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Mottness-induced healing in strongly correlated superconductors

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We study impurity healing effects in models of strongly correlated superconductors. We show that in general both the range and the amplitude of the spatial variations caused by nonmagnetic impurities are significantly suppressed in the superconducting as well as in the normal states. We explicitly quantify the weights of the local and the nonlocal responses to inhomogeneities and show that the former are overwhelmingly dominant over the latter. We find that the local response is characterized by a well-defined healing length scale, which is restricted to only a few lattice spacings over a significant range of dopings in the vicinity of the Mott insulating state. We demonstrate that this healing effect is ultimately due to the suppression of charge fluctuations induced by Mottness. We also define and solve analytically a simplified yet accurate model of healing, within which we obtain simple expressions for quantities of direct experimental relevance.

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Introduction. Strong electronic correlations are believed to be essential for a complete understanding of many classes of unconventional superconductors, such as the cuprates [1–4], heavy fermion superconductors [5], organic materials [6,7], and iron pnictides [8]. Among the many puzzling features of these systems is their behavior in the presence of disorder. In the case of the cuprates, experiments have shown that these d-wave superconductors are quite robust against disorder as introduced by carrier doping [3,9,10]. In particular, there seems to be a "quantum protection" of the d-wave nodal points [11]. Other anomalies were found in the organics [12] and the pnictides [13]. Although it is controversial whether conventional theory is able to explain these features [14], strong electronic interactions can give rise to these impurity screening effects. Indeed, they have been captured numerically by the Gutzwiller-projected wave function [15–17], even though a deeper insight into the underlying mechanism is still lacking. Similar impurity screening phenomena have been found as a result of strong correlations in the metallic state of the Hubbard model [18].

Despite this progress, it would be desirable to understand to what extent this disorder screening is due only to the presence of strong correlations or whether it is dependent on the details of the particular model or system. For example, are the effects of the intersite superexchange, crucial to describe the cuprates, essential for this phenomenon? To address these issues, it would be fruitful to have an analytical treatment of the problem. We will describe in this Rapid Communication how an expansion in the disorder potential is able to provide important insights into these questions. In particular, we show that the "healing" of the impurities is a sheer consequence of the strong correlations and depends very little on the symmetry of the superconducting (SC) state or the inclusion of intersite magnetic correlations.

We considered dilute nonmagnetic impurities in an otherwise homogenous, strongly correlated electronic state. We avoided complications related to the nucleation of possible different competing orders by the added impurities, such as fluctuating or static charge- and spin-density waves [19–22] or the formation of local moments [23]. Therefore, we focused only on how a given strongly correlated state readjusts itself in the presence of the impurities. We used a spatially inhomogeneous slave boson treatment [4,24–27], which allowed us to perform a complete quantitative calculation. We have allowed for either or both of d-wave SC and s-wave resonating valence bond (RVB) orders.

Our analytical and numerical results demonstrate that (i) for sufficiently weak correlations we recover the results of the conventional theory [14], in which the variations of the different fields induced by the impurities show oscillations with a long-ranged power-law envelope; (ii) for strong interactions and in several different broken symmetry states, the amplitude of the oscillations is strongly suppressed by a common prefactor x, the deviation from half filling; (iii) the spatial disturbances of the SC gap are healed over a precisely defined length scale, which does not exceed a few lattice parameters around the impurities; and (iv) this "healing effect" is intrinsically tied to the proximity to the Mott insulating state, even though it survives up to around 30% doping.

Model and method. We study the t-t'-J model on a cubic lattice in d dimensions with dilute nonmagnetic impurities,

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + J\sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i (\epsilon_i - \mu_0) n_i, \quad (1)$$

where t_{ij} are the hopping matrix elements between nearest-neighbor (t) and second-nearest-neighbor (t') sites, $c^{\dagger}_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator of an electron with spin projection σ at site i, J is the superexchange coupling constant between nearest-neighbor sites, $n_i = \sum_\sigma c^{\dagger}_{i\sigma} c_{i\sigma}$ is the number operator, μ_0 is the chemical potential, and ϵ_i is the impurity potential. The no-double-occupancy constraint ($n_i \leqslant 1$) is implied. We set the nearest-neighbor hopping t as the energy unit and choose $t' = -0.25t$. To treat this model, we employ the $U(1)$ slave boson theory [4,24,26,28]. Details can be found in Ref. [4] and we only describe it very briefly here. It starts with the replacement $c^{\dagger}_{i\sigma} = f^{\dagger}_{i\sigma} b_i$, where $f^{\dagger}_{i\sigma}$ and b_i are auxiliary fermionic (spinon) and bosonic fields, and the representation is faithful in the subspace $n_i \leqslant 1$ if the constraint $\sum_\sigma f^{\dagger}_{i\sigma} f_{i\sigma} + b^{\dagger}_i b_i = 1$ is enforced. This is implemented by a Lagrange multiplier λ_i on each site. The J term is then decoupled by Hubbard-Stratonovich fields in the particle-particle (Δ_{ij}) and particle-hole (χ_{ij}) channels. The auxiliary bosonic fields are all treated in the saddle-point approximation: $\langle b_i\rangle = r_i = \sqrt{Z_i}$ gives the quasiparticle residue, $\langle\lambda_i\rangle$ renormalizes the site energies, and $\chi_{ij} = \sum_\sigma \langle f_{i\sigma}^\dagger f_{j\sigma}\rangle$ and $\Delta_{ij} = \langle f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow}\rangle$ describe, respectively, the strength of a spinon singlet and the pairing amplitude across the corresponding bonds. Note that we do not assume these values are spatially uniform. This treatment is equivalent to the Gutzwiller approximation [2,15]. In terms of Gorkov's spinor notation [29] with $\Psi_i(i\omega_n) = [f_{i\uparrow}^\dagger(i\omega_n)\, f_{i\downarrow}(-i\omega_n)]^\dagger$, where ω_n is the fermionic Matsubara frequency, the spinon Green's function is a 2×2 matrix: $[G_{ij}(i\omega_n)]_{ab} = -\langle\Psi_i(i\omega_n)\Psi_j^\dagger(i\omega_n)\rangle_{ab}$. Defining $h_{ij} \equiv -t_{ij}$, the saddle-point equations read as follows:

$$\chi_{ij} = 2T\sum_n (G_{ij})_{11}, \tag{2}$$

$$\Delta_{ij} = -2T\sum_n (G_{ij})_{12}, \tag{3}$$

$$\left(r_i^2 - 1\right) = -2T\sum_n (G_{ii})_{11}, \tag{4}$$

$$\lambda_i r_i = -2T\sum_{nl} h_{il} r_l (G_{il})_{11} = -\sum_l h_{il} r_l \chi_{il}. \tag{5}$$

Note that we used Eq. (2) in the second equality of Eq. (5). At $T=0$ and in the clean limit $\epsilon_i = 0$, we have $Z = Z_0 = x$. The Mott metal-insulator transition is signaled by the vanishing of the quasiparticle weight $Z_0 \to 0$ at half filling. It will be interesting to compare the results of the above procedure with the ones obtained from solving only Eqs. (2) and (3) while setting $Z_i = 1$ and $\lambda_i = 0$. The two sets will be called correlated and noncorrelated, respectively. In order to be able to compare them, we set $J = t/3$ in the correlated case and adjusted J in the noncorrelated case in such a way that the two clean dimensionful SC gaps coincide, as discussed in Ref. [15].

Healing. Although the detailed solutions of Eqs. (2)–(5) can be straightforwardly obtained numerically, we will focus on the case of weak scattering by dilute impurities and expand those equations up to first order in ε_i around the homogeneous case. It has been shown and we confirm that disorder induces long-ranged oscillations in various physical quantities, especially near the nodal directions in the d-wave SC state [14]. The linear approximation we employ is quite accurate for these extended disturbances far from the impurities, since these are always small. Besides, it provides more analytical insight into the results.

In general, we can expand the spatial variations of the various order parameters in different symmetry channels through cubic harmonics, $\delta\varphi_{ij} = \sum_g \delta\varphi_i \Gamma(g)_{ij}$, where $\varphi_{ij} = \chi_{ij}$ or Δ_{ij} and $\Gamma(g)_{ij}$ are the basis functions for cubic harmonic g of the square lattice.[1] In the current discussion, we choose $\delta\chi_{ij} = \delta\chi_i\Gamma(s)_{ij}$ and $\delta\Delta_{ij} = \delta\Delta_i\Gamma(d_{x^2-y^2})_{ij}$, as we are interested in oscillations with the same symmetry as the ground state [4,24,26,28]. We also assume there is no phase difference between order parameters on different bonds linked to same site. Then, we can define "local" spatial variations of the order parameters as $\delta\chi_i \equiv \frac{1}{2d}\sum_j \delta\chi_{ij}\Gamma(s)_{ij}$ and $\delta\Delta_i \equiv \frac{1}{2d}\sum_j \delta\Delta_{ij}\Gamma(d_{x^2-y^2})_{ij}$. Details of the calculation can be found in the Supplemental Material [30].

We find that both $\delta\chi_{ij}$ and $\delta\Delta_{ij}$, as well as the impurity-induced charge disturbance δn_i, are proportional to $Z_0 = x$, indicating the importance of strong correlations for the healing effect. Indeed, we can trace back this behavior to the readjustment of the r_i and λ_i fields, as encoded in Eqs. (4) and (5). Besides, this $O(x)$ suppression is a generic consequence of the structure of the mean-field equations and holds for different broken symmetry states, such as the flux phase state, s-wave superconductivity, etc.

Let us focus in more detail on the spatial variations of the local pairing field $\delta\Delta_i$. In the first column of Fig. 1 we show results for $\delta\Delta_i$ for three identical impurities. The "crosslike" tails near the nodal directions [31] are conspicuous in the absence of correlations (bottom) but are strongly suppressed in their presence (top). While this suppression is further enhanced as the Mott metal-insulator transition is approached ($x \to 0$), it is still quite significant even at optimal doping ($x = 0.2$). This is the "healing" effect previously reported [15–17]. In order to gain insight into its underlying mechanism, we look at the spatial correlation function of local gap fluctuations,

$$\left\langle \frac{\delta\Delta_i}{\Delta_0}\frac{\delta\Delta_j}{\Delta_0}\right\rangle_{\text{disorder}} = f\left(\mathbf{r}_i - \mathbf{r}_j\right), \tag{6}$$

where the brackets denote an average over disorder, after which lattice translation invariance is recovered. The Fourier transform of $f(\mathbf{r})$ can be written in the linear approximation as

$$f(\mathbf{k}) = \alpha W^2 S(\mathbf{k}), \tag{7}$$

where W is the disorder strength, α depends on the detailed bare disorder distribution, and the "power spectrum" (PS) $S(\mathbf{k})$ is related to gap linear response function $M_\Delta(\mathbf{k})$ by $S(\mathbf{k}) = M_\Delta^2(\mathbf{k})$. The latter is defined by Fourier transforming the kernel in $\delta\Delta_i = \Delta_0\sum_j M_\Delta(\mathbf{r}_i - \mathbf{r}_j)\varepsilon_j$, which in turn can be easily obtained from the solution of the linearized equations [30]. Inspired by the strongly localized gap fluctuations at the top left of Fig. 1, we define the local component of the PS, $S_{\text{loc}}(\mathbf{k}) \equiv M_{\Delta,\text{loc}}^2(\mathbf{k})$, where $M_{\Delta,\text{loc}}(\mathbf{k})$ is obtained by *restricting the lattice sums up to the second-nearest-neighbor distance* ($\sqrt{2}a$) in the linearized equations [30]. We also define $S_{\text{nonloc}}(\mathbf{k}) = M_{\Delta,\text{nonloc}}^2(\mathbf{k}) \equiv [M_\Delta(\mathbf{k}) - M_{\Delta,\text{loc}}(\mathbf{k})]^2$. In the last three columns of Fig. 1, we show, in this order, $S(\mathbf{k})$, $S_{\text{loc}}(\mathbf{k})$, and $S_{\text{nonloc}}(\mathbf{k})$ for the correlated (top) and noncorrelated (bottom) cases at $x = 0.2$. Clearly, in the presence of correlations, the local PS is characterized by a smooth, spherically symmetric bell-shaped function, whereas the nonlocal part is highly anisotropic. Besides, and more importantly, the nonlocal PS is negligibly small in the correlated case. The full PS is thus *overwhelmingly dominated* by the local part, unlike in the noncorrelated case. In the Supplemental Material [30], we extend the analysis to the underdoped and overdoped regimes, where very similar behavior is found, even up to dopings of $x = 0.3$.

[1] s, $d_{x^2-y^2}$, d_{xy}, etc., with basis functions expressed as $\cos k_x + \cos k_y$, $\cos k_x - \cos k_y$, and $\sin k_x \sin k_y$, etc.

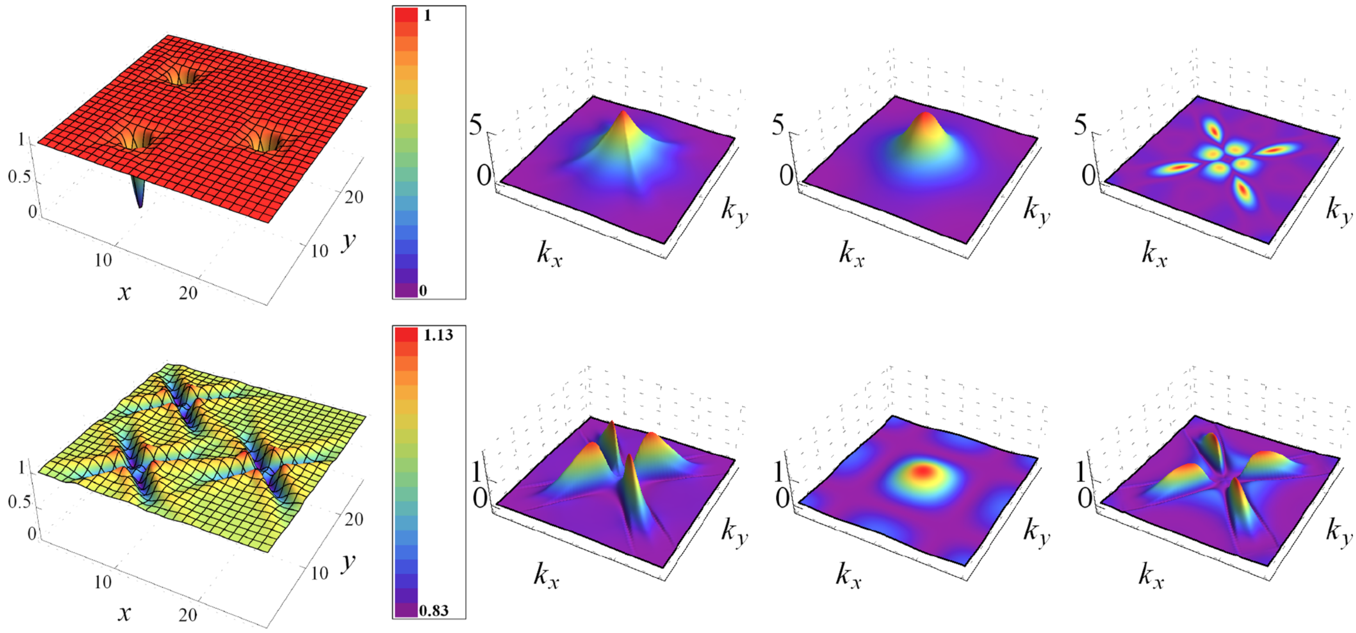

FIG. 1. (Color online) Spatial variations of normalized local SC gap $\frac{\Delta_i}{\Delta_0}$ for three impurities (first column) and the corresponding power spectra $S(\mathbf{k})$, $S(\mathbf{k})_{\rm loc}$, and $S(\mathbf{k})_{\rm nonloc}$ (second to fourth columns), in the presence (top) and in the absence (bottom) of correlations for $x = 0.2$. The strong suppression of gap oscillations by correlations can be traced to the dominance of the local, spherically symmetric power spectrum $[S_{\rm loc}(\mathbf{k})]$ over the nonlocal anisotropic part $[S_{\rm nonloc}(\mathbf{k})]$.

In order to quantify the localized nature of the healing effect, we are led to a natural definition of a "healing factor" h in the d-wave SC state,

$$h = \frac{\int S_{\rm nonloc}(\mathbf{k}) d^2k}{\int S_{\rm loc}(\mathbf{k}) d^2k}, \tag{8}$$

where the integration is over the first Brillouin zone. It measures the relative weight of nonlocal and local parts of the gap PS. The healing factor as a function of doping is shown in the left panel of Fig. 2 for the noncorrelated (blue) and correlated (red) cases. The contrast is striking. When correlations are present, h is extremely small up to 30% doping and the gap disturbance is restricted to a small area around the impurities. In contrast, without correlations, significant pair fluctuations occur over quite a large area for all dopings shown. We conclude that the strong dominance of the local part over the highly anisotropic nonlocal contribution caused by correlations is the key feature behind the healing process.

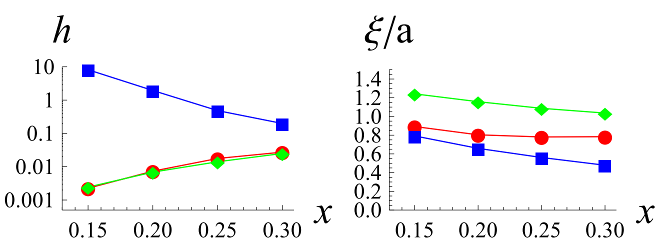

FIG. 2. (Color online) Left: The healing factor h as a function of doping in the uncorrelated case (blue curve with squares), in the correlated case (red curve with circles), and in the correlated case without $\delta\chi_i$ fluctuations (green curve with diamonds). Right: Doping dependence of the SC (ξ_S, red curve with circles) and normal state (ξ_N, blue curve with squares) healing lengths. The green curve with diamonds gives ξ_S calculated within the minimal model (see text).

The shape of $S_{\rm loc}(\mathbf{k})$ shows that the gap disturbance created by an impurity is healed over a well-defined distance, the "healing length" ξ_S. This length scale can be obtained by expanding the inverse of $M_{\Delta,{\rm loc}}(\mathbf{k})$ [or, equivalently, $M_\Delta(\mathbf{k})$] up to second order in k^2, thus defining a Lorentzian in $\mathbf{k}$ space,

$$M_{\Delta,{\rm loc}}(\mathbf{k}) \approx \frac{1}{A + Bk^2}. \tag{9}$$

The SC healing length is then given by $\xi_S = \sqrt{B/A}$. The x dependence of ξ_S is shown in red in the right panel of Fig. 2. It is of the order of one lattice spacing in the relevant range $0.15 < x < 0.3$. It should be noted that precisely the same length scale also governs the healing of charge fluctuations in the SC state, showing that this phenomenon is generic to the strongly correlated state. A similar procedure can be carried out for the charge fluctuations in the normal state, thus defining a normal state healing length ξ_N [30]. The blue curve of the right panel of Fig. 2 shows the x dependence of ξ_N, which is also of the order of one lattice spacing.

Mottness-induced healing. The healing effect we have described comes almost exclusively from the δr_i and $\delta\lambda_i$ fluctuations: h is hardly affected by the $\delta\chi_i$ field. If we suppress the $\delta\chi_i$ fluctuations completely [30], there is only a tiny change in the results, as shown by the green curve in the left panel of Fig 2. The same is not true, however, if we turn off either δr_i or $\delta\lambda_i$ or both. We conclude that the healing effect in the d-wave SC state originates from the strong correlation effects alone, rather than the spinon correlations.

Within the linear approximation we are employing, all fluctuation fields ($\delta\Delta$, δr, etc.) are proportional, in $\mathbf{k}$ space, to the disorder potential $\varepsilon(\mathbf{k})$. Therefore, they are also proportional

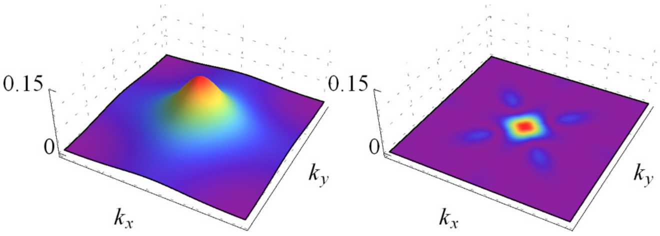

FIG. 3. (Color online) Local (left) and nonlocal (right) parts of the charge-fluctuation power spectra $N(\mathbf{k})_{\text{loc}}$ and $N(\mathbf{k})_{\text{nonloc}}$ in the presence of strong correlations for $x = 0.2$.

to each other. In particular, given the centrality of the strong correlation fields, it is instructive to write the gap fluctuations in terms of the slave boson fluctuations,

$$\delta\Delta(\mathbf{k}) = -2\chi_{\text{pc}}(\mathbf{k})r\delta r(\mathbf{k}) = \chi_{\text{pc}}(\mathbf{k})\delta n(\mathbf{k}). \qquad (10)$$

In the last equality, we used $n_i = 1 - r_i^2$, which enables us to relate two physically transparent quantities: the gap and the charge fluctuations. Indeed, this will provide crucial physical insight into the healing process. By focusing on the linear charge response to the disorder potential $\delta n(\mathbf{k}) = n_0 M_n(\mathbf{k})\varepsilon(\mathbf{k})$, we can, in complete analogy with the gap fluctuations, define a PS for the spatial charge fluctuations, $N(\mathbf{k}) = M_n^2(\mathbf{k})$. This PS can also be broken up into local $[N_{\text{loc}}(\mathbf{k}) = M_{n,\text{loc}}^2(\mathbf{k})]$ and nonlocal $\{N_{\text{nonloc}}(\mathbf{k}) = [M_n(\mathbf{k}) - M_{n,\text{loc}}(\mathbf{k})]^2\}$ parts, as was done for the gap-fluctuation PS. These two contributions, obtained from the solution of the full linearized equations, are shown in Fig. 3. The charge PS in the correlated d-wave SC state is also characterized by a smooth, almost spherically symmetric local part and a negligibly small anisotropic nonlocal contribution. Note also the strong similarity between the local PS for gap (top row of Fig. 1) and charge fluctuations. This shows a strong connection between the gap and charge responses. Evidently, this is also reflected in real space, where the charge disturbance is healed in the same strongly localized fashion as the gap disturbance [30]. In fact, the local part of the charge response function $M_{n,\text{loc}}(\mathbf{k})$ can be shown to be well approximated by a Lorentzian [30] and we can write for small $\mathbf{k}$,

$$\delta\Delta_{\text{loc}}(\mathbf{k}) \approx -\chi_{\text{pc}}(\mathbf{k}=0)\,\frac{8r^2/\lambda}{k^2 + \xi_S^{-2}}\,\varepsilon(\mathbf{k}), \qquad (11)$$

where the SC healing length ξ_S can be expressed in terms of the Green's functions of the clean system [30]. The relations implied by Eqs. (10) and (11), as well as the doping dependence of the quantities in them, could be tested in scanning tunneling microscopy (STM) studies and would constitute an important test of this theory.

Equations (10) and (11) allow us to obtain a clear physical picture of the healing mechanism. The spatial gap fluctuations can be viewed as being ultimately determined by the charge fluctuations. Furthermore, their ratio $\chi_{\text{pc}}(\mathbf{k})$, which is essentially a pair-charge correlation function, is a rather smooth function *of order unity,only weakly renormalized by interactions*. Therefore, it is the strong suppression of charge fluctuations by "Mottness," as signaled by the r^2 factor in Eq. (11), which is behind the healing of gap fluctuations. This elucidates the physics of healing previously found numerically [15–17]. It also suggests that the healing phenomenon is generic to Mott systems [18] and is not tied to the specifics of the cuprates.

A minimal model. Interestingly, the crucial role played by the strong correlation fields (r_i and λ_i) suggests a "minimal model" (MM) for an accurate description of the healing process, which we define as follows: (i) The spatially fluctuating strong correlation fields r_i and λ_i are first calculated for the self-consistently determined, *fixed, uniform* Δ and χ, and then (ii) the effects of their spatial readjustments are fed back into the gap equation (3) in order to find $\delta\Delta_i$ [30]. The accuracy of this procedure can be ascertained by the behavior of the healing factor: It is *numerically indistinguishable* from the green curve in the left panel of Fig. 2. Furthermore, the value of ξ_S calculated within the MM differs from the one obtained from the solution of the full linearized equations by at most 20% (red and green curves in the right panel of Fig. 2). Besides its accuracy, the advantage of this MM description lies in the simplicity of the analytical expressions obtained. As shown in the Supplemental Material [30], it provides simple expressions for the important quantities $\chi_{\text{pc}}(\mathbf{k})$ and ξ_S.

Conclusions. In this Rapid Communication, we have found an inextricable link between the healing of gap and charge disturbances in strongly correlated superconductors, suggesting that this phenomenon is generic to any system close to Mott localization. An important experimental test of this link would be provided by STM studies of the organic superconductors [12] and maybe the pnictides [13]. Whether it is also relevant for heavy fermion systems [32] is an open question left for future study.

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