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Interplay between magnetism and superconductivity in the iron pnictides

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We consider phase transitions and potential coexistence of spin-density-wave (SDW) magnetic order and extended s-wave (s^+) superconducting order within a two-band itinerant model of iron pnictides in which SDW magnetism and s^+ superconductivity are competing orders. We show that depending on parameters, the transition between these two states is either first order or involves an intermediate phase in which the two orders coexist. We demonstrate that such coexistence is possible when SDW order is incommensurate.

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I. INTRODUCTION

Iron-based pnictide superconductors—oxygen containing 1111 materials RFeAsO (R=La, Nd, Sm) and oxygen-free 122 materials AFe_2As_2 (A=Ba, Sr, Ca)—are at the center of experimental and theoretical activities at the moment because of high potential for applications and for the discovery of new mechanisms of superconductivity. Most of the parent compounds of Fe pnictides are magnetically ordered. Upon doping, magnetism disappears and superconductivity emerges, but the nature of this transition remains unclear. Some experiments on fluoride-doped 1111 materials indicate that the transition is first order,[1] some show behavior more consistent with a quantum-critical point separating magnetic and superconducting (SC) states,[2] and some show a coexistence of magnetism and SC in both classes of materials.[3–5]

It is by now rather firmly established that Fe pnictides are metals in a paramagnetic phase for all dopings, with two sets of (almost) doubly degenerate Fermi surface (FS) pockets—a hole pocket centered at (0,0) and an electron pocket centered at $\boldsymbol{\pi}=(\pi,\pi)$ in the folded Brillouin zone. To a good approximation, one hole FS and two electron FSs are near nested, i.e., the hole FS strongly overlaps with both electron FSs when shifted by π.[6–11] Like in chromium,[12] this nesting geometry is favorable to a spin-density-wave (SDW) ordering at $\boldsymbol{\pi}$ as the corresponding susceptibility logarithmically diverges at $T=0$,[12] and a small repulsive interaction in the particle-hole channel at momentum transfer $\boldsymbol{\pi}$ already gives rise to a SDW instability at $T=T_s$. If the interaction is attractive in a SC pairing channel, then the SC pairing susceptibility also diverges logarithmically at $T=0$ and the system becomes a SC at $T=T_c$, unless magnetism interferes.

Previous studies of an itinerant model of small electron and hole FSs have found that the *same* interaction, interband Josephson-type pair hopping, gives rise to a SDW order and to superconductivity with extended s-wave (s^+) symmetry of the SC order parameter [$\Delta(k)\propto\cos k_x+\cos k_y$ in the folded Brillouin zone],[13,14] leading to competition between the two orders. The full interactions in SDW and s^+ channels also involve interband forward scattering and intraband Hubbard interaction, respectively, and the full interaction is larger in the SDW channel.[13] Then at zero doping, which we associate with near-perfect nesting, the highest instability temperature is that of a SDW state. At a nonzero doping x, nesting is destroyed (either the hole or electron pocket gets relatively larger), and SDW susceptibility no longer diverges. Magnetic $T_s(x)$ then goes down with doping, and beyond a particular value of x the first instability upon cooling is at T_c into the s^+ SC state. The superconducting T_c is only weakly affected by doping.

The goal of the present work is to understand how the system evolves from a SDW antiferromagnet to an s^+ superconductor. For this we derive and solve a set of coupled nonlinear BCS-type equations for SC and SDW order parameters. We assume that the interactions in the two channels are comparable in strength and that $T_c\lesssim T_s$, where T_s is the transition temperature at zero doping, $T_s=T_s(x=0)$.

We report two results. First, when T_s/T_c is close to unity, the system displays second-order SDW and SC transitions at $T_s(x)$ and T_c, whichever is larger. The SDW state is commensurate, with momentum $\boldsymbol{\pi}$. At smaller T, the transition between SDW and SC upon changing x is first order, and there is no stable coexistence region (Fig. 1). This is similar to the phase diagram reported for $LaFeAsO_{1-x}F_x$ in Ref. 1. Second, when T_s/T_c gets larger, SDW order becomes incommensurate with momentum $\mathbf{Q}=\boldsymbol{\pi}+\mathbf{q}$ below some $T_s^*=0.56T_s>T_c$ (a SDW_q phase[15,16]). We argue that in this situation SDW_q and SC states coexist in some range of T and δ. The coexistence region is initially confined to a small region below T_c, while at lower T the system still displays a first-order transition between a commensurate SDW and SC states. As the ratio T_s/T_c increases, the coexistence region extends down to lower T and eventually reaches $T=0$ (Figs. 2 and 3).

An incommensurate SDW_q state at finite dopings has been studied in connection with theoretical models for chromium and its alloys by Rice[15] and others,[12] and in connection to pnictides by Cvetkovic and Tesanovic.[16] Such a state is a magnetic analog of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state[17] for which doping plays the same role as a magnetic field in a paramagnetically limited superconductor.[15] We found that such a SDW_q state exists alone in some T range above T_c, but at smaller T it exists only in combination with s^+ superconductivity.

II. MODEL AND EQUATIONS

We neglect double degeneracy of hole and electron states, which does not seem to be essential for the pnictides,[14,18] and consider a weak-coupling model with two families of fermions, near one hole and one electron FSs of small and near-

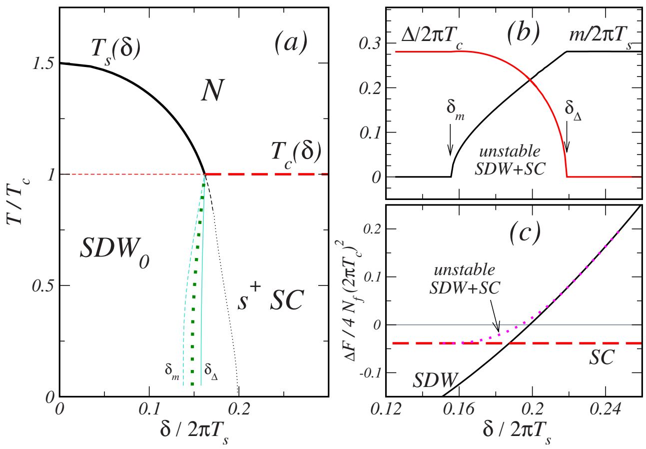

FIG. 1. (Color online) (a) Phase diagram for $T_s/T_c=1.5$ as a function of δ controlled by doping. Thick solid and dashed lines are second-order SDW and SC transitions at $T_s(\delta)$ and T_c, and dotted line—first-order transition between commensurate SDW_0 and s^+ SC. Thin lines—physically inaccessible transitions. The pure magnetic $T_s(\delta)$ line follows the curve of "paramagnetically limited superconductivity." The superconducting T_c is independent of δ in our model. Light lines, denoted δ_Δ and δ_m, are instability lines of SC and SDW states. (b) SDW and SC order parameters and (c) free energy for SDW, SC, and unstable mixed phases at $T/T_c=0.1$.

equal sizes. The free-electron part of the Hamiltonian is $\mathcal{H}_0 = \Sigma_{\mathbf{k}}[\xi_c(\mathbf{k})c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha}+\xi_f(\mathbf{k})f^\dagger_{\mathbf{k}\alpha}f_{\mathbf{k}\alpha}]$, where operators $c_{\mathbf{k}\alpha}$ and $f_{\mathbf{k}\alpha}$ describe fermions near (0,0) and (π,π), respectively (the momentum $\mathbf{k}$ in $f_{\mathbf{k}\alpha}$ is a deviation from $\boldsymbol{\pi}$). The dispersions $\xi^{f,c}(\mathbf{k}) = \pm\xi_{\mathbf{k}}+\delta$, where $\xi_{\mathbf{k}}=v_F(k-k_F)$, and δ measures a deviation from a perfect nesting and may be tuned by doping (x) or pressure. The four-fermion part contains interactions in SDW and SC channels and in mean-field (BCS) approximation reduces to the effective quadratic form $\mathcal{H} = \frac{1}{2}\Sigma_{\mathbf{k}\alpha\beta}\bar{\Psi}_{\mathbf{k}\alpha}\hat{\mathcal{H}}\Psi_{\mathbf{k}\beta}$, with $\bar{\Psi}_{\mathbf{k}\alpha}=(c^\dagger_{\mathbf{k}\alpha},c_{-\mathbf{k}\alpha},f^\dagger_{\mathbf{k}+\mathbf{q}\alpha},f_{-\mathbf{k}-\mathbf{q}\alpha})$ (Ψ is a conjugated column)

$$\hat{\mathcal{H}} = \left(\begin{array}{cc|cc} \xi^c(\mathbf{k}) & \Delta^c i\sigma^y_{\alpha\beta} & m_{\mathbf{q}}\sigma^z_{\alpha\beta} & 0 \\ -\Delta^{*c}i\sigma^y_{\alpha\beta} & -\xi^c(-\mathbf{k}) & 0 & -m_{\mathbf{q}}\sigma^z_{\alpha\beta} \\ \hline m^*_{\mathbf{q}}\sigma^z_{\alpha\beta} & 0 & \xi^f(\mathbf{k}+\mathbf{q}) & \Delta^f i\sigma^y_{\alpha\beta} \\ 0 & -m^*_{\mathbf{q}}\sigma^z_{\alpha\beta} & -\Delta^{*f}i\sigma^y_{\alpha\beta} & -\xi^f(-\mathbf{k}-\mathbf{q}) \end{array}\right). \tag{1}$$

The two diagonal blocks of the matrix $\hat{\mathcal{H}}$ include the s^+ SC order parameter $\Delta^c=-\Delta^f=\Delta$ for two FS pockets, and two off-diagonal blocks contain SDW parameter $m_{\mathbf{q}}$; $\xi^f(\mathbf{k}+\mathbf{q}) = \xi_{\mathbf{k}}+\delta+\mathbf{v}_F\mathbf{q}$ for $q \ll k_F$. The values of $m_{\mathbf{q}}$ and Δ are determined by conventional self-consistency equations

$$m_{\mathbf{q}} = V^{\mathrm{SDW}}\sum_{\mathbf{k}} \sigma^z_{\alpha\beta}\langle f^\dagger_{\mathbf{k}+\mathbf{q}\alpha}c_{\mathbf{k}\beta}\rangle, \tag{2a}$$

$$\Delta = V^{\mathrm{SC}}\sum_{\mathbf{k}} (-i\sigma^y)_{\alpha\beta}\langle c_{-\mathbf{k}\alpha}c_{\mathbf{k}\beta}\rangle, \tag{2b}$$

where the sums are confined to only the (0,0) FS pocket, V^{SDW} and V^{SC} are the couplings in the particle-hole SDW channel and in the particle-particle SC s^+ channel.[13] Taken alone, V^{SC} leads to an s^+ SC state with critical temperature T_c, while V^{SDW} leads to a SDW state with transition temperature T_s at $\delta=0$. The SDW order yields a real magnetization $M(R)\sim\cos\mathbf{QR}$ at wave vector $\mathbf{Q}=\boldsymbol{\pi}+\mathbf{q}$. The couplings V^{SDW} and V^{SC} undergo logarithmic renormalizations from fermions with energies between ϵ_F and much larger bandwidth W and flow to the same value when $W/\epsilon_F\to\infty$.[13] For any finite W/ϵ_F, V^{SDW} is the largest of the two.

The correlators in Eq. (2) are related to components of the Green's function $\hat{G}(\mathbf{k},\tau)_{\alpha\beta}=-\langle T_\tau\Psi(\tau)_{\mathbf{k}\alpha}\bar{\Psi}(0)_{\mathbf{k}\beta}\rangle$, defined as the inverse of $\hat{G}^{-1}=i\varepsilon_n-\hat{\mathcal{H}}$, where $\varepsilon_n=\pi T(2n+1)$ are the Matsubara frequencies. The Green's functions in Eq. (2) can be explicitly integrated over $\xi_-=[\xi^f(\mathbf{k}+\mathbf{q})-\xi^c(\mathbf{k})]/2=\xi_{\mathbf{k}}+\frac{1}{2}\mathbf{v}_F\mathbf{q}$. Removing the coupling constants $2N_f|V^{\mathrm{SC}}|$ and $2N_f|V^{\mathrm{SDW}}|$ (N_f is the density of states at the Fermi surface per

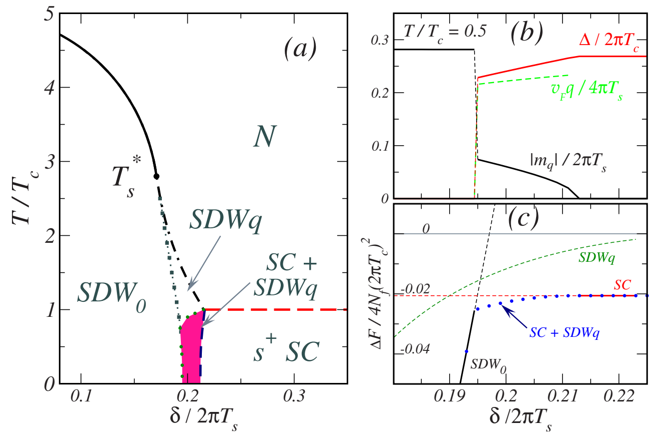

FIG. 2. (Color online) (a) Same as in Fig. 1 but for $T_s/T_c=5$. An incommensurate SDW_q order appears below $T_s(\delta)$ once it becomes smaller than $T^*_s=0.56T_s>T_c$. Below T_c, a new mixed phase appears in which incommensurate SDW_q order coexists with SC. At small T, there is no SDW_q state without superconductivity. (b), (c) The transitions into the mixed state are second order from a SC state and first order from a commensurate SDW_0 state. The free energy now shows that near $\delta/2\pi T_s=0.2$ a mixed state has lower energy than the two pure states.

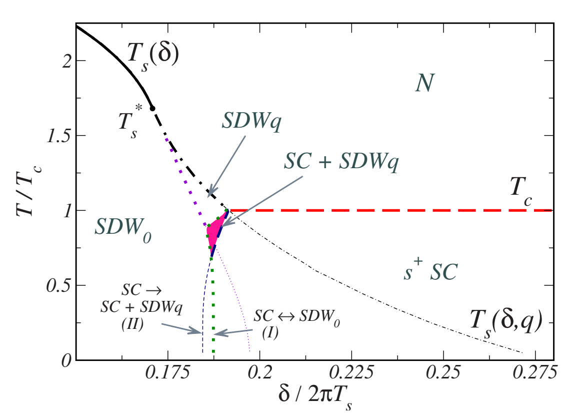

FIG. 3. (Color online) Same as in the previous two figures, but for intermediate $T_s/T_c=3$. Mixed phase appears only in a tiny region near the point where T_c and $T_s(\delta,q)$ cross. At smaller T, the system still displays a first-order transition (dotted line) between a commensurate SDW_0 state and a SC state.

spin) and the upper cutoffs of the frequency sums in favor of the transition temperatures $T_{c,s}$, we obtain from Eq. (2)

$$\ln\frac{T}{T_c} = 2\pi T \sum_{n>0} \mathrm{Re}\left\langle \frac{(E_n + i\delta_{\mathbf{q}})/E_n}{\sqrt{(E_n + i\delta_{\mathbf{q}})^2 + m_q^2}} - \frac{1}{|\varepsilon_n|} \right\rangle \tag{3a}$$

and

$$\ln\frac{T}{T_s} = 2\pi T \sum_{n>0} \mathrm{Re}\left\langle \frac{1}{\sqrt{(E_n + i\delta_{\mathbf{q}})^2 + m_q^2}} - \frac{1}{|\varepsilon_n|} \right\rangle, \tag{3b}$$

where angle brackets denote the Fermi surface average, $E_n=\sqrt{\varepsilon_n^2+|\Delta|^2}$, $\delta_{\mathbf{q}}=[\xi^c(\mathbf{k})+\xi^f(\mathbf{k}+\mathbf{q})]/2=\delta+\frac{1}{2}\mathbf{v}_F\mathbf{q}$, and T_s and T_c are solutions of the linearized equations, respectively, for SDW ($\Delta=\delta=0$) and SC ($m_q=0$). This system of equations is solved to find all possible uniform SC and (generally) incommensurate SDW states.

Note that for $\Delta=0$, Eq. (3b) for SDW order coincides with the gap equation for a paramagnetically limited superconductor with m_q instead of a superconducting order parameter, δ instead of magnetic field H, and incommensurateness vector $\mathbf{q}$ instead of the total momentum of a Cooper pair.[12,15,16]

We will also need the free energy $F(\Delta,m_q)$ for these mean-field order parameters to pick out the state with the lowest F. We find $F(\Delta,m_q)$ in two complementary approaches: by differentiating with respect to interaction parameters[19] and by using Luttinger-Ward functional and extending to a finite m_q the derivation of the condensation energy for a BCS SC.[20,21] Both methods yield

$$\begin{aligned}\frac{\Delta F(\Delta,m_q)}{4N_f} &= \frac{|\Delta|^2}{2}\ln\frac{T}{T_c} + \frac{m_q^2}{2}\ln\frac{T}{T_s} \\ &\quad - \pi T\sum_{\varepsilon_n} \mathrm{Re}\Big\langle \sqrt{(E_n + i\delta_{\mathbf{q}})^2 + m_q^2} \\ &\quad - |\varepsilon_n| - \frac{|\Delta|^2}{2|\varepsilon_n|} - \frac{m_q^2}{2|\varepsilon_n|}\Big\rangle,\end{aligned} \tag{4}$$

where $\Delta F(\Delta,m_q)=F(\Delta,m_q)-F(0,0)$. For each T and δ we solve self-consistency Eq. (3) for Δ and m_q for various q's and select the solution with the smallest free energy.

III. RESULTS

The results of our calculations are shown in Figs. 1–3. We find that the system behavior depends on the ratio $T_s/T_c > 1$. When this ratio is close to unity, the system only develops a commensurate SDW order with $m_{q=0}=m$ (see Fig. 1). The SDW and SC transitions at $T_s(\delta)$ and T_c [which is independent of δ; see Eq. (3a) with $m_{\mathbf{q}}=0$] are of second order. Below the tricritical point at which $T_s(\delta)=T_c$, the transition between the states ($m\neq 0,\Delta=0$) and ($\Delta\neq 0,m=0$) is first order [Fig. 1(c)] and there is no region where m and Δ coexist.

The first-order transition at $T=0$ can be understood analytically. Setting $q=0$ and subtracting Eq. (3a) from Eq. (3b), we obtain for small δ,

$$\ln\frac{T_s}{T_c} = \frac{\delta^2}{m^2 + \Delta^2}. \tag{5}$$

Setting $\Delta^2=0$ yields a linearized SC gap [Eqs. (3)]. We see that in the presence of a nonzero $m_0=m(T=0)$, Δ first appears at $\delta_\Delta^2=m_0^2\ln(T_s/T_c)$. Similarly, for nonzero Δ_0, the SDW order grows from $\delta_m^2=\Delta_0^2\ln(T_s/T_c)$. Their ratio $\delta_\Delta/\delta_m=m_0/\Delta_0=T_s/T_c>1$, implying that Δ nucleates in the SDW phase at a higher doping whereas m develops in the SC state at lower δ [see Fig. 1(b)]. This contradicts the very fact that the SDW state is stable at smaller dopings than the SC state. The solution with $\Delta,m\neq 0$ then grows in the "wrong" direction of δ, and we explicitly verified that it has a higher energy than pure states and therefore is unstable [see Fig. 1(c)]. As both $q=0$ SDW and SC gaps cover the entire FS, the absence of the state where the two coexist implies that fully gapped SC and SDW orders cannot coexist, and only one of these two states is present at a given δ. A first-order transition between the SDW and SC states occurs at $\delta=\delta_{cr}$, when their free energies coincide. This happens when $-m_0^2/2+\delta_{cr}^2=-\Delta_0^2/2$; hence,

$$\delta_{cr}^2 = \frac{m_0^2}{2}\left[1 - \left(\frac{T_c}{T_s}\right)^2\right], \tag{6}$$

which is in between the two second-order instability points δ_m and δ_Δ.

The situation changes when T_s/T_c gets larger, and there appears a wider range of dopings where $T_s(\delta)>T_c$. If only commensurate magnetic order SDW_0 was possible, magnetic transition would become first order below a certain $T_s^*=0.56T_s$, which at large enough T_s/T_c becomes greater than T_c. In reality, the system avoids a first-order transition and extends the region of magnetic order by forming an incommensurate SDW_q state below T_s^* (see Figs. 2 and 3).[12,15,16] The transition from the normal state to the SDW_q state is second order, and the subsequent transition to the commensurate SDW_0 state is first order. Once m_q is developed, the actual solution is more complex and includes harmonics with multiple q,[12] but we ignore this for now.

Our main result is the prediction of coexistence of incommensurate SDW_q order with an s^+ SC order below T_c. Physically, the key reason for the appearance of such a phase is that incommensurate SDW_q order does not gap the excitations on the entire FS—the system remains a metal albeit with a modified, smaller FS.[16,22,23] Once the Fermi surface survives, an attractive pairing interaction gives rise to SC below T_c. Alternatively speaking, for SDW_q order, some parts of the FS become inaccessible to magnetic "pairing," and the SC order takes advantage of this (cf. Refs. 24 and 25).

At large enough T_s/T_c, the coexistence phase extends to $T=0$ (see Fig. 2 for $T_s/T_c=5$). In Fig. 2(b) we show order parameters at $T=T_c/2$. The transition from a commensurate SDW state into a mixed state is first order with both Δ and the amount of incommensurateness q jumping to finite values. The transition from a SDW_q state into a mixed state as well as the transition from a mixed state into a pure SC state are of second order with m_q gradually vanishing. Figure 2(c) shows the corresponding free energies of all states. Comparing it with Fig. 1(c) we see that now the SC state becomes unstable at a higher δ and the mixed state now has lower energy than pure SC or SDW states.

The behavior at somewhat smaller T_s/T_c is intermediate between those in Figs. 1 and 2. In Fig. 3 we show the phase diagram for intermediate $T_s/T_c=3$. We still have $T^*>T_c$, and the mixed phase still exists, but it now appears only as a small pocket near the point where $T_s(\delta)=T_c$. At smaller T, the system shows the same behavior as at $q=0$, i.e., a first-order transition between commensurate SDW and SC states.

IV. CONCLUSIONS

To conclude, in this Rapid Communication we considered the interplay between itinerant SDW and s^+ SC orders in a two-band model for the pnictides. The SDW magnetism emerges first at T_s for $\delta=0$, where δ is the measure of FS mismatch $[T_s=T_s(0)]$, but $T_s(\delta)$ decreases when the FS nesting is reduced by doping or pressure. Superconductivity emerges at T_c which weakly depends on doping. We assume $T_s>T_c$, but T_c becomes the highest at large dopings. We found that the transition between s^+ SC and SDW is first order, if T_s and T_c are close, and the SDW order is commensurate. At larger T_s/T_c, the system develops an incommensurate SDW_q order at some nonzero δ. Such a state does not gap the whole FS and allows for a coexistence of magnetism and superconductivity. The mixed phase first appears in a small pocket near $T_s(\delta)=T_c$ but extends down to $T=0$ as T_s/T_c increases. The transition from the mixed phase to a commensurate SDW phase is first order, and that to the SC phase is second order.

This phase diagram is in qualitative agreement with experiments on the pnictides,[1–5] which is a good indication that our mean-field model captures the basic physics of the transformation from an SDW to a SC state upon doping. For quantitative in-depth comparisons one has to include fine details of the electronic structure, e.g., the presence of two hole and two electron FSs and the fact that even the undoped samples do not have a perfect nesting, $\delta\neq 0$. This, however, requires more extensive numerical investigation.

Finally, here we only considered a mixed state with a uniform SC order (zero total momentum of a pair). In principle, an inhomogeneous SC state (a true FFLO state) is possible because incommensurate SDW_q order breaks the symmetry between FS points with $\mathbf{k}$ and $-\mathbf{k}$. This, however, should not change the phase diagram as a nonuniform SC state may only exist at large enough m_q, i.e., near a first-order transition into a commensurate SDW phase, possibly extending a mixed state into the SDW_0 region. For large m_q, an approximation by a single q is not sufficient. A more sophisticated analysis in this region is called for.

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