Electronic Structure of Fe-Based Superconductors

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The electronic structure of the Fe-based superconductors is discussed, mainly from the point of view of first principles calculations in relation to experimental data. Comparisons and contrasts with cuprates are made. The problem of reconciling experiments indicating an s symmetry gap with experiments indicating line nodes is discussed and a possible

Key words: iron-pnictide, electronic structure, Fermi surface, magnetism

Abstract
The electronic structure of the Fe-based superconductors is calculations in relation to experimental data. Compariso reconciling experiments indicating an *s* symmetry gap with resolution is given. *Key words:* iron-pnictide, electronic structure, Fermi surfa *PACS:* 74.25.Jb, 74.25.Kc, 74.70.Dd **1. Introduction**Superconductivity is fundamentally an electronic phenomena, and is in particular an instability of the metallic Fermi surface due to interactions. Therefore understanding the electronic structure, especially the low energy electronic structure at and near the Fermi energy, as well as the interactions that may lead to superconductivity is essential to unraveling the physics of a superconducting material. This includes developing understanding of the details of the interactions in relation to competing or cooperating states such as magnetic orderings and lattice distortions. The purpose of this paper is to discuss the electronic structure of the Fe-based superconductors (FeSC), [1, 2] mainly from the perspective of first principles calculations in relation to experiment. **2. Crystal Structure and Chemistry**Since the discovery of superconductivity in electron doped oxy-pnictides, prototype LaFeAs(O,F), high temperature superconductivity has been discovered in three additional families of iron compounds: ThCr₂Si₂ structure materials, prototype BaFe₂As₂, with either hole or electron doping, [3] the LiFeAs family, [4, 5, 6] and the α-PbO structure iron chalcogenides, prototype Fe_{1+x}Se. [7, 8] Remarkably, superconductivity can be produced by electron doping on the Fe site itself, with either Co or Ni. [9, 10, 11] In addition, superconductivity has been found in the corresponding pure Ni based compounds, both the oxy-

[9, 10, 11] In addition, superconductivity has been found in the corresponding pure Ni based compounds, both the oxypnictides and in the $ThCr_2Si_2$ structure. [12, 13, 14, 15] However, the superconductivity in these compounds can be understood as ordinary electron-phonon superconductivity, [16, 17, 18] in contrast to the Fe-based materials, which cannot be understood in this way. [19, 20] The related Co compounds are not superconducting and are either ferromagnetic or near ferromagnetism. [21, 22] Here we focus on the Fe-based phases.

The basic structural feature connecting these compounds is the presence of square planar sheets of Fe coordinated tetrahedrally by pnictogens or chalcogens and nominal Fe valence near Fe^{2+} . We begin with FeSe, which is the simplest of the compounds. Its structure is depicted in Fig. 1. This structure consists of square planes of Fe with Se atoms arranged above and below the planes in such as way as to tetrahedrally coordinate the iron. The arrangement of Se above and below the Fe plane leads to a c(2x2) doubling of the unit cell compared to the Fe square lattice, so the actual unit cell contains two Fe atoms. The lattice may also be regarded as a tetragonally distorted close packed lattice of Se, with Fe inside tetrahedral holes arranged so that the Fe atoms are in a square plane.

The other FeSC compounds may be regarded as based on the same square planar sheets with Se replaced by As and counter-ions inserted in such a way as to maintain the nominal Fe valence. For example, LiFeAs may be regarded as FeSe with Se replaced by As and Li inserted between the layers. In the ThCr₂Si₂ structure, e.g. BaFe₂As₂, the FeAs planes have Ba between them, and the stacking is changed from simple tetragonal, as in LiFeAs, FeSe and LaFeAsO, to body centered tetragonal, thus providing a better coordination for Ba.

This type of structure is an important difference from cuprates. In particular, because of the larger size of Se and As anions, relative to O, tetrahedral coordination is preferred, leading to a structure composed of edge sharing tetrahedra. In cuprates the structural motif is that of corner sharing octahedra. This is important for two reasons. First of all, in materials built from corner sharing octahedra the metal - metal distance is much longer than the metal ligand distance (by a factor of two for an undistorted perovskite) so that direct metal - metal interactions typically play a very minor role compared to hopping through the ligands, e.g. in band formation and magnetic interactions. Secondly, structures built from cor-



Figure 1: (Color online) Crystal structure of α -FeSe shown along a (120) direction using sphere sizes proportional to the Shannon ionic radii of high spin Fe²⁺ and Se²⁻. The inset (not to scale) shows the Fe plane with coordinating Se atoms above (+) and below (-) the plane. Note the resulting c(2x2) doubling of the cell (dashed line) with respect to the Fe square lattice.

ner sharing octahedra almost invariably are prone to structural distortions e.g. in order to accommodate counter ions with sizes that are not perfectly matched to their sites. Thus the ideal cubic perovskite $(Pm3m, BaZrO_3)$ structure is relatively uncommon, while distorted perovskite structures (e.g. Pnma, CaTiO₃) are very common. These distortions typically couple strongly to electronic structure, and to magnetic and other properties, as might be anticipated based on the fact that metal - O - metal hopping plays a key role in band formation. Similarly, some of the most studied cuprates, particularly the Bi compounds (e.g. Bi₂Sr₂CaCu₂O₈, BISCO) and the "214" family (e.g. $La_{2-x}Sr_xCuO_4$) show strong lattice distortions that greatly complicate the interpretation of experimental results. One instructive example is provided by the longstanding misinterpretation of the shadow bands in BISCO as being a novel manifestation of strong correlation effects, when in fact they are just a band structure effect arising from the complex lattice distortion in that compound. [23, 24, 25] The key point is that the structures of the FeSC are much simpler, and in particular these compounds are not prone to complex lattice distortions. This should greatly facilitate experimental studies of these materials and comparison of theoretical and experimental results. Also, we note that the structure places the Fe atoms closer together than in a perovskite, so that direct Fe - Fe interactions may be (and are, see below) important.

The electronic structures of the various compounds as obtained within density functional theory have been reported by a number of authors. [20, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51] While these differ in detail a number of common features are present. Fig. 2 shows the electronic density of states (DOS) of FeSe as obtained in



Figure 2: (Color online) Calculated electronic density of states for FeSe and projections onto atom centered spheres of radius 2.1 Bohr following Ref. [41]. Note that the p orbitals of Se are extended, and so the projection is proportional to, but underestimates the Se p contribution.

the local density approximation (LDA) without including magnetism. [41] As may be seen, the main Se p bands are well below the Fermi energy (between 3 eV and 6 eV binding energy) and the DOS from -2.5 eV to 2 eV is dominated by Fe d states, with only a modest admixture of Se character, similar to the level of covalency in typical oxides. The arsenides are similar as shown in Fig. 3 for LaFeAsO. In that compound the main As p bands occur between ~ -5.5 and -2 eV with respect to the Fermi energy, E_F and again the bands near E_F are dominated by Fe d character. This implies that from a crystal chemical point of view the Se and As are anionic, Se^{2-} and As^{3-} and that the electronic structure near E_F should be regarded as derived from metallic square lattice sheets of Fe²⁺ embedded in tetrahedral holes of the anion lattice. This picture has been confirmed by core-level and valence photoemission experiments, which show the bands near E_F to be predominantly Fe in character. [52] We note that this modest d - p hybridization is common to the Fe, Co and Ni materials in this structure and is in strong contrast with the behavior of the corresponding Mn compounds. [53]

An examination of the DOS (Figs. 2 and 3) shows that Fe *d* manifold is split into to main peaks. These are separated by a rather prominent pseudogap, with E_F occurring towards the bottom. This pseudogap occurs at an electron count of six per Fe, corresponding to the *d* electron count of Fe²⁺. Importantly, a tetrahedral crystal field scheme, such as might arise if the Fe - As (Se) interactions were dominant, would have a gap at four electrons per Fe, since in a tetrahedral ligand field the e_g levels would be below the t_{2g} levels. Instead, the position of the pseudogap shows the importance of direct Fe-Fe interactions in the formation of the band structure. This in contrast to cuprate superconductors, where the Cu ions are contained within distorted corner sharing octahedra, and hopping through O plays the critical role in band formation, conduction and



Figure 3: (Color online) Calculated electronic density of states for LaFeAsO and projections onto atom centered spheres of radius 2.1 Bohr as in Fig. 2, following Ref. [27].

magnetic exchange interactions.

Calculations have also been performed using methods that incorporate an explicit Hubbard-like Coulomb term, U, via the dynamical mean field theory (DMFT). [54, 55] Those calculations, as is usual when incorporating an additional on-site Coulomb repulsion, yield a strong shift of Fe d spectral weight away from the region around E_F to Hubbard bands at binding energies corresponding to U. Additionally, it is claimed that the metallic state is destroyed in favor of a total incoherent state. [55] This disagrees qualitatively with experimental data, which show a metallic state, including observation of quantum oscillations, [56, 57, 58] metallic-like band dispersions around E_F , [34, 59] and critically the non-observation of Hubbard bands. [60] From this perspective the FeSC behave very differently from cuprate superconductors. At first sight, this may seem surprising as one might wonder how adding the U could degrade results. However, it is to be emphasized that density functional theory does already contain some correlations and as a result the addition of U can lead to double counting of correlations with detrimental effects in band-like metals. It should also be noted that arguments as to why correlation effects should be weak have been advanced by Nakamura and co-workers, [61] and also by Anisimov and co-workers, [62] based on a Wannier function analysis. In any case, considering the non-observation of the Hubbard bands and the non-observation of the associated strong spectral weight shifts into them as predicted by current DMFT calculations with substantial U we do not discuss these further here.

3. Band Structure and Fermi Surface

The non-spin-polarized LDA band structure for FeSe is shown in Fig. 4, following Ref. [41]. The corresponding Fermi surface is shown in Fig. 5. As may be seen the band structure is semi-metallic, with small Fermi surface sections, in contrast to cuprates. [63] While the lay-



Figure 4: Calculated band structure for FeSe following Ref. [41].

ered crystal structure is reflected in the cylindrical shape of the Fermi surface, there is clear three dimensionality. The amount of three dimensionality varies from compound to compound, but is particularly pronounced in ThCr₂Si₂ structure BaFe₂As₂, [36, 47] where one of the hole sections shows rather strong k_z dispersion near $k_z=1/2$. Nonetheless, considering the Fermi surface, the FeSC are substantially less anisotropic than the cuprates, including the simplest tetragonal one layer compounds, Tl₂Ba₂CuO₆, [64] and HgBa₂CuO₄, [65] and even considering YBa₂Cu₃O₇, which is one of the least anisotropic cuprates.

The relatively low anisotropy of the FeSC is of potential practical importance. In particular, flux pinning is an important issue in applications of superconductivity, and this is greatly facilitated in low anisotropy materials. The lower anisotropy of FeSC is supported by several experiments, and in fact favorable results for flux pinning have been obtained in FeSC samples. [66, 67, 68, 69]

The basic structure of the Fermi surface is similar in all the FeSC. It consists of two electron cylinders centered at the zone corner, compensated by hole sections around the zone center. Both are primarily derived from Fe d_{xz} and d_{yz} orbitals (with the reference frame have z normal to the Fe planes). In addition, in some compounds, an additional heavy d_{z^2} derived heavy hole section is predicted at the zone center. [26, 27] As mentioned, there is hybridization between Fe and the ligands, albeit modest. In particular, the d bands at E_F have antibonding character with the As / Se ligands.

The electron sections may be regarded [20, 70] as deriving from the 2D zone boundary $(\pi, 0)$ and $(0, \pi) d_{xz}$ and d_{yz} bands in the simple one Fe unit cell that would exist without the As / Se atoms above and below the plane. Both of these points are folded to the 2D zone corner (π, π) point in the c(2x2) unit cell of the compound. Since these bands arise from the zone boundary of the Fe lattice, they have antibonding character between the Fe atoms and are more dispersive than the d_{xz}/d_{yz} bands at the zone center, which are bonding in character and heavier.



Figure 5: (Color online) Calculated Fermi surface for FeSe following Ref. [41].

This basic Fermi surface structure with small disconnected hole and electron Fermi surfaces at the zone center and zone corner, respectively, is confirmed by photoemission experiments. [34, 59, 71, 72, 73, 74] Furthermore, high field measurements show two gap superconductivity, [75] with the implication that both sets of Fermi surface are present and play a role in the superconducting phase.

Finally, it is important to emphasize that although the Fermi surface is small, and therefore the carrier density is low in the FeSC, this does not mean that the Fermi level density of states, $N(E_F)$ is low. In fact, it is high, and in particular higher than in cuprates. Depending on the specific compound and details of the structure used in the calculation, $N(E_F)$ can exceed 2 eV⁻¹ on a per Fe both spins basis. For example, the calculated value for LaFeAsO is $N(E_F)=2.6 \text{ eV}^{-1}$. Considering that the DOS near E_F is mainly from Fe, this places the FeSC near itinerant magnetism, based on nearness to the Stoner criterion. Thus based on the band structure, these materials should be characterized as low carrier density, high density of states metals, near itinerant magnetism. This is in contrast to cuprate superconductors, which for optimum doping are high carrier density, moderate density of states materials, and are far from itinerant magnetism. Consequences of the heavy bands in the FeSC relative to cuprates are short superconducting coherence lengths and high superfluid densities.

4. Magnetism

Besides the high values of $N(E_F)$ in the FeSC, which place them in proximity to itinerant magnetism in general, the Fermi surface itself is nested. In particular, the approximately compensating cylindrical hole and electron sections match reasonably well if translated by (π,π,k_z) for arbitrary k_z , and in addition they have similar d_{xz}/d_{yz} orbital character. This leads to a peak in the Lindhard susceptibility, [20, 39, 70, 28] which with Stoner enhancement is sufficient to result in a magnetic instability. This is a spin density wave (SDW) instability of the Fermi surface driven by electrons at and near E_F . This provides an explanation for the experimentally observed SDW order found in most of the undoped FeSC. [76, 77] This SDW shows an evolution of the order parameter with temperature consistent with the expected behavior of an SDW, and optical spectroscopy shows gapping of the Fermi surface and reduction of the scattering rate consistent with a Fermi surface driven SDW. [78] This is consistent with transport data, which show a reduction in both resistivity and Hall carrier concentration in the ordered state. [79] Importantly, although most of the Fermi surface is gapped by the SDW in the FeSC, there are remaining carriers, and these are unambiguously metallic, as shown by the observation of quantum oscillations in the SDW state. [56] This is in contrast to cuprates, where the undoped materials are antiferromagnetic Mott insulators.

Furthermore, we emphasize that these materials are not near a Mott insulator in the normal sense. In particular, a wide range of chemical space has been explored so far, including substitution of the counter-ions, such as various rare earths in the oxy-pnictides, different alkaline earths in the $\text{Th}Cr_2Si_2$ structure materials, replacement of As by P, and also chalcogens, (S,Se,Te), and also alloying on the Fe site with Co and Ni. This implies exploration of substantial parameter space, but nonetheless, the compounds are practically all metallic and in particular no Mott insulator has been found as a function of doping, pressure or chemical substitution.

The density functional electronic structure also provides a qualitative understanding of the phase diagrams. In particular, magnetic order arises in general when the Lindhard function, $\chi_0(\mathbf{q},\omega=0)$ at the ordering wavevector \mathbf{q} exceeds a critical value so that there is a divergence of the Stoner enhanced susceptibility, $\chi_S(\mathbf{q}) = \chi_0(\mathbf{q})[1 - \chi_0(\mathbf{q})]$ $I(\mathbf{q})\chi_0(\mathbf{q})^{-1}$. Here the Stoner enhancement parameter, $I(\mathbf{q})$ is a smooth function of \mathbf{q} , reflecting the \mathbf{q} dependence of the band character, while χ_0 can be a strongly **q** dependent function reflecting the Fermi surface. Besides the Stoner enhancement, in certain materials near a magnetic critical point, as in e.g. weak itinerant magnets, such as Ni₃Al and $Sr_3Ru_2O_7$, [80, 81] there can be a suppression due to spin-fluctuations. In this regard, high $\chi_S(\mathbf{q})$ at **q** away from the ordering wavevector can lead to spin fluctuations that compete with the ordered state. [80, 82, 83, 84]

In any case, this sharp peak due to nesting of cylinders is at the 2D wavevector that separates the axes of the cylinders, i.e. (π,π) in the FeSC, and with no k_z dependence for true cylinders. Thus one obtains a commensurate SDW at the zone corner. This is different from Cr metal, where nesting vector is determined by a spanning vector on the Fermi surface and is not set by symmetry. yielding an incommensurate SDW. [85] With doping the relative sizes of the hole and electron Fermi surface sections must change in order to satisfy Luttinger's theorem. For example, with hole doping the electron sheets would become smaller, while the hole surfaces would expand and in fact this is what is observed experimentally. [59] For nested cylinders with radii differing by small δq , the sharp peak at (π,π) will be smeared out to yield a plateau with diameter $2\delta q$, thus reducing the peak value of χ_0 , while retaining a large area integrated χ_0 in the region around the zone corner. This is as found in calculations of the Lindhard function for the doped FeSC. [20] Thus the doping induced size mismatch between the electron and hole Fermi surfaces will lower the peak value of χ_0 . Since this is what controls magnetic ordering, it is qualitatively expected that doping will work against the SDW state.

While this is what is observed generally in the FeSC, Fe_{1+x} Te is an exception. That material, which is doped by excess Fe outside the Fe square lattice layers, shows an incommensurate SDW at high doping (x=0.165), which becomes commensurate as the doping level is reduced. [86] Density functional calculations show that FeTe, while sharing the same basic electronic structure features with the FeSC, has larger Fermi surfaces, with a greater tendency towards magnetism, and additionally that the excess Fe in the doped compound carries magnetic moments, which may further stabilize ordered states. [41, 87] Significantly, if magnetism persists to high doping, where there is a large size mismatch δq between the electron and hole Fermi surface sections then an incommensurate SDW is expected. In that case (specifically when radius of the smaller cylinder becomes half the radius of the larger cylinder), a dip in the center of the (π,π) centered plateau in χ_0 results, so that the maximum in χ_0 is no longer at the zone corner explaining the incommensurate SDW, and leading to the expectation of a doping dependent wavevector.

This type of itinerant mechanism is distinct from local moment magnetism, where moment formation is a result of on-site interactions and magnetism is a consequence of weaker inter-site interactions, e.g. superexchange. Itinerant magnetism differs from local moment magnetism in that the physics involves the Fermi surface and is therefore long range, and in the itinerant case longitudinal degrees of freedom can be important, while in local moment magnets only transverse degrees of freedom are important at low energy.

This is not to say that the Hund's coupling, which arises from on-site atomic-like interactions, is not important in itinerant magnets. It is after all the origin of the Stoner enhancement and without it (i.e. $I(\mathbf{q})=0$) there would be no magnetic instability at all. This is important because it means that electronic states away from the Fermi energy are involved in the magnetism and will be coupled to the SDW through the exchange interaction, and furthermore this may be observable in spectroscopy. In fact, for bcc Cr [85] changes in the optical spectrum are seen extending up to ~ 0.5 eV upon the onset of the SDW.

However, while density functional calculations provide a qualitative description of the properties of the FeSC, there are significant quantitative problems. These show that the physics of these materials is far from simple. Experimentally, normal state of the doped superconducting FeSC is paramagnetic, while the SDW ground states have varying magnetic moments, but these are generally small, e.g. $\sim 0.4 \ \mu_B$ in LaFeAsO. [76] Therefore, one may expect that structural parameters, such as bond lengths, obtained within density functional calculations without including magnetism will be in good agreement with experimental values. This is not the case. For example, in the prototype, LaFeAsO, the refined As height above the Fe plane is 1.31 Å, measured by neutron diffraction at 4 K, i.e. in the ordered SDW state, 1.32 Å, measured at 175 K, i.e. in the metallic state above the SDW ordering temperature, and 1.32 Å, at 10 K, measured for the F doped superconducting material. [76] In contrast, LDA calculations without including magnetism yield 1.16 Å, i.e. an underestimate of ~ 0.15 Å. [27, 31] Similar large underestimates of the ligand height are found for the other FeSC compounds, including FeSe. [41]

The problem is apparently magnetic in origin. The FeSC show a very strong interplay of structure and magnetism as was demonstrated by detailed calculations. [30, 31] This leads to an anomalous pressure dependence of the structure with a collapse in the c-axis lattice parameter of $CaFe_2As_2$, for example. [88, 89] In particular, the magnetism is strongly coupled to the ligand height and the stability of magnetic states is greatly enhanced as the ligand height is increased. This interplay between magnetism and structure (via hybridization) was discussed in a local picture by Wu and co-workers. [90] In any case, larger equilibrium ligand heights are obtained when magnetism is included in the calculations, and guite reasonable agreement with experiment is obtained, especially if calculations are done using generalized gradient approximations (GGA), which more strongly stabilize magnetism compared to the LDA for these compounds. However, this comes at a price. In particular, while the structure is improved, and the SDW type ordering remains the predicted ground state the magnetism is far too stable, with moments of $\sim 2 \ \mu_B$ as compared to experimental moments of less that 1 μ_B in most compounds. For comparison, standard GGA calculations for Fe metal give a moment that is within 0.1 μ_B of experiment. [91] Furthermore, in the FeSC a magnetic state is then incorrectly predicted to be the ground state independent of doping.

Thus within density functional theory, the predicted ground state of the FeSC is strongly magnetic, whereas experimentally the ground state is a paramagnetic metal (doped) or a much more weakly magnetic SDW state that can be destroyed in favor of a paramagnetic superconductor with moderate pressure. [92, 93, 94] Furthermore, at least in LaFeAsO and other oxy-pnictides, the SDW is preceded by a structural distortion that lowers the symmetry to that of the SDW state, but at a higher temperature than the long range magnetic orderings, [76] and importantly the largest signatures in transport and other properties are at the structural transition. The structural transition is explainable within DFT as a consequence of the magnetic ordering (with large moments), [29, 51] and it has been argued that its occurrence reflects a fluctuating magnetic state closely related to the SDW but without long range static order. [95]

The type of error found in density functional calculations for the FeSC is very different in nature from cuprates and other materials where localization due to Coulomb repulsions plays the key role. In those materials, the meanfield-like LDA treatment yields insufficient localization and less tendency towards moment formation. This is the case in the cuprates and in Mott insulators in general. Cases where the LDA overestimates the tendency towards magnetism are much less common and generally occur in materials near quantum critical points, e.g. Ni₃Al and $Sr_3Ru_2O_7$. These are materials where magnetic ordering is suppressed by quantum fluctuations, which are beyond the scope of standard density functional theory. Therefore we take the discrepancy of ligand position as obtained in non-magnetic density functional theory from the experimental value, in combination with the overly magnetic ground state as evidence for the presence of strong spin fluctuations associated with the SDW. It is worth noting that at the GGA level, using experimental ligand positions, these materials are unstable against magnetism in general, including various antiferromagnetic configurations other than the SDW ordering, though the SDW remains the lowest energy state. This may be important in understanding the strong suppression of magnetism relative to such calculations, since this general magnetic instability does provide a large phase space for competing fluctuations.

This is supported by several pieces of experimental evidence. In several compounds, including both undoped and superconducing samples, the susceptibility $\chi(T)$ is an increasing function of temperature up to high temperatures. [79, 96, 97] This shows the presence local antiferromagnetic correlations that persist up to high temperature. Fe exchange multiplets, demonstrating strong local fluctuating magnetism, were found in non-magnetic superconducting CeFeAsO_{0.89}F_{0.11} by x-ray absorption spectroscopy. [98] The other case where this is observed in a non-magnetic Fe compound is NbFe₂, [99] which is an itinerant magnetic in close proximity to a quantum critical point. [100] Furthermore, the scattering rate indicated by optics and by transport is high in the normal state and decreases strongly at the SDW onset. [78, 79] Returning to the Hund's coupling, the implication of the large dynamical spin fluctuations that would needed to suppress the overly stable magnetism in the mean-fieldlike GGA ground state, is that correspondingly strong electronic signatures should be present. This is consistent with the observation of exchange splitting of $\sim 3 \text{ eV}$ in the Fe 3s spectra of paramagnetic CeFeAsO_{0.89}F_{0.11}. [98] Considering that these are dynamical fluctuations, one may then expect shifts in spectral weight accompanied by increases in the scattering rate within the Fe derived valence bands up to eV energies.

5. Superconductivity

At this time the mechanism for superconductivity has not yet been established. Detailed calculations have shown that the superconductivity cannot be understood in terms of standard electron-phonon theory. [19, 20] Also, there is a clear association, e.g. in the phase diagrams, between superconductivity and suppression of the SDW, either by doping or by pressure. Considering the evidence for spin fluctuations in the normal state and the similarity of the normal states above the SDW transition and above the superconducting transition it is tempting to consider pairing based on spin fluctuations. Key points are that the pairing interaction will have a shape closely related to the real part of the susceptibility (but more strongly peaked in weak coupling), and that spin fluctuations are repulsive in a singlet channel. [101, 102] Therefore the strongest interaction will be at (π,π) similar to the SDW, and will favor opposite sign order parameters on Fermi surface sections separated by this wavevector. Furthermore, the nesting related peak in $\chi(\mathbf{q})$ does not show strong fine structure on the scale of the small (electron or hole) Fermi surfaces nor is there strong k_z dependence. Therefore the itinerant spin fluctuations do not provide a driving force for changes in the order parameter within a given Fermi surface section, either along k_z or in the (k_x, k_y) plane. Therefore, within the simplest scenario an s symmetry state with opposite sign order parameters on the electron and hole sections might be expected. This is the s_+ state proposed by Mazin and co-workers and by Kuroki and co-workers. [20, 70] Experimental tests to determine the symmetry of the order parameter are needed to confirm whether this is the actual superconducting state. In any case, within such a framework, the same electrons that drive the spinfluctuations (i.e. those on the nested Fermi surface) are the electrons that are involved in either the SDW order or the superconductivity. Therefore, both the SDW and superconductivity are Fermi surface instabilities, driven by the same interaction and competing for the same electrons.

As mentioned, both the superconducting and SDW orders arise from a normal state that already has strong antiferromagnetic correlations and so perhaps may be regarded as related. In this case, while there is clearly a competition for electrons between the two orders, one may ask whether they can co-exist. A trivial possibility is that there is a first order line separating the SDW and superconducting states, so that there is some region of two phase co-existence, i.e. nanoscale phase separation with superconducting and magnetic nanoregions. Even without a first order line, local variations in the doping level may be expected to lead to a mixed state with superconducting and magnetic regions on a nanoscale near the boundary between these two states in the FeSC. This is especially likely in the FeSC because of the heavy band masses and resulting short coherence lengths, which mean that statistical variations in dopant concentration within a volume defined by the coherence length will be substantial. For example the estimated in-plane coherence length of $BaFe_{1.8}Co_{0.2}As_2$ is ~ 28 Å. [103] If the coherence length out-of-plane is half the in-plane value, then the corresponding volume would be $\sim 10^4 \text{ Å}^3$, which would contain ~ 200 transition metal atoms, and on average 20 Co atoms and therefore with local \sqrt{n} variations in the doping level of ~ 20%.

A more interesting possibility is that there may be a coexistence on the Fermi surface. In general, very soft fluctuations (energy below the gap) are pair breaking in superconductivity since the superconducting state is unstable against condensation of the fluctuations (i.e. magnetic order). This could lead to a situation where part of the Fermi surface is gapped by the condensation of spin fluctuations (i.e. magnetism) and part is gapped by superconductivity, with a node separating these regions. This is somewhat analogous to one picture of the cuprate pseudogap state based on angle resolved photoemission experiments. [104] Such a state would be one way to reconcile conflicts between experiments suggesting line nodes and experiments suggesting s symmetry. In this regard, we note that there is conflicting experimental evidence regarding the gap in the FeSC. Various experiments, including Andreev spectroscopy and photoemission strongly suggest an s wave gap, [71, 74, 73, 72, 105] while at the same time nuclear magnetic resonance (NMR) measurements show a T^3 dependence of the relaxation rate going to very low T. This excess NMR relaxation rate is generally a clear signature of line nodes, inconsistent with a simple s (including s_{+}) gap. [106, 107, 108, 109, 110] A similar conclusion is reached from penetration depth measurements, i.e. that a non-exponential density of states is present. [111] While an explanation in terms of a very strongly anisotropic swave gap [112] may be possible, the persistence of the excess NMR relaxation to very low temperature in samples with scattering as indicated by the resistivity, may require a different explanation, one possibility being the scenario outlined above. Also, it should be mentioned that some of the data could perhaps be explained by scattering effects. [111] In any case, it will be of great interest to examine the phase boundary between the superconducting and SDW states in detail.

6. Summary and Conclusions

The discovery of the FeSC provides us with the second example of superconductivity above 50 K. Thus the relationship between the FeSC and the cuprates is of considerable interest. It is perhaps premature to make definitive connections between these materials, considering that the pairing mechanism has not been conclusively established in either material, and in fact at this time not even the pairing symmetry is clearly established in the FeSC. Nonetheless, it still of interest to note similarities and differences.

Starting with similarities, neither the cuprates nor the FeSC can be understood as conventional electron phonon superconductors and both materials have both antiferromagnetic and superconducting phases in doping dependent phase diagrams. However, the differences appear to be more significant. In the cuprates the antiferromagnetic phases are Mott insulators arising from the effects of Coulomb correlations. These have substantial gaps and local moment magnetism. In the FeSC the antiferromagnetic phases are more directly connected with the normal state, as they are metallic and arise from an SDW instability of the Fermi surface. Unlike cuprates, superconductivity can be produced in the FeSC by destroying the SDW state without doping. Interestingly, the signatures of spin fluctuations are much more apparent in the FeSC than in the normal state of the cuprates, especially if one considers optimal doping. Finally, much of the physics of the FeSC appears to be related to itinerant electrons and the Fermi surface.

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