Theory of Multiband Superconductivity in Spin-Density-Wave Metals

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We study the emergence of multiband superconductivity with s- and d-wave symmetry on the background of a spin density wave (SDW). We show that the SDW coherence factors renormalize the momentum dependence of the superconducting (SC) gap, yielding a SC state with an *unconventional* s-wave symmetry. Interband Cooper pair scattering stabilizes superconductivity in both symmetries. With increasing SDW order, the s-wave state is more strongly suppressed than the d-wave state. Our results are universally applicable to two-dimensional systems with a commensurate SDW.

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Understanding the microscopic origin of thermodynamic phases with multiple order parameters (OP) is one of the central issues in condensed matter physics. This topic is particularly important for describing the complex phase diagram of many correlated metals such as the high-T_c cuprates, ferropnictides, and heavy fermion compounds, in which it was suggested that superconductivity coexists with a rich variety of other states, such as charge, spin, or orbital density wave states. In such coexistence phases, the presence of a density wave immediately leads to multiband superconductivity due to the folding of the electronic bands. The relative phase of the superconducting (SC) order parameters in multiband superconductors was originally studied in Ref. [1], and has attracted significant interest recently in MgB_2 [2] and the ferropnictides [3]. The growing experimental evidence for the coexistence of superconductivity and a spin density wave (SDW) in the n-type (i.e., electron-doped) cuprates [4–6], heavy fermion [7], and organic superconductors [8] raises the question of how phase locking occurs in such systems. This question is of particular interest in the n-type cuprates where experiments suggest a transition from a SC with a $d_{x^2-y^2}$-wave symmetry in the underdoped materials to either an s- or a $(d + is)$-wave symmetry in the optimally doped ones [4]. However, some disagreement remains since other measurements suggest the existence of a $d_{x^2-y^2}$-wave OP with higher harmonics over the entire doping range [4].

Motivated by these observations, we study in this Letter the emergence of two-band superconductivity with $d_{x^2-y^2}$- or s-wave symmetry [9–11] on the background of a commensurate SDW with imperfect nesting. We show that the SDW coherence factors renormalize the momentum dependence of the SC gap. This yields an *unconventional* s-wave OP with a π-phase shift between the two bands, line nodes along the boundary of the reduced Brillouin zone (RBZ), and a sign change between momenta connected by the SDW ordering momentum $\mathbf{Q}$. In contrast, in the $d_{x^2-y^2}$-wave state, the OP is locked in-phase, with no *additional* line nodes. While in both cases, superconductivity is stabilized by interband Cooper pair scattering, the s-wave state is suppressed more quickly than the $d_{x^2-y^2}$-wave state with increasing SDW OP. To demonstrate the generality of our results, we consider both n- and p-type doping, leading to different evolutions of the Fermi surface (FS) in the SDW state.

Our starting point for investigating the coexistence of superconductivity and SDW order is the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k},\mathbf{k}'} U c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}+\mathbf{Q}\uparrow} c^{\dagger}_{\mathbf{k}'+\mathbf{Q}\downarrow} c_{\mathbf{k}'\downarrow} + \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q},\uparrow} c^{\dagger}_{\mathbf{p}-\mathbf{q},\downarrow} c_{\mathbf{p},\uparrow} c_{\mathbf{k},\downarrow}, \quad (1)$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ ($c_{\mathbf{k}\sigma}$) creates (annihilates) an electron with spin σ and momentum $\mathbf{k}$. We consider a two-dimensional system with $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - \mu$ being the normal state tight-binding energy dispersion on a square lattice, and hopping matrix elements $t = 250$ meV, $t'/t = 0.4$, and $t''/t = 0.1$, in accordance with ARPES experiments [12]. The chemical potentials $\mu/t = -0.32$ and $\mu/t = -1.09$ describe the slightly underdoped n- and p-type cuprates, respectively, and the corresponding FS in the paramagnetic state are shown in Figs. 1(a) and 1(b). The second and third term of Eq. (1) give rise to a commensurate SDW and superconductivity, respectively. Here, the assumption of a SC pairing interaction in the (transverse) spin-flip channel is natural for the $d_{x^2-y^2}$-wave case where pairing is likely mediated by spin waves, and the longitudinal spin mode is gapped in the SDW state. For the s-wave case, this distinction is irrelevant since both pairing channels lead to identical results. Finally, while we take the interactions in Eq. (1) to be independent of each other, the question of whether they possess different microscopic origins, as is likely for the s-wave case, or originate from the same one, albeit renormalized differently by vertex corrections, as

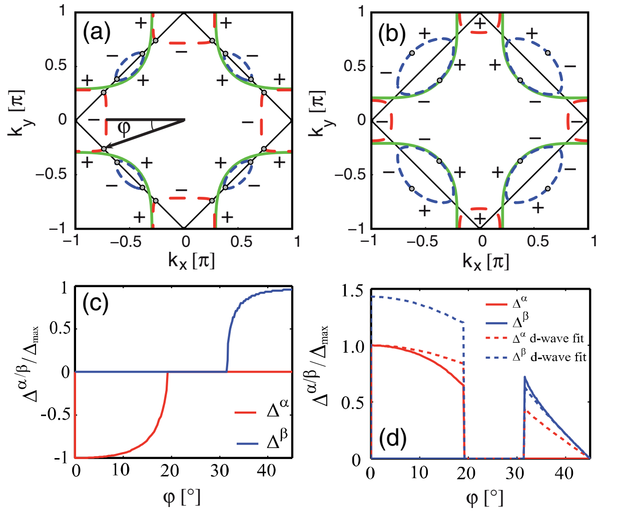

FIG. 1 (color online). FS (green solid lines) for the n-type (a) and p-type (b) cuprates ($x = 0.12$) in the paramagnetic state. In the SDW state ($W_0 = 0.1$ eV), the α band possesses electron pockets (red long-dashed area) and the β-band hole pockets (blue dashed area). The RBZ is shown as a thin black line. The phase of the (a) *unconventional s* and (b) $d_{x^2-y^2}$ SC OPs (of the c electrons) are denoted by $+/-$. (c),(d) Angular dependence of the SC OP in the *unconventional* s-wave and $d_{x^2-y^2}$-wave channels for n-type doping close to T_c.

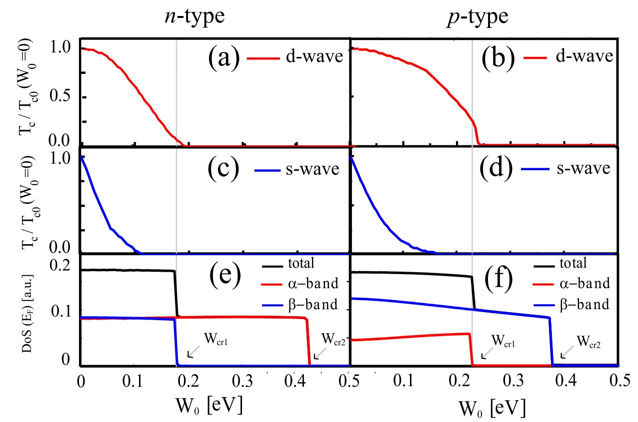

FIG. 2 (color online). T_c for *unconventional* s- and d-wave symmetries, as well as the DOS, as a function of W_0 at fixed chemical potential and for (a),(c),(e) n- and (b),(d),(f) p-type cuprates. We set $W_0 = 0.1$ eV, and for the n-type (p-type) cuprates $V_d = -2$ eV ($V_d = -1.2$ eV) and $V_s = -0.6$ eV ($V_s = -0.47$ eV).

suggested for the d-wave case [13], is beyond the scope of this study.

In what follows, we study the coexistence phase in the limit $T_c \ll T_{\rm SDW}$, and diagonalize the Hamiltonian in two steps. We first derive the electronic spectrum of the SDW state by decoupling the second term of Eq. (1) *via* a mean-field (MF) approximation, and then diagonalize it together with the first term using a unitary SDW transformation, introducing new quasiparticle operators $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$ for the two resulting bands with dispersions $E^{\alpha,\beta}_{\mathbf{k}} = \varepsilon^+_{\mathbf{k}} \pm \sqrt{(\varepsilon^-_{\mathbf{k}})^2 + W_0^2}$. Here, $W_0 = U/2\sum_{\mathbf{k},\sigma}\langle c^\dagger_{\mathbf{k}+\mathbf{Q},\sigma}c_{\mathbf{k},\sigma}\rangle \mathrm{sgn}\sigma$ is the SDW OP with ordering momentum $\mathbf{Q} = (\pi, \pi)$, and $\varepsilon^\pm_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} \pm \varepsilon_{\mathbf{k}+\mathbf{Q}})/2$. Because of imperfect nesting the α band exhibits electron pockets around $(\pm\pi, 0)$ and $(0, \pm\pi)$ while the β band possesses hole pockets around $(\pm\pi/2, \pm\pi/2)$, as shown in Figs. 1(a) and 1(b) for the n- and p-type cuprates, respectively. The size of these pockets decreases with increasing W_0. At $W_0 = W_{\rm cr1} \approx 0.23$ eV ($W_{\rm cr1} \approx 0.19$ eV), the hole (electron) pockets disappear first for the n-type (p-type) cuprates, followed by the vanishing of the electron (hole) pockets at $W_{\rm cr2} > W_{\rm cr1}$, as follows from the evolution of the density of states (DOS) in Figs. 2(e) and 2(f). For $W_0 > W_{\rm cr2}$, the system is an antiferromagnetic insulator (AFI). Note that $W_{\rm cr1,2}$ is solely determined by the band structure in the paramagnetic state.

Applying the unitary SDW transformation to the SC pairing interaction [third term in Eq. (1)], and subsequently performing a MF decoupling in the particle-particle channel, we keep only anomalous expectation values of the form $\langle\alpha^\dagger_{\mathbf{k},\uparrow}\alpha^\dagger_{-\mathbf{k},\downarrow}\rangle$ and $\langle\beta^\dagger_{\mathbf{k},\uparrow}\beta^\dagger_{-\mathbf{k},\downarrow}\rangle$. The resulting MF Hamiltonian is diagonalized by two independent Bogolyubov transformations, yielding the energy dispersions $\Omega^\gamma_{\mathbf{k}} = \sqrt{(E^\gamma_{\mathbf{k}})^2 + (\Delta^\gamma_{\mathbf{k}})^2}$ ($\gamma = \alpha, \beta$). The SC gaps, $\Delta^{\alpha,\beta}_{\mathbf{k}}$ are determined self-consistently from two coupled gap equations given by (at $T = 0$ K)

$$\Delta^\alpha_{\mathbf{k}} = -\sum_{\mathbf{p}\in\mathrm{RBZ}}\left[L^{\alpha\alpha}_{\mathbf{k},\mathbf{p}}\frac{\Delta^\alpha_{\mathbf{p}}}{2\Omega^\alpha_{\mathbf{p}}} + L^{\alpha\beta}_{\mathbf{k},\mathbf{p}}\frac{\Delta^\beta_{\mathbf{p}}}{2\Omega^\beta_{\mathbf{p}}}\right],$$
$$\Delta^\beta_{\mathbf{k}} = -\sum_{\mathbf{p}\in\mathrm{RBZ}}\left[L^{\beta\alpha}_{\mathbf{k},\mathbf{p}}\frac{\Delta^\alpha_{\mathbf{p}}}{2\Omega^\alpha_{\mathbf{p}}} + L^{\beta\beta}_{\mathbf{k},\mathbf{p}}\frac{\Delta^\beta_{\mathbf{p}}}{2\Omega^\beta_{\mathbf{p}}}\right], \qquad (2)$$

where $L^{\alpha\alpha}_{\mathbf{k},\mathbf{p}} = L^{\beta\beta}_{\mathbf{k},\mathbf{p}} = (V_{\mathbf{k}-\mathbf{p}}F^{u,v}_{\mathbf{k},\mathbf{p}} - V_{\mathbf{k}-\mathbf{p}+\mathbf{Q}}F^{v,u}_{\mathbf{k},\mathbf{p}})$, $L^{\alpha\beta}_{\mathbf{k},\mathbf{p}} = L^{\beta\alpha}_{\mathbf{k},\mathbf{p}} = (V_{\mathbf{k}-\mathbf{p}}N^{v,u}_{\mathbf{k},\mathbf{p}} - V_{\mathbf{k}-\mathbf{p}+\mathbf{Q}}N^{u,v}_{\mathbf{k},\mathbf{p}})$ with $N^{x,y}_{\mathbf{k},\mathbf{p}}, F^{x,y}_{\mathbf{k},\mathbf{p}} = u^2_{\mathbf{k}}x^2_{\mathbf{p}} \pm 2u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{p}}v_{\mathbf{p}} + v^2_{\mathbf{k}}y^2_{\mathbf{p}}$, x, $y = u$, v, $u_{\mathbf{k}}v_{\mathbf{k}} = W_0/2\Lambda_k$, and $u^2_{\mathbf{k}}$, $v^2_{\mathbf{k}} = [1 \pm \varepsilon^-_{\mathbf{k}}/\Lambda_k]/2$, with $\Lambda_k = \sqrt{(\varepsilon^-_{\mathbf{k}})^2 + W_0^2}$. The coupling of the OPs in the α and β bands results from terms of the form $\langle\alpha^\dagger_{\mathbf{k},\uparrow}\alpha^\dagger_{-\mathbf{k},\downarrow}\rangle\beta_{\mathbf{k}+\mathbf{q},\uparrow}\beta_{-\mathbf{k}-\mathbf{q},\downarrow}$ describing momentum dependent interband Cooper pair scattering in the MF Hamiltonian. Below, we use $V(\mathbf{k}, \mathbf{k}') = V_s$ and $V(\mathbf{k}, \mathbf{k}') = V_d\varphi_{\mathbf{k}}\varphi_{\mathbf{k}'}/4$ with $\varphi_{\mathbf{k}} = \cos k_x - \cos k_y$ as the pairing interactions in the s- and $d_{x^2-y^2}$-wave channel, respectively. We checked that in the limit considered here, i.e., $\Delta_{\rm sc} \ll W_0$, feedback effects of superconductivity on the SDW order are negligible, and that pairing terms of the form $\langle\alpha^\dagger_{\mathbf{k},\uparrow}\beta^\dagger_{-\mathbf{k},\downarrow}\rangle$ are irrelevant due to the FS mismatch between the α and β bands.

We begin by discussing the form of the SC OP. In the s-wave case, the SDW coherence factors entering the gap equation, Eq. (2), can be factorized and one finds $\Delta^\alpha_{\mathbf{k}} = D^\alpha_k\Delta^\alpha_0(u^2_{\mathbf{k}} - v^2_{\mathbf{k}})$ with $\Delta^\alpha_0 = F^\alpha - F^\beta$, and $\Delta^\beta_{\mathbf{k}}$ follows *via*

$\alpha \leftrightarrow \beta$. Here, $F^\gamma = V_s \sum_{\mathbf{p}} D^\gamma_{\mathbf{p}} (u^2_{\mathbf{p}} - v^2_{\mathbf{p}}) \frac{\Delta^\gamma_{\mathbf{p}}}{2\Omega^\gamma_{\mathbf{p}}} \tanh(\frac{\Omega^\gamma_{\mathbf{p}}}{2T})$ with $\gamma = \alpha, \beta$. Moreover, $D^\gamma_{\mathbf{k}}$ is unity if $|E^\gamma_{\mathbf{k}}| \leq \hbar\omega_D$, and zero otherwise, with ω_D being the Debye frequency. The above form of the SC gap yields three important results. First, the s-wave gap is dressed by the SDW coherence factors, and hence acquires line nodes along the RBZ boundary where $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 0$ [11]. Second, there is a π-phase shift between the SC OP in the α and β bands, as well as within the same band between momenta connected by $\mathbf{Q}$, i.e., $\Delta^\gamma_{\mathbf{k}} = -\Delta^\gamma_{\mathbf{k}+\mathbf{Q}}$. As a result, the s-wave symmetry of the SC OP is *unconventional*, as summarized in Fig. 1(a). Third, while Δ^γ_0 needs to be calculated self-consistently, its temperature dependence does not affect the momentum dependence of the SC OP.

In the d-wave case, the SDW coherence factors can again be factorized, and one finds from Eq. (2) $\Delta^\gamma_{\mathbf{k}} = \varphi_{\mathbf{k}}(\Delta^\gamma_0 + u_{\mathbf{k}} v_{\mathbf{k}} \Delta^\gamma_1)$ with $\Delta^\gamma_0 = F^\alpha_0 + F^\beta_0$, $\Delta^\alpha_1 = -\Delta^\beta_1 = F^\beta_1 - F^\alpha_1$. Here, $F^\gamma_0 = \frac{V_d}{4} \sum_{\mathbf{p}} D^\gamma_{\mathbf{p}} \varphi_{\mathbf{p}} \frac{\Delta^\gamma_{\mathbf{p}}}{2\Omega^\gamma_{\mathbf{p}}} \tanh(\frac{\Omega^\gamma_{\mathbf{p}}}{2T})$ and $F^\gamma_1 = V_d \sum_{\mathbf{p}} D^\gamma_{\mathbf{p}} \varphi_{\mathbf{p}} u_{\mathbf{p}} v_{\mathbf{p}} \frac{\Delta^\gamma_{\mathbf{p}}}{2\Omega^\gamma_{\mathbf{p}}} \tanh(\frac{\Omega^\gamma_{\mathbf{p}}}{2T})$. Since $|\Delta^\gamma_1| < |\Delta^\gamma_0|$, the SC OP in the α and β bands are in phase with no *additional* line nodes, in contrast to the s-wave case. The resulting phase of the SC OP is shown in Figs. 1(b). Note that the temperature evolution of the self-consistently determined $\Delta^\gamma_{0,1}$ can lead to changes in the momentum dependence of the d-wave OP. Finally, we find that for both SC symmetries, the SC OP evolves continuously into that of the paramagnetic state, obtained in the limit $W_0 \to 0$ in which the folded parts of the FS disappear. In particular, for the s-wave case, the same sign of the SC gap is restored over the entire (large) FS. Moreover, it follows from the gap equation, Eq. (2) and the subsequent discussion, that the renormalization of the SC order parameter due to the SDW order is tied to the symmetry of the pairing interaction alone, while its particular momentum dependence can only introduce higher harmonics into the superconducting gap.

We next study the dependence of T_c on the SDW order parameter, W_0. To this end, we solve Eq. (2) iteratively in the RBZ on a 500×500 lattice, setting $\omega_D = 0.1$ eV. This approach also yields the momentum dependence of the SC gap at $T \leq T_c$. A study of the temperature induced changes in the momentum dependence of the d-wave OP will be reserved for future work. In Figs. 2(a)–2(d) we present $T_c(W_0)/T_c(W_0 = 0)$ for fixed chemical potential as a function of W_0 for the $d_{x^2-y^2}$- and s-wave channels and the n- and p-type cuprates. In both channels, T_c decreases with increasing W_0. For the d-wave symmetry, we find that T_c becomes exponentially suppressed once W_0 exceeds W_{cr1}, where the first FS pockets disappear in the pure SDW state. In order to understand this rapid decrease of T_c around W_{cr1}, we present in Fig. 3 the dependence of the effective intra- and interband interaction projected onto the s- or d-wave channel, defined via $V^{\text{intra}}_{\text{eff}} = \sum'_{\mathbf{k},\mathbf{p}} L^{\alpha\alpha}_{\mathbf{k},\mathbf{p}} \phi_{\mathbf{k}} \phi_{\mathbf{p}}$ and $V^{\text{inter}}_{\text{eff}} = \sum'_{\mathbf{k},\mathbf{p}} L^{\alpha\beta}_{\mathbf{k},\mathbf{p}} \phi_{\mathbf{k}} \phi_{\mathbf{p}}$, where $\phi_{\mathbf{k}} = 1$ for the s-wave case, and $\phi_{\mathbf{k}} = \cos k_x - \cos k_y$ for the d-wave case. For the d-wave case [Fig. 3(a)], $V^{\text{intra}}_{\text{eff}}$ decreases with increasing W_0, due to the vanishing of the SDW coherence factors in $L^{\alpha\alpha}_{\mathbf{k},\mathbf{p}}$ for $\mathbf{k} - \mathbf{p} = \mathbf{Q}$, in agreement with previous results [13]. The same argument, however, does not apply to $V^{\text{inter}}_{\text{eff}} = 2 - V^{\text{intra}}_{\text{eff}}$ which increases with increasing W_0, thus stabilizing the SC state. Once the FS of one of the bands disappears at W_{cr1} (independent of whether these are the electron or hole pockets), the channel for interband Cooper pair scattering, and hence T_c, become rapidly suppressed and vanish slightly above W_{cr1} due to the finite Debye frequency. While one might expect to find an exponentially suppressed, but nonzero T_c as long as the system is metallic, i.e., for $W_{\text{cr1}} < W_0 < W_{\text{cr2}}$, its resolution is currently beyond our numerical capabilities. This strong suppression of T_c around W_{cr1} provides an explanation for the experimental observations that the emergence of hole pockets in n-type cuprates coincides approximately with the onset of superconductivity on the underdoped side [4,6,14]. For the s-wave case, T_c decreases more rapidly than for the d-wave case, and becomes smaller than our numerical resolution already for W_0 considerably smaller than W_{cr1}. This behavior does not arise from a change in the DOS, which remains almost unchanged for $W_0 < W_{\text{cr1}}$ [see Figs. 2(e) and 2(f)], but is due to a decreasing magnitude of the effective interaction, $V^{\text{intra}}_{\text{eff}} = -V^{\text{inter}}_{\text{eff}}$, with increasing W_0, as shown in Fig. 3(b). This decrease arises since the contributions to Eq. (2) coming from the folding of the original BZ onto the RBZ is repulsive and thus pair-breaking. In contrast, in the d-wave case, all contributions have the same sign and thus are attractive.

Finally, in Figs. 1(c) and 1(d), we present the momentum dependence of the SC gaps for both symmetries along the electron and hole FS pockets as depicted in Fig. 1(a). In agreement with the above discussion, the s-wave OP is *unconventional* in that it possesses a π-phase shift between the α and β bands, and line nodes along the RBZ boundary. In the $d_{x^2-y^2}$-wave case, the gap is nodeless on the α band and possesses a line node in the β band. While both SC OP possess line nodes, the slope of the gaps near the line nodes is considerably larger in the s-wave case, where it is determined by the Fermi velocity, than in the d-wave case, where it is set by the gap velocity, $v_\Delta = \partial\Delta_k/\partial k$ [see Fig. 1(c) and 1(d)]. As a result, the DOS in both cases scales linearly at small energies, however, with a much smaller slope in the s-wave than in the d-wave case. In

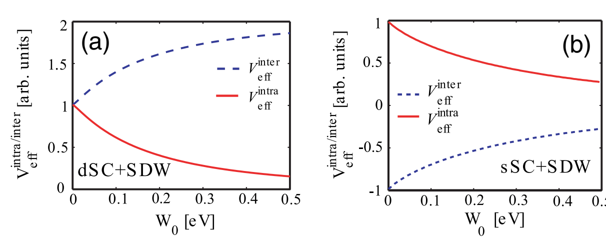

FIG. 3 (color online). The projected inter- and intraband effective interactions as a function of W_0.

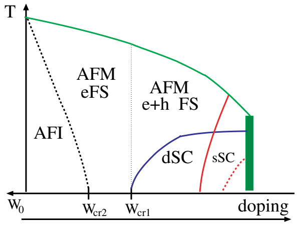

FIG. 4 (color online). Synopsis of our results shown as a schematic phase diagram. The system is an antiferromagnetic metal with electron pockets for $W_{cr1} < W_0 < W_{cr2}$ ($e-$ FS), and with electron and hole pockets for $W_0 < W_{cr1}$ ($e+h-$ FS).

thermodynamic measurements, it might therefore be difficult to distinguish between the *unconventional* s-wave OP discussed above, and a conventional, constant s-wave OP. We stress that the inclusion of the SDW coherence factors in the gap equation is crucial in determining the W_0 dependence of T_c, and momentum dependence of the SC OP. Our results therefore lead to new properties of the coexistence phase, not discussed in earlier studies [15,16].

The synopsis of our results is shown in form of a schematic phase diagram for n-type doping in Fig. 4. The system is an antiferromagnetic insulator for $W_0 > W_{cr2}$, and becomes metallic with the emergence of electron pockets in the α band at $W_0 = W_{cr2}$. While single-band superconductivity may occur for $W_{cr1} < W_0 < W_{cr2}$, the interaction necessary to achieve any appreciable T_c is necessarily large rendering this possibility unlikely in real systems. However, the appearance of hole pockets in the β band at W_{cr1} allows for the emergence of two-band superconductivity with d-wave symmetry (blue curve). Upon further decreasing W_0, the current experimental results suggest one of two scenarios. First, superconductivity with an s-wave symmetry remains the subdominant OP, implying $T^s_{c0} < T^d_{c0}$ even for $W_0 \to 0$ (red dashed curve). Second, if, as suggested by experiments, there is a transition of the SC symmetry from d to s wave (red solid curve), then this would naturally occur with decreasing W_0 if for $W_0 \to 0$ one has $T^s_{c0} > T^d_{c0}$. It is interesting to note that the experimentally observed transition in the n-type cuprates between a state with well-defined nodes to a state with large gapped phase space is consistent with this second scenario. Moreover, the observation of pair-breaking peaks in electronic Raman scattering which occur at similar energies in both B_{1g} and B_{2g} channels [14], would also suggest similar gap magnitudes, consistent with the form of the SC gap in the s-wave case [see Fig. 1(c)]. Clearly, further experiments are required to clarify the SC symmetry over the entire doping range.

In conclusion, we have studied the emergence of multiband superconductivity with s- and d-wave symmetries in the presence of an SDW state. In both cases, the momentum dependence of the SC OP is strongly renormalized by the SDW coherence factors. In the s-wave case, this leads to an unconventional OP which acquires line nodes along the boundary of the RBZ, and a π-phase shift between the α and β bands. For both symmetries, interband Cooper pair scattering stabilizes the superconducting order. Moreover, with increasing W_0, the SC state with s-wave symmetry is more strongly suppressed than that with d-wave symmetry. Our results are universally applicable to any (quasi-) two-dimensional system with commensurate SDW order in which the folding of the original BZ leads to separate FS pockets in both bands. Finally, we note that our results can be straightforwardly generalized to the coexistence of superconductivity with a commensurate charge or orbital density wave state [17].

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