PHYSICAL REVIEW B **82**, 060507(R) (2010)

Nodal-antinodal dichotomy from pairing disorder in *d*-wave superconductors

Dimitrios Galanakis[1] and Stefanos Papanikolaou[2]
[1]*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*
[2]*Department of Physics, Cornell University, Ithaca, New York 14853-8150, USA*
(Received 22 April 2010; published 10 August 2010)

We study the basic features of the local density of states (LDOS) observed in scanning tunnel microscope experiments on high-T_c *d*-wave superconductors in the context of a minimal model of a *d*-wave superconductor which has *weakly* modulated off-diagonal disorder. We show that the low- and high-energy features of the LDOS are consistent with the observed experimental patterns and, in particular, the anisotropic local domain features at high energies. At low energies, we obtain not only the scattering peaks predicted by the octet model [Y. Kohsaka *et al.*, Science **315**, 1380 (2007)], but also weak features that should be experimentally accessible. Finally, we show that the emerging features of the LDOS lose their correspondence with the features of the imposed disorder, as its complexity increases spatially.

DOI: 10.1103/PhysRevB.82.060507   PACS number(s): 74.20.Mn, 74.72.−h, 79.60.−i

In recent years, the effect of underlying inhomogeneities in superconductors has been studied intensively. In the context of high-temperature superconductors (SCs), checkerboard local density of states (LDOS) oscillations and strong nanoscale gap inhomogeneity have been observed in scanning tunneling spectroscopy (STS) experiments,[1] and signals in dynamical susceptibility measured by neutron scattering have been interpreted as stripelike nanoscale modulations of charge and spin degrees of freedom.[2] Even though it is still not clear whether these modulations are intrinsic or driven entirely by disorder, it seems plausible that the magnitude of T_c might be strongly related to the very existence of inhomogeneity on the coherence length scale,[3,4] and therefore a deeper understanding of the source of inhomogeneities is important. In the cases of the compounds $La_{2-x}Ba_xCuO_4$ and $La_{2-x}Sr_xCuO_4$ (with Nd or Eu codoping), inhomogeneities take the form of static long-range stripelike spin and charge modulations.[5–8]

Tunneling spectroscopy has been used to probe states in different regions of momentum and energy by the help of the Fourier-transform STS (FT-STS) and the high-energy features of the LDOS. At low energies, in the *d*-wave superconducting state near optimal doping, quasiparticle interference observed by FT-STS is dominated by peaks at well-defined wave vectors $\mathbf{q}_i$ which are consistent with a simple model of Bogoliubov quasiparticles, called the octet model.[9,10] Even though the qualitative features of the octet model are experimentally robust, a quantitative understanding of the amplitude, location, and width of the peaks is not straightforward to obtain and depends rather sensitively on the nature of the scattering medium.[11] A pointlike scatterer, for example, in an otherwise homogeneous *d*-wave SC leads to a landscape of some spotlike and some arclike dispersive features close to $\mathbf{q}_i$ in the FT-STS images,[12] whereas experimental data appear mostly spotlike. At high energies, local unidirectionality has been observed in domains with size approximately $5a_0$, close to the superconductor's coherence length and the domains typically alternate in orientation. This behavior is usually attributed to a disordered charge-density wave (CDW) with some success on demonstrating the emergence of the LDOS patterns from the underlying CDW order.[13]

In Refs. 14 and 15 it was shown that generic off-diagonal disorder (coupling of the nodal *d*-wave quasiparticles to an *s*-wave order parameter Δ_s) is a relevant operator that leads to a first-order transition in a system with tetragonal-orthorhombic symmetry breaking. Therefore, off-diagonal disorder presents the dominating effect for superconductors with tendency toward orthorhombic symmetry breaking. However, when the orthorhombic symmetry is not broken (due to frustration effects), it is expected that modulated forms of the expected disorder should be present, with no effect at large length scales. In this Rapid Communication we present an explicit model with off-diagonal, modulated disorder, which unifies the basic features of the scanning tunnel microscope (STM) observations into a consistent framework.

In this model, itinerant fermions are coupled to weak, off-diagonal disorder, modulated in well-defined domains. Such a state is characterized by a density wave order. We motivate the existence of such disorder on the basis of (i) a phenomenological theory of competing *s*- and *d*-order parameters and (ii) recent mean-field studies on more detailed states, supporting a modulation of the off-diagonal disorder.[13] First, we show by using first-order perturbation theory, that the spectrum at low energies and the position of the nodes remains unchanged, an expected result since at long length scales the disorder averages to zero. Second, we find that at low energies the Fourier maps of the LDOS have peaks that are dispersing according to the octet-model scattering,[11] given that $\Delta^{(s)}/\Delta_d \ll 1$ with the addition of weak static peaks, bearing strong similarities to the STM experiments' observations.[16] In addition there are static peaks close to $(\pm 3\pi/5, \pm \pi/5)$, but these peaks are very weak (since $\Delta^{(s)}$ is very small) and if spatial disorder exists, span a large region around these wave vectors. Third, we show that at high energies the LDOS acquires a domain structure that is locally anisotropic and highly similar to the observed STM patterns. The order parameter[17] we use to identify the anisotropy, shows that by increasing the disorder amplitude, the anisotropy becomes noticeable at higher energies. Such anisotropy is not evident in a system with disorder that respects the *d*-wave symmetry. Finally, we show that disorder with irregular features, coming, for example, from an off-critical system, has *no direct correspondence* to the LDOS patterns, and at high energies there are no local anisotropic features, due to the complexity of the high-energy spectrum and induced bound states.[18]

To motivate the presence of modulated off-diagonal disorder, we consider a system that can potentially support both s- and d-wave orders $\Psi_s=|\Psi_s|e^{i\phi_s}$ and $\Psi_d=|\Psi_d|e^{i\psi_d}$, respectively, and can be described by the Ginsburg-Landau (GL) functional,

$$F[\Psi_d,\Psi_s]=-a_d|\Psi_d|^2+\frac{b_d}{2}|\Psi_d|^4+K_d|\nabla\Psi_d|^2-a_s|\Psi_s|^2 +\frac{b_s}{2}|\Psi_s|^4+K_s|\nabla\Psi_s|^2+a_{sd}(\Psi_s\Psi_d^*+\text{c.c.}) +b_{sd}|\Psi_s|^2|\Psi_d|^2, \tag{1}$$

where the first and second lines are the d- and s-wave order GL functionals, respectively, with $a_{s,d},b_{s,d},K_{s,d}>0$. The coupling $b_{sd}>0$ is the magnitude of the repulsive interaction which suppresses the s-d mixing. The term proportional to a_{sd} can be written as $a_{sd}|\Psi_s||\Psi_d|\cos(\phi_s-\phi_d)$ and is extremized when $a_{sd}e^{i(\phi_s-\phi_d)}=-|a_{sd}|$. For simplicity, in what follows we assume that $a_{sd}<0$ and $\phi_s=\phi_d$ and ignore this term.

In the case of a homogeneous system we may drop the spatial derivatives in the GL functional, Eq. (1), and minimize it with the choice,

$$|\Psi_d^B|^2=\frac{a_d}{b_d}\frac{1-b_0/\lambda}{1-b_0^2}, \tag{2}$$

$$|\Psi_s^B|^2=\frac{a_s}{b_s}\frac{1-b_0\lambda}{1-b_0^2}, \tag{3}$$

where $\lambda=\frac{a_d\sqrt{b_s}}{a_s\sqrt{b_d}}$ and $b_{sd}=b_0\sqrt{b_sb_d}$.

In an inhomogeneous system and for an appropriate choice of the parameters, the minimization of the functional in Eq. (1), results in rendering domain walls along which $\Psi_s=0$, asymptotically of zero energy. In this parameter regime, domain walls are in competition with the homogeneous state, and their emergence depends sensitively on microscopic disorder effects, present in the system. In order to demonstrate this feature, we consider a single boundary along the y axis and assume that $\Psi_s(x)=\Psi_s^Bf(x)$, where $f(x)$ is an arbitrary decreasing function, defined in $[0,\infty)$ and $f(0)=0$, $f(\infty)=1$. Also, we assume naturally that $\Psi_s(-x)=-\Psi_s(x)$. For simplicity, we assume that Ψ_d does not vary spatially across the boundary ($K_d\gg K_s$) so that we can replace $|\Psi_d|$ with its bulk value. Replacing this form in Eq. (1) we get the energy E_b of the boundary

$$E_b=F[\Psi_d^B,\Psi_s]-F[\Psi_d^B,\Psi_s^B] =C_1|\Psi_s^B|^2[K_sC_3+b_s|\Psi_s^B|^2(1-C_2)], \tag{4}$$

where $C_1=\int_0^\infty dx[1-f^2(x)]$, $C_2=\frac{1}{2}C_1^{-1}\int_0^\infty dx[1-f^4(x)]$, and $C_3=C_1^{-1}\int_0^\infty dx[\partial_xf(x)]^2$. If $f(x)<1$ then $C_2<\frac{1}{2}$ and the energy is positive. However the energy of the boundary vanishes in the limit of high s-d repulsive interactions $b_{sd}/K_s\to 0$ and therefore it should be stabilized by infinitesimal lattice disorder. These domain walls which are competing with the homogeneous state can be present at distances only larger than the coherence length scale such that the off-diagonal order parameter Δ_s is modulated accordingly. Beyond our calculation, additional motivation for the consideration of modulated mixed SC order parameter comes from microscopically motivated mean-field states,[13] where the coexistence of modulated mixed order parameters is necessary.

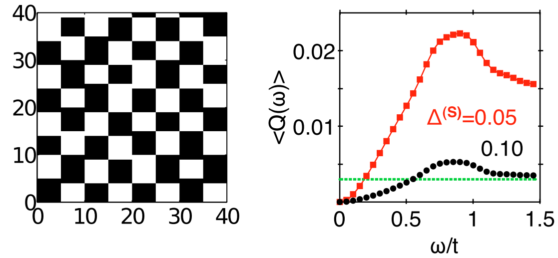

FIG. 1. (Color online) Off diagonal disorder and the anisotropy. (a) A spatial map of the employed off-diagonal disorder for $L=40$ sites, where black corresponds to $+\Delta_s$ and white to $-\Delta_s$. The off-diagonal component has a weakly disordered modulation wavelength which is assumed to be close to the superconducting coherence length. In (b), the order parameter $Q(r)$ of Eq. (9) averaged over 100 disorder configurations. It shows a strong a peak at $0.8t$ and decays slowly at higher energies. The decay is associated with the fact that the domains become internally homogeneous at very high energies, even though there is a remaining anisotropy. Given an experimental resolution, it is clear that decreasing the magnitude of Δ_s makes the anisotropy observable at higher energies.

In order to study the effects of such modulations on the experimentally studied LDOS, we consider an explicit model of lattice itinerant fermions, in which the Hamiltonian takes the form,

$$H_{\mathrm{F}}=-t\sum_{\langle\mathbf{ij}\rangle\sigma}(c_{\mathbf{i}\sigma}^{\dagger}c_{\mathbf{j}\sigma}+\text{H.c.})+\sum_{\mathbf{i},\alpha}(\Delta_{\mathbf{i}\alpha}c_{\mathbf{i}\uparrow}c_{\mathbf{i}+\alpha\downarrow}+\text{H.c.}) +\sum_{\mathbf{i}}(\Delta_{\mathbf{i}}^{(s)}c_{\mathbf{i}\uparrow}c_{\mathbf{i}\downarrow}+\text{H.c.}), \tag{5}$$

where $c_{\mathbf{i}\sigma}$ are fermionic operators and $\Delta_{\mathbf{i}\alpha}=\beta|\Delta_{\mathbf{i}}|e^{i\phi_{\mathbf{i}}}$ are complex numbers for the d-wave SC order parameter defined now at the links $(\mathbf{i},\mathbf{i}+\alpha)$ [α=unit vector along the x or y direction; $\beta=1(-1)$ for α along x (y)]. The order parameter $\Delta_{\mathbf{i}}^{(s)}$ is chosen to be modulated in space and take the values $\pm|\Delta^{(s)}|$ in short-range domains[19] [cf. Fig. 1(a)].

For $\Delta^{(s)}\to 0$ this model can be studied in perturbation theory. If $\Delta_{s,d}(k)$ are the Fourier transform of the s and d wave order parameters, the first order correction to the Green function is

$$G^1(\omega,\mathbf{k})=\Delta_s(0)\Delta_d(\mathbf{k})\frac{\omega+\epsilon_{\mathbf{k}}}{(\omega^2-E_{\mathbf{k}}^2)^2}, \tag{6}$$

which has poles at the same frequencies, $\omega=\pm E_{\mathbf{k}}=\pm\sqrt{\epsilon_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$, as the unperturbed system. This result shows that for weak disorder amplitudes, the low-energy properties of the superconductor and the positions of the nodal points are unaffected, as it is a well-known experimental fact for the cuprates.[20]

In the following, we go beyond perturbation theory and we study both low- and high-energy features of the model by

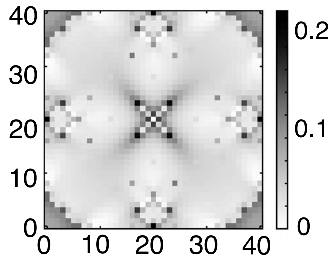

FIG. 2. LDOS at low energies. Typical map of the Fourier transform of LDOS at a low energy $\omega=0.75\Delta_d$ is shown, for the pure $5a_0$ density wave model, and where a potential impurity is added, in order to compare with the results of Ref. 22. The amplitude of the Fourier transform of the patterns shows a number of peaks that are not dispersing with the energy change but their amplitude is weak and close to the experimentally resolved q_2 wave vector (Ref. 16). The origin of the peaks is associated with the allowed scattering wave vectors for a d-wave superconductor in the presence of a density wave similar with Ref. 22. In that case, the wave vector is $(\pm\pi/4,0)$ and $(0,\pm\pi/4)$, here it is $(\pm\pi/5,\pm 3\pi/5)$ and $(\pm 3\pi/5,\pm\pi/5)$, very close to what has been labeled experimentally as q_2.

solving it in a self-consistent mean-field manner[21] using exact diagonalization on systems of size $L\times L$. The relevant parameters to our calculation satisfy the hierarchy $\Delta^{(s)} \ll \Delta^{(d)} \ll t$ with $t\sim 400$ meV and $\Delta^{d}\sim 60-100$ meV, which we believe to be consistent with the cuprates. Equation (5) can be diagonalized by using a Bogoliubov transformation. The corresponding Bogoliubov de Gennes equations are solved iteratively, for fixed $\Delta^{(s)}$ fixed until a self-consistent solution is found for the d-wave order parameter $\Delta_{\mathbf{i}\alpha} = g\langle c^{\dagger}_{\mathbf{i}+\alpha\downarrow} c^{\dagger}_{\mathbf{i}\uparrow}\rangle$,

$$\begin{pmatrix} \hat{\xi}_{\uparrow} & \hat{\Delta} \\ \hat{\Delta}^{*} & -\hat{\xi}^{*}_{\downarrow} \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \qquad (7)$$

The mean-field parameters are updated after each iteration using the equation

$$\Delta_{\mathbf{i}\alpha} = g\sum_{n} (u_{n,i}v^{*}_{n,i+\alpha} + u_{n,i+\delta}v^{*}_{n,i})\tanh\left(\frac{E_n}{2T}\right), \qquad (8)$$

where the nearest-neighbor interaction $g<0$ has to be attractive in order for the d-wave superconductor to be stable. The coupling g was chosen $g\equiv g_0=-2.5t$ so that the self-consistent average d-wave gap $\Delta^{(d)}$ is $0.26t$. The amplitude of the s-wave disorder is chosen as $|\Delta_s|=0.05t$, unless stated otherwise.

At low energies, the spectral function of the model [cf. Fig. 1(a)] is similar to the unperturbed d-wave SC. In order to study the low-energy features of the LDOS and compare to the unperturbed case,[11,22] we consider a single-site potential impurity (a change in the chemical potential) of strength $U=0.5t$. As shown in Fig. 2, the LDOS contains similar peaks as the unperturbed system,[11] which resemble the basic features of the octet model.[11,16] In addition, there are more *nondispersing* peaks at $\mathbf{Q}=(\pm\pi/5,\pm 3\pi/5)$ and $(\pm 3\pi/5,\pm\pi/5)$. These peaks signify the emergence of the locally anisotropic density wave, which at low energies has very weak features. In the presence of spatial disorder, as in the model of Fig. 1, these peaks cluster around the denoted wave vectors $\mathbf{Q}$. Experimentally, Kohsaka *et al.*[16] showed that the observed FT-STS peaks $\mathbf{q_i}$ are somewhat consistent with scattering of nodal quasiparticles from the edges of their equal energy contours. However, the predicted dispersion of the peaks as a function of energy is clearly inconsistent with the experimental data with some of the peaks being almost *static* (e.g., $\mathbf{q}_2$). Such inconsistencies might be due to the presence of the additional peaks that our model predicts: in particular, we predict that the peaks around $\mathbf{Q}$ might be present, experimentally, in the region around the observed wave vector $\mathbf{q}_2$.[16] The clear distinction of these disorder peaks should validate the present model.

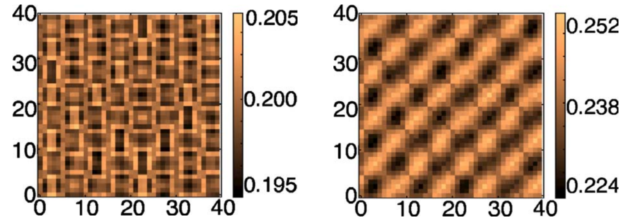

FIG. 3. (Color online) LDOS at high energies. Spatial map of the LDOS at $\omega=0.7t\sim 2.7\Delta_d$ is shown in (a). The pattern that emerges has strong anisotropic features similar to the experimentally observed ones. Notice the bond-based structure and the local anisotropy that forms in this case. Such features are robust under weak disorder. In (b), the form of the LDOS when the disorder respects the d-wave symmetry has no evident anisotropic features at $\omega=t$ but only a natural modulation, imposed by the modulation of the coupling.

The weak disorder we described is adequate to induce local anisotropic features at high energies. As shown in Fig. 3(a), the LDOS shows strong anisotropic features and internal domain structure that resembles the experimental observations. The large intensity near the domain walls on linelike structures and the similarity to large parts of the observed STM maps, signify that our toy description captures important experimental facts. Moreover, we define a local order parameter of the anisotropy[17] applied on the LDOS $F(r)$,

$$Q(r) = [(\partial_x^2 - \partial_y^2)F(r)]^2 + 4[(\partial_x\partial_y)F(r)]^2. \qquad (9)$$

This order parameter, averaged spatially and over disorder configurations, distinguishes between anisotropic fluctuations of the LDOS. As shown in Fig. 1(b), the anisotropy increases monotonically until $E_{th}\simeq 0.8t$ and then decays slowly at higher energies. The energy threshold where the anisotropy is maximally visible, is almost *independent* of the amplitude of the disorder, but dependent on the d-wave gap scale ($E_{th}\sim 2\Delta_d$). Assuming that the experimental resolution allows for a low threshold on the identification of the order parameter [horizontal line in Fig. 1(b)] indicates that the smaller the amplitude of the off-diagonal disorder, the higher the energy where the locally anisotropic features of the domains become visible. This observation signifies that the energy scale ($\sim 2\Delta_d$) where the high-energy domains in STM experiments become visible can be much larger than the ac-

RAPID COMMUNICATIONS

tual energy scale which leads to their formation, which it is just $\sim 0.2\Delta_d$.

Another form of possible superconducting disorder is a pair-density wave (PDW) such as the one proposed in association to experiments in $La_{2-x}Ba_xCuO_4$ (Ref. 23) and $Bi_2Sr_2CaCu_2O_{8+\delta}$.[24] We investigated the behavior of LDOS in the presence of such a PDW, by setting $\Delta^{(s)}=0$ and modulating the coupling $g=g_0+\delta g$, where δg follows the pattern of Fig. 1(a) and has a maximum $|\delta g|_{\max}=0.05t$. As seen in Fig. 3(b), there is no evidence of local anisotropy due to the presence of such disorder.

Given that off-diagonal disorder generates high-energy bound states which distort the LDOS in complex ways,[18] we studied the behavior of the LDOS in cases where the spatial form of the disorder has jerky features or where the amplitude has strong variations. We find that when the defined domains have *jerky* features, as in a conserved-order parameter Ising model near its critical point, the LDOS high-energy features have complex characteristics with no local anisotropy at regions where large domains exist [cf. Figs. 4(a) and 4(b)]. However, amplitude (with no spatial jerkiness) variations in the off-diagonal disorder, as soon as they have zero global average, do not affect our qualitative conclusions.

In conclusion we studied a simple phenomenological model of itinerant fermions which is able to capture different features appearing in the STM experiments. The key component of the model is the off-diagonal disorder, which is known to be ubiquitous in systems with tendency toward orthorhombic distortions (such as $Y_{2-x}Ba_xCuO_4$ and $La_{2-x}Sr_xCuO_4$), and in other less distorted systems, such as $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$. In our model this disorder takes the form of an inhomogeneous *s*-wave disorder modulated over distances of a few sites. We find that in the presence of this disorder the model can explain the nondispersive features, which arise from scattering of quasiparticles on the order parameter, the dispersive features which are the result of quasiparticle interference and more importantly the bond based anisotropy of the LDOS. We also see that an off-diagonal disorder of this type does not distort the form of the LDOS at large distances and low energies, in

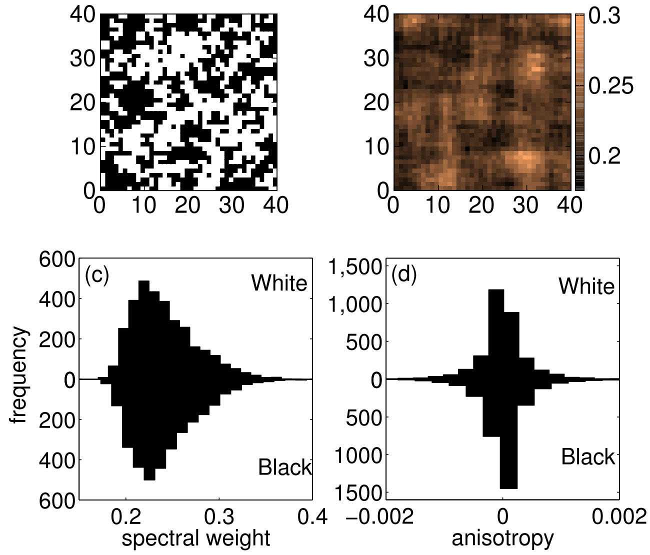

FIG. 4. (Color online) Stability of the anisotropy under strong spatial disorder. A typical off-critical $(T=1.4T_c)$ spatial map of a conserved order-parameter Ising model is shown in (a), which represents a typical form of strong spatial disorder. Spatial map of the corresponding LDOS for $\omega=t$ is shown in (b). A histogram of the spectral weight (c) and the anisotropy from Eq. (9) (d) is plotted for the sites that are labeled black and white in (a). There is no correlation between the positions of the domains and the value of anisotropy of the LDOS, as it can be seen by comparing the statistical profile of the anisotropy, due to the presence of a large collection of bound states generated by the jerky features of the order parameter, as discussed in Ref. 18.

contrast to potential impurities.[25] We believe that its effect on the features of the LDOS, should not depend on the driving mechanism, which could be purely electronic as discussed in Ref. 13.

We would like to acknowledge rather helpful discussions with E. A. Kim, P. Phillips, S. Sachdev, and J. P. Sethna. This research was partially supported by NSF under Grant No. DMR-0706379 (D.G.) and DOE-BES through Grant No. DE-FG02-07ER46393 (S.P.).

[1] O. Fischer *et al.*, Rev. Mod. Phys. **79**, 353 (2007).
[2] J. M. Tranquada, *Handbook of High-Temperature Superconductivity* (Springer-Verlag, Berlin, 2007).
[3] I. Martin *et al.*, Phys. Rev. B **72**, 060502 (2005).
[4] E. Arrigoni and S. A. Kivelson, Phys. Rev. B **68**, 180503 (2003).
[5] J. M. Tranquada *et al.*, Phys. Rev. Lett. **78**, 338 (1997).
[6] S. Wakimoto *et al.*, Phys. Rev. B **64**, 174505 (2001).
[7] V. J. Emery *et al.*, Proc. Natl. Acad. Sci. U.S.A. **96**, 8814 (1999).
[8] N. B. Christensen *et al.*, Phys. Rev. Lett. **98**, 197003 (2007).
[9] J. E. Hoffman *et al.*, Science **297**, 1148 (2002).
[10] K. McElroy, Phys. Rev. Lett. **94**, 197005 (2005).
[11] B. Andersen and P. Hirschfeld, Phys. Rev. B **79**, 144515 (2009).
[12] L. Capriotti *et al.*, Phys. Rev. B **68**, 014508 (2003).
[13] M. Vojta and O. Rosch, Phys. Rev. B **77**, 094504 (2008).
[14] M. Vojta *et al.*, Phys. Rev. Lett. **85**, 4940 (2000).
[15] M. Vojta *et al.*, Int. J. Mod. Phys. B **14**, 3719 (2000).
[16] Y. Kohsaka *et al.*, Science **315**, 1380 (2007).
[17] S. A. Kivelson *et al.*, Rev. Mod. Phys. **75**, 1201 (2003).
[18] B. M. Andersen *et al.*, Phys. Rev. Lett. **96**, 097004 (2006).
[19] The size of the domains has been chosen to be $5a_0\times 5a_0$, which is experimentally relevant. Variations around this size in one or both linear dimensions (an example of such a variation is shown in Fig. 1, where the linear size fluctuates between 4 and 6 in the y direction) do not affect conclusions and neither do random fluctuations in the magnitude of the disorder $\Delta^{(s)}$ (where $\Delta_d^{(s)}=0.05t+\delta$ with $\delta^{\max}=0.025t$).
[20] A. Damascelli *et al.*, Rev. Mod. Phys. **75**, 473 (2003).
[21] W. A. Atkinson *et al.*, Phys. Rev. Lett. **85**, 3922 (2000).
[22] Q.-H. Wang and D.-H. Lee, Phys. Rev. B **67**, 020511 (2003).
[23] E. Berg *et al.*,Phys. Rev. B **79**, 064515 (2009).
[24] B. M. Andersen *et al.*, Phys. Rev. B **76**, 020507 (2007).
[25] A. V. Balatsky *et al.*, Rev. Mod. Phys. **78**, 373 (2006).