

Coexistence between superconducting and spin density wave states in iron-based superconductors: Ginzburg–Landau analysis

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 Supercond. Sci. Technol. 23 054011

(<http://iopscience.iop.org/0953-2048/23/5/054011>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 216.165.143.4

The article was downloaded on 28/05/2010 at 20:54

Please note that [terms and conditions apply](#).

Coexistence between superconducting and spin density wave states in iron-based superconductors: Ginzburg–Landau analysis

M G Vavilov¹, A V Chubukov¹ and A B Vorontsov²

¹ Department of Physics, University of Wisconsin, Madison, WI 53706, USA

² Department of Physics, Montana State University, Bozeman, MT 59717, USA

Received 17 December 2009, in final form 5 February 2010

Published 23 April 2010

Online at stacks.iop.org/SUST/23/054011

Abstract

We consider the interplay between superconducting (SC) and commensurate spin-density-wave (SDW) orders in iron pnictides by analyzing a multiple-order Ginzburg–Landau free energy. We are particularly interested in whether the doping-induced transition between the two states is first order or whether the two pure phases are separated by an intermediate phase with coexisting SC and SDW orders. For perfect nesting, the two orders do not coexist, because SDW order, which comes first, gaps the full Fermi surface leaving no space for SC to develop. When nesting is not perfect due to either ellipticity of electron bands or doping-induced difference in chemical potentials for holes and electrons, SDW order still leaves modified Fermi surfaces for not too strong SDW magnetism and the SC order may develop. We show that the two orders coexist only when certain relations between ellipticity and doping are met. In particular, in a compensated metal, ellipticity alone is not sufficient for coexistence of the two orders.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In the phase diagram of recently discovered iron-based pnictide materials superconducting (SC) and spin-density-wave (SDW) states are close neighbors [1]. The interplay between these two orders has been the focus of numerous experimental and theoretical studies. Superconductivity and magnetic ordering are normally mutually exclusive states of electronic systems, and a first-order transition between SC and SDW orders has been reported in some pnictides, e.g. for $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$ [2]. However, recent nuclear magnetic resonance (NMR) [3], specific heat, susceptibility, Hall coefficient [4, 5] and neutron scattering experiments [6] on $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ indicate that SDW and SC phases coexist over some doping range.

The electronic spectrum of the pnictides results in two hole pockets centered at $(0, 0)$ and two electron pockets centered at $(0, \pi)$ and $(\pi, 0)$ in the unfolded Brillouin zone (BZ) [7–16]. Multiple Fermi surfaces (FSs) create a number of different possibilities [17, 18] for electron ordering in

the form of SDW, charge-density-wave (CDW) states and a superconducting state with extended s-wave symmetry in which the gaps on the hole and electron FSs are of different signs (an s^{+-} state) [16, 19–25]. When one order develops, electron states are reorganized and either favor or hinder the development of other orders. Specifically, in the case of a compensated metal and a perfect nesting (all FSs are cylinders of equal radii) an SDW order comes first and completely gaps all Fermi surfaces, preventing the system from developing SC or CDW orders. The situation is different, however, if electron and hole pockets are not ideal circles and intersect at certain points when the two FSs are centered at the same momentum. This is what is actually observed in the pnictides: hole FSs have circular cross sections, while electron FSs have elliptic ones. In this case the SDW order modifies the Fermi surfaces and leaves ungapped electronic states that may develop superconducting instability [26]. Another possibility for coexistence is the formation of an SDW order with an incommensurate wavelength on circular hole and electron

FSs of different radii. Again, strong nesting of electronic states occurs only on a small part of the FS, leaving other parts available for the SC pairing [27]. The persistence of the (modified) FS into the SDW phase, however, only implies that a superconducting order may develop within the SDW phase [26, 27]. The relative thermodynamic stability of different phases (SC, SDW, SC + SDW) can only be determined from analysis of the free energy.

In the present paper we report an analytical study of the nature of the phase transition between SC and SDW states in iron pnictide materials. We demonstrate that SDW and extended s^{+-} SC orders may coexist, but only in a situation when both ellipticity *and* a difference $\delta\mu$ in electron and hole chemical potentials are present. If either ellipticity or $\delta\mu$ are small, SDW and SC states are separated by a first-order phase transition. In particular, if the system remains a compensated metal, the transition is first order, even when electron bands are elliptical.

We also discuss the s^{++} order parameter (ordinary s -wave). The authors of [6] argued that for this order parameter coexistence is impossible for any FS geometry. The argument was based on the observation that the transition is strongly first order at a perfect nesting, and on numerical results for a finite ellipticity and a finite $\delta\mu$. We analyzed this issue analytically and confirmed that the transition between SDW and s^{++} SC states is indeed first order.

We follow earlier works [6, 26, 27] and consider a simplified model with one circular hole and one elliptical electron FS, separated by, for example, $(0, \pi)$ in the unfolded BZ or (π, π) in the folded zone. This momentum is also the ordering momentum of the commensurate SDW state [28, 29]. The inclusion of another hole and electron FSs does not affect either superconductivity [21–24, 30, 31] or magnetic order [32–36]. We will also assume that SDW order at a finite doping remains commensurate. This is true if SDW and SC instabilities, when taken separately, occur not far from each other (we set the condition below). If this condition is not met, SDW order becomes incommensurate even before SC develops, and the interplay between SDW and superconductivity has to be re-evaluated. For circular FSs this has been done in [24, 27] and the result is that an incommensurate SDW order and an s^{+-} superconductivity do coexist, at least near T_s .

2. General form of the free energy

We first present a general analysis of the free energy for a system characterized by two scalar order parameters, which we denote as Δ for an SC order and M for an SDW order. We assume that Δ has the same momentum-independent magnitude, but may have either equal signs (s^{++} state) or opposite signs (s^{+-} state) on the hole and electron FSs. We comment below on the case when superconducting gaps on hole and electron FSs have different magnitudes.

The free energy $\mathcal{F}(\Delta, M)$ to the fourth order in parameters (Δ, M) can be written in the form

$$\mathcal{F} = -\alpha_s \Delta^2 - \alpha_m M^2 + A \Delta^4 + B M^4 + 2C \Delta^2 M^2. \quad (1)$$

Below we find from microscopic considerations how all five prefactors in equation (1) depend on doping and ellipticity. But for the moment we simply assume that α_s , A , B and C are positive constants and α_m varies from $\alpha_m > \alpha_s$ to $\alpha_m = 0$. This mimics the system behavior upon doping, see section 3.

The free energy extrema are found for three different cases.

- Pure SC state, $M = 0$, $\partial\mathcal{F}/\partial\Delta = 0$, is given by

$$\mathcal{F}_s = -\frac{\alpha_s^2}{4A}, \quad \Delta^2 = \frac{\alpha_s}{2A}. \quad (2)$$

- Pure SDW state, $\Delta = 0$, $\partial\mathcal{F}/\partial M = 0$, is given by

$$\mathcal{F}_m = -\frac{\alpha_m^2}{4B}, \quad M^2 = \frac{\alpha_m}{2B}. \quad (3)$$

- Mixed SC + SDW state, $\Delta \neq 0$, $M \neq 0$, found from the conditions $\partial\mathcal{F}/\partial\Delta = \partial\mathcal{F}/\partial M = 0$, which, when solved for Δ and M , give

$$M^2 = \frac{\alpha_m A - \alpha_s C}{2(AB - C^2)}, \quad \Delta^2 = \frac{\alpha_s B - \alpha_m C}{2(AB - C^2)}. \quad (4)$$

The corresponding free energy is

$$\begin{aligned} \mathcal{F}_c &= \mathcal{F}_s - \frac{1}{4A} \frac{(\alpha_m A - \alpha_s C)^2}{AB - C^2} \\ &= \mathcal{F}_m - \frac{1}{4B} \frac{(\alpha_s B - \alpha_m C)^2}{AB - C^2}. \end{aligned} \quad (5)$$

These solutions are only meaningful when both $M^2 > 0$ and $\Delta^2 > 0$.

To describe the system behavior with decreasing α_m , we also introduce the free energy $\mathcal{F}(M)$ as a function of M only, obtained from equation (1) by substituting

$$\Delta^2(M) = \frac{\alpha_s}{2A} - \frac{C}{A} M^2 \quad (6)$$

as a solution to $\partial\mathcal{F}/\partial\Delta = 0$. This gives

$$\begin{aligned} \mathcal{F}(M) &= \mathcal{F}_s + \gamma M^2 + \beta M^4, \quad \gamma = -\alpha_m + \alpha_s C/A, \\ \beta &= B - C^2/A. \end{aligned} \quad (7)$$

The condition $\Delta^2(M) \geq 0$ determines the upper limit on a value of the SDW order, $M_m^2 = \alpha_s/(2C)$. The extremum of $\mathcal{F}(M)$, if it exists below M_m , yields the free energy in the coexistence state, \mathcal{F}_c . Equation (5) shows that the free energy in the mixed state is the lowest of the three when $\chi \equiv AB - C^2$ is positive or $\beta > 0$ in equations (7).

First, we consider the case $\chi > 0$. Combining $AB - C^2 > 0$ with the conditions that the mixed phase only exists when $\Delta^2 > 0$ and $M^2 > 0$, we show the behavior of values $\mathcal{F}_{s,m,c}$ as functions of α_m in the top panel of figure 1. We also plot $\mathcal{F}(M)$ for three values of α_m : (A) $\alpha_m = \alpha_s B/C$, (B) $\alpha_m = \alpha_s \sqrt{B/A}$ and (C) $\alpha_m = \alpha_s C/A$. The triangle symbol (Δ) in these plots at $M = M_m$ is the value of \mathcal{F}_m from equations (3) corresponding to the extremum of the free energy at $\Delta \equiv 0$. In general, \mathcal{F}_m is different from $\mathcal{F}(M_m)$, both of which are obtained from equation (1) with $\Delta = 0$, but $M = \sqrt{\alpha_m/2B}$ or $M = \sqrt{\alpha_s/2C}$, respectively.

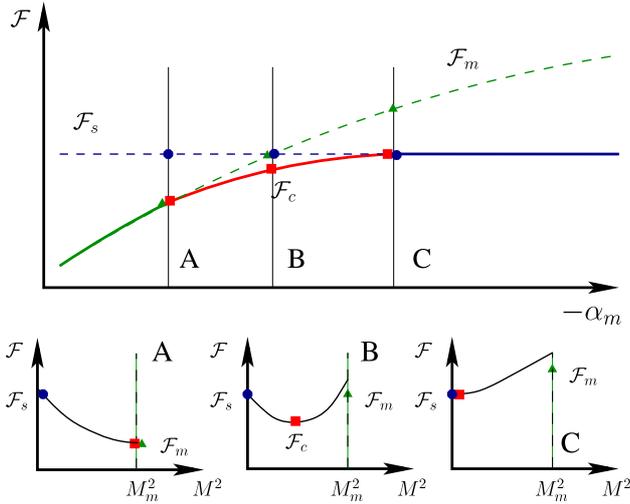


Figure 1. Top: evolution of the extreme values of the free energy, $\mathcal{F}_{s,c,m}$, as a function of α_m for $\chi = AB - C^2 > 0$. When the local extremum for $\Delta \neq 0$ and $M \neq 0$ appears, it becomes the global minimum and describes a thermodynamically stable phase with coexisting SC and SDW orders. Bottom: dependence of the free energy along the trajectory $\Delta(M)$, see equation (6), and the values of \mathcal{F}_s (O), \mathcal{F}_m (Δ) and \mathcal{F}_c (\square). (A) $\alpha_m = \alpha_s B/C$, when a small SC order appears within the SDW phase, $\mathcal{F}_m = \mathcal{F}_c$; $\alpha_m = \alpha_s \sqrt{B/A}$, when the mixed phase is the global minimum, $\mathcal{F}_m = \mathcal{F}_s > \mathcal{F}_c$; and (C) $\alpha_m = \alpha_s C/A$, when the SDW order disappears, $\mathcal{F}_s = \mathcal{F}_c$.

At large $\alpha_m > \alpha_s B/C$, the system is in the SDW phase and $\mathcal{F}(M)$ monotonically decreases with increasing M to $\mathcal{F}(M_m)$, but \mathcal{F}_m has an even smaller value than $\mathcal{F}(M_m)$. In this case $\gamma < 0$ and $\beta > 0$ in equations (7). At such α_m the solution corresponding to the coexistence state does not exist because the condition $\Delta^2 > 0$ is not yet satisfied. At $\alpha_m \leq \alpha_s B/C$, and the minimum of $\mathcal{F}(M)$ takes place at M , given by equations (4), for $0 < M < M_m$ when the coexistence state develops (still, we have $\gamma < 0$ and $\beta > 0$ in equations (7)). The minimum splits from $\Delta = 0$ at $\alpha_m = \alpha_s B/C$ via a continuous second-order transition. When α_m decreases further, but still $\alpha_m > \alpha_s C/A$, the minimum shifts to smaller M , and eventually, at $\alpha_m = \alpha_s C/A$, reaches the value \mathcal{F}_s at $M = 0$. At even smaller α_m , the global minimum corresponds to \mathcal{F}_s , i.e. the system gradually transforms from the mixed state into the superconducting state. The overall evolution of the system has two second-order transitions at $\alpha_m = \alpha_s B/C$ and $\alpha_m = \alpha_s C/A$, and the intermediate mixed state at $\alpha_s C/A < \alpha_m < \alpha_s B/C$.

In the opposite case, $AB - C^2 < 0$, the free energy of the ‘coexistence’ state is always larger than the free energy of pure SDW or SC states, i.e. the ‘coexistence’ state corresponds to a saddle point of the free energy and does not represent an actual thermodynamic state of the system. The evolution of $\mathcal{F}_{s,m,c}$ is shown in figure 2. At large $\alpha_m > \alpha_s C/A$, the free energy reaches its minimum at $\Delta = 0$, $M^2 = \alpha_m/(2B)$ and the system is in the pure SDW phase. In this case, $\gamma > 0$ and $\beta < 0$ in equations (7). The ‘coexistence’ state solution does not exist because it formally corresponds to $\Delta^2 < 0$. At $\alpha_m = \alpha_s C/A$, \mathcal{F}_c and \mathcal{F}_s coincide. At smaller α_m the mixed state solution becomes real, in the sense that it corresponds to $\Delta^2 > 0$, and $\mathcal{F}(M)$ develops a maximum at M , defined

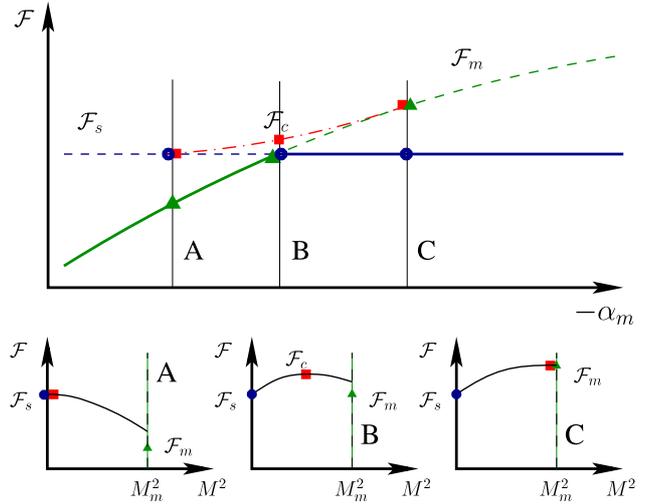


Figure 2. Top: evolution of the extreme values of the free energy, $\mathcal{F}_{s,c,m}$, as a function of α_m for $\chi = AB - C^2 < 0$. The local extremum \mathcal{F}_c for $\Delta \neq 0$ and $M \neq 0$ corresponds to a local maximum and represents a thermodynamically unstable state. Bottom: dependence of the free energy along the trajectory $\Delta(M)$, see equation (6), and the values of \mathcal{F}_s (O), \mathcal{F}_m (Δ) and \mathcal{F}_c (\square). (A) $\alpha_m = \alpha_s C/A$. The local extremum \mathcal{F}_s appears at this point, but the pure SDW state has a smaller energy $\mathcal{F}_s = \mathcal{F}_c > \mathcal{F}_m$; (B) $\alpha_m = \alpha_s \sqrt{B/A}$. At this point, $\mathcal{F}_m = \mathcal{F}_s < \mathcal{F}_c$, and the system undergoes a first-order transition between SC and SDW states, (C) $\alpha_m = \alpha_s C/A$. The local extremum now corresponds to a weak SC order, but the pure SC state has a lower free energy, $\mathcal{F}_m = \mathcal{F}_c > \mathcal{F}_s$.

by equations (4). As α_m decreases, the maximum moves to larger M and simultaneously \mathcal{F}_m increases. At $\alpha_m = \alpha_s \sqrt{B/A}$, the free energies for pure states, \mathcal{F}_m and \mathcal{F}_s become equal, while the ‘coexistence’ state has a higher energy. At even smaller α_m , $\mathcal{F}_m > \mathcal{F}_s$ and the pure SC phase is a true thermodynamic equilibrium state. The magnetic state remains a local minimum of $\mathcal{F}(\Delta, M)$ and the ‘coexistence’ state remains a local maximum of $\mathcal{F}(M)$ down to $\alpha_m = \alpha_s B/C$. At even smaller α_m the coefficient γ changes sign and the ‘coexistence’ solution disappears.

3. Application to pnictides

We now apply the above analysis of the two-parameter model to the pnictide superconductors. We approximate the electronic structure of pnictides by a model of two families of fermions, which form one hole and one electron FSs of approximately equal sizes. We assume that the hole FS is circular and the dispersion of fermions near this FS is

$$\varepsilon_h = \mu_h - \frac{k^2}{2m_h}. \quad (8)$$

The electronic FS is an ellipse, and the dispersion of fermions near this FS is

$$\begin{aligned} \varepsilon_e = & -\mu_e + \frac{k_x^2}{2m_x} + \frac{k_y^2}{2m_y} = -\varepsilon_h + \mu_h - \mu_e \\ & + \frac{k^2}{2} \left[\frac{(m_x + m_y)}{2m_x m_y} - \frac{1}{m_h} \right] + \frac{k_x^2 - k_y^2}{2} \frac{m_y - m_x}{2m_x m_y}. \end{aligned} \quad (9)$$

The last three terms represent different deviations from perfect nesting: (i) the change in chemical potentials $\delta\mu = \mu_h - \mu_e$, (ii) the difference in the electron and hole masses, $m_{x,y} \neq m_h$, and (iii) ellipticity, $m_x \neq m_y$. We will see that typical ε_h are of the order of the temperature T . We assume that the chemical potential μ is much larger than T and neglect all terms arising due to deviations from perfect nesting with the contribution to the free energy small in the parameter T/μ_h . Within this approximation, we can set $k = k_F = \sqrt{2m_h\mu_h}$ in the two terms in the last line of equation (9). Then $\varepsilon_e = -\varepsilon_h + 2\delta_\varphi$, where

$$\delta_\varphi = \delta_0 + \delta_2 \cos 2\varphi, \quad \delta_2 = \frac{k_F^2}{8} \frac{m_y - m_x}{m_x m_y}, \quad (10)$$

$$\delta_0 = \frac{\mu_h - \mu_e}{2} + \frac{k_F^2}{4} \left(\frac{m_x + m_y}{2m_x m_y} - \frac{1}{m_h} \right). \quad (11)$$

Within this approximation, the two dispersions differ by a term $2\delta_\varphi$ which depends on the angle along the FS but does not depend on ε_h . One can verify that, with these ε_h and ε_e , superconducting gaps along the hole and electron FSs are equal in magnitude and different in sign if, indeed, the pairing interaction is approximated by a constant and μ is set to be much larger than T .

The free energy for the case when the two dispersions differ by a constant was presented in [27] for circular FSs, when $\delta_\varphi = \delta_0$ is just a constant. Extending the expression for the free energy to the case when δ_φ depends on φ due to ellipticity, we obtain

$$\begin{aligned} \frac{\mathcal{F}(\Delta, M)}{4N_f} &= \frac{|\Delta|^2}{2} \ln \frac{T}{T_s} + \frac{M^2}{2} \ln \frac{T}{T_m} + \pi T \sum_{\omega_m} \frac{|\Delta|^2 + M^2}{2|\omega_m|} \\ &- \pi T \sum_{\omega_m} \text{Re} \sqrt{(E_m + i\delta_\varphi)^2 + M^2 - |\omega_m|}_\varphi, \end{aligned} \quad (12)$$

where $E_m = \sqrt{\omega_m^2 + \Delta^2}$, $\omega_m = \pi T(2m + 1)$ are the Matsubara frequencies and $\langle \dots \rangle_\varphi$ imply averaging over the direction φ on the Fermi surface. Temperatures T_s and T_m are transition temperatures to SC or SDW states for ‘pure’ cases when interactions are exclusively in the SC or SDW channels.

Expanding the free energy, equation (12), up to the fourth order in M and Δ and comparing the result with equation (1) we obtain

$$A = \frac{\pi T}{4} \sum_{m \geq 0} \frac{1}{\omega_m^3}, \quad (13)$$

$$B = \frac{\pi T}{4} \sum_{m \geq 0} \left\langle \omega_m \frac{\omega_m^2 - 3\delta_\varphi^2}{(\omega_m^2 + \delta_\varphi^2)^3} \right\rangle, \quad (14)$$

$$C = \frac{\pi T}{4} \sum_{m \geq 0} \left\langle \frac{\omega_m^2 - \delta_\varphi^2}{\omega_m(\omega_m^2 + \delta_\varphi^2)^2} \right\rangle \quad (15)$$

and

$$\alpha_s = \frac{1}{2} \ln(T_s/T), \quad (16)$$

$$\alpha_m = \frac{1}{2} \ln \frac{T_m}{T} - \pi T \sum_{m \geq 0} \left\langle \frac{\delta_\varphi^2}{\omega_m(\omega_m^2 + \delta_\varphi^2)} \right\rangle. \quad (17)$$

The superconducting part of the free energy, expressed via α_s and A , is independent of δ_φ , but the magnetic part and the

mixed $\Delta^2 M^2$ term depend on δ_φ . The expansion makes sense if Δ , M are of the same order, i.e. if T_s and T_m do not differ much, which we assume henceforth.

For perfect nesting $\delta_\varphi \equiv 0$ and we have $A = B = C$, i.e. $\chi = 0$, as was explicitly stated in [6]. Furthermore, the interaction term in the free energy is $A(\Delta^2 + M^2)^2$ and does not favor either SC or SDW orders even beyond the expansion to the fourth order [27]. The transition occurs into a state with a higher transition temperature T_s or T_m , and once either SDW or SC order develops, the other order does not appear simply because the quadratic term favors either $\Delta = 0$ or $M = 0$, and the interaction term is isotropic. If $T_s = T_m$, the free energy given by equation (12) is $SO(5)$ symmetric and extra terms are needed to break this symmetry.

As we said, we consider the case when $T_m > T_s$, such that at perfect nesting the system develops an SDW order. Deviations from perfect nesting lead to two effects. First, the magnitude of α_m is reduced, which is the manifestation of the fact that SDW instability is suppressed when nesting becomes non-perfect. Superconducting α_s is not affected by δ_φ , and at large δ_φ superconductivity is the only possible state. Second, coefficients B and C evolve with δ_φ , and $\chi = AB - C^2$ becomes non-zero when δ_φ is finite. The question is: what is the sign of this term? We recall that, when $\chi > 0$, the system evolves from SDW to SC via two second-order transitions and the intermediate coexistence phase, while for $\chi < 0$, there is no mixed state and SDW and SC phases are separated by a first-order transition.

To get an insight into how χ evolves at non-zero δ_φ , we first consider δ_φ as a small parameter and expand A , B and C in powers of δ_φ . Collecting terms up to fourth order in δ_φ , we obtain

$$\chi = \frac{1}{32\pi^8 T^8} (s_1 \langle \delta_\varphi^4 \rangle - s_2 \langle \delta_\varphi^2 \rangle^2), \quad (18)$$

where

$$\begin{aligned} s_1 &= 5 \left(\sum_{m \geq 0} \frac{1}{(2m+1)^3} \right) \left(\sum_{m \geq 0} \frac{1}{(2m+1)^7} \right), \\ s_2 &= 9 \left(\sum_{m \geq 0} \frac{1}{(2m+1)^5} \right)^2. \end{aligned} \quad (19)$$

The sums are expressed in terms of the Riemann zeta function and give $s_1 \approx 5.26$ and $s_2 \approx 9.08$. Substituting δ_φ from (11) and averaging, we obtain

$$\chi \approx \frac{1}{32\pi^8 T^8} (-3.82\delta_0^4 + 6.70\delta_0^2\delta_2^2 - 0.30\delta_2^4). \quad (20)$$

We emphasize that, in the two limits when either $\delta_2 = 0$ or $\delta_0 = 0$, $\chi < 0$, i.e. the transition is first order. The first limit corresponds to circular FSs with different chemical potentials, while the second limit corresponds to the case when the chemical potential remains equal but electron dispersion becomes elliptical. In both cases, the SDW order opens gaps for some fermionic excitations, but still preserves low-energy fermionic states near the modified FSs. Fermions near these FSs still have a non-zero s^{+-} SC solution: however, this solution represents an energetically unfavorable state. We

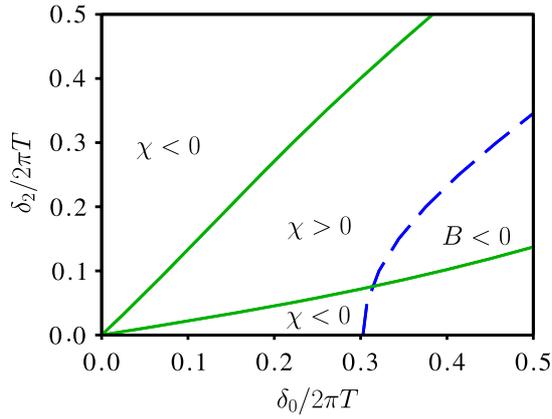


Figure 3. Contour plot of the sign of $\chi = AB - C^2$, where A , B and C are given by equations (13)–(15). The area between the two solid lines corresponds to positive values of χ , where the coexistence between the SDW and SC phases is possible. Below the dashed line the value of B is negative and the system undergoes a transition from the normal state to the incommensurate SDW state. The mixed phase between SC and incommensurate SDW orders does exist [27], but its boundaries are shifted compared to the ones for commensurate SDW.

particularly emphasize that the ellipticity of electron dispersion taken alone (i.e. $\delta_0 = 0$) is not sufficient for the appearance of the coexistence phase.

When both δ_0 and δ_2 are non-zero, there is a relatively broad range $0.76 < \delta_2/\delta_0 < 4.68$ where $\chi > 0$ and the transformation from pure SDW to SC phases occurs via a coexistence phase. To verify that this statement holds at larger values of δ_0 and δ_2 , we computed $\chi = \chi(\delta_0, \delta_2)$ without expanding in δ_φ . We plot the sign of $\chi(\delta_0, \delta_2)$ in figure 3. We obtained the same result as above, namely, for $\delta_0 = 0$ or $\delta_2 = 0$, $\chi < 0$ and the transition between SDW and SC states is of first order, while when both δ_0 and δ_2 are non-zero, there exists a region with $\chi(\delta_0, \delta_2) > 0$. In this parameter range, the transformation from SDW to SC phases involves a coexistence phase.

Two remarks are in order here. In our analysis of the free energy we assumed that B given by equation (14) is positive. This is, however, only true if δ_0 and δ_2 are below certain thresholds, see the dashed line in figure 3. At larger δ_0 and δ_2 , the coefficient B becomes negative and the analysis has to be modified. This is the condition where instability with respect to the formation of an incommensurate SDW order occurs, much like the Fulde–Ferrell–Larkin–Ovchinnikov phase in superconductors. In particular, for $\delta_2 = 0$, B becomes negative for $\delta_0/2\pi T \approx 0.304$ [24, 27]. This order develops at a temperature above T_s if $T_s < 0.56 T_m$. We also note that equation (20) is obtained under the assumption that $T \ll \mu$, which allowed us to restrict the contributions to $T^4\chi$ from terms that scale as $(\delta_\varphi/T)^4$ and neglect terms which scale as powers of $(\delta_\varphi/\mu_h)^2$. It is unlikely but, in principle, possible that the expansion of the full χ in powers of δ_φ begins with the quadratic term $(1/T^4)(\delta_\varphi/\mu_h)^2$, i.e. $T^4\chi = c_2(\delta_\varphi/\mu_h)^2 + c_4(\delta_\varphi/T)^4 + \dots$. If this is the case and $c_2 > 0$, the mixed phase exists in a tiny range of δ_φ , where $\chi < 0$ without the c_2 term.

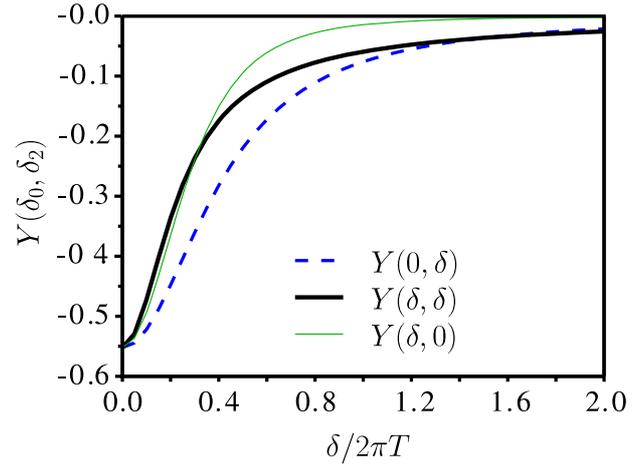


Figure 4. The behavior of $Y(\delta_0, \delta_2)$ for three cases: $Y(\delta, 0)$, $Y(0, \delta)$ and $Y(\delta, \delta)$. In all cases $Y(\delta_0, \delta_2)$ monotonically increases with increasing argument, but remains negative.

4. Conventional two-band s-superconductivity

For completeness, we also consider the case when the superconducting order parameter in a conventional s-wave, i.e. the sign of Δ , is the same on hole and electron FSs. This case has been considered in [6] and the conclusion was that the transition from the SDW to SC phase is always of first order, regardless of ellipticity or the shift of chemical potentials. This result implies that the very coexistence between SDW and SC in Fe-pnictides is an implication that the pairing state is not a conventional s^{++} state.

The analysis in [6] was based on the observation that for the s^{++} gap, $\chi < 0$ already for circular FSs and perfect nesting, and in numerical calculations of χ for some cases when nesting is not perfect. We analyze this issue analytically.

The free energy for the s^{++} SC gap can be derived using the same approach as in [27] and has the form

$$\begin{aligned} \frac{\mathcal{F}^{++}(\Delta, M)}{4N_f} &= \frac{|\Delta|^2}{2} \ln \frac{T}{T_s} + \frac{M^2}{2} \ln \frac{T}{T_m} \\ &+ \pi T \sum_{\omega_m} \frac{|\Delta|^2 + M^2}{2|\omega_m|} - \frac{\pi T}{2} \sum_{\omega_m} \sum_{\pm} \left\{ (\omega_m^2 + \Delta^2 + M^2 \right. \\ &\left. - \delta_\varphi^2 \pm 2\sqrt{\Delta^2 M^2 - \delta_\varphi^2(\omega_m^2 + \Delta^2)})^{1/2} - |\omega_m| \right\}_\varphi. \end{aligned} \quad (21)$$

Expanding this free energy in powers of Δ^2 and M^2 and comparing the result with equation (1), we find that coefficients A and B are still given by equations (13) and (14), but the coefficient C is modified to

$$C = \frac{\pi T}{4} \sum_{m \geq 0} \left\langle \frac{3\omega_m^2 + \delta_\varphi^2}{\omega_m(\omega_m^2 + \delta_\varphi^2)^2} \right\rangle. \quad (22)$$

We now have $\chi = Y(\delta_0, \delta_2)/\pi^4 T^4$. At perfect nesting, $Y(0, 0) = -(7\zeta(3)/8)^2/2 < 0$ and the transition is of first order. When $\delta_{0,2}$ increases, the magnitude of $\chi \propto Y(\delta_0, \delta_2)$ is reduced, but we found that its sign remains negative for arbitrary values of δ_0 and δ_2 . In figure 4, we show the behavior of $Y(\delta_0, \delta_2)$ for three cases: $Y(\delta, 0)$, $Y(0, \delta)$ and $Y(\delta, \delta)$. We

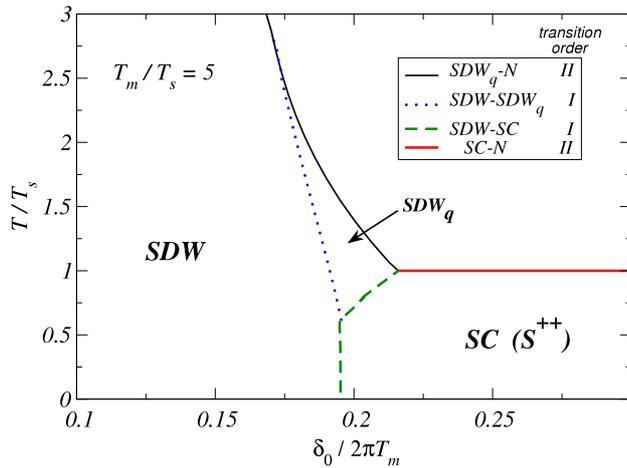


Figure 5. The phase diagram for $T_m/T_s = 5$ for s^{++} superconductivity for two circular Fermi surfaces as a function of δ_0 . The solid curved line is the transition between the normal and (in)commensurate SDW_q states. The dotted line is the first-order transition line between commensurate and incommensurate SDW phases. The solid horizontal line is the second order normal–SC transition. The transitions between both, incommensurate and commensurate SDW phases, and the SC phase are first order (dashed lines), and the mixed phase does not appear.

see that in all cases $Y(\delta_0, \delta_2)$ remains negative for arbitrary magnitudes of $\delta_{0,2}$. We computed the sign of χ everywhere in the (δ_0, δ_2) plane and found that it is always negative. Therefore, we confirm the result of [6] that there is no mixed phase if the SC gap has s^{++} symmetry on both FSs.

We went a step further and analyzed what happens when T_m is much greater than T_s , and magnetic order becomes incommensurate at high temperatures $T > T_s$. The results are presented in figure 5. We observe that, even when magnetic order is incommensurate, the transition between SDW and SC phases remains of first order, shown by the dashed line in figure 5, and the mixed state does not occur. In contrast, for an s^{++} SC, once the SDW order becomes incommensurate, the transformation from incommensurate SDW to SC involves the coexistence phase even though the transition from commensurate SDW to SC phase would be of first order.

5. Conclusions

In this paper we studied analytically the interplay between a commensurate SDW magnetism and superconductivity in the model for Fe-pnictides. The conventional wisdom is that the transition from SDW to SC should be of first order in the case of a perfect nesting, because then the SDW order fully gaps electronic states, leaving no space for SC, but should involve a coexistence phase for non-perfect nesting because then SDW order leaves modified FSs on which an SC order may develop. We show that the situation is more complex and the presence of FSs in the SDW phase is not a sufficient condition for the mixed state to emerge. We show explicitly that the transition remains of first order when doping shifts hole and electron bands, but the bands remain circular, and when the electron

band becomes elliptical, but the chemical potential does not shift (the material remains a compensated metal). Only when both ellipticity and a shift of the chemical potential are present, we found the mixed state for some range of parameters.

We also analyzed the case when the SC order has a conventional, sign-preserving s^{++} symmetry on the two FSs and confirmed analytically the result of [6] that the transition between SDW and SC phases is always of first order, and the mixed phase does not appear. We argue that this is the case even when the SDW order becomes incommensurate.

Acknowledgments

We thank I Eremin, R Fernandes, I Mazin, J Schmalian, O Sushkov and Z Tesanovic for useful discussions. MG V acknowledges the Donors of the American Chemical Society Petroleum Research Fund for partial support and AVC acknowledges the support from NSF-DMR 0906953.

References

- [1] Kamihara Y, Watanabe T, Hirano M and Hosono H 2008 *J. Am. Chem. Soc.* **130** 3296
- [2] Luetkens H *et al* 2009 *Nat. Mater.* **8** 305
- [3] Laplace Y, Bobroff J, Rullier-Albenque F, Colson D and Forget A 2009 *Phys. Rev. B* **80** 140501
- [4] Chu J-H, Analytis J G, Kucharczyk C and Fisher I R 2009 *Phys. Rev. B* **79** 014506
- [5] Rotter M, Tegel M and Johrendt D 2008 *Phys. Rev. Lett.* **101** 107006
- [6] Fernandes R M *et al* 2009 arXiv:0911.5183
- [7] Liu C *et al* 2008 *Phys. Rev. Lett.* **101** 177005
- [8] Evtushinsky D V *et al* 2009 *Phys. Rev. B* **79** 054517
- [9] Hsieh D, Xia Y, Wray L, Qian D, Gomes K, Yazdani A, Chen G F, Luo J L, Wang N L and Hasan M Z 2008 arXiv:0812.2289v1
- [10] Ding H *et al* 2008 arXiv:0812.0534
- [11] Zabolotny V B *et al* 2009 *Nature* **457** 569
- [12] Coldea A I, Fletcher J D, Carrington A, Analytis J G, Bangura A F, Chu J H, Erickson A S, Fisher I R, Hussey N E and McDonald R D 2008 *Phys. Rev. Lett.* **101** 216402
- [13] Coldea A I, Andrew C M J, Analytis J G, McDonald R D, Bangura A F, Chu J-H, Fisher I R and Carrington A 2009 *Phys. Rev. Lett.* **103** 026404
- [14] Singh D J and Du M H 2008 *Phys. Rev. Lett.* **100** 237003
- [15] Boeri L, Dolgov O V and Golubov A A 2008 *Phys. Rev. Lett.* **101** 026403
- [16] Mazin I I, Singh D J, Johannes M D and Du M H 2008 *Phys. Rev. Lett.* **101** 057003
- [17] Chubukov A V, Efremov D and Eremin I 2008 *Phys. Rev. B* **78** 134512
- [18] Chubukov A V 2009 *Physica C* **469** 640
- [19] Kuroki K, Onari S, Arita R, Usui H, Tanaka Y, Kontani H and Aoki H 2008 *Phys. Rev. Lett.* **101** 087004
- [20] Barzykin V and Gorkov L P 2008 *JETP Lett.* **88** 131
- [21] Maier T A, Graser S, Scalapino D J and Hirschfeld P J 2009 *Phys. Rev. B* **79** 224510
- [22] Chubukov A V, Vavilov M G and Vorontsov A B 2009 *Phys. Rev. B* **80** 140515
- [23] Thomale R, Platt C, Hu J, Honerkamp C and Bernevig B A 2009 *Phys. Rev. B* **80** 180505
- [24] Cvetkovic V and Tesanovic Z 2009 *Europhys. Lett.* **85** 37002
- [25] Stanev V, Kang J and Tesanovic Z 2008 *Phys. Rev. B* **78** 184509

- [26] Parker D, Vavilov M G, Chubukov A V and Mazin I I 2009 *Phys. Rev. B* **80** 100508
- [27] Vorontsov A B, Vavilov M G and Chubukov A V 2009 *Phys. Rev. B* **79** 060508
- [28] de la Cruz C *et al* 2008 *Nature* **453** 899
- [29] Klauss H-H *et al* 2008 *Phys. Rev. Lett.* **101** 077005
- [30] Wang F, Zhai H, Ran Y, Vishwanath A and Lee D-H 2009 *Phys. Rev. Lett.* **102** 047005
- [31] Platt C, Honerkamp C and Hanke W 2009 *New J. Phys.* **11** 055058
- [32] Lorenzana J, Seibold G, Ortix C and Grilli M 2008 *Phys. Rev. Lett.* **101** 186402
- [33] Brydon P and Timm C 2009 *Phys. Rev. B* **79** 180504
- [34] Johannes M D and Mazin I I 2009 *Phys. Rev. B* **79** 220510
- [35] Mazin I I and Johannes M D 2009 *Nat. Phys.* **5** 141
- [36] Eremin I and Chubukov A V 2010 *Phys. Rev. B* **81** 024511