Multiband Superconductivity in Spin Density Wave Metals

J.-P. Ismer$^{1,2}$, Ilya Eremin$^{1,2}$, Enrico Rossi$^{3,*}$, Dirk K. Morr$^3$, G. Blumberg$^4$

$^1$Max-Planck-Institut für Physik komplexer Systeme, 10117 Dresden, Germany
$^2$Institut für Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany
$^3$Department of Physics, University of Illinois at Chicago, Chicago, IL 60607, USA
$^4$Department of Physics and Astronomy, The State University of New Jersey, Piscataway, NJ 08854, USA

(Dated: July 9, 2009)

We study the emergence of multiband superconductivity with $s$- and $d$-wave symmetry on the background of 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.

PACS numbers: 74.72.-h, 75.40.Gb, 74.20.Rp, 74.20.Fg

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. Interestingly enough, 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 superconductivity was originally studied in Ref. [1], and has attracted significant interest recently in the context of MgB$_2$ [2] and the ferropnictides [3], in which in-phase and out-of-phase locking, respectively, of the OPs has been found.

The growing experimental evidence for the coexistence of superconductivity and a spin density wave (SDW) in the $n$-type (i.e., electron-doped) cuprates [1, 2, 3] of some heavy fermion [4] and organic superconductors [5] raises the question of how phase-locking occurs in such systems. This question is of particular interest in the $n$-type cuprates due to a possible transition of the SC symmetry from $d$-wave to $s$-wave with increasing doping. However, there remains experimental disagreement regarding this transition. While some measurements are consistent with a transition from a SC $d_{x^2-y^2}$-wave symmetry in the underdoped materials to either an $s$- or a $(d+is)$-wave symmetry in the optimally and overdoped ones, other results suggest the existence of a $d_{x^2-y^2}$-wave OP with higher harmonics for the entire doping range [4].

In this Letter, we study the emergence of two-band superconductivity with $d_{x^2-y^2}$- or $s$-wave symmetry on the background of a commensurate SDW state with imperfect nesting, using the $n$-type cuprates as a particular example. We show that the SDW coherence factors renormalize the momentum dependence of the SC gap. This yields an $s$-wave OP which is unconventional, in that it acquires a $\pi$-phase shift between the two bands, line nodes along the boundary of the reduced Brillouin zone (RBZ), and changes sign 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. In both cases, superconductivity is stabilized by interband Cooper pair scattering. With increasing SDW OP, the unconventional $s$-wave state is suppressed more quickly than the $d_{x^2-y^2}$-wave state. In the latter case, the vanishing of $T_c$ coincides approximately with the disappearance of the first of the two Fermi surfaces (FS). To demonstrate the generality of our results for other materials, we consider both $n$- and $p$-type doping, leading to different evolutions of the FS in the SDW state.

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

$$
\mathcal{H} = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_{k,k',\sigma} U c_{k\sigma}^\dagger c_{k+Q\sigma}^\dagger c_{k'+Q\sigma} c_{k'\sigma} + \sum_{k,\mathbf{Q},\sigma} V_{Q} c_{k+\mathbf{Q}\sigma}^\dagger c_{\mathbf{p}-\mathbf{Q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\sigma}
$$

(1)

where $c_{k\sigma}^\dagger$ ($c_{k\sigma}$) creates (annihilates) an electron with spin $\sigma$ and momentum $\mathbf{k}$. We consider a two-dimensional system with the normal state tight-binding energy dispersion $\varepsilon_k = -2t (\cos k_x + \cos k_y) + \Delta \cos k_x \cos k_y - 2t'' (\cos 2k_x + \cos 2k_y) - \mu$, with hopping matrix elements $t = 250$ meV, $t'/t = 0.4$, and $t''/t = 0.1$. 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 (b). The second and third terms in Eq. (1) give rise to a commensurate SDW and superconductivity, respectively. While it is generally assumed that both phases emerge from the same underlying interaction, its renormalization due to vertex corrections gives rise to two different effective interactions, $U$ and...
values of the form $\langle \alpha_{k,\sigma}^\dagger, \alpha_{-k,\sigma}^\dagger \rangle$ and $\langle \beta_{k,\sigma}^\dagger, \beta_{-k,\sigma}^\dagger \rangle$, and their complex conjugates. The resulting MF Hamiltonian can be diagonalized by two independent Bogoliubov transformations, yielding $\Omega_k \gamma = \sqrt{(E_k^\gamma)^2 + (\Delta_k^\gamma)^2}$ ($\gamma = \alpha, \beta$) as the energy dispersion of the two bands. The SC gaps, $\Delta_k^\alpha, \beta$ are determined self-consistently from two coupled gap equations given by (at $T = 0$ K)

$$
\Delta_k^\alpha = - \sum_{p \in RBZ} \left[ L_{k,p}^{\alpha \alpha} \frac{\Delta_p^\alpha}{2\gamma_p^\alpha} + L_{k,p}^{\beta \beta} \frac{\Delta_p^\beta}{2\gamma_p^\beta} \right],
$$

$$
\Delta_k^\beta = - \sum_{p \in RBZ} \left[ L_{k,p}^{\alpha \beta} \frac{\Delta_p^\alpha \Delta_p^\beta}{2\gamma_p^\alpha \gamma_p^\beta} \right],
$$

where $L_{k,p}^{\alpha \alpha} = L_{k,p}^{\beta \beta} = (V_{k-p} - E_{\alpha}^u - E_{\alpha}^v - Q^\nu_{k,p})$, $L_{k,p}^{\alpha \beta} = L_{k,p}^{\beta \alpha} = (V_{k-p} - E_{\alpha}^u - E_{\alpha}^v - Q^\nu_{k,p})$ with $N_{k,p}^\nu_{k,p} = u_{k,p}^u u_{k,p}^v \pm 2u_{k,p} u_{k,p}^u$, $x, y = u, v$, $u_{k,p}^u = \frac{1}{2} \frac{1 + \sqrt{(\varepsilon_k^\gamma + W_D^2)}}{\varepsilon_k^\gamma + W_D^2}$, and $\varepsilon_k = \frac{1}{2} \frac{1 + \sqrt{(\varepsilon_k^\gamma + W_D^2)}}{\varepsilon_k^\gamma + W_D^2}$.

The coupling of the OPs in the $\alpha$ and $\beta$ bands results from momentum dependent interband Cooper pair scattering described by terms of the form $\langle \alpha_{k,\sigma}^\dagger, \alpha_{-k,\sigma}^\dagger \rangle \beta_{k+\mathbf{Q},\sigma}^\dagger \beta_{-k-\mathbf{Q},\sigma}$. In the MF Hamiltonian, we use $V_{k, k'} = V_s$ and $V_{k, k'} = V_d \varphi_k \varphi_{k'}/4$ with $\varphi_k = \cos k_x - \cos k_y$ 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., $\Delta_{sc} \ll W_0$, feedback effects of superconductivity on the SDW order are negligible, and moreover, pairing terms of the form $\langle \alpha_{k,\sigma}^\dagger, \beta_{-k,\sigma}^\dagger \rangle$ are irrelevant due to the FS mismatch between the $\alpha$ and $\beta$ 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 $\Delta_k^\alpha = D_{k}^\alpha \Delta_0^\alpha (1 - v_{k,\sigma}^d)^2$ with $\Delta_0^\alpha = F_{\alpha} - F_{\beta}^\alpha$, and $\Delta_0^\beta$ follows via $\alpha \leftrightarrow \beta$. Here, $F_{\alpha} = V_s \sum_{\mathbf{p}} D_{p,\mathbf{k}}^\alpha (u_{k,p}^u - v_{k,p}^v) \frac{T_{\mathbf{p}}}{T_{\mathbf{p}}} \tanh (\frac{\gamma_{k,p}^\alpha}{2T})$ with $\gamma = \alpha, \beta$. Moreover, $D_{k}^\alpha$ is unity if $|E_{k,p}^\gamma| \leq \hbar \omega_D$, and zero otherwise, with $\omega_D$ 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 lines nodes along the RBZ boundary where $v_{k,\sigma} = 0$. Second, there is a $\pi$-phase shift between the SC OP in the $\alpha$- and $\beta$-bands, as well as within the same band between momenta connected by $\mathbf{Q}$, i.e., $\Delta_{k,\sigma}^\gamma = -\Delta_{k+\mathbf{Q},\sigma}^\gamma$. As a result, the $s$-wave symmetry of the SC OP is unconventional, as summarized in Fig. 1(a). Third, while $\Delta_0^\beta$ 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) $\Delta_k^\alpha = D_{k}^\alpha \Delta_0^\alpha (1 - v_{k,\sigma}^d)^2$ with $\Delta_0^\alpha = F_{\alpha} - F_{\beta}^\alpha$, and $\Delta_0^\beta$ follows via $\alpha \leftrightarrow \beta$. Here, $F_{\alpha} = V_s \sum_{\mathbf{p}} D_{p,\mathbf{k}}^\alpha (u_{k,p}^u - v_{k,p}^v) \frac{T_{\mathbf{p}}}{T_{\mathbf{p}}} \tanh (\frac{\gamma_{k,p}^\alpha}{2T})$ with $\gamma = \alpha, \beta$. Moreover, $D_{k}^\alpha$ is unity if $|E_{k,p}^\gamma| \leq \hbar \omega_D$, and zero otherwise, with $\omega_D$ 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 lines nodes along the RBZ boundary where $v_{k,\sigma} = 0$. Second, there is a $\pi$-phase shift between the SC OP in the $\alpha$- and $\beta$-bands, as well as within the same band between momenta connected by $\mathbf{Q}$, i.e., $\Delta_{k,\sigma}^\gamma = -\Delta_{k+\mathbf{Q},\sigma}^\gamma$. As a result, the $s$-wave symmetry of the SC OP is unconventional, as summarized in Fig. 1(a). Third, while $\Delta_0^\beta$ needs to be calculated self-consistently, its temperature dependence does not affect the momentum dependence of the SC OP.

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 $\Delta_k^\alpha = D_{k}^\alpha \Delta_0^\alpha (1 - v_{k,\sigma}^d)^2$ with $\Delta_0^\alpha = F_{\alpha} - F_{\beta}^\alpha$, and $\Delta_0^\beta$ follows via $\alpha \leftrightarrow \beta$. Here, $F_{\alpha} = V_s \sum_{\mathbf{p}} D_{p,\mathbf{k}}^\alpha (u_{k,p}^u - v_{k,p}^v) \frac{T_{\mathbf{p}}}{T_{\mathbf{p}}} \tanh (\frac{\gamma_{k,p}^\alpha}{2T})$ with $\gamma = \alpha, \beta$. Moreover, $D_{k}^\alpha$ is unity if $|E_{k,p}^\gamma| \leq \hbar \omega_D$, and zero otherwise, with $\omega_D$ 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 lines nodes along the RBZ boundary where $v_{k,\sigma} = 0$. Second, there is a $\pi$-phase shift between the SC OP in the $\alpha$- and $\beta$-bands, as well as within the same band between momenta connected by $\mathbf{Q}$, i.e., $\Delta_{k,\sigma}^\gamma = -\Delta_{k+\mathbf{Q},\sigma}^\gamma$. As a result, the $s$-wave symmetry of the SC OP is unconventional, as summarized in Fig. 1(a). Third, while $\Delta_0^\beta$ needs to be calculated self-consistently, its temperature dependence does not affect the momentum dependence of the SC OP.
The momentum dependence of the self-consistently determined $\Delta_0$ Figs. 1(b). Note that the temperature evolution of the case. The resulting phase of the SC OP is shown in FIG. 2: (color online) $T_{sc}$ symmetries, as well as the DOS, as a function of $W_0$ 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).

$$\varphi_k = (\Delta_{01}^u + u_k \Delta_{01}^v)$$ with $\Delta_{01}^u = F_0^a + F_0^b$, $\Delta_{01}^v = -\Delta_{01}^b = F_0^a - F_0^b$. Here, $F_0^\alpha = \frac{V}{T} \sum_{p} D_p^\alpha v_p^{\alpha} \tanh \left( \frac{\alpha \Omega}{2T} \right)$ and $F_1^\gamma = \frac{V}{T} \sum_{p} D_p^\gamma v_p^{\gamma} \tanh \left( \frac{\gamma \Omega}{2T} \right)$. Since $|\Delta_0^v| < |\Delta_0^u|$, the SC OP in the $\alpha$ and $\beta$-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. (1b), Note that the temperature evolution of the self-consistently determined $\Delta_{01}^u$ 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.

We next study the dependence of $T_c$ on the SDW order parameter, $W_0$. To this end, we linearize Eq. (2), and solve it iteratively in the RBZ on a 500 $\times$ 500 lattice, setting $\omega_D = 0.1$ eV. This approach also yields the momentum dependence of the SC gap at $T_c - 0^+$. 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) - (d) we present $T_c(W_0)/T_c(W_0 = 0)$ 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(a) the dependence of the effective intra- and interband interaction projected onto the s- or d-wave channel, defined via $V_{eff}^{intra} = \sum_{k,p} L_{k,p}^{\alpha \alpha} \phi_k \phi_p$ and $V_{eff}^{inter} = \sum_{k,p} L_{k,p}^{\alpha \beta} \phi_k \phi_p$ where $\phi_k = 1$ for the s-wave case, and $\phi_k = \cos k_x - \cos k_y$ for the d-wave case. For the d-wave case, $V_{eff}^{intra}$ decreases with increasing $W_0$, due to the vanishing of the SDW coherence factors in $L_{k,p}^{\alpha \alpha}$ for $k - p = Q$, in agreement with previous results [9]. The same argument, however, does not apply to $V_{eff}^{inter} = 2 - V_{eff}^{intra}$ 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 non-zero $T_c$ as long as the system is metallic, i.e., for $W_{cr1} < W_0 < W_{cr2}$, its resolutions 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 [11, 12, 10]. 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 $W_0 < W_{cr1}$ [see Figs. 2(e) and (f)], but is due to a decreasing magnitude of the effective interaction, $V_{eff}^{inter} = -V_{eff}^{intra}$, with increasing $W_0$, as shown in Fig. 3(b). This decrease arises since the contributions to Eq. (4) coming from the folding of the original BZ onto the RBZ, are pairbreaking. In contrast, in the d-wave case, these contributions have the same sign as those coming from the RBZ, and thus are not pairbreaking.

Finally, in Fig. 3(c) and (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 $\pi$-phase shift between the $\alpha$- and $\beta$-bands, and lines nodes along the RBZ boundary. In the $d_{x^2-y^2}$-wave case, the gap is nodeless on the $\alpha$-band and possess a line node in the $\beta$-band. While both the unconventional s- as well as the d-wave SC OP possess line nodes the slope with which the gaps increase as one moves away from 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 [see Fig. 1 (c) and (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 thermodynamic measurements, it is therefore 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 [11, 12].

The synopsis of our results, applied to the n-type cuprates, is shown in form of a schematic phase diagram 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 $\alpha$-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 highly unlikely for both SC symmetries in real systems. However, the appearance of hole pockets in the $\beta$-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 $T_{c0}^s < T_{c0}^d$ even for $W_0 \to 0$ (red dashed curve). Second, if, as suggest 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 $T_{c0}^d > T_{c0}^s$. 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 [10], 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, in particular, phase sensitive experiments are required to clarify the SC symmetry over the entire doping range.

In conclusion, we have studied the emergence of multi-band 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 $\pi$ phase shift between the $\alpha$ and $\beta$ 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 [13].

We thank A.V. Chubukov, M. Vavilov, and P. Grigoriev for the fruitful discussions. This work is supported by the Volkswagen Foundation (1/82203), NSF-DMR (0645461), the RMES Program (N 2.1.1/2985) (I.E.), and by the U.S. Department of Energy under Award No. DE-FG02-05ER46225 (D.M.). D.M. and G.B. would like to acknowledge the hospitality of the MPI-PKS where the final stages of this manuscript were completed.

[1] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. 3, 552 (1959); A. J. Leggett, Prog. Theor. Phys. 36, 901 (1966).
[2] G. Blumberg et al., Phys. Rev. Lett. 99, 227002 (2007).
[3] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. 101, 057003 (2008).
[4] N. P. Armitage, P. Fournier, and R. L. Greene, arXiv:0906.2931 and refs. therein.
[5] P. Li, F.F. Balakirev, and R.L. Greene, Phys. Rev. Lett. 99, 047003 (2007); W. Yu, J.S. Higgins, P. Bach, and R.L. Greene, Phys. Rev. B 76, 020503 (2007); Y. Dagan and R.L. Greene, Phys. Rev. B 76, 024506 (2007).
[6] H. Matsui et al., Phys. Rev. Lett. 94, 047005 (2005).
[7] C. Pfeiferer, arXiv:0905.2625 (unpublished).
[8] The Physics of Organic Superconductors and Conductors, A.G. Lebed (Ed.), Springer Series in Materials Science, Vol. 110, (2008).
[9] J.R. Schrieffer, X.G. Wen, and S. C. Zhang, Phys. Rev. B 39, 11663 (1989).
[10] M. M. Qazilbash et al., Phys. Rev. B 72, 214510 (2005).
[11] T. Das, R.S. Markiewicz, and A. Bansil, Phys. Rev. B 74, 020506(R) (2006).
[12] X.-Z. Yan, Q. Yuan, and C.S. Ting, Phys. Rev. B 74, 214521 (2006).

[13] J.-P. Ismer et al., unpublished.