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Strong coupling critique of spin fluctuation driven charge order in underdoped cuprates

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Charge order has emerged as a generic feature of doped cuprates, leading to important questions about its origin and its relation to superconductivity. Recent experiments on two classes of hole doped cuprates indicate a novel d-wave symmetry for the order. These were motivated by earlier spin fluctuation theoretical studies based on an expansion about hot spots in the Brillouin zone that indicated such an order would be competitive with d-wave superconductivity. Here, we reexamine this problem by solving strong coupling equations in the full Brillouin zone for experimentally relevant parameters. We find that bond-oriented order, as seen experimentally, is strongly suppressed. We also include coupling to B_{1g} phonons and do not see any qualitative change. Our results argue against an itinerant model for the charge order, implying instead that such order is likely due to Coulombic phase separation of the doped holes.

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Following earlier NMR studies [1], recent x-ray experiments on underdoped cuprates have detected short range charge density wave (CDW) order with a period of three to five lattice spacings in $YBa_2Cu_3O_{7-x}$ (YBCO) [2–4], and in Bi based [5,6] and Hg based cuprates [7]. For YBCO, the doping range where the charge order has been observed [8] coincides with the doping range where quantum oscillation experiments detect reconstruction of the Fermi surface [9]. In conventional CDW systems, the charge order is thought to have s-wave symmetry [10]. In contrast, scanning tunneling microscopy [11] and resonant soft x-ray scattering [12,13] data have revealed a novel d-wave symmetry, where the two oxygen ions in a CuO_2 unit are out of phase. This charge order differs from the more robust stripe order seen earlier in La based compounds [14–16], which appears to have s-wave symmetry instead [13]. In all cases, though, the wave vector is oriented along the bond direction [17].

The search for d-wave symmetry was motivated by earlier theoretical studies of Metlitski and Sachdev [18,19]. They have shown that charge order is competitive with d-wave superconductivity in a spin fluctuation model. This instability has a d-wave form factor, with a diagonal wave vector that spans Fermi surface points (hot spots) that intersect the antiferromagnetic zone boundary of the undoped phase (Fig. 1). The subsequent observation of charge order in YBCO motivated a number of followup studies [20–24]. Most of these studies are either based on an expansion around the hot spots, with the Fermi surface curvature treated as a perturbation [20,22,24], or rely on a weak coupling approximation. So, the question arises whether these results survive in a strong coupling treatment where these approximations are not made.

Here, we solve the strong coupling instability equation for the charge order in the entire Brillouin zone, including the full momentum and frequency dependence of the bosonic and fermionic spectra. This formalism has been used in the past to study d-wave superconductivity originating from spin fluctuations [25,26]. It has also been used to study instabilities in the particle-hole channel [27]. Recently, this formalism was used by us to examine the effect of the pseudogap on spin fluctuation mediated pairing [28]. The one approximation we make is that the bosonic and fermionic spectra are taken from experiment rather than self-consistently calculated. We find that bond-centered charge order is completely suppressed, and inclusion of the dressed fermion Green's function additionally suppresses diagonal charge order, with the only robust order in this model for experimentally relevant parameters being d-wave superconductivity.

Our starting point is the linearized equation for the anomalous self-energy in the particle-hole channel,

$$T\sum_{k',\omega_m} V(k-k',i\omega_n - i\omega_m)\mathcal{P}^Q(k',i\omega_m)\Phi^Q(k',i\omega_m) = \lambda\Phi^Q(k,i\omega_n). \quad (1)$$

Here, Q is the ordering vector, V is the interaction. and $\mathcal{P}^Q$ is the CDW particle-hole kernel,

$$\mathcal{P}^Q(k',i\omega_m) = G\left(k'-\frac{Q}{2},i\omega_m\right)G\left(k'+\frac{Q}{2},i\omega_m\right), \quad (2)$$

where G is the fermion Green's function. Because of the complexity of the strong coupling equations, as a first approximation, we do not include the frequency dependence of the fermion self-energy, and thus set $G(k,i\omega) = (i\omega - \xi_k)^{-1}$. For ξ_k, we consider a renormalized dispersion that fits low energy angle-resolved photoemission spectroscopy (ARPES) data for $Bi_2Sr_2CaCu_2O_{8+\delta}$ (the tb2 dispersion of Ref. [29]). Later in this Rapid Communication, we will include the fermion self-energy as well. The interaction assumed here is

$$V(k,i\Omega_n) = \int_{-\infty}^{\infty}\frac{dx}{\pi}\frac{V''(k,x)}{i\Omega_n - x}, \quad (3)$$

where V'' is proportional to the imaginary part of the dynamic spin susceptibility. We consider the phenomenological form [30]

$$V''(k,\Omega) = \frac{3}{2}g_{sf}^2\chi_Q\frac{\Omega\Omega_{sf}}{\chi_k^2\Omega_{sf}^2+\Omega^2},$$
$$\chi_k = (\xi_{AF}/a)^{-2} + 2 + \cos k_x a + \cos k_y a, \quad (4)$$

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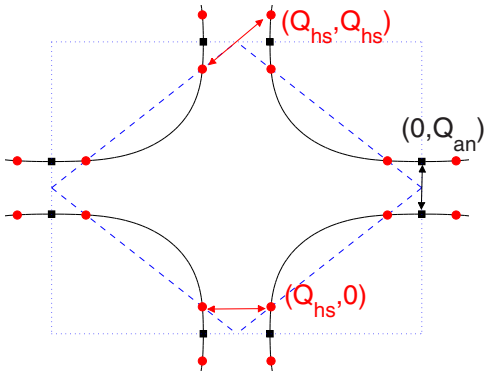

FIG. 1. (Color online) Fermi surface for the tight binding dispersion considered in this work. The dashed lines show the antiferromagnetic Brillouin zone and the dotted lines the structural one. Solid circles denote the hot spots and solid squares the antinodal points. The wave vectors studied here are indicated by the arrows.

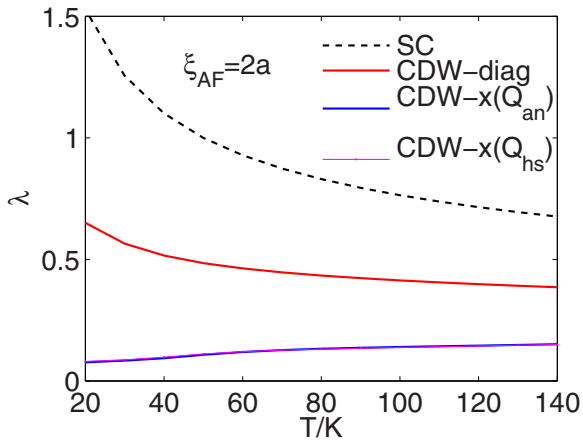

FIG. 2. (Color online) Temperature dependence of the leading eigenvalues for the superconducting d-wave state (SC), the diagonal CDW state (CDW-diag), and the bond-oriented CDW state (CDW-x), in an approximation where G is based on a renormalized dispersion taken from ARPES data. The ordering vector for CDW-diag is (Q_{hs},Q_{hs}). For CDW-x, two vectors were considered, $(Q_{an},0)$ and $(Q_{hs},0)$.

where g_{sf} is the spin-fermion coupling constant, ξ_{AF} is the antiferromagnetic correlation length, χ_Q is the static susceptibility at $Q_{AF}=(\pi/a,\pi/a)$, and Ω_{sf} is the characteristic spin fluctuation energy scale. Because of the $1/\Omega$ decay of V'', we impose a frequency cutoff Ω_c. We use $\Omega_c = 300$ meV, $\Omega_{sf} = 100$ meV, $g_{sf}^2\chi_Q = 0.9$ eV, and $\xi_{AF} = 2a$, where a is the lattice constant. The values of ξ_{AF} and Ω_{sf} are motivated from inelastic neutron scattering studies of the magnetic excitations of underdoped YBCO near Q_{AF} [31,32]. Ω_c is motivated from recent resonant inelastic x-ray scattering studies of the higher energy excitations away from Q_{AF} [33,34]. The value of $g_{sf}^2\chi_Q$ was chosen to obtain a superconducting T_c of 50 K, typical for underdoped YBCO. At the transition, the leading eigenvalue λ in Eq. (1) reaches 1, with its eigenvector giving the structure of the CDW order parameter.

We consider the CDW instabilities for the diagonal CDW case (CDW-diag) with ordering vector (Q_{hs},Q_{hs}), and for the bond-oriented case (CDW-x) with vectors $(Q_{an},0)$ and $(Q_{hs},0)$, as shown in Fig. 1. We perform our calculations with a $0.02\pi/a$ momentum grid with 32 Matsubara frequencies, which is sufficient for the convergence of the eigenvalues for the temperature range studied here (see the Supplemental Material [35]). Figure 2 shows the temperature dependence of the leading eigenvalue for the different CDW cases along with the d-wave superconducting case.

As expected, the eigenvalue for the superconducting case exhibits a logarithmic divergence in T. This is present as well for CDW-diag order, though we find it to be significantly reduced relative to the superconducting one. The CDW-diag state has d-wave (B_{1g}) symmetry with a momentum dependence that is well described by $\cos(k_xa)-\cos(k_ya)$, as can be seen in Fig. 3(a). Increasing the antiferromagnetic coherence length does not change our findings. The CDW-diag instability becomes stronger with longer ξ_{AF}, but it always remains subdominant relative to d-wave superconductivity (see the Supplemental Material [35]).

We now focus on the bond-oriented CDW states, since experimental evidence for diagonal-oriented order is lacking. The T dependence of the leading eigenvalues for CDW-x are also plotted in Fig. 2. They are almost identical for vectors $(Q_{hs},0)$ and $(Q_{an},0)$. The eigenvalues vary little with temperature, showing no evidence for a log in the temperature range studied. This is one of our main results, and differs from an analytic approximation quoted in earlier work [24]. The lack of a log divergence in our case is likely due to the curvature coming from the experimentally determined Fermi surface. Moreover, our bosonic spectrum is based on inelastic neutron and x-ray scattering measurements. Hence, we are not in the extreme quantum critical regime considered in Ref. [24].

We next look at the structure of the CDW-x state. Figure 3(b) shows the momentum dependence of the eigenvector corresponding to the leading eigenvalue, and can be well fit by a sum of a constant (s), $\cos(k_xa)+\cos(k_ya)$ (s'), and $\cos(k_xa)-\cos(k_ya)$ (d), with the d-wave component dominant, consistent with earlier studies [21].

We now turn to the influence of the fermion self-energy. The fermion self-energy in a lowest order approximation is

$$\Sigma(k,i\omega) = T\sum_{k',\omega'} V(k-k',i\omega-i\omega')G_0(k',i\omega') \qquad (5)$$

$$= T\sum_{k',\omega'} V(k-k',i\omega-i\omega')\frac{-i\omega'-\xi_{k'}}{\omega'^2+\xi_{k'}^2}, \qquad (6)$$

where G_0 is the bare Green's function. Since our previous ξ_k was based on ARPES data, we scale it by a factor of 2 to get an approximation to the bare dispersion, with a bare nodal Fermi velocity $v_F^{\rm node} = 3.2$ eVÅ. For the spin fluctuation interaction, we use $g_{sf}^2\chi_Q = 3.2$ eV and keep the rest of the parameters the same as before. This coupling strength renormalizes the nodal Fermi velocity to 1.8 eVÅ, which is comparable to the experimental value. To keep the shape of the Fermi surface intact, we drop the term proportional to $\xi_{k'}$ in the self-energy calculation [Eq. (6)]. We now use this dressed Green's function $[G^{-1}(k,i\omega) = i\omega-\xi_k-\Sigma(k,i\omega)]$ for the instability analysis in Eq. (1). Its effect (Fig. 4) is to additionally suppress the diagonal charge order (presumably due to the energy

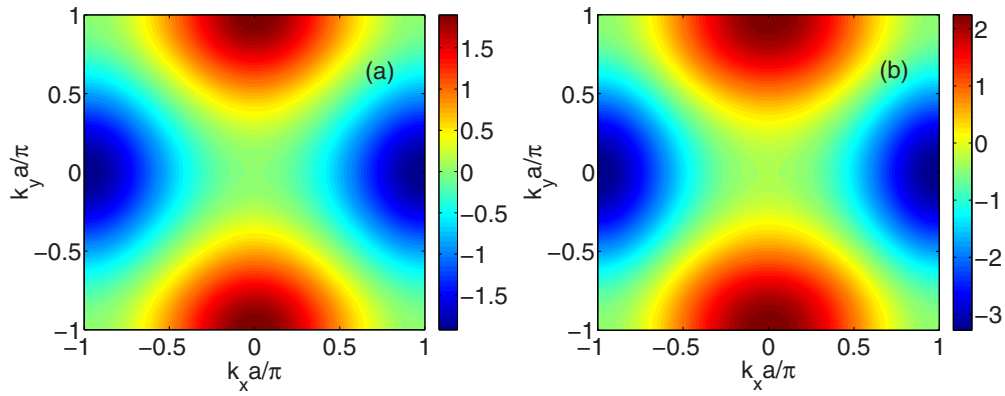

FIG. 3. (Color online) The momentum dependence of the eigenvectors at the lowest Matsubara frequency ($T = 40$ K) corresponding to leading eigenvalues (Fig. 2) for the (a) CDW-diag and (b) CDW-x states. For CDW-x, the ordering vector is $(Q_{an},0)$, though the eigenvector for $(Q_{hs},0)$ is similar. A normalization condition of $T\sum_{\omega_n,k}|\Phi^Q(k,i\omega_n)|^2 = 1$ is employed.

smearing of G). As a consequence, for experimentally relevant parameters, only d-wave superconductivity remains as a robust instability in this model.

Our results cast doubt on an itinerant spin fluctuation mediated origin for the observed charge order. On the other hand, the dependence of the observed wave vector on doping [8] is suggestive that the Fermi surface is playing some role as in classic CDW systems. This is in contrast to the La based cuprates whose doping dependence is opposite to this, as would be expected from a real-space picture where the wave vector is proportional to the doping. In classic CDW systems such as $2H$-$NbSe_2$, phonons play an important role [36]. Hence, one could think that this might be the case in the cuprates as well, where anomalies have been seen in both optic [37] and acoustic [38] phonon modes near the charge ordering vector. It is interesting to note that B_{1g} phonon modes have been postulated to be responsible for dispersion anomalies seen in photoemission near the antinodes [39], and perhaps their d-wave symmetry is related to that of the charge order. In support of this, several theoretical studies have suggested that coupling of the electrons to such modes can cause d-wave charge order [40,41]. We examine this idea by including the phonon mediated interaction along with the spin fluctuation mediated interaction in the CDW instability equation. Under the assumption that the electron-phonon interaction is modest, we do not find that its addition has sufficient strength to cause a CDW instability either (see the Supplemental Material [35]).

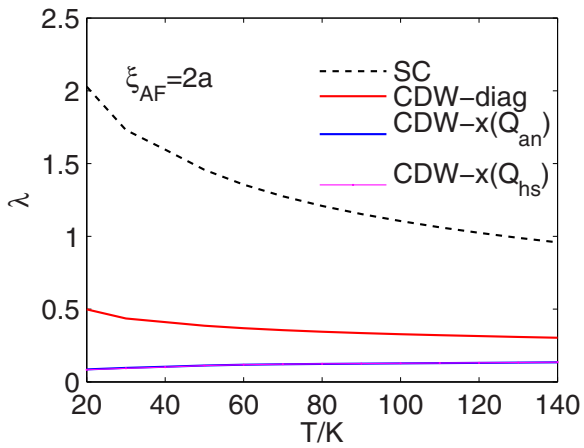

FIG. 4. (Color online) Temperature dependence of the leading eigenvalues for the superconducting d-wave state (SC), the diagonal CDW state (CDW-diag), and the bond-oriented CDW state (CDW-x), obtained using dressed Green's functions.

None of the above means that spin mediated interactions are irrelevant for the charge order, but our results indicate that an itinerant treatment of the problem in a parameter range appropriate to experiment is not adequate to capture the resulting physics. In that context, we point to real-space treatments of the t-J model such as the density matrix renormalization group (DMRG), which indicate a strong tendency to bond-centered charge order in the underdoped regime [42], with the d-wave structure likely due to Coulomb repulsion which acts to enforce charge neutrality in each unit cell.

Note added. Recently, a critique of this work has been offered by Wang and Chubukov [43,44]. Their primary criticism revolves around two points—that in the original submission, we neglected the fermion self-energy that they argue lessens the detrimental impact of the Fermi surface curvature, and that our value of Ω_{sf} is too small by an order of magnitude. In regards to the first point, using dressed Green's functions, we now find strong suppression of the charge order, even for diagonal wave vectors. In regards to the second point, our value of Ω_{sf} is based on experiment, and an order of magnitude larger value would lead to a spin fluctuation energy scale at the Γ point of the zone of 4 eV, in gross disagreement with inelastic x-ray scattering data. We also comment that the logarithmic temperature divergence of the eigenvalue derived for bond-centered charge order in their work is based on analytic approximations which we feel are not valid for experimentally realistic parameters. Certainly, we find no evidence for a log in our own numerical studies, even for a ξ_{AF} as large as $10a$ (see the Supplemental Material [35]). As an additional note, our results are consistent with recent findings based on a real-space version of Eliashberg theory [45].

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