Pairing Mechanism in Fe-Based Superconductors

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Abstract
I review recent works on the symmetry and the structure of the superconducting gap in Fe-based superconductors (FeSCs) and on the underlying pairing mechanism in these systems. The experimental data on superconductivity show very rich behavior, with potentially different symmetry of a superconducting state for different compositions of the same material. The variety of different pairing states raises the issue of whether the physics of FeSCs is model dependent or is universal, governed by a single underlying pairing mechanism. I argue that the physics is universal and that all pairing states obtained so far can be understood within the same universal pairing scenario and are well described by the effective low-energy model with small numbers of input parameters.
1. INTRODUCTION

The discovery in 2008 of superconductivity in Fe-based pnictides (1) (binary compounds of the elements from the fifth group: N, P, As, Sb, Bi) was, arguably, among the most significant breakthroughs in condensed matter physics during the past decade. Major efforts by the condensed matter community have been devoted in the few years since the discovery to understanding the normal state properties of these materials, the pairing mechanism, and the symmetry and structure of the pairing gap.

The family of Fe-based superconductors (FeSCs) is already quite large and keeps growing. It includes various Fe-pnictides such as 1111 systems RFeAsO (R = rare earth element) (1–4), 122 systems XFe$_2$As$_2$ (X = alkaline earth metals) (5–7), 111 systems such as LiFeAs (9), and also Fe-chalcogenides (Fe-based compounds with elements from the sixteenth group: S, Se, Te) such as FeTe$_{1-x}$Se$_x$ (10) and AFe$_x$Se$_2$ (A = K, Rb, Cs) (11, 12).

Parent compounds of FeSCs are metals, in distinction to cuprate superconductors for which parent compounds are Mott insulators. Still, similar to the cuprates, in most cases these parent compounds are antiferromagnetically ordered (for the latest results on magnetic measurements, see Reference 13 and references therein). Because electrons that carry magnetic moments still travel relatively freely from site to site, the magnetic order is often termed as a spin-density wave (SDW), by analogy with, e.g., antiferromagnetic Cr, rather than with Heisenberg antiferromagnetism (the latter term is reserved for systems in which electrons are nailed down to particular lattice sites by very strong Coulomb repulsion).

Superconductivity (SC) in FeSCs emerges upon either hole or electron doping (see Figure 1) but can also be induced by pressure or by isovalent replacement of one pnictide element by another, e.g., As by P (8). In some systems, such as LiFeAs (9) and LaFePO (14), SC emerges already at zero doping instead of magnetic order.

![Figure 1](image_url)

**Figure 1**

Schematic phase diagram of Fe-based pnictides upon hole or electron doping. In the shaded region, superconductivity (SC) and antiferromagnetism coexist. Not all details/phases are shown. Superconductivity can be initiated not only by doping but also by pressure and/or isovalent replacement of one pnictide element by another (8). The nematic phase at $T > T_N$ is the subject of debate. Superconductors at large doping are KFe$_2$As$_2$ for hole doping (42, 43) and A$_x$Fe$_{2-x}$Se$_2$ (A = K, Rb, Cs) for electron doping (11, 12). Whether superconductivity in pnictides exists at all intermediate dopings is not clear yet. Taken from Reference 24.
The magnetism, the electronic structure, the normal state properties of FeSCs, and the interplay between FeSCs and cuprate superconductors have been reviewed in several recent publications (15–25). This review is an attempt to summarize our current understanding of the pairing mechanism and the symmetry and structure of the pairing gap at various hole and electron dopings.

The phenomenon of SC has a long history. SC was discovered by Kamerlingh Onnes (26) exactly a century ago. It was explained in general terms nearly 50 years later, in 1957, by Bardeen, Cooper, and Schrieffer (BCS), who demonstrated that an arbitrary weak attractive interaction between low-energy fermions is sufficient to pair them into a bound state. At weak coupling, paired fermions immediately form a Bose-Einstein condensate, behave as one single macroscopic quantum object, and move coherently under the applied electric field, i.e., superconduct. In \( d \)-dimensional electronic systems low-energy fermionic states are located in momentum space near particular \( d - 1 \) dimensional surfaces, called Fermi surfaces (FSs), on which fermionic energy is zero relative to the chemical potential. At weak/moderate coupling, the pairing problem is confined to a near vicinity of an FS. The interaction between fermions is generally nonsingular with respect to variations of the distance to the FS and can be approximated by its value right on the FS.

What causes the attraction between fermions is a more subtle question, and the nature and the origin of the pairing glue have been the subject of great debates in the condensed matter community over the past 50 years. BCS attributed the attraction between fermions to the underlying interaction between electrons and phonons (27) (the two electrons interact with each other by emitting and absorbing the same phonon that then serves as a glue that binds electrons into pairs). The electron-phonon mechanism has been successfully applied to explain SC in a large variety of materials, from Hg and Al to recently discovered and extensively studied MgB\(_2\) with the transition temperature \( T_c = 39 \) K (28). Nonphononic mechanisms of the pairing have also been discussed, most notably in connection with superfluidity in \(^3\)He (29), but did not become the mainstream before the discovery of SC in LaBaCuO in 1986 (30). That discovery and subsequent discoveries of superconductivity at higher \( T_c \) in other cuprates signaled the beginning of the new era of high-temperature superconductivity to which FeSCs added a new avenue with quite high traffic over the past three years.

Superconductivity is a quite robust phenomenon. It has been known since the early sixties (31) that in isotropic systems the equation for superconducting \( T_c \) factorizes if one expands the interaction between the two fermions in partial components corresponding to interactions in the subspaces with a given angular momentum of the two interacting fermions \( l = 0, 1, 2, 3, \) etc. (In spatially isotropic systems the \( l = 0 \) component is called \( s \)-wave, the \( l = 1 \) component is called \( p \)-wave, the \( l = 2 \) component is called \( d \)-wave, etc.) If just one component with some \( l \) is attractive, the system undergoes a SC transition at some temperature \( T = T_c \). For phonon-mediated superconductors, \( s \)-wave superconductivity is the most likely outcome. In the cuprates, however, the pairing symmetry has been firmly established as \( d \)-wave. The vast majority of researchers believe that such pairing is not caused by phonons and emerges instead due to screened Coulomb interaction between electrons. The screened Coulomb interaction \( U(r) \) is constant and repulsive at short distances but has a complex dependence on \( r \) at large distances and may develop an attractive component at some \( l \). One solid reason for the attraction, at least at large \( l \), was identified by Kohn & Luttinger (32) back in 1965.

In lattice systems, angular momentum is no longer a good quantum number, and the equation for \( T_c \) only factorizes between different irreducible representations of the lattice space group. In tetragonal systems, which include both cuprates and FeSCs, there are four one-dimensional irreducible representations, \( A_{1g}, B_{1g}, B_{2g}, \) and \( A_{2g} \), and one two-dimensional...
representation, $E_{2g}$. Each representation has an infinite set of eigenfunctions. The eigenfunctions from $A_{1g}$ are invariant under symmetry transformations in a tetragonal lattice: $x \rightarrow -x$, $y \rightarrow -y$, $x \rightarrow y$; the eigenfunctions from $B_{1g}$ change sign under $x \rightarrow y$, etc. If a superconducting gap has $A_{1g}$ symmetry, it is often called $s$-wave because the first eigenfunction from the $A_{1g}$ group is just a constant in momentum space (a $\delta$-function in real space). If the gap has $B_{1g}$ or $B_{2g}$ symmetry, it is called $d$-wave ($d_{x^2-y^2}$ or $d_{xy}$), because in momentum space the leading eigenfunctions in $B_{1g}$ and $B_{2g}$ are $\cos k_x - \cos k_y$ and $\sin k_x \sin k_y$, respectively, and these two reduce to $l = 2$ eigenfunctions $\cos 2\theta$ and $\sin 2\theta$ in the isotropic limit.

In the cuprates, the superconducting gap has been proved experimentally to have $B_{1g}$ symmetry (see, e.g., Reference 33 and references therein). The gap with this symmetry appears quite naturally in the cuprates, in the doping range where they are metals, if one assumes that the glue that binds fermions together is a spin-fluctuation exchange rather than a phonon (see Figure 2). The notion of a spin-fluctuation exchange is a convenient way to describe multiple Coulomb interactions between fermions. It is believed, although not proved rigorously, that in systems located reasonably close to a magnetic instability, the fully screened Coulomb interaction between fermions can be approximated by an effective interaction in which fermions exchange quanta of their collective fluctuations in the spin channel. That a $B_{1g}$ gap is selected is not a surprise because such a gap $\Delta(k) \propto \cos k_x - \cos k_y$ changes sign not only under $k_x \rightarrow k_y$ but also between $k$ and $k' = k + Q$, where $Q = (\pi, \pi)$ is the momentum at which spin fluctuation–mediated pairing interaction $U(k, k')$ is peaked. This sign change is the crucial element for any electronic mechanism of superconductivity because one needs to extract an attractive (negative) component from the repulsive (positive) screened Coulomb interaction. For the $B_{1g}$ gap such a

Figure 2

A comparison of the pairing state from spin-fluctuation exchange in cuprate SCs and in Fe-based superconductors (FeSCs). In the cuprates (a) the Fermi surface (FS) is large, and antiferromagnetic $Q = (\pi, \pi)$ connects points on the same FS. Because spin-mediated interaction is positive (repulsive), the gap must change sign between FS points separated by $Q$. Consequently, the gap changes sign twice along the FS. This implies a $d$-wave gap symmetry. In FeSCs (b) scattering by $Q$ moves fermions from one FS to the other. In this situation, the gap must change sign between different FSs but to first approximation remains a constant on a given FS. By symmetry, such a gap is an $s$-wave gap. It is called $s^{\pm}$ because it changes sign between different FSs.

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resolved photoemission spectroscopy (ARPES) data on moderately doped KFe$_2$As$_2$ and BaFe$_2$(As$_{1-x}$P$_x$)$_2$, which detected only a small variation of the gap along the FSs centered at (0,0) (40), and with the evolution of the tunneling data in a magnetic field (41). [However, for heavily hole-doped KFe$_2$As$_2$ various experimental probes (42) indicate the presence of gap nodes, which for the FS geometry in these materials (43) are consistent with a $d$-wave gap.] For the doping range where the gap is very likely an $s$-wave, the data on some FeSCs were interpreted as evidence for the full gap (44–47), whereas the data for other FeSCs were interpreted as evidence that the gap has nodes (48, 49) or deep minima (50–52). In addition, recent nuclear magnetic resonance (NMR) experiments on LiFeAs have been interpreted in favor of a $p$-wave gap (53).

In this review, I argue that all these seemingly very different gap structures (with the exception of a $p$-wave gap) actually follow quite naturally from the same underlying physics idea that FeSCs can be treated as moderately interacting itinerant fermionic systems with multiple FS sheets and effective four-fermion intraband and interband interactions in the band basis.
I introduce the effective low-energy model with small numbers of input parameters (54) and use it to study the doping evolution of the pairing in hole- and electron-doped FeSCs. It has been argued (54) that various approaches based on the underlying microscopic model in the orbital basis reduce to this model at low energies.

The review is organized as follows. In Section 2 I discuss general aspects of the pairing in FeSCs. I briefly review the band structure of FeSCs and show that it contains several bands of low-energy excitations. I then present generic symmetry considerations of the pairing in a multiband superconductor. I show that a conventional wisdom that an $s$-wave gap is nodeless along the FSs, that a $d$-wave gap has four nodes, etc., has only limited applicability in multiband superconductors, and there are cases when the gap with four nodes has an $s$-wave symmetry, and the gap without nodes has a $d$-wave symmetry. In Section 3 I discuss the interplay between intraband and interband interactions, first for a toy two-pocket model and then for realistic multipocket models, and set the conditions for an attraction in an $s$-wave or a $d$-wave channel.

I consider a five-orbital model with local interactions, convert it into a band basis, and argue that for most input parameters the bare interaction is repulsive in all channels due to strong intrapocket Coulomb repulsion. In Section 4 I discuss the ways to overcome Coulomb repulsion. I review random phase approximation (RPA) and renormalization group (RG) approaches and show that magnetic fluctuations enhance inter-pocket interaction, if this interaction is positive, and this enhancement gives rise to an attraction in both $s^\pm$ and $d_{x^2-y^2}$ channels. I briefly discuss $s^+s^+$ pairing, which emerges if input parameters are such that inter-pocket interaction is negative. In Section 5 I use a combination of RPA and leading angular harmonic approximation (LAHA) to analyze the pairing in $s$- and $d$-wave channels at different dopings. I show that magnetically mediated pairing leads to (a) an $s^\pm$ superconductivity with nodes on electron pockets for moderate electron doping, (b) an $s^\pm$ superconductivity without nodes for moderate hole dopings, (c) a nodeless $d$-wave superconductivity for strong electron doping (except, possibly, small nodal regions near $k_z = \pi/2$), and (d) a nodal $d$-wave superconductivity for strong hole doping. I briefly review the experimental situation in Section 6 and present concluding remarks in Section 7. I list separately the summary points and future issues.

2. GENERIC ASPECTS OF PAIRING IN Fe-BASED SUPERCONDUCTORS

2.1. The Electronic Structure

The electronic structure of FeSCs at low energies is rather well established by ARPES (55) and quantum oscillation measurements (56). In weakly and moderately electron-doped materials, such as BaFe$_{1-x}$Co$_x$Fe$_2$As$_2$, the FS contains several quasi-2D warped cylinders centered at $k = (0,0)$ and $k = (\pi,\pi)$ in a 2D cross section, and may also contain a quasi-3D pocket near $k_z = \pi$ (Figure 3). The fermionic dispersion is electron-like near the FSs at $(\pi,\pi)$ (filled states are inside an FS) and hole-like near the FSs centered at $(0,0)$ (filled states are outside an FS). In heavily electron-doped FeSCs, such as A$_x$Fe$_{1-x}$Se$_2$ (A = K, Rb, Cs), only electron pockets remain, according to recent ARPES studies (11). In weakly and moderately hole-doped FeSCs, such as Ba$_{1-x}$K$_x$Fe$_2$As$_2$, the electronic structure is similar to that at moderate electron doping, however the spherical FS becomes the third quasi 2D hole FS centered at $(2\pi,0) = (0,0)$. In addition, new low-energy hole states likely appear around $(\pi,\pi)$ and squeeze electron pockets (57). At strong hole doping, electron FSs disappear and only hole FSs are present (43). These electronic structures agree well with first-principle calculations (17, 58, 59), which is another argument to treat FeSCs as itinerant fermionic systems. The measured FS reflects the actual crystal structure of
FeSCs in which there are two nonequivalent positions of a pnictide above and below an Fe plane, and, as a result, there are two Fe atoms in the unit cell (this actual BZ is called a folded BZ). From a theoretical perspective, it would be easier to work in the BZ that contains only one Fe atom in the unit cell (this theoretical BZ is called an unfolded BZ). I illustrate the difference between folded and unfolded BZs in Figure 4. In general, only a folded BZ is physically meaningful. However, if for some reason a potential from a pnictogen (or chalcogen) can be neglected, the difference between the folded and the unfolded BZs becomes purely geometrical: The momenta \( \mathbf{k}_x \) and \( \mathbf{k}_y \) in the folded BZ are linear combinations of \( \mathbf{k}_x \) and \( \mathbf{k}_y \) in the unfolded BZ: \( \mathbf{k}_x = \mathbf{k}_x + \mathbf{k}_y \), \( \mathbf{k}_y = \mathbf{k}_x - \mathbf{k}_y \). In this situation, folded and unfolded BZs become essentially equivalent.

Most of the existing theoretical works on the pairing mechanism and the structure of the SC gap analyze the pairing problem in the unfolded BZ, in which two hole pockets are centered at (0,0) and one at \( (\pi, \pi) \), and the two electron pockets are at (0,0) and (\( \pi, \pi \)). It became increasingly clear recently that the interaction via a pnictogen/chalcogen and also 3D effects do play some role in the pairing, particularly in strongly electron-doped systems (60, 61). However, it is still very likely that the key aspects of the pairing in FeSCs can be understood by analyzing a pure 2D electronic structure with only Fe states involved. Below I assume that this is the case and consider a 2D model in the unfolded BZ with hole FSs near (0,0) and \( (\pi, \pi) \) and electron FSs at (0,0) and \( (\pi, \pi) \).

### 2.2. The Structure of \( s \)-Wave and \( d \)-Wave Gaps in a Multiband Superconductor

I now use the multiband electronic structure as input and consider the pairing problem at weak coupling. I show that an \( s \)-wave gap generally has angle dependence on electron FSs and may even have nodes, whereas a \( d \)-wave gap, which is normally assumed to have nodes, may in fact be nodeless on the same electron FSs.

A generic low-energy BCS-type model in the band basis is described by

\[
\mathcal{H} = \sum_{i,k} \epsilon_i(k) a_{i,k}^\dagger a_{i,k} + \sum_{i,j,k,p} \Gamma_{ij}(k,p) a_{j,k}^\dagger a_{i,p} a_{j,-p}. \tag{1}
\]

The quadratic term describes low-energy excitations near hole and electron FSs, labeled \( i \) and \( j \), and the four-fermion term describes the scattering of a pair \( (k^\uparrow, -k^\uparrow) \) on the FS \( i \) to a pair \( \ldots \)
These interactions are either intrapocket interactions (hole-hole $G_{hh}$ or electron-electron $G_{ee}$) or interpocket interactions (hole-electron $G_{eh}$, hole-hole $G_{hh}$, and electron-electron $G_{ee}$). I illustrate this in Figure 5.

Assume for simplicity that the frequency dependence of $\Gamma$ can be neglected and low-energy fermions are Fermi-liquid quasiparticles with Fermi velocity $v_{k_F}$. In this situation, the gap $\Delta(k)$ also does not depend on frequency, and the linearized gap equation becomes the eigenfunction/eigenvalue problem

$$\lambda_i \Delta_i(k) = - \int \frac{dp}{4\pi^2 v_{p_F}} \Gamma(k_F, p_F) \Delta_i(p),$$

where $\Delta_i$ are eigenfunctions and $\lambda_i$ are eigenvalues. The system is unstable toward pairing if one or more $\lambda_i$ are positive. The corresponding $T_{c,i}$ scale as $T_{c,i} = \Lambda_i e^{-1/\lambda_i}$. Although $\Lambda_i$ are...
Generally different for different $i$, the exponential dependence on $1/\lambda_i$ implies that, most likely, the solution with the largest positive $\lambda_i$ emerges first and establishes the pairing state, at least immediately below $T_c$.

As I discussed in the Introduction, the vertex $\Gamma(k,p)$ can be decomposed into representations of the tetragonal space group (one-dimensional representations are $A_{1g}$, $B_{1g}$, $B_{2g}$, and $A_{2g}$). Basis functions from different representations do not mix, but each contains an infinite number of components. For example, $s$-wave components, and even for $s$-wave, $G_{e_1,b}$ and $G_{e_1,c}$ depend on the angles along electron FSs. Taken from Reference 66.

For simplicity, only one hole Fermi surface (FS) is shown. $\Gamma$, $X$, and $Y$ points are $(0,0)$, $(\pi,0)$, and $(0,\pi)$, respectively. $G_{e_1,b}$ is the interaction within the hole pocket; $G_{e_1,b}$ and $G_{e_2,b}$ are the interactions between a hole and an electron pocket; and $G_{e_1,c}$, $G_{e_2,c}$, and $G_{e_1,c}$ are intrapocket and interpocket interactions involving the two electron pockets. Each interaction contains $s$-wave and $d$-wave components, and even for $s$-wave, $G_{e_1,b}$ and $G_{e_1,c}$ depend on the angles along electron FSs.

**Figure 5**

Intrapocket and interpocket interactions in a four-band 2D model for Fe-based superconductors (FeSCs). For simplicity, only one hole Fermi surface (FS) is shown. $\Gamma$, $X$, and $Y$ points are $(0,0)$, $(\pi,0)$, and $(0,\pi)$, respectively. $G_{e_1,b}$ is the interaction within the hole pocket; $G_{e_1,b}$ and $G_{e_2,b}$ are the interactions between a hole and an electron pocket; and $G_{e_1,c}$, $G_{e_2,c}$, and $G_{e_1,c}$ are intrapocket and interpocket interactions involving the two electron pockets. Each interaction contains $s$-wave and $d$-wave components, and even for $s$-wave, $G_{e_1,b}$ and $G_{e_1,c}$ depend on the angles along electron FSs. Taken from Reference 66.
The hole FSs can be approximated by an angle-independent $\Gamma_{h,h}^s(k,p) = U_{h,h} (h, \text{ label different hole FSs})$, whereas $d$-wave ($B_{1g}$) interaction can be approximated by $\Gamma_{h,h}^d(k,p) = \tilde{U}_{h,h} \cos 2\phi_h \cos 2\phi_p$.

The situation changes, however, when we consider the pairing component involving fermions from electron FSs. Suppose that $k$ is still near the center of the BZ, but $p$ is near one of the two electron FSs, say the one centered at $(0,\pi)$. Consider all possible $\Psi_n(p)$ with $A_{1g}$ symmetry. A simple experimentation with trigonometry shows that there are two different subsets of basis functions:

subset I: $1, \cos p_x \cos p_y, \cos 2p_x + \cos 2p_y$ and subset II: $\cos p_x + \cos p_y, \cos 3p_x + \cos 3p_y$.

For a circular FS centered at $(0,\pi)$, the functions from subset I can be again expanded in a series of $\cos 4\phi_p$ with integer $l$. The functions from subset II are different—they all vanish at $(0,\pi)$ and are expanded in a series of $\cos(2\phi_p + 4l\phi_p)$ (the first term is $\cos 2\phi_p$, the second is $\cos 6\phi_p$, etc.). For elliptic FSs $\cos 4\phi_p$ and $\cos(2\phi_p + 4l\phi_p)$ terms appear in both subsets. In both cases, the total is (66, 67):

$$\Psi_n^s(p) = a_m + \tilde{a}_m \cos 4\phi_p + \tilde{b}_m \cos 8\phi_p + \ldots$$

$$+ \tilde{a}_m \cos 2\phi_p + \tilde{b}_m \cos 6\phi_p + \tilde{c}_m \cos 10\phi_k + \ldots$$

For the other electron FS, $\Psi_n^s(p)$ is the same, but momentum components $p_x$ and $p_y$ are interchanged; hence, the sign of all $\cos(2\phi_p + 4l\phi_p)$ components changes.

Let us make the same approximation as before and keep only the leading components in each subset. Then

$$\Psi_n^s(p) = \tilde{a}_m \pm a_m \cos 2\phi_p,$$

where the upper sign is for one electron FS and the lower for the other. The angle-independent term and the $\cos 2\phi_p$ term have to be treated on equal footing because each is the leading term in the corresponding series. Combining Equation 8 with the fact that $\Psi_n^s(k)$ on a hole FS can be approximated by a constant, we obtain a generic form of the $s$-wave component of the interaction between fermions near hole and electron FSs:

$$\Gamma_{e_1,e_2}^s(k,p) = U_{e,e} \left( 1 + 2\xi_{e,e} \cos 2\phi_{p_1} + \ldots \right)$$

$$\Gamma_{e_1,e_2}^s(k,p) = U_{e,e} \left( 1 - 2\xi_{e,e} \cos 2\phi_{p_2} + \ldots \right),$$

where dots stand for $\cos 4\phi_h$, $\cos 4\phi_p$, $\cos 6\phi_p$, etc., terms.

By the same reasoning, $s$-wave components of interpocket and intrapocket interactions between fermions from electron FSs are

$$\Gamma_{e_1,e_2}^s(k,p) = U_{e,e} \left( 1 + 2\xi_{e,e} \left( \cos 2\phi_{k_1} + \cos 2\phi_{p_1} + \ldots \right) + 4\beta_{e,e} \cos 2\phi_{k_1} \cos 2\phi_{p_1} + \ldots \right)$$

$$\Gamma_{e_2,e_2}^s(k,p) = U_{e,e} \left( 1 - 2\xi_{e,e} \left( \cos 2\phi_{k_2} + \cos 2\phi_{p_2} + \ldots \right) + 4\beta_{e,e} \cos 2\phi_{k_2} \cos 2\phi_{p_2} + \ldots \right)$$

$$\Gamma_{e_1,e_2}^s(k,p) = U_{e,e} \left( 1 + 2\xi_{e,e} \left( \cos 2\phi_{k_1} - \cos 2\phi_{p_1} + \ldots \right) - 4\beta_{e,e} \cos 2\phi_{k_1} \cos 2\phi_{p_1} + \ldots \right).$$
Once the pairing interaction has the form of Equations 9 and 10, the gaps along the hole FSs are angle independent (modulo cos 4\phi terms), but the gaps along the two electron FSs are of the form

$$\Delta^e_{\pm}(k) = \Delta_e \pm \bar{\Delta}_e \cos 2\phi_k.$$  \hspace{1cm} 11.

When \bar{\Delta}_e is small compared to \Delta_e, the angle dependence is weak, but when |\bar{\Delta}_e| > |\Delta_e|, s-wave gaps have nodes at accidental values of \phi, which differ between the two electron FSs.

A similar consideration holds for the \textit{d}$_{x^2-y^2}$ gap. Within the same approximation of leading angular momentum harmonics, we have

$$\Gamma^d_{e_1, e_2}(k, p) = \tilde{U}_{e_1 e_2} \cos 2\phi_k \left(1 + \tilde{z}_{e_1 e_2} \cos 2\phi_{p_1}\right) + \ldots$$

$$\Gamma^d_{e_1, h_1}(k, p) = \tilde{U}_{e_1 h_1} \cos 2\phi_k \left(-1 + \tilde{z}_{e_1 h_1} \cos 2\phi_{p_1}\right) + \ldots$$ \hspace{1cm} 12.

and

$$\Gamma^d_{e_2, e_2}(k, p) = \tilde{U}_{e_2 e_2} \left(1 + 2\tilde{z}_{e_2 e_2} \cos 2\phi_{k_1} + \cos 2\phi_{p_1}\right) + 4\tilde{\beta}_{e_2} \cos 2\phi_{k_1} \cos 2\phi_{p_1} + \ldots$$

$$\Gamma^d_{e_1, e_1}(k, p) = \tilde{U}_{e_1 e_1} \left(1 - 2\tilde{z}_{e_1 e_1} \cos 2\phi_{k_1} + \cos 2\phi_{p_1}\right) + 4\tilde{\beta}_{e_1} \cos 2\phi_{k_1} \cos 2\phi_{p_1} + \ldots$$

The solution of the gap equation then yields the gap in the form

$$\Delta^e_{\pm}(k) = \bar{\Delta}_e \cos 2\phi_k$$

$$\Delta^e_{\pm}(k) = \pm \bar{\Delta}_e + \tilde{\Delta}_e \cos 2\phi_k.$$  \hspace{1cm} 14.

Along the hole FS, the gap behaves as a conventional \textit{d}-wave gap with four nodes along the diagonals. Along electron FSs, the two gaps differ in the sign of the angle-independent terms and have in-phase cos 2\phi oscillating components. When \bar{\Delta}_e << \Delta_e the two electron gaps are simply plus and minus gaps, but when \bar{\Delta}_e > \bar{\Delta}_e, each has accidental nodes, again along different directions on the two electron FSs.

We see therefore that the geometry of the FSs in FeSCs affects the gap structure in a fundamental way: Because electron FSs are centered at the \textit{k} points that are not along BZ diagonals, s-wave gaps on these FSs have cos 2\phi oscillations that one normally would associate with a \textit{d}-wave symmetry, and \textit{d}-wave gaps have constant (plus-minus) components that one would normally associate with an \textit{s}-wave symmetry. When these wrong components are large, the gaps have accidental nodes. These nodes may be present or absent for both \textit{s}-wave and \textit{d}-wave gaps, i.e., symmetry constraints play no role here.

An \textit{s}-wave gap with nodes is one of the exotic options specific to the electronic structure of FeSCs. Another exotic option is a \textit{d}-wave state without nodes. In heavily electron-doped FeSCs, hole states are gapped, and only electron FSs remain. The \textit{d}-wave gaps on these two FSs have no nodes if the cos 2\phi oscillation component is smaller than a constant term; hence, the system displays a behavior typical for a fully gapped SC despite the gap actually having a \textit{d}-wave symmetry. There are even more exotic options offered by the actual three-dimensionality of the electronic structure and/or the hybridization of the electron FSs due to interaction via a pnictide/chalcogen. One RPA calculation (61) places the nodes of the \textit{s}$^\pm$ gap on hole pockets,
near particular $k_z$. Another study (60) argues that a $d$-wave gap for heavily electron-doped FeSCs must have nodes near $k_z = \pi/2$.

It is essential, however, that either a more conventional one or a more exotic pairing state develop only if the corresponding eigenvalue $\lambda_i$ is positive. To understand under what conditions $\lambda_i > 0$ we now have to consider specific models for FeSCs.

### 3. THE INTERPLAY BETWEEN INTRAPOCKET AND INTERPOCKET INTERACTIONS

In this section we make the first step in the analysis of what causes the attraction in FeSCs and consider how the sign and magnitude of $\lambda_i$ depend on the interplay between intrapocket and interpocket interactions.

#### 3.1. The Toy Two-Pocket Model

As a warm-up, consider first an idealized two-pocket model (68) consisting of two identical circular pockets: a hole pocket at (0,0) and an electron pocket at $(p, p)$. Because the electron FS is centered at $k$ along the diagonal, the cos $2\phi$ terms in the electronic gap are no longer present, so some part of the physics of FeSCs is lost. Still, this idealized model is a good starting point to consider the interplay between intrapocket and interpocket interactions.

For a two-pocket model Equations 9–13 reduce to

$$
G_{hh}^{s} = U_{hh}, \quad G_{he}^{s} = U_{he}, \quad G_{ee}^{s} = U_{ee}$$

and

$$
G_{hh}^{d}(k_F, p_F) = \tilde{U}_{hh} \cos 2\phi k \cos 2\phi p, \quad G_{he}^{d}(k_F, p_F) = \tilde{U}_{he} \cos 2\theta k, \quad G_{ee}^{d} = U_{ee}.
$$

The eigenvalue problem, Equation 2, reduces to the set of two coupled equations in each channel. Solving them, we obtain

$$
\lambda_{s,1,2} = \frac{-(u_{hh} + u_{ee}) \pm \sqrt{(u_{hh} - u_{ee})^2 + 4u_{he}^2}}{2}
$$

and

$$
\lambda_{d,1,2} = \frac{-(\tilde{u}_{hh} + \tilde{u}_{ee}) \pm \sqrt{(\tilde{u}_{hh} - \tilde{u}_{ee})^2 + 4\tilde{u}_{he}^2}}{4}
$$

where $u_{ij} = U_{ij}N_F$ and $N_F = n(2\pi)$ is the density of states per spin projection.

We see that a solution with a positive $\lambda$ in either an $s$- or a $d$-wave channel exists if the interpocket interaction is larger than intrapocket interactions. Specifically, one needs

$$
u_{he}^2 > u_{ee}u_{hh} \text{ or } \tilde{u}_{he}^2 > \tilde{u}_{ee}\tilde{u}_{hh}.
$$

If this condition is not met, the system remains in the normal state down to $T = 0$.

If Equation 17 is satisfied and $u_{he} > 0$, $s$-wave solution with $\lambda^s > 0$ yields a plus-minus gap, $\Delta_e = -\Delta_h$ ($s^\pm$ state). If $u_{he} < 0$ (what requires intraband attraction), the $s$-wave solution is a conventional one, with $\Delta_e = \Delta_h$. Similarly, $d$-wave solutions yield cos $2\phi$ gaps on the hole and electron FSs with either zero or $\pi$ phase shifts.

#### 3.2. Multiband Models

Consider next a more realistic case of two electron FSs centered at $(0, \pi)$ and $(\pi, 0)$. Now hole-electron and electron-electron interactions have cos $2\phi$ terms, and the eigenvalue/eigenfunction problem, Equation 2, reduces to the set of either four (or five) coupled equations in either
s-wave or d-wave channels: Two (or three) $\Delta$s are the gaps on the hole FSs, and two other $\Delta$s are angle-independent and $\cos 2\phi$ components of the gaps on the electron FSs. Accordingly, there are either four or five different $\lambda_i$'s and $\lambda_d$'s.

The analysis of $4 \times 4$ or $5 \times 5$ gap equations is tedious but straightforward. I do not discuss it in length (for a detailed discussion see References 54 and 66) but rather focus on whether the interpocket interaction $u_{be}$ is required to exceed the threshold set by intrapocket hole-hole and electron-electron interactions. Interestingly enough, this may no longer be necessary. To illustrate this, consider the case of an $s$-wave pairing in a four-pocket model and assume for simplification that only one hole pocket is relevant to the pairing. Then the eigenvalue problem reduces to the set of three equations for $\Delta_h$, $\Delta_e$, and $\Delta_c$ [Equation 15]. I illustrate this in Figure 6.

In other words, for one of the $s$-wave solutions, $\lambda^i > 0$ even if intrapocket repulsions are the largest. The full solution of the $3 \times 3$ set with $\Delta_e = \beta_{ee} = 0, \lambda^i > 0$ no matter what the ratio is of $u_{be}$ and $u_{he}$. In particular, for $u_{be} < u_{ee}u_{hh}$ (and, hence, $\lambda_{1,2} < 0$), $\lambda_3^i$ is positive or negative depending on whether or not $A > 0$, where

$$
A = 4u_{ee}u_{hh}(x_e^2 - \beta_{ee}) + u_{he}^2(x_{he}^2 + 2\beta_{ee} - 3\Delta_h\Delta_e).$$

When the angle dependence of the electron-electron interaction can be neglected, i.e., $\Delta_{ee} = \beta_{ee} = 0, \lambda^i > 0$ no matter what the ratio is of $u_{be}$ and $u_{ee}u_{hh}$. In particular, for $u_{he}u_{ee} > u_{he}$ and $\Delta_{he} << 1$,

$$
\lambda_3^i = x_{he}^2 \frac{2u_{he}u_{hh}}{u_{hh}u_{ee} - u_{be}} > 0.
$$

In other words, for one of the $s$-wave solutions, $\lambda^i > 0$ even if intrapocket repulsions are the largest. The full solution of the $3 \times 3$ set with $\Delta_e = \beta_{ee} = 0$ shows that two $\lambda$'s are repulsive and one is attractive for arbitrary $u_{he}^2/u_{ee}u_{hh}$. When the ratio is small, the attractive solution is close to Equation 19; when the ratio is large, the attractive solution is close to $\lambda_3^i$ in Equation 15. I illustrate this in Figure 6.

There is, however, one essential difference between the $u_{he}^2/u_{ee}u_{hh} > 1$ and $u_{he}^2/u_{ee}u_{hh} < 1$ cases. In the first case, momentum dependence of the interaction just modifies the plus-minus solution that already existed for momentum-independent interaction. In this situation, the gap along electron FSs gradually acquires some $\cos 2\phi$ variation and remains nodeless for small $\Delta_{he}$. In the second case, the solution with $\lambda > 0$ is induced by the momentum dependence of the interaction, and the eigenvalue corresponding to $\lambda_3^i$ necessarily has $\Delta_c > \Delta_e$, i.e., the $s$-wave gap has nodes along the electron FS (67). In other words, the pairing occurs for all parameters but whether the gap is nodal at small $\Delta_{he}$ depends on the relative strength of intrapocket and interpocket interactions. When intrapocket interaction dominates, the gap adjusts and develops a strong $\cos 2\phi$ component that does not couple to a momentum-independent $u_{ee}$ term and as such effectively reduces the strength of electron-electron repulsion.

The same reasoning holds for two nonequivalent hole FSs, five-pocket models, and the $d$-wave channel. For all cases, the solution with $\lambda > 0$ may exist even when intrapocket interactions are the largest, but in this situation the gaps on the hole FSs have accidental nodes. The existence or nonexistence of the solution at strong intrapocket repulsion depends on the complex interplay between the prefactors of $\cos 2\theta$ terms in electron-hole and electron-electron pairing vertices (see Equation 18).

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3.3. How to Extract $\Gamma_{ij}(\mathbf{k}, \mathbf{p})$ from the Orbital Model?

Thus far in our discussion $u_{ij}$, $x_{ij}$ etc., are treated as some phenomenological inputs. To obtain the actual values of these parameters, one needs a microscopic model. The most commonly considered model for FeSCs is an effective five-orbital model for Fe atoms with local intraorbital and interorbital hopping integrals and intraorbital and interorbital density-density (Coulomb) repulsions, Hund-rule exchange, and the pair hopping term

$$H_{\text{int}} = \sum_{i} U_{ii} n_{i,s} n_{i\bar{s}} + \sum_{i,s,t \neq s} \frac{V_{st}}{2} n_{i,s} n_{i\bar{t}} - \sum_{i,s,t \neq s} \frac{J_{st}}{2} \mathbf{S}_{i,s} \cdot \mathbf{S}_{i,\bar{t}} + \frac{1}{2} \sum_{i,s,t \neq s} J'_{st} \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma},$$

where $n_{i,s} = n_{i,s\uparrow} + n_{i,s\downarrow}$.

The Hamiltonian $H_{\text{int}}$ can be equivalently reexpressed via spin-independent interactions as

$$H_{\text{int}} = \sum_{i,s} U_{ii} n_{i,s} n_{i\bar{s}} + \sum_{i,s,t \neq s} \frac{\bar{U}_{st}}{2} n_{i,s} n_{i\bar{t}} + \sum_{i,s,t \neq s} \frac{J_{st}}{4} c_{i\sigma}^\dagger c_{i\sigma} c_{i\bar{\sigma}} c_{i\bar{\sigma}} + \frac{1}{2} \sum_{i,s,t \neq s} J'_{st} \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} c_{i\bar{\sigma}} c_{i\bar{\sigma}},$$

where $\bar{U}_{st} = V_{st} + J_{st}/4$.

The hopping integrals (36 total) are obtained from the fit the band structure obtained in the density functional theory (69). For the interaction parameters, the most common approximation is to assume that $\bar{U}_{st}$, $J_{st}$ and $J'_{st}$ are independent of the orbital indices $s$ and $t$, as long as $s \neq t$. The model can also be extended to include nonlocal Fe-Fe interactions via a pnictide (70).

The bare parameters in Equations 20 and 21 are interrelated due to local spin-rotation invariance (19, 35), but that invariance is broken if we view these equations as effective low-energy models in which the interactions are dressed by the renormalizations coming from fermions with energies of the order of the bandwidth. For this reason, in most studies $U$, $\bar{U}$, $J$, and $J'$ are treated as independent parameters.

We now need to convert Equations 20 and 21 into the band basis and reexpress the result in the form of Equation 1. This is done by introducing new, hybridized operators, which
diagonalize the quadratic form, and reexpressing the interaction terms in Equation 20 or 21 in terms of these new operators. The end result of this procedure is the effective Hamiltonian in the band basis that in the momentum space has the form of Equation 1 with $G_{ij}(k, k')$ given by

$$
G_{ij}(k, k') = \text{Re} \sum_{stpq} \alpha_{j}^{s}(\mathbf{k}) \alpha_{j}^{p}(\mathbf{k}) \left[ \Gamma_{ij}^{st}(k, k')^{*} \right] \times \alpha_{i}^{q}(\mathbf{k}') \alpha_{i}^{p}(\mathbf{k})^{*},
$$

where $[\Gamma_{ij}^{st}(k, k')]$ are linear combinations of $U, \tilde{U}, J,$ and $\tilde{J},$ and $\alpha_{j}^{s}$ is the matrix element connecting the original fermionic operator $c_{p}$ in the orbital basis with the new fermionic operator $a_{j}$ on FS $j$ in the band basis. The matrix elements $\alpha_{j}^{s}$ contain information, which orbitals mostly contribute to a particular segment of a particular FS (19, 20). Because of this, the interaction $\Gamma_{ij}(k, p)$ in the band basis generally depends on the angles along different FSs and contains components in all representations of the tetragonal $D_{4h}$ group.

The angle dependence of $s$-wave and $d_{xy}$ vertices agrees by symmetry with Equations 9–13. What is a priori unknown is how well the interactions can be approximated by the leading angle harmonics, i.e., whether the terms labeled as ... in Equations 9–13 can actually be neglected. This issue was analyzed in detail in Reference 54, and the answer is affirmative—LAHA works rather well. In Figure 7 I show representative fits for a particular set of parameters. In Table 1 I show $u_{he}$ and other parameters extracted from the fit [in the lines marked NSF, meaning that this is for the bare interaction, without extra spin-fluctuation components (see below)]. The results vary somewhat depending on the values of $U, V, J,$ and $J'$, but in general intraband interactions in the $s$-wave channel, $u_{he}$ and $u_{hb}$, exceed interband $u_{hhe}$. This is not surprising because $u_{he}$ and $u_{hb}$ are essentially Coulomb interactions at small momentum transfers, whereas $u_{hhe}$ is the interaction at large momentum transfers, and it should be smaller in general. Only when $V = J = J' = 0$ does the interaction in the band basis become independent

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7.png}
\caption{Representative fits of the interactions $\Gamma_{ij}(k_{F}, p_{F})$ by leading angular harmonic approximation for the four-pocket model. $\Gamma_{ij}$ is obtained by converting the Hamiltonian (Equations 20 and 21) from the orbital to the band basis. The symbols represent interactions computed numerically for the five-band orbital model using RPA; the gray lines are the fits using Equations 9–13. The fit is for the sets $U = 1.67, J = J' = 0.21, V = 1.46$, and $\mu = 0.08$ (all in eV). A positive $\mu$ corresponds to electron doping. $k_{F}$ in $\Gamma_{ij}(k_{F}, p_{F})$ is selected along the $y$ direction on either an electron or a hole Fermi surface (FS) (its location is specified on top of each panel), and $p_{F}$ is varied along each of the FSs. The angle $\phi$ is measured relative to $k_{F}$.}
\end{figure}
on the momentum \( \mathbf{q} \), i.e., \( \Sigma_{ee} = \Sigma_{bb} = \Sigma_{hc} \) (this was termed Coulomb avoidance in Reference 23). As shown in Table 1, intraband interactions are also larger in the \( d \)-wave channel, \( \Sigma_{he} \gg \Sigma_{he} \), although the reasons why are not transparent.

According to the analysis in Section 2, as long as intraorbital interactions exceed interorbital interactions, \( \lambda_i \) are negative (repulsive) even if we neglect \( \cos 2\phi \) terms in \( \Gamma_{ij} \). If we keep these terms, \( \lambda_i \) can be positive even for small \( u_{he} \) or \( \bar{u}_{he} \) but this requires that angle-dependent terms satisfy the inequality in Equation 18. The values of \( \alpha, \beta \), etc., depend on the model parameters. For the particular set of parameters that I considered, the \( \alpha_{del}, \beta_{ee} \), and their \( d \)-wave analogs in Table 1 are such that for the bare interaction neither \( s \)-wave nor \( d \)-wave pairing is possible.

Varying system parameters (e.g., making \( J \) larger) one can, in principle, meet the condition in Equation 18 and obtain either \( s \)-wave or \( d \)-wave solution with a positive \( \lambda_i \) already at the bare level. But even if some \( \lambda_i \) are positive, they are quite small by absolute magnitude \( (67) \), i.e., \( T_c \) obtained using bare interaction is very low.

### 4. HOW TO OVERCOME INTRAPOCKET REPULSION

How to overcome strong intrapocket repulsion is the major issue for FeSCs. A conventional McMillan-Tolmachev renormalization \( (71) \) that reduces Coulomb repulsion and allows electron-phonon attraction to overcome it does not help at this stage because both \( u_{ee} u_{hh} \) and \( u_{hc}^2 \) renormalize in the same way. If the repulsive \( u_{ee} u_{hh} \) part is initially stronger, the renormalization just reduces the strength of the total repulsive interaction but does not change its sign.

The generic idea of how to overcome Coulomb repulsion goes back to the Kohn-Luttinger approach to superconductivity \( (32) \). The pairing interaction I have considered so far is the bare interaction between fermions. The actual pairing interaction \( \Gamma_{ij}(\mathbf{k},\mathbf{p}) \) is given by the fully renormalized irreducible vertex in the particle-particle channel. This irreducible vertex is the sum of the original (bare) interaction and terms of second and higher order in \( U, V \), etc. Part of these higher-order terms accounts for the screening of the original Coulomb interaction by particle-hole pairs; another part can be recast as effective interactions mediated by collective bosonic degrees of freedom in either the charge or the spin channel. The issue I discuss now is how to obtain these dressed pairing vertices.

#### 4.1. The Random Phase Approximation Approach

One route is to adopt a semiphenomenological approach and assume that the system is reasonably close to a particular density-wave-ordered phase, such that the strongest component of the

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Table for ( s )-wave and ( d )-wave parameters for the same set as in Figure 7</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \tilde{u}_{bb} )</td>
</tr>
<tr>
<td>NSF</td>
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</tr>
<tr>
<td>SF</td>
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<tr>
<td>NSF</td>
<td>0.7</td>
</tr>
<tr>
<td>SF</td>
<td>1.50</td>
</tr>
</tbody>
</table>

*\( ^a \)Bare interaction without the spin-fluctuation component.  
*\( ^b \)Full interaction.
Pairing Mechanism in FeSCs

enhanced interaction is mediated by near-gapless fluctuations of this density-wave order. The approach goes back to Berk & Schrieffer (72), who considered effective pairing interaction mediated by ferromagnetic spin fluctuations. In recent years it has been applied to cuprates (see, e.g., Reference 73) and other correlated electron materials (74). Most parent compounds of FeSCs possess long-range SDW order, and it is natural to assume that magnetically mediated pairing interaction plays a central role.

There is no rigorously justified diagrammatic derivation of an effective fermion-fermion interaction mediated by collective modes, except for special cases (76). The pragmatic approach is to select a set of ladder-type or bubble-type diagrams that give rise to a density-wave order above some interaction threshold and to use the same set of diagrams below the threshold. This approach is termed RPA by analogy with the screening problem. A generic way to apply RPA is to antisymmetrize the original interaction, decompose it into spin and charge channels, and renormalize each interaction in a ladder/bubble approximation, neglecting cross-terms. Each four-fermion interaction component \((\Gamma_{\text{AF}})_{ij}^{\text{SDW}}\) then contains two combinations of fermionic spin indices: \(\delta_{\sigma_0}^{\sigma_\uparrow} \delta_{\sigma_\downarrow}^{\sigma_\uparrow}\) and \(\delta_{\sigma_0}^{\sigma_\downarrow} \delta_{\sigma_\uparrow}^{\sigma_\uparrow}\), where \(\sigma\) are Pauli matrices. These two combinations have to be convoluted with the spin structure \(i\omega_n\) of the two-particle anomalous pairing vertex. Using \(\sigma_{\sigma_0}^{\sigma_\uparrow} \delta_{\sigma_0}^{\sigma_\downarrow} \delta_{\sigma_\uparrow}^{\sigma_\uparrow} = \sigma_{\sigma_0}^{\sigma_\downarrow} \delta_{\sigma_0}^{\sigma_\uparrow} \delta_{\sigma_\downarrow}^{\sigma_\uparrow} = -3 \sigma_{\sigma_0}^{\sigma_\uparrow} \delta_{\sigma_0}^{\sigma_\downarrow} \delta_{\sigma_\uparrow}^{\sigma_\downarrow}\) and incorporating the factor \(-3\) into the spin part of the effective pairing vertex, one obtains in the orbital basis

\[
\Gamma_{ij}^{\text{RPA}}(k,p) = \left[ \frac{1}{4} \Gamma^s + \frac{3}{4} \Gamma^c + \frac{3}{2} (\Gamma^s)^2 \chi_s^{\text{RPA}}(k-p) \right]_{pq}.
\]

where \(\Gamma^s\) and \(\Gamma^c\) are spin and charge components of the bare antisymmetrized interaction, \(\chi_s^{\text{RPA}}\) is the dressed static spin susceptibility, and \(\chi_c^{\text{RPA}}\) is the dressed static charge susceptibility. The interaction, Equation 23, is then converted into the band basis using Equation 22, and the pairing in different channels is analyzed in the same way as it was done for the bare interaction, i.e., either by explicitly solving the integral equation on \(\lambda_s\) in a particular channel (19–21, 75, 76) or by approximating \(\Gamma_{ij}(k,p)\) by the leading angular harmonics and solving \(4 \times 4\) or \(5 \times 5\) gap equations (see Section 5 below). The full analysis of the pairing problem often requires one to know the frequency dependence of \(\chi_s\), but for the analysis of the pairing symmetry and the momentum dependence of the gap the frequency dependence is not overly relevant and I neglect it.

In all model calculations, the spin susceptibility \(\chi_s^{\text{RPA}}\) is enhanced due to close proximity to SDW order, while the charge susceptibility \(\chi_c^{\text{RPA}}\) remains small and can be neglected. How \((\Gamma^s)^2 \chi_s^{\text{RPA}}\) in Equation 23 modifies \(u_{he}\) depends on the type of SDW order. For moderately doped FeSCs \(\chi_s^{\text{RPA}}(q)\) is peaked at \((0,\pi)\) and \((\pi,0)\), which are the two momenta separating hole and electron FSs. Not surprisingly, electron-hole interaction \(u_{he}\) is enhanced relative to \(u_{hh}\) and \(u_{ee}\). For less obvious reasons, the \(d\)-wave component of electron-hole interaction \(u_{he}\) is also enhanced, although not as strongly as \(u_{hh}\). In the rows marked as SF in Table 1, I show renormalized interactions for the same set of input parameters that were considered in the previous section. Clearly, \(u_{he}\) and \(u_{he}\) are enhanced. If the enhancement is strong enough, either Equation 18 becomes valid or \(u_{he}^{2}/u_{ee}u_{hh}\) becomes larger than one (or \(u_{he}^{2}/u_{ee}u_{hh}\) becomes larger than one), and the system becomes unstable toward \(s\)-wave or \(d\)-wave superconductivity, depending on which \(\lambda_s\) is the largest.

This scenario requires bare \(\Gamma^s\) to be positive. Only then is spin susceptibility \(\chi_s^{\text{RPA}}(q)\) enhanced. In the orbital basis, this requirement essentially means that intraorbital Coulomb
repulsion $U$ must be larger than interorbital $\bar{U}$. In the band basis, the same requirement implies that bare $u_{he}$ must be positive (68). What if bare $u_{he}$ is negative? Then $|u_{he}|$ may still get an enhancement within RPA, but the enhancement now comes from charge (orbital) fluctuations (36). The latter are strong if the system is close to a state with an orbital order. [Some propose (37) that broken rotational invariance observed above $T_N$ in most FeSCs (77) is due to orbital order, others argue (38, 61) that the order above $T_N$ is an Ising order associated with $Z_2$ degree of freedom separating $(0, \pi)$ and $(\pi, 0)$ spin configurations.] If $u_{he}^2$ is enhanced by orbital fluctuations such that it exceeds $u_{ee} u_{bb}$, $s$-wave SC again develops, but the eigenvalue now corresponds to a conventional $s^{++}$ gap, with the same sign along hole and electron FSs (36). I compare experimental evidence for $s$ versus $s^{++}$ gaps in Section 6. For the rest of this section I assume that $u_{he} > 0$, i.e., the attractions are due to spin fluctuations.

There are two underlying assumptions in the RPA approach. The obvious one is the selection of only ladder or bubble diagrams in the absence of a small parameter. The less obvious assumption is the very idea that the pairing can be viewed as mediated by collective density-wave bosonic excitations, because mediation implies that density-wave fluctuations develop at energies well above relevant energies for the pairing. This last idea is reasonably well justified for the cuprates, in which magnetic fluctuations develop at energies of a few thousand Kelvin, well above $T_c$. Whether this is also the case for FeSCs is less obvious, as magnetism in most of these materials is itinerant (parent compounds are metals), and the highest $T_c$ is at dopings at which SC and SDW ordering temperatures almost coincide. Whether in this situation spin fluctuations can be viewed as preexisting for the SC problem is not obvious. In this situation, it is instructive to consider also an alternative approach that treats magnetic and SC fluctuations on equal footing. This alternative approach is based on the RG technique and is thus termed the RG approach.

4.2. The Renormalization Group Approach

The RG approach is unbiased in the sense that it does not assume that the pairing is mediated by a collective bosonic degree of freedom. Rather, it departs from a bare Hamiltonian with the original four-fermion interaction and studies how particle-particle and particle-hole susceptibilities evolve as one progressively integrates out contributions from fermions with energies larger than some running scale $E$. This should, in principle, address the issue of whether spin fluctuations develop at a larger $E$ than pairing fluctuations. In practice, this approach is also an approximate one because even at weak coupling one cannot explicitly sum up contributions from fermions with energies between the bandwidth $W$ and running energy $E$. This can be done rigorously only if the renormalizations depend on the running scale logarithmically, i.e., whether they are the functions of $L = \log W/E$. Then the flow of the couplings can be described by a set of differential equations $du_i/dL = f(u_{int})$, where $u_{int}$ are renormalized interactions at the running scale $L$.

Renormalizations in a superconducting channel indeed depend on $L$, but renormalizations in other channels are in general nonlogarithmical. In this respect FeSCs are gifts from nature because density-wave renormalizations involving fermions near hole and electron FSs also scale as $\log W/E$, as long as $E$ is above the threshold set by nonperfect nesting (68, 78). Then one can obtain a set of coupled RG equations for pairing and density-wave vertices. This set is called parquet because the renormalizations in the particle-particle channel are often represented as horizontal ladder diagrams, renormalizations in the particle-hole (density-wave) channel as
vertical ladder diagrams, and taking both on an equal footing amounts to building perturbatively a parquet pattern.

From a physics perspective, the key feature of the RG approach is that the pairing, SDW, and charge density wave (CDW) fluctuations all talk to each other at intermediate energies. In particular, not only are pairing fluctuations enhanced by SDW fluctuations, but also SDW and CDW fluctuations are affected by pairing fluctuations.

To get an idea of how the RG works in FeSCs, consider momentarily a toy two-pocket model (68). In Section 3.1, I introduced three interactions that contribute to the pairing: intrapocket hole-electron and electron-electron interactions \( u_{he} \) and \( u_{ee} \) and inter-pocket hole-electron interaction \( u_{be} > 0 \). Suppose that bare electron-hole interaction is weak and the bare \( \lambda^s < 0 \). Now let us add two other interactions that do not directly contribute to the pairing but contribute to density-wave instability: density-density and exchange interactions between fermions from hole and electron pockets, \( u_{dd} \) and \( u_{ex} \), respectively. The coupling in the SDW channel is \( \lambda^{SDW} = u_{dd} + u_{be} \) and the coupling in the CDW channel is \( \lambda^{CDW} = u_{dd} + u_{be} - 2u_{ex} \). As one progressively integrates out contributions from high energies, all couplings evolve and obey

\[
\begin{align*}
\dot{u}_{dd} &= u_{dd}^2 + u_{be}^2 \\
\dot{u}_{ex} &= 2u_{ex}(u_{dd} - u_{ex}) \\
\dot{u}_{be} &= u_{be}(4u_{dd} - 2u_{ex} - u_{bb} - u_{ee}) \\
\dot{u}_{bb} &= -u_{bb}^2 - u_{bb}^2 \\
\dot{u}_{ee} &= -u_{ee}^2 - u_{ee}^2
\end{align*}
\]

where the derivatives are with respect to \( L = (1/2) \log W/E \). We see that \( u_{be} \) gets a boost from \( u_{eb} \), which is a part of the SDW vertex, and in turn \( u_{dd} \) gets a boost from \( u_{be} \). Solving the set, we find that \( u_{be} \) grows under the RG while \( u_{bb} \) and \( u_{ee} \) decrease (and eventually change sign), such that below some \( E_0 \) the running \( \lambda^s \) changes sign and becomes attractive.

The physics behind the sign change of \( \lambda^s \) is essentially the same as in RPA analysis—\( u_{eb} \) gets a boost from SDW fluctuations. But RG analysis also addresses the issue of the interplay between SDW and SC orders, as both are determined by the running interactions that push each other (CDW coupling decreases when \( u_{be} \) increases). For the two-pocket model the SDW eigenvalue \( \lambda^{SDW} \) remains larger than \( \lambda^s \) along the whole RG trajectory (Figures 8a,b), but in multipocket systems more complex behavior is possible (66, 79) (see Figures 8c,d and Figure 9).

The ability to address in an unbiased way what kind of order develops first is an obvious advantage of the RG approach. At the same time, the parquet RG has only limited applicability range because Equation 24 and the analogous equations for multipocket models (66) are valid only when the running \( E \) is larger than the Fermi energy \( E_F \). This would not be an obstacle if the RG instability in FeSCs developed already at \( E > E_F \) (68, 80, 81). But this is unlikely given that \( E_F \sim 10^2 \) meV is an order of magnitude larger than \( T_N \) and \( T_c \). One then has to extend the analysis to \( E < E_F \). It turns out that at such \( E \) renormalizations in the SDW and SC channels decouple from each other (22, 66), and each \( \lambda^r \) evolves according to \( d\lambda^r_i/dL = (\lambda^r_i)^2 \) (where now \( L = \log W/E \)). Then, at perfect nesting, SDW or SC instability occurs first depending on which \( \lambda^r \) (either \( \lambda^{SDW} \) or \( \lambda^s \)) is larger at \( E_F \). Away from a perfect nesting, the logarithmical RG flow of \( \lambda^{SDW} \) is cut below some scale \( E_{bs} \), while \( \lambda^s \) continues to grow and definitely becomes the leading instability above a certain doping. I illustrate this in Figure 9.

This consideration shows that what the parquet RG actually provides are the values of the dressed interactions \( u_{ij} \) at the scale of \( E_F \). Below this scale, SDW order develops without input from the SC channel, and SC develops in a BCS fashion, without input from the SDW channel. If the doping is such that SC instability is the leading instability in the problem, the symmetry and the structure of the SC gap are analyzed in the same way as in Section 3, only \( u_{ij} \) and \( \tilde{u}_{ij} \) are
now dressed interactions, renormalized by the RG flow between $W$ and $E_F$. From this perspective, RPA and RG approaches are similar in the sense that the end result of both approaches is the effective BCS Hamiltonian at $E_F$ with renormalized interactions, some of which are pushed up by SDW fluctuations.

There is another issue with the RG, related to angle dependencies of the interactions (see Section 3.3). A conventional logarithmic RG is applicable only when $x$ and $\beta$ terms in Equations 9–13 are small. To order $O(x)$ and $O(\beta)$, angle dependencies remain intact; only the overall factors $u_{ij}$ flow (66). Beyond this order, logarithmic and nonlogarithmic terms mix, and the selection of diagrams can no longer be rigorously justified. One way to proceed in this situation is to keep the angle dependence intact by hand and use the same equations for $u_{ij}$ as if the interactions were angle independent (66). Another way is to partition each FS into patches and write a larger set of RG equations for the interactions between different patches. This last

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**Figure 8**

Running vertices in spin-density wave (SDW) and superconducting (SC) $s^\pm$ channels for the two-pocket model $(a,b)$ and the four-pocket model $(c,d)$, as functions of the renormalization group (RG) parameter $L = \log W/E$. For the two-pocket model $\lambda_{SDW}^*$ is the largest along the whole RG flow at perfect nesting $(a)$, but $\lambda_{\text{SC}}^*$ eventually wins at a finite doping when $\lambda_{SDW}^*$ is cut below some $E_b$. For the four-pocket model, $\lambda_{\text{SC}}^*$ can be the largest coupling already at perfect nesting $(c)$, or can exceed $\lambda_{SDW}^*$ above some critical doping $(d)$. Taken from Reference 66.
This approach is called the functional RG (fRG) (see References 79, 82, 83, and 84; for a general discussion on the fRG, see Reference 85). The fRG is not an exact approach, as it mixes logarithmical and nonlogarithmical terms, but it is nevertheless a very powerful numerical technique to analyze the interplay between density-wave and superconducting instabilities in systems with angle-dependent interactions.

The majority of the results obtained so far on FeSCs using the RPA, the fRG and the logarithmic RG fully agree on (a) the interplay between SDW and SC instabilities, (b) the symmetry of the SC state at different dopings, and (c) the structure of the SC gap. This is good news because it likely implies that the underlying physics of FeSCs is quite robust. In particular, both the fRG (79) and the conventional RG (66) show that in four-band systems SC may be the leading instability even without doping, whereas in two-band and five-band systems SDW is the leading instability at zero doping, and SC emerges only upon doping. RPA, the fRG, and the conventional RG all show that the $s^\pm$ gap has nodes along electron FSs in a much wider parameter range in four-pocket than in five-pocket systems because the additional hole FS at $(\pi,\pi)$ tends to stabilize nodeless gap. Yet another example

![Figure 9](https://www.annualreviews.org/doi/10.1146/annurev-conmatphys-030411-143258)

(Top panel) The phase diagram of the four-pocket model at zero doping as the function of the strength of the angle-dependent component of the interaction, $\alpha$, and $L_{E_F} = \log W/E_F$, where $W$ is the bandwidth and $E_F$ is the Fermi energy. (Lower panels) The phase diagrams as functions of doping for different $L_{E_F}$. The superconducting gap in the $s^\pm$ state may be nodeless or have nodes along electron Fermi surfaces. In the region labeled SDW, SC emerges only at a finite doping, when SDW instability is cut. In the region labeled SC, the SC state emerges already at zero doping. Taken from Reference 66. Abbreviations: SC, superconductivity; SDW, spin-density wave.
is the equivalence between RPA (86) and fRG (83) results for heavily electron-doped systems, in which only electron pockets remain—both approaches yield a $d$-wave gap with no nodes.

5. DOPING DEPENDENCE OF THE COUPLINGS

In this section I assume that SC is the leading instability and briefly review how the gap symmetry and structure evolve with doping. For definiteness I use the RPA approach combined with LAHA (see Section 3). The results differ for electron and hole dopings, and I consider them separately.

5.1. Electron Doping

For small and moderate electron dopings, the FS consists of four pockets—two hole FSs at (0,0) and two electron FSs at $(0,\pi)$ and $(\pi,0)$. Typical fits by LAHA, the parameters extracted from the fits, and the solutions in $s$-wave and $d$-wave channels are shown in Figure 10 and in Table 2. It turns out (66) that some system properties are sensitive to the choice of parameter, but some are quite universal. The parameter-sensitive properties are the presence or absence of accidental nodes in the $s$-wave gap (although for most parameters the gap does have nodes, as in Figure 10) and the gap symmetry itself, because for most input parameters and dopings, $\lambda$ and $\lambda'$ remain comparable as long as both hole and electron FSs are present (see Table 2). That the $d$-wave state is a strong competitor in four-pocket systems was first emphasized in References 19 and 35. The authors of Reference 19 suggested that different FeSCs may have different symmetry even for the same FS topology.

The universal observation is that the driving force for attraction in both $s$-wave and $d$-wave channels is strong interpocket electron-hole interaction ($u_{ee}$ and $u_{he}$ terms) no matter how small the hole pockets are. The gap structure does not change much with doping as long as both hole and electron pockets are present.

The situation changes qualitatively once the hole pockets disappear (Figure 11). It is clear from Table 2 that now a direct $d$-wave electron-electron interaction $u_{ee}$ becomes strong and attractive. The argument as to why this happens is as follows (54): $u_{ee}$ is an antisymmetric combination of intrapocket and interpocket electron-electron interactions $u_{ee} = u_{ee}^{\text{intra}} - u_{ee}^{\text{inter}}$. Both $u_{ee}^{\text{intra}}$ and $u_{ee}^{\text{inter}}$ are positive (repulsive), but the sign of $u_{ee}$ depends on the interplay between $u_{ee}^{\text{intra}}$ and $u_{ee}^{\text{inter}}$. As long as hole FSs are present, spin fluctuations are peaked near $q = (0,\pi)$ and $(\pi,0)$, which is an equal distance from the relevant momenta $q = 0$ for $u_{ee}^{\text{intra}}$ and $q = (\pi,\pi)$ for $u_{ee}^{\text{inter}}$. In this situation, $u_{ee}^{\text{intra}}$ and $u_{ee}^{\text{inter}}$ remain close in magnitude, and $u_{ee}$ is small. Once the hole pockets disappear, the peak in the RPA spin susceptibility shifts toward $(\pi,\pi)$ (86), and $u_{ee}^{\text{inter}}$ increases stronger due to the spin-fluctuation exchange than $u_{ee}^{\text{intra}}$. A negative $u_{ee}^{\text{intra}} - u_{ee}^{\text{inter}}$ then gives rise to a plus-minus gap on the two electron FSs. The gap changes sign under $k_x \rightarrow -k_x$ and therefore has $d_{x^2-y^2}$ symmetry. This pairing mechanism is essentially identical to the spin-fluctuation scenario for $d$-wave pairing in the cuprates (73).

A different proposal has been put forward in References 87 and 88. These authors argued that the gap symmetry may be a nodeless $s$-wave [equal sign of the gaps on the pockets at $(0,\pi)$ and $(\pi,0)$]. According to (87, 88) such $s$-wave pairing emerges, in some range of parameters, if one uses for electron-electron interaction the orbital version of the $J_1 - J_2$ model. Yet another proposal for strongly electron-doped FeSCs is $s^{++}$ pairing driven by orbital fluctuations (89).
5.2. Hole Doping

For small and moderate hole doping, the FS contains five pockets—two hole pockets at (0,0), two electron pockets at (0,\pi) and (\pi,0), and one more hole pocket at (\pi,\pi). Representative FSs for hole doping, typical fits by LAHA, the parameters extracted from the fit, and the solutions in s-wave and d-wave channels are shown in Figure 12 and in Table 3. As with electron doping, there are universal and parameter-sensitive features. The parameter-sensitive property is again the presence or absence of accidental nodes in the s-wave gap along the electron FSs. However, for most of the parameters, the gap does not have nodes (see Figure 12) because the total \( u_{pe} \) increases once it acquires an additional contribution \( H_{b1e} \).

![Figure 10](image)

**Figure 10**
Representative case of small/moderate electron doping, when both hole and electron pockets are present. (a) The Fermi surface. (b) Representative fits of the interactions by leading angular harmonic approximation (LAHA) [the dots are random phase approximation results; the lines are LAHA expressions (Equations 9–13)]. (c,d) The eigenfunctions in s-wave and d-wave channels for the largest \( l_s \) and \( l_d \). Taken from Reference 54.
There are two universal features. First, the $s$-wave eigenvalue is enhanced relative to a $d$-wave one and becomes the leading instability as long as both hole and electron pockets are present. Second, the driving force for the attraction in both $s$- and $d$-channels is again strong interpocket electron-hole interaction (the $u_{bc}$ and $u_{be}$ terms), no matter how small the electron pockets are.

The situation again changes rapidly once electron pockets disappear (see Figure 13). Now electron-hole interaction becomes irrelevant, and the attractive pairing interaction may only be due to intra- and interpocket interactions involving hole pockets.

Table 2 Some of the leading angular harmonic approximation (LAHA) parameters extracted from the LAHA fit in Figures 10 and 11 for electron doping

<table>
<thead>
<tr>
<th></th>
<th>$u_{bc}$</th>
<th>$u_{be}$</th>
<th>$\alpha_{bc}$</th>
<th>$\alpha_{be}$</th>
<th>$\lambda_s$</th>
<th>$u_{ee}$</th>
<th>$\alpha_{ee}$</th>
<th>$\lambda_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s$-wave</td>
<td>0.8</td>
<td>0.79</td>
<td>-0.19</td>
<td>0.91</td>
<td>0.05</td>
<td>0.25</td>
<td>3.65</td>
<td>0.20</td>
</tr>
<tr>
<td>$d$-wave</td>
<td>0.50</td>
<td>-0.39</td>
<td>-0.46</td>
<td>-0.04</td>
<td>1.5</td>
<td>0.37</td>
<td>-2.57</td>
<td>0.29</td>
</tr>
</tbody>
</table>

$a$ Table taken from Reference 66.

$b$ Column i corresponds to Figure 10.

$c$ Column ii corresponds to Figure 11 (no hole pockets).

Figure 11

The fits of the random phase approximation interactions by leading angular harmonic approximation and the structure of $s$-wave and $d$-wave gaps for the case of heavy electron doping, when only electron Fermi surfaces are present. Taken from Reference 54.

There are two universal features. First, the $s$-wave eigenvalue is enhanced relative to a $d$-wave one and becomes the leading instability as long as both hole and electron pockets are present. Second, the driving force for the attraction in both $s$- and $d$-channels is again strong interpocket electron-hole interaction (the $u_{bc}$ and $u_{be}$ terms), no matter how small the electron pockets are.

The situation again changes rapidly once electron pockets disappear (see Figure 13). Now electron-hole interaction becomes irrelevant, and the attractive pairing interaction may only be due to intra- and interpocket interactions involving hole pockets.
Figure 12

Representative case of small/moderate hole doping, when both hole and electron pockets are present. (a) The Fermi surface. (b) Representative fits of the interactions by leading angular harmonic approximation (LAHA) [the symbols are random phase approximation results; the lines are LAHA expressions (Equations 9–13)]. (c,d) The eigenfunctions in $s$-wave and $d$-wave channels for the largest $l_s$ and $l_d$. Taken from Reference 54.

Table 3  Some of the leading angular harmonic approximation parameters extracted from the fits in Figures 12 and 13 for hole doping

<table>
<thead>
<tr>
<th></th>
<th>$s$-wave</th>
<th></th>
<th>$d$-wave</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$u_{h_1b_1}$</td>
<td>$u_{h_1e}$</td>
<td>$\alpha_{h_1e}$</td>
</tr>
<tr>
<td></td>
<td>0.86</td>
<td>0.92</td>
<td>-0.18</td>
</tr>
<tr>
<td>$d$-wave</td>
<td>$\tilde{u}_{h_1b_1}$</td>
<td>$\tilde{u}_{h_1e}$</td>
<td>$\tilde{\alpha}_{h_1e}$</td>
</tr>
<tr>
<td></td>
<td>0.51</td>
<td>-0.45</td>
<td>-0.48</td>
</tr>
</tbody>
</table>

*Column i corresponds to Figure 12 (hole and electron pockets are present).

*Column ii corresponds to Figure 13 (no electron pockets).
LAHA analysis shows (54) that, at least in some range of parameters, there is an attraction in both $s$-wave and $d$-wave channels, and furthermore $\lambda_d/C_24$, (see Figure 13). The near-equivalence of $s$-wave and $d$-wave eigenvalues was also found in a recent unrestrictive RPA study (90). Within LAHA, the attractive $\lambda_d$ is due to strong intra-pocket interaction between the two hole pockets centered at $(0,0)$. The $s$-wave gap then changes sign between these two hole pockets. The gap along the $(\pi,\pi)$ pocket is induced by a weaker inter-pocket interaction and is much smaller. The attractive $\lambda_d$ emerges for two reasons (54). First, the $d$-wave intrapocket interaction $\tilde{u}_{b_1b_1}$ becomes negative. Second, the interpocket interaction $\tilde{u}_{b_1b_2}$ between the two pockets at $(0,0)$ becomes larger in magnitude than repulsive $\tilde{u}_{b_2b_2}$ and $\tilde{u}_{b_3b_3}$ (see Table 3). The solutions with $\lambda_d > 0$ then exist separately for FSs $b_{1,2}$ and $b_3$; the residual interpocket interaction just sets the relative magnitudes and phases between the gaps at $b_3$ and $b_{1,2}$. The $d$-wave gap with the same structure has been obtained in the fRG analysis at large hole doping (84). That study found less competition with $s$-wave than in RPA-based studies.

6. EXPERIMENTAL SITUATION

Experimental study of FeSCs has been one of the major research topics in condensed matter physics since 2008, and several detailed reviews have already appeared in the literature (15, 16, 18, 24, 25). Here I briefly discuss the experimental situation concerning the symmetry and the structure of the SC gap.
As of today, there is no “smoking gun” experiment that could carry the same weight as phase-sensitive measurements of $d_{xy}$ gap symmetry in the cuprates (33). Still, there is enough experimental data to minimize the number of possible gap structures. The theoretical proposals for the gap symmetry and structure are summarized in Section 5. The proposed symmetry is different for weakly/moderately doped systems with hole and electron FSs and for strongly doped systems where FSs of only one type are present. It is therefore instructive to consider weak/moderate and strong doping separately.

6.1. Moderate Doping: Gap Symmetry

The candidates are $s$-wave (either $s^\pm$ or $s^{++}$) or $d_{xy}$ gaps. The two behave very differently along the hole FSs centered at (0,0)—the $s$-wave gap is nodeless with $\cos 4\phi$ variations, whereas the $d$-wave gap has nodes along $k_x = \pm k_y$. ARPES measurements, both from synchrotron (57, 91–93) and laser light (40), show quite convincingly that the gap along hole FSs is nodeless in both hole- and electron-doped FeSCs. This unambiguously selects an $s$-wave gap. Additional evidence in support of $s$-wave pairing comes from the very flat low-temperature behavior of the penetration depth in the highest $T_c$ 1111 FeSC systems (94).

6.2. Moderate Doping: $s^\pm$ versus $s^{++}$

The distinction between $s^\pm$ and $s^{++}$ gaps is a more subtle issue, particularly given that both belong to the same $A_{1g}$ representation and also because in general the $A_{1g}$ gap on electron pockets may have strong oscillating components. In general, the gaps on electron and hole FSs have nonequal magnitudes, and the issue of whether the gap is $s^\pm$ or $s^{++}$ reduces to whether the gap averaged over an electron FS has the same sign or opposite sign as the gap averaged over a hole FS. This is not a fundamental symmetry issue and, moreover, when $\cos 2\phi$ oscillations are strong, one may switch from equal to opposite signs of the averaged gaps by a small change in parameter (66) or by adding impurities (95). Still, when oscillations are not very strong, whether the eigenfunction has an $s^\pm$ or $s^{++}$ character is essential because it determines, to a large extent, whether the pairing is driven by spin or by orbital fluctuations (see Section 4).

The experimental data most frequently cited in support of the $s^\pm$ gap are the observations of a magnetic resonance in neutron scattering (13, 96). If, as many researchers believe, the resonance is a spin exciton, it exists at a momentum $Q$ if the gaps at FS momenta $k_F$ and $k_F + Q$ are of opposite sign. Experimentally, the resonance is observed (13, 96) near $Q = (\pi,\pi)$ in the folded BZ, which in this zone is precisely the distance between electron and hole FSs. The excitonic resonance then exists if the gap changes sign between hole and electron pockets and does not exist if the gap does not change sign. A similar reasoning has been used in identifying the resonance seen in the cuprates with a fingerprint of $d_{xy}$ gap symmetry (see, e.g., Reference 97 and references therein).

From the experimental perspective, the neutron peak is the resonance if it is narrow and is located below twice the gap value. The argument made by the supporters of the $s^{++}$ scenario (36) is that the observed neutron peak is more broad than the resonance seen in the cuprates and that there is no firm evidence that the peak energy is below $2\Delta$ for the minimum gap. For the $s^{++}$ gap structure, there is no resonance, but there is a redistribution of the neutron spectral weight immediately above $2\Delta$, which gives rise to a local maximum in the magnetic structure factor (36, 98, 99). Still, the majority of researchers do believe that the observed neutron peak is a resonance, and that it is quite broad is at least partly due to $\cos 2\phi$ gap variations along the electron FSs (99).
Further rather strong evidence in support of the $s^\pm$ gap is the observed variation of the quasiparticle interference pattern in a magnetic field (41), although the interpretation of the data has been the subject of debates (100). It was also argued (101) that the very presence of the coexistence region between SC and stripe magnetism in FeSCs is a fingerprint of an $s^\pm$ gap, because for an $s^{++}$ gap a first-order transition between a pure magnetic and a pure SC state is much more likely.

6.3. Moderate Doping: Nodal versus Nodeless $s^\pm$ Gaps

Assume for definiteness that the pairing is driven by spin fluctuations and the gap has an $s^\pm$ structure. In the 2D scenario, such a gap has $\cos 2\phi$ variations along electron FSs, which, according to theory, can be rather strong, particularly in electron-doped FeSCs. Experimental data show that whether the gap is nodeless or has nodes depends on the material, the doping, and whether SC coexists with SDW order.

6.3.1. Hole doping. For hole-doped FeSCs (e.g., for Ba$_{1-x}$K$_x$Fe$_2$As$_2$) the data indicate that the gap is nodeless, at least away from the coexistence region. This is consistent with the theory (see Section 5). ARPES experiments do not show any angular variation of the gap along either hole or electron FSs (57, 91), but it is not entirely clear whether ARPES can at present distinguish between the gaps on the two electron FSs, which in folded zone are both centered at $(\pi,\pi)$. Thermal conductivity data show that $\kappa/T$ tends to zero in the limit of $T = 0$, in line with what one should expect for a nodeless SC (102). Specific heat data also show nodeless behavior (103). The interpretation of the penetration depth data requires more care, as the data do show a power-law behavior $\lambda(T) - \lambda(0) \propto T^\alpha$ with $\alpha \sim 2$ (104). Such behavior is expected for an SC with point nodes, but it is also expected in a wide range of $T$ for a nodeless $s^\pm$ SC in the presence of modest interband scattering by nonmagnetic impurities (105). Penetration depth measurements on artificially irradiated samples (106) support the idea that the gap is nodeless and the power-law $T^\alpha$ behavior of $\lambda(T) - \lambda(0)$ is due to impurities.

6.3.2. Electron doping. For electron-doped FeSCs, e.g., 122 materials such as Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ or 1111 materials such as NdFeAsO$_{1-x}$F$_x$, ARPES shows no-nodal gaps along hole FSs (92, 93), but there are no data on the gaps along each of the two electron FSs. At optimal doping, the data on both thermal conductivity (107, 108) and penetration depth (108, 109) are consistent with no-nodal gaps. However, the data for overdoped Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ indicate that gap nodes may develop: The behavior of $\lambda(T)$ becomes more steep, and $\kappa/T$ now tends to a finite value (107) expected for an SC with line nodes. The data also show $\sqrt{H}$ behavior of $\kappa$ in a magnetic field (107) also expected for an SC with line nodes (110), but it was argued that the behavior resembling $\sqrt{H}$ can be obtained even if the $s^\pm$ gap has no nodes (111). There is also clear anisotropy between in-plane conductivity and conductivity along the $z$ direction, which was interpreted (107) as an indication that the nodes may be located near particular $k_z$. Specific heat data in overdoped Ba(Fe$_{0.9}$Co$_{0.1}$)$_2$As$_2$ were also interpreted as evidence for the nodes (112).

The development of the nodes in the $s^\pm$ gap upon electron doping is in line with the theory. The farther the system moves away from the SDW phase, the weaker is the increase of intraband electron-hole interaction and hence the stronger is the competition for intraband repulsion. As I discussed in Section 3, the gap adjusts to this change by increasing its $\cos 2\phi$ component to reduce the effect of the intraband repulsion in the gap equation.
There is also experimental evidence for $\cos 2\phi$ gap oscillations from the observed oscillations (113) of the field-induced component of the specific heat $C(H,T)$ in superconducting FeTe$_{1-x}$Se$_x$ ($x \sim 0.5$). The measured $C(H,T)$ oscillates with the direction of the applied field as $\cos 4\phi$. In theory, such an oscillation is related to the behavior of $\Delta^2(\phi)$ (64); hence, $\cos 2\phi$ gap oscillations in $\Delta$ lead to $\cos 4\phi$ oscillations in $C(H,T)$. The observed field and temperature dependence of the prefactor for $\cos 4\phi$ terms are consistent with the idea that the oscillations are caused by $\cos 2\phi$ terms in $\Delta$. These data were also interpreted as evidence for a no-nodal gap because if $\cos 2\phi$ gap oscillations were strong and the gap had nodes at accidental points, the behavior of $\Delta^2$ would be more complex than the observed $a + b \cos 4\phi$.

For LiFeAs, which is undoped but has an FS structure similar to electron-doped FeSCs, no-nodal behavior has been observed in ARPES (114), specific heat (115), penetration depth (116), and NMR (53, 117) measurements. The NMR data, however, were interpreted (53) as evidence for a possible $B$-type $p$-wave gap ($p_x + ip_y$). Whether this is the case remains an open issue. In any event, the evidence for a no-nodal gap in this material is overwhelming.

6.3.3. Coexistence region. Taken at face value, thermal conductivity and penetration depth data indicate that the gap becomes nodal in the coexistence regime in both hole-doped and electron-doped FeSCs. The most striking evidence comes from thermal conductivity (102, 107)—in the coexistence regime $\kappa/T$ tends to a finite value at $T \to 0$ and shows $\sqrt{H}$ behavior, both characteristics are typical for an SC with line nodes. There is no theoretical understanding at present as to why the SC gap develops nodes in the coexistence regime [for a toy two-pocket model, theory predicts that the gap should have no nodes (118)], so this is another open issue.

6.3.4. Isovalent doping. Electron or hole doping is not the only way to change the properties of FeSCs. Another method is to replace one pnictide with the other. The most common replacement is As $\to$ P. P-containing materials include the very first FeSC, LaFeOP, with $T_c \leq 5$ K (119); the family BaFe$_2$As$_{1-x}$P$_x$ with the highest $T_c$ around 30 K (120); and LiFeP (T. Shibauchi, private communication). Penetration depth, thermal conductivity, specific heat, and NMR data (121) in these materials all show behavior consistent with line nodes. In particular, $\kappa$ scales linearly with $T$ at low $T$ and displays $\sqrt{H}$ behavior in a magnetic field, and $\lambda(T) - \lambda(0)$ is also linear in $T$ down to very low $T$. Laser ARPES data (40) show that the gap along FSs is nodeless, so the nodes likely are located on electron FSs.

As we discussed above, the existence of the nodes on electron FSs is generally in line with theory predictions. It has been argued (35) that a replacement of As by P changes the height of a pnictide with respect to Fe plane, which effectively reduces interpocket electron-hole interaction, in which case the gap develops nodes to reduce the effect of intrapocket repulsion. However, this argument is only suggestive, and it is not entirely clear at the moment why all P-based FeSCs have nodes. One way to analyze this semi-quantitatively is to study the correlation between $2\Delta/T_c$ on the hole FSs and the presence of nodes on electron FSs. This study (122) shows that from this perspective P-based FeSCs are most likely to have the gap nodes.

Another open issue is the location of the nodes along the $z$ direction. Oscillations of thermal conductivity with the direction of a magnetic field have been measured recently (123), and the $\cos 4\phi$ component of these oscillations has been interpreted using the modified 2D form $\Delta_\phi(k_z) = \Delta_0(1 + \alpha(k_z) \cos 2\phi)$. The best fit to the data yields $\alpha(k_z) > 1$ for some $k_z$ and $\alpha(k_z) < 1$ for others, in which case the nodes form patches along $k_z$. However, whether this is the only explanation of the data is debatable.

I caution that although the presence of nodes on electron FSs is likely, they have not been directly observed yet; it is still possible that the nodes are located on a hole FS, near
particular $k_z$, as some 3D theories suggest (61). Another possibility, which is also not entirely ruled out, is that the system behavior near the surface, probed by ARPES, is not the same as in the bulk. The probability that this is the case is not high, however, because ARPES data are obtained using a laser light that probes states located farther from the surface than in conventional synchrotron-based ARPES.

6.4. Strongly Doped Fe-Based Superconductors

The situation is more complex at strong hole doping and at strong electron doping. In the first case, electron pockets disappear and only hole pockets are present; in the second case only electron pockets remain.

6.4.1. Electron doping. Strongly electron-doped materials, of which $K_{0.8}Fe_{1.7}Se_2$ is the most studied, belong to the family of $A_xFe_{2-y}Se_2$ ($A = K$, Rb, Cs) (11, 12). $T_c$ in $A_xFe_{2-y}Se_2$ is rather high, almost 40 K. ARPES shows (12) that only electron FSs are present in $A_xFe_{2-y}Se_2$, whereas hole pockets are at least 60 meV from the FS; however, hole dispersion above 60 meV is still clearly visible in ARPES. Two electron FSs are at $(0, \pi)$ and $(\pi, 0)$, as in other FeSCs, and there is, possibly, another electron FS at $(0, 0)$. RPA, LAHA, and some fRG calculations for these systems predict that the gap should have a $d$-wave symmetry, at least when the FSs are at $(0, \pi)$ and $(\pi, 0)$ only. A $d$-wave symmetry in this situation means that the gaps on the two electron FSs behave as $\Delta_0(\pm 1 + \cos 2\varphi)$, and all calculations yield $\Delta_0 < 1$, i.e., no nodes (neglecting 3D effects). The theoretical alternative is $s^\pm$ symmetry for one reason (89) or the other (87, 88). At present, both ARPES and specific heat data indicate that the gap is nodeless, at least for most $k_z$ values, but whether the gap is an $s$-wave or a nodeless $d$-wave remains to be seen.

6.4.2. Hole doping. A strongly hole-doped system is $KFe_2As_2$ ($T_c = 3$ K), which is at the opposite end of the $BaFe_2As_2$ parent in the $K_xBa_{1-x}Fe_2As_2$ family. According to ARPES (43), this system has only hole pockets at $(0, 0)$. There may also be additional hole pockets [hole blades (57)], but this is not entirely clear. Both thermal conductivity and penetration depth measurements clearly point to nodal behavior (42). There is, however, no “smoking gun” symmetry-sensitive measurement, so whether the gap is a $d$-wave or an $s$-wave with nodes on hole FSs due to strong $\cos 4\varphi$ gap component (124) remains an open issue.

6.5. Summary

Overall, the agreement between theory and experiment with respect to gap symmetry and structure is reasonably good. Theory predicts that the gap symmetry in weakly and moderately doped FeSCs is an $s$-wave. This is consistent with ARPES data. Many theorists argue that an $s$-wave gap changes sign between hole and electron FSs. Quasiparticle interference and neutron scattering data are consistent with this idea, if, indeed, the neutron peak is the resonance. Further, theory predicts that the $s^\pm$ gap has oscillations along electron FSs, and these oscillations give rise to accidental nodes, which are more likely for systems with two-hole and two-electron cylindrical FSs than in systems with an additional-hole cylindrical FS. This is also generally consistent with the experiments, although at present the agreement is more qualitative than quantitative. For strongly electron-doped FeSCs, the theory based on RPA, LAHA, and the fRG predicts a nodeless $d$-wave gap, except, perhaps, in the region near $k_z = \pi/2$. This is neither confirmed nor disproved by the experiments. For strongly hole-doped FeSCs, with only hole pockets, experiments point to the presence of the nodes, but whether the gap is a $d$-wave or a
nodal s-wave has not been firmly established. Finally, in the coexistence region of SC + SDW, theory prediction for a two-band toy model is a nodeless $s^\pm$ gap. This is apparently inconsistent with the data that show nodal behavior. What the gap structure is in the coexistence region of realistic four-band and five-band models remains to be seen.

7. CONCLUSION

The analysis of the gap symmetry and structure in FeSCs is a fascinating subject because of the multiorbital/multiband nature of these materials. It is now well understood that in multiband systems a conventional notion that the $s$-wave gap is nodeless, the $d$-wave has four nodes, etc., does not work, and the $s$-wave gap may have nodes, whereas the $d$-wave gap may remain nodeless. Furthermore, nodes may appear or disappear, depending on doping and other external conditions. Another peculiarity of FeSCs is a close proximity between pairing eigenvalues $\lambda_i$ and different symmetry representations, e.g., $A_{1g}$ and $B_{1g}$. Because of proximity, even the gap symmetry may change upon doping or other external perturbation. Also, below $T_c$, the system may lower the energy by moving into a mixed state with, e.g., $s + id$ gap function. To analyze this issue, one needs to go beyond the analysis presented in this review and solve the full nonlinear gap equation.

The existence of superconductivity at the end points of the phase diagram, when only hole pockets or electron pockets are present, is another fascinating issue. There are competing proposals for the gap symmetry at strong electron doping, and so far experiments cannot distinguish between these proposals. Finally, the gap structure in the coexistence regime with SDW is yet another fascinating unexplored issue, and comprehensive analysis of SC in the coexistence phase is clearly called for.

**SUMMARY POINTS**

1. For weakly and moderately electron-doped FeSCs, $s^\pm$ and $d_{x^2-y^2}$ pairing channels are nearly degenerate. The driving force for the pairing in both channels is inter-pocket electron-hole interaction, enhanced by spin fluctuations. The $d$-wave gap has nodes at $k_x = \pm k_y$ on the hole Fermi surfaces (FSs); the $s^\pm$ gap has cos $2\phi$ variations on electron FSs and may have nodes. The probability that the $s^\pm$ gap has nodes increases with electron doping.

2. For strongly electron-doped FeSCs, when only electron pockets remain, the gap has $d$-wave symmetry, which in this situation implies that the angle-independent component of the gap changes sign between the two electron pockets. The driving mechanism for the pairing is a direct $d$-wave attraction between electron pockets, again enhanced by spin fluctuations. The gap is nodeless but may acquire nodes near $k_z = \pi/2$ when 3D effects and/or hybridization between electron pockets are included. A competing theory proposal, based on the orbital $J_1 - J_2$, is that the gap is a sign-preserving $s$-wave.

3. For weakly and moderately hole-doped FeSCs, $s^\pm$ pairing is the dominant instability. The driving force is again inter-pocket electron-hole interaction, enhanced by spin fluctuations. The gap has cos $2\phi$ variation along electron FSs but likely does not have nodes.

4. For strongly hole-doped FeSCs, when only hole FSs remain, the gap symmetry may be $d$-wave, with nodes at $k_x = \pm k_y$ on all hole FSs. The $d$-wave pairing mechanism is the combination of a $d$-wave attraction within the hole pocket at $(\pi, \pi)$ and a strong intrapocket $d$-wave interaction between the two hole pockets centered at $(0,0)$.
A competing theory proposal is that the gap is s-wave, with potential nodes due to strong cos 4\( \phi \) variation along hole FSs centered at (0,0). To what extent this attraction is induced by spin fluctuations is unclear.

5. For real 3D systems, one scenario is that the 2D picture survives, and nodes, if present, are vertical nodes, located on electronic FSs at given \( k_x \) and \( k_y \) but arbitrary \( k_z \). Another scenario is that nodes on electron FSs exist only in some ranges of \( k_z \). And the third, more radical, scenario is that the nodes appear as horizontal nodes near particular \( k_z \), either on electron or on hole FSs.

6. An alternative scenario for all FeSCs is that the gap is a conventional, sign-preserving \( s^{++} \) gap but still may have cos 2\( \phi \) oscillations on electron FSs. Such a gap appears if the inter-pocket electron-hole interaction \( \mu_{he} \) is negative (attractive) and is enhanced by charge (orbital) fluctuations and phonons.

FUTURE ISSUES
1. What would be the “smoking gun” experiment to distinguish between \( s^{\pm} \) and \( s^{++} \) gaps?
2. Why do all P-based FeSCs appear to have nodes, and where are these nodes located?
3. What is the structure of the superconductivity (SC) gap in the coexistence region with spin-density wave (SDW) order?
4. What are the pairing mechanism, gap symmetry, and structure in heavily electron-doped K\(_{x}\)Fe\(_{2} \)–\( \delta \)Se\(_{2} \) and heavily hole-doped KFe\(_{2}\)As\(_{2} \)?
5. Is there a mixed \( s + id \) SC state in FeSCs at \( T = 0 \)?
6. Is there a FeSC with a \( p \)-wave symmetry?

DISCLOSURE STATEMENT
The author is not aware of any affiliations, memberships, funding, or financial holdings that might be perceived as affecting the objectivity of this review.

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