of great current interest in the field of spin electronics and quantum information technology [11].

To study the electronic structure of quantum corrals and the creation of quantum mirages, we employ a generalized $\hat{T}$-matrix formalism [6,9,12,13]. For a fully gapped SSC, it was shown [14] that the coupling J between an impurity spin and delocalized electrons needs to exceed a critical value J_c before a Kondo effect can occur. We thus consider only $J < J_c$, and hence treat magnetic impurities with spin S as classical variables [12], in full agreement with experiment [15] (see also below). In the Nambu formalism, the electronic Green's function in the presence of N impurities located at $\mathbf{r}_i$ is

$$\hat{G}(\mathbf{r}, \mathbf{r}', \omega_n) = \hat{G}_0(\mathbf{r}, \mathbf{r}', \omega_n) + \sum_{i,j=1}^{N} \hat{G}_0(\mathbf{r}, \mathbf{r}_i, \omega_n)\hat{T}(\mathbf{r}_i, \mathbf{r}_j, \omega_n) \times \hat{G}_0(\mathbf{r}_j, \mathbf{r}', \omega_n), \tag{1}$$

where one has for the $\hat{T}$ matrix

$$\hat{T}(\mathbf{r}_i, \mathbf{r}_j, \omega_n) = \hat{V}_i\, \delta_{i,j} + \hat{V}_i \sum_{l=1}^{N} \hat{G}_0(\mathbf{r}_i, \mathbf{r}_l, \omega_n)\hat{T}(\mathbf{r}_l, \mathbf{r}_j, \omega_n), \tag{2}$$

and

$$\hat{G}_0^{-1}(\mathbf{k}, i\omega_n) = [i\omega_n\tau_0 - \epsilon_{\mathbf{k}}\tau_3]\sigma_0 + \Delta_0\tau_2\sigma_2; \quad \hat{V}_i = \frac{1}{2}(U_i\sigma_0 + J_iS\sigma_3)\tau_3. \tag{3}$$

$\hat{G}_0(\mathbf{k}, i\omega_n)$ is the electronic Green's function of the unperturbed (clean) system in momentum space, $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$ are the Pauli matrices in spin and Nambu space, respectively, and Δ_0 is the SC gap. For simplicity, we consider a corral that is embedded in a 2D SSC whose normal state dispersion is given by $\epsilon_{\mathbf{k}} = k^2/2m - \mu$ ($\hbar = 1$), where

$\mu = k_F^2/2m$ is the chemical potential and $k_F = \pi/2$ is the Fermi wave vector (lattice constant $a_0 = 1$). Qualitatively similar results to the ones shown below are expected when the quantum corral is located in a 3D SSC [16]. We set $1/(m\Delta_0) = 30$, yielding a SC coherence length of $\xi_c = k_F/(m\Delta_0) = 15\pi$. Moreover, $\hat{V}_i$ is the scattering matrix at $\mathbf{r}_i$, with U_i and J_i being the potential and magnetic scattering strengths of the impurity, respectively. Unless otherwise noted, we take for definiteness $U_i/\Delta_0 = 30$ ($J_i = 0$) for nonmagnetic impurities and $J_iS/\Delta_0 = 30$ ($U_i = 0$) for magnetic impurities. These values are taken to demonstrate the qualitative features of our results which are *robust* against changes in the scattering strengths or in the form of the fermionic dispersion. The DOS, $N(\mathbf{r}, \omega)$, is obtained from a numerical computation of Eqs. (1) and (2) with $N(\mathbf{r}, \omega) = A_{11} + A_{22}$, $A_{ii}(\mathbf{r}, \omega) = -\mathrm{Im}\hat{G}_{ii}(\mathbf{r}, \omega + i\delta)/\pi$, and $\delta = 0.02\Delta_0$.

We first study an elliptical corral with semiaxes $a = 20$, $b = 15$, and eccentricity $e = \sqrt{7}/4$, that consists of 100 *nonmagnetic* impurities. In the absence of magnetic impurities, no eigenmodes exist for frequencies $|\omega| < \Delta_0$, i.e., inside the SC gap. Defining the center of the corral as $(0, 0)$, we place a magnetic impurity in the corral's focus at $f_+ = (13, 0)$, while leaving the other focus at $f_- = (-13, 0)$ empty. As expected, the magnetic impurity induces a bound state whose spectroscopic signature are a particlelike and holelike peak in the DOS at frequencies $\Omega_b^{(1,2)}/\Delta_0 = \mp 0.4$ [see Fig. 1(a)]. The presence of a bound state allows an eigenmode of the corral to exist inside the SC gap, leading to spatial oscillations in the DOS, as shown in Fig. 1(b) for $\Omega_b^{(2)} < \Delta_0$ [all spatial DOS plots shown in the following possess the same intensity scale to facilitate a direct comparison, with light (dark) color indicating a large (small) DOS]. This eigenmode, in turn, creates a quantum mirage of the DOS bound state peaks in the empty focus at f_- [Fig. 1(a)]. The presence of two bound state peaks at $\Omega_b^{(1,2)}$ permits us to study eigenmodes at different excitation energies. Note, e.g., that the spectral weight in the DOS at $\Omega_b^{(1)}$ [Fig. 1(c)] is much more concentrated around f_+ than at $\Omega_b^{(2)}$ [Fig. 1(b)] concomitant with a weaker excited eigenmode and quantum mirage. It was noted earlier [10] that eigenmodes can be excited only if the excitation (via the impurity bound state) takes place at a position where the spectral weight of the eigenmode is large, and if the excitation energy, i.e., $\Omega_b^{(1,2)}$, is close to the eigenmode's energy (note that due to the corral wall's porosity and its finite scattering potential, the eigenmodes possess a substantial frequency width [10]). While two eigenmodes exist outside the SC gap at $\Omega_m^{(\pm)}/\Delta_0 = \pm 1.1$, the mode's amplitude at $\Omega_m^{(+)}$ in the vicinity of the foci is considerably larger than that at $\Omega_m^{(-)}$, yielding a weaker eigenmode, a weaker quantum mirage and a concentration of spectral weight around f_+ at $\Omega_b^{(1)}$. This demonstrates that the eigenmodes act as "waveguides" for the projection of the bound state peaks into a quantum image [1,10].

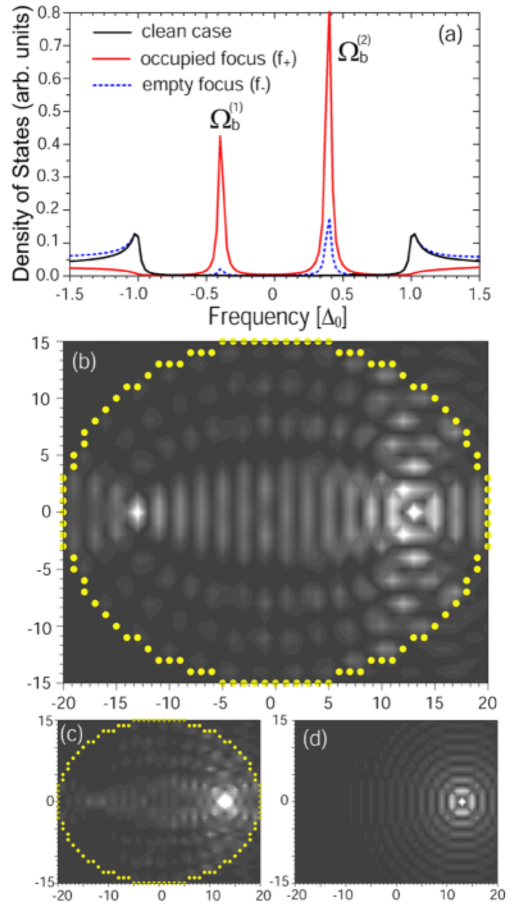

FIG. 1 (color online). (a) DOS in the occupied [solid gray (red) line] and empty focus [dotted (blue) line] for a nonmagnetic corral with a magnetic impurity located at f_+. Solid black line: DOS of the clean system. (b),(c) DOS inside the quantum corral [the filled gray (yellow) circles represent the corral impurities] for (b) $\Omega_b^{(2)}/\Delta_0 = 0.4$ and (c) $\Omega_b^{(1)}/\Delta_0 = -0.4$. (d) DOS at $\Omega_b^{(2)}/\Delta_0 = 0.575$ for a magnetic impurity at f_+ without corral.

The effect of a corral on the DOS strongly depends on the ratio of the decay length, $\xi_d = \xi_c/\sqrt{1 - (\Omega_b/\Delta_0)^2}$, and the corral's semiaxes. In the above case, $\Omega_b^{(1,2)}/\Delta_0 = \pm 0.4$, $\xi_d = 16.4\pi \gg a, b$, and the spatial DOS pattern at $\Omega_b^{(2)}$ is significantly different for a magnetic impurity at f_+ with [Fig. 1(b)] and without a corral [Fig. 1(d)]. Of particular importance is the observation that the presence of a corral shifts $\Omega_b^{(1,2)}$ from $\Omega_b^{(1,2)}/\Delta_0 = \pm 0.575$ (no corral) to $\Omega_b^{(1,2)}/\Delta_0 = \pm 0.4$, which is a *qualitatively* new feedback effect of the corral on the impurity bound state. In contrast, if $\xi_d \ll a, b$, the bound state wave function at the position of the corral wall is exponentially suppressed, no eigenmodes can be excited, and the spatial DOS pattern of a single magnetic impurity remains unchanged in the presence of a quantum corral [16]. Hence by varying JS and thus ξ_d, the spatial DOS pattern inside the corral can be changed.

The DOS changes considerably when the magnetic impurity is moved off the focus, as shown in Fig. 2 for

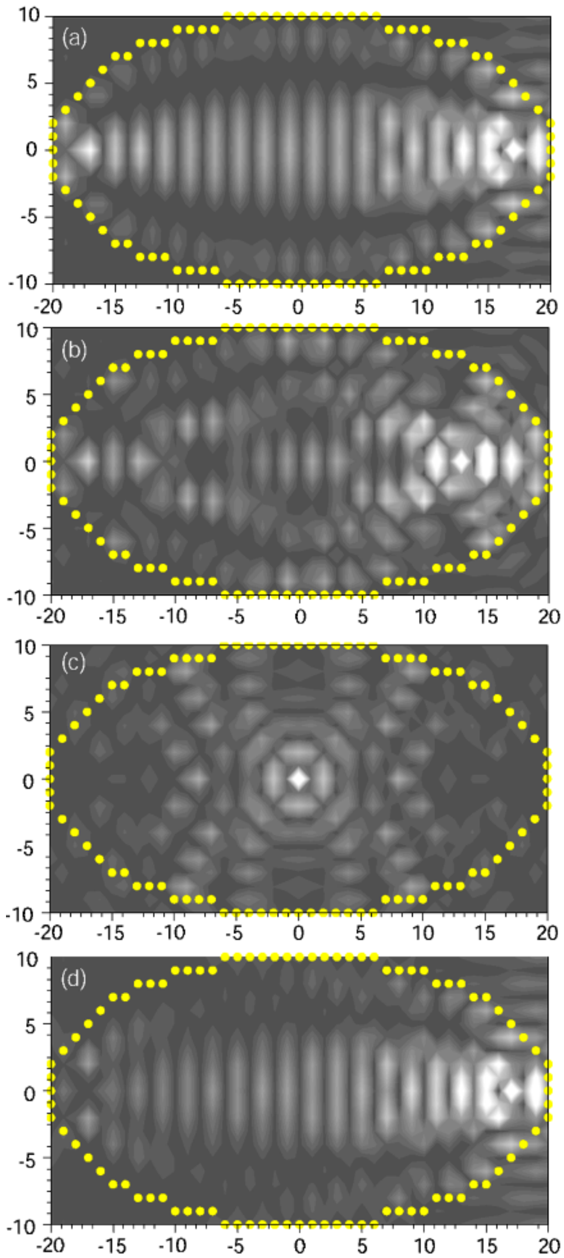

FIG. 2 (color online). DOS at $\Omega_b^{(2)}$ for a magnetic impurity located at (a) $f_+ = (17, 0)$, (b) $\mathbf{r} = (13, 0)$, and (c) $\mathbf{r} = (0, 0)$. (d) DOS for an oscillating impurity potential along the corral wall with $U(\phi) = U_0 \cos\phi$ and $U_0/\Delta_0 = 30$.

a corral with 88 impurities, $a = 20$, $b = 10$, eccentricity $e = \sqrt{3}/2$ and $f_\pm = (\pm 17, 0)$. For a magnetic impurity located at f_+ and $\Omega_b^{(2)}/\Delta_0 = 0.475$ [Fig. 2(a)], the DOS exhibits a similar pattern, including a quantum mirage at f_-, as in Fig. 1(b), albeit with only one instead of three "side wings" in the excited eigenmode. When the impurity is off the focus at $(13, 0)$ [Fig. 2(b)], the bound state energy increases to $\Omega_b^{(1,2)}/\Delta_0 = \mp 0.5$, and only a much weaker quantum mirage emerges at f_-. A completely different eigenmode is excited when the impurity is located in the corral's center at $(0, 0)$ [Fig. 2(c)] with $\Omega_b^{(1,2)}/\Delta_0 = \mp 0.725$. Thus, changing the location of the impurity leads to different excited eigenmodes and a simultaneous shift in $\Omega_b^{(1,2)}$. In Fig. 2(d) we plot the DOS for an oscillating impurity potential in the corral's wall with $U(\phi) = U_0 \cos\phi$, $U_0/\Delta_0 = 30$, and ϕ being the angle between the x axis and the line connecting the center of the ellipse with the impurity. Such a corral potential, arising, e.g., from charge oscillations in its wall, weakens the eigenmodes, particularly along the vertical axis of the corral where $U(\phi)$ is small, and almost completely destroys the quantum mirage of the bound state peak [compare Figs. 2(a) and 2(d)].

Quantum interference effects between two magnetic impurities in an s-wave superconductor lead to a frequency splitting of the bound state peaks through the formation of bonding and antibonding bound states [8,9]. This splitting, which is a direct measure of the interaction between the impurities, can be enhanced if the magnetic impurities are placed in the foci of a corral. We consider the corral of Fig. 1 and assume for definiteness that the impurity spins are parallel; however, qualitatively similar results are obtained for an arbitrary angle between the spins. In the absence of a quantum corral (Fig. 3), the splitting of the bound state peaks is small, $\delta\Omega_b/\Delta_0 = 0.1$, due to the large distance between the impurities. In the presence of the corral the splitting increases to $\delta\Omega_b'/\Delta_0 = 0.65$, implying that the interaction between the two magnetic impurities is enhanced. This splitting therefore provides a *direct* and *unambiguous* probe for the strength of the interaction between magnetic impurities, in contrast to the effects expected in the normal state [17]. For the oscillating impurity potential of Fig. 2(d), the splitting decreases to $\delta\Omega_b''/\Delta_0 = 0.175$; i.e., the interaction between the impurities is weakened. Thus quantum corrals provide a novel approach for manipulating the interaction between magnetic impurities.

In Fig. 4 we present the DOS inside a quantum corral ($a = 20, b = 10$) consisting of 88 magnetic impurities. The corral's impurity spins are antiferromagnetically aligned (the total spin of the corral is zero) and an additional magnetic impurity is located at $f_+ = (17, 0)$. Since

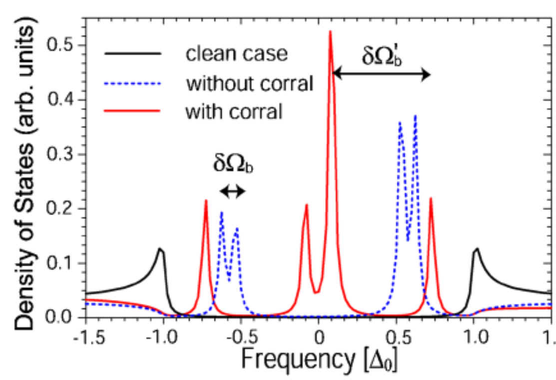

FIG. 3 (color online). Splitting of the bound state peaks in the DOS at $f_- = (-13, 0)$ with and without a quantum corral for two magnetic impurities with parallel spins.

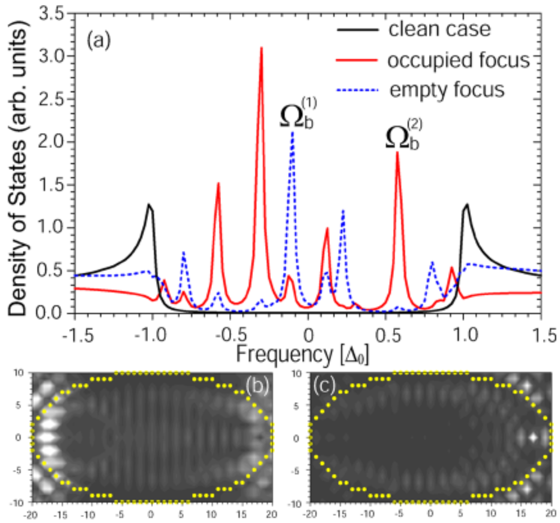

FIG. 4 (color online). (a) DOS at $f_\pm$ for a magnetic corral. Spatial DOS pattern for (b) $\Omega_b^{(1)}/\Delta_0 = -0.1$ and (c) $\Omega_b^{(2)}/\Delta_0 = 0.575$ [see (a)].

the bound states associated with the magnetic impurities are coupled, the DOS exhibits a large number of peaks [Fig. 4(a)], but no well defined quantum image in the empty focus. The DOS pattern changes qualitatively between different bound state energies, as seen in Figs. 4(b) and 4(c) for the DOS at $\Omega_b^{(1)}/\Delta_0 = -0.1$ and $\Omega_b^{(2)}/\Delta_0 = 0.575$. For $\Omega_b^{(1)}$ the spectral weight of the excited eigenmode is predominantly centered around the empty focus, while for $\Omega_b^{(2)}$ most of the spectral weight is located in the vicinity of the occupied focus. Thus, in contrast to nonmagnetic corrals, the spectral weight of eigenmodes in a magnetic corral can be concentrated near the occupied *or* empty focus.

Finally, we comment on the relevance of pair-breaking effects near magnetic impurities. Since the suppression of the SC gap close to a single magnetic impurity does not alter the DOS's qualitative features [13], our results for a single or two widely spaced magnetic impurities presented in Figs. 1–3 are likely robust against pair-breaking effects. In magnetic corrals, on the other hand, the suppression of the SC gap is potentially relevant and could lead to the emergence of a Kondo effect for the entire corral. However, for an antiferromagnetic quantum corral with *zero* total spin, as the one discussed above, no Kondo effect is expected if the antiferromagnetic coupling I between the impurity spins is large enough (i.e., $I \gg J$), in analogy to the two impurity Kondo effect [18]. In the T-matrix approach, the coupling I is not directly considered, but assumed to lead to a relative orientation of the spin impurities, such as the above antiferromagnetic alignment. Whether or not a Kondo effect occurs in the weak-coupling limit $J < J_C$ for a quantum corral with *nonzero* total spin embedded in an s-wave superconductor is at present unclear; work is currently under way to study the significance of pair-breaking effects, and the possibility for a Kondo effect in this case [16].

In summary, we demonstrate that a quantum mirage of an impurity bound state peak can be projected from the occupied into the empty focus of a nonmagnetic quantum corral via the excitation of the corral's eigenmodes. We observe an enhanced interaction between magnetic impurities inside the corral, which can be tuned through oscillations in the corral's impurity potential. This provides a novel tool to manipulate the interaction between magnetic impurities, a topic of great relevance in spin electronics and quantum information technology [11].

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[1] H. C. Manoharan, C. P. Lutz, and D. M. Eigler, Nature (London) **403**, 512 (2000).
[2] A. W. Holleitner *et al.*, Phys. Rev. Lett. **87**, 256802 (2001).
[3] D. J. Derro *et al.*, Phys. Rev. Lett. **88**, 097002 (2002).
[4] C. Chicanne *et al.*, Phys. Rev. Lett. **88**, 097402 (2002).
[5] K.-F. Braun and K.-H. Rieder, Phys. Rev. Lett. **88**, 096801 (2002).
[6] D. K. Morr and A. V. Balatsky, Phys. Rev. Lett. **90**, 067005 (2003).
[7] D. K. Morr and N. Stavropoulos, Phys. Rev. B **66**, 140508(R) (2002); U. Michelucci *et al.*, J. Phys. Chem. Solids **63**, 2283 (2002); L. Zhu *et al.*, Phys. Rev. B **67**, 094508 (2003); B. M. Andersen and P. Hedegard, Phys. Rev. B **67**, 172505 (2003).
[8] M. E. Flatte and D. E. Reynolds, Phys. Rev. B **61**, 14 810 (2000).
[9] D. K. Morr and N. A. Stavropoulos, Phys. Rev. B **67**, 020502(R) (2003).
[10] G. A. Fiete *et al.*, Phys. Rev. Lett. **86**, 2392 (2001); A. A. Aligia, Phys. Rev. B **64**, 121102 (2001); K. Hallberg, A. A. Correa, and C. A. Balseiro, Phys. Rev. Lett. **88**, 066802 (2002); D. Porras *et al.*, Phys. Rev. B **63**, 155406 (2001); O. Agam and A. Schiller, Phys. Rev. Lett. **86**, 484 (2001); Y. Shimada *et al.*, Surf. Sci. **514**, 89 (2002); M. Weissmann and H. Bonadeao, Physica (Amsterdam) **10E**, 544 (2001).
[11] S. A. Wolf *et al.*, Science **294**, 1488 (2001); B. E. Kane, Nature (London) **393**, 133 (1998).
[12] Y. Lu, Acta Phys. Sin. **21**, 75 (1965); H. Shiba, Prog. Theor. Phys. **40**, 435 (1968).
[13] M. I. Salkola, A. V. Balatsky, and J. R. Schrieffer, Phys. Rev. B **55**, 12 648 (1997).
[14] K. Satori *et al.*, J. Phys. Soc. Jpn. **61**, 3239 (1992).
[15] A. Yazdani *et al.*, Science **275**, 1767 (1997).
[16] D. K. Morr and N. A. Stavropoulos (to be published).
[17] A. Correa *et al.*, Europhys. Lett. **58**, 899 (2002); G. Chiappe and A. A. Aligia, Phys. Rev. B **66**, 075421 (2002).
[18] C. Jayaprakash *et al.*, Phys. Rev. Lett. **47**, 737 (1981); B. A. Jones and C. M. Varma, Phys. Rev. Lett. **58**, 843 (1987); B. A. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988); I. Affleck *et al.*, Phys. Rev. B **52**, 9528 (1995); J. B. Silva *et al.*, Phys. Rev. Lett. **76**, 275 (1996).