A unified description of cuprate and iron arsenide superconductors

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We propose a unified description of cuprate and iron-based superconductivity. Consistency with magnetic structure inferred from neutron scattering implies significant constraints on the symmetry of the pairing gap for the iron-based superconductors. We find that this unification requires the orbital pairing formfactors for the iron arsenides to differ fundamentally from those for cuprates at the microscopic level.

Keywords iron arsenide superconductor, cuprate superconductor, pairing formfactor, SU(4) dynamical symmetry

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1 Introduction

In a 2004 paper [1] we proposed that an SU(4) dynamical symmetry introduced in Refs. [2−4] had two properties important for understanding high-temperature superconductivity (SC). The first was that the SU(4) algebra imposed no double occupancy by symmetry, not projection. Thus superconductivity emerges naturally from an antiferromagnetic (AF) Mott insulator state at half filling. The second was that SU(4) symmetry alone is sufficient to guarantee many essential features of cuprate superconductivity, irrespective of microscopic details such as pairing formfactors (except to the extent that these are broadly consistent with an emergent SU(4) symmetry).

This led us to propose that cuprate superconductivity was a new kind of superconductivity characterized by more complex behavior than normal BCS superconductivity because the symmetry structure associated with the superconductivity was non-abelian. The physical content of this mathematical statement is that the non-abelian algebra imposes dynamical constraints on the interaction of collective degrees of freedom such as magnetism and charge with superconductivity. Because of the key dynamical role played by the commutators, we termed this behavior non-abelian superconductivity.

We demonstrated in Ref. [1], and amplified in more recent papers [5−10], that any microscopic structure consistent with an algebra having non-abelian subalgebras can lead to the complex behavior observed for cuprate superconductors. In Ref. [1] we predicted that there could be other compounds rather different from cuprate superconductors in microscopic details that could exhibit properties analogous to cuprate superconductors, provided that they realized in their emergent properties a symmetry, such as SU(4), having non-abelian subgroups and thus non-trivial commutators between pairing and other degrees of freedom.

In early 2008 a series of experiments initiated in Japan and China demonstrated a surprising new class of high-temperature superconductors based on iron arsenides [11−20]. These compounds have achieved critical temperatures $T_c \sim 55$ K that are surpassed only by cuprates. These Fe-based superconductors have an atomic structure differing from that of the cuprates in significant details, yet there are many similarities when compared with the cuprates. This has led to a flurry of efforts to determine whether these two classes of superconductors share a similar origin. At stake is the mechanism for Fe-based superconductivity, but perhaps a deeper understanding of that for cuprate superconductivity as well.

In understanding the cuprates a key role was played by the realization that superconductivity is dominated
by singlet $d$-wave pairs. Hence, a major emphasis for the new Fe-based superconductors has been to determine the symmetry of the pairing gap. Experimentally, the situation remains somewhat unclear. There is substantial evidence that the pairing gap is spin singlet [21–23], but the gap orbital symmetry remains unsettled. Many experiments suggest that there are no gap nodes on the Fermi surfaces but some find evidence for nodes [21, 24–39], suggesting that there may be more than one orbital gap symmetry playing a role in the FeAs compounds.

Many theoretical proposals have been made for the gap symmetry (see, for example, Refs. [40–54]). These typically start from assumptions about microscopic structure and interactions near the Fermi surface and attempt to predict the likely orbital and spin structure for pairs. This is a complex problem and different authors reach different conclusions concerning the gap symmetry.

In this paper we propose that the Fe-based superconductors are a second example (after cuprates) of the non-abelian superconductivity predicted in Ref. [1]. We further propose that the similarity of cuprate and Fe-based phenomenology indicates that non-abelian superconductivity for the FeAs superconductors is based on the same $SU(4)$ symmetry that explains the phenomenology of the cuprates, thus providing a unified picture of Cu- and Fe-based superconductors. We argue that this is the case even if the microscopic pairing mechanism in the two cases were to turn out to be different. Indeed, we shall provide evidence that unification at the emergent degrees of freedom level is possible only if the two classes of high temperature superconductors have different microscopic pairing structures. Finally, we use the non-abelian symmetry to predict the orbital and spin symmetries possible for the Fe-based compounds by requiring consistency between observed pairing and magnetic properties.

2 Cuprate and Fe-based phenomenology

Many experiments suggest strong similarities between cuprate and Fe-based superconductors. Both appear to be mediated by electron-electron correlations rather than phonons (some dispute this), and to involve the close proximity of antiferromagnetism (AF) and superconductivity (SC). In both, the superconductivity occurs often (but not always) in 2-dimensional (2-D) conducting planes and corresponds to superconductors with low carrier density, and the superconductors emerge from the parent compounds upon either hole or particle doping from donor planes. On the other hand, some things seem rather different between the two classes of superconductors. Specifically, if we wish to address how similar the cuprate and FeAs superconductors are, the following issues are perhaps relevant:

a. Multiband physics

There is uniform agreement that FeAs superconductivity is multiband and many think that this is crucial to the physics. The main disagreement is over whether one must treat all five Fe bands near the Fermi surface, or whether a simplified model with say two bands captures most of the physics. Thus, there are multiple sheets for the Fermi surface and the microscopic pairing formfactor for an $n$-band model is actually an $n \times n$ matrix.

b. Multigap physics

Related to the question of multiband physics is the question of multigap physics. From the microscopic point of view, if there are multiple bands near the Fermi surface that can contribute to the pairing interaction, the orbital formfactor for the pairing gap becomes a matrix, which implies that there can be more than one observable pairing gap. Various experiments in the FeAs compounds see evidence for two or more pairing gaps, differing in size by as much as a factor of two. For example, the ARPES measurements of Ref. [24] find evidence for four Fermi surface sheets in $\text{Ba}_0.6\text{K}_0.4\text{Fe}_2\text{As}_2$, and four corresponding gaps, with the largest and smallest gaps differing by about a factor of two in size.

c. Singlet gap or triplet gap

On general grounds we would expect that the pairing gap could be either spin singlet or triplet, depending on the nature of the appropriate effective interaction. This is supported by the numerical calculations of the Moreo–Dagotto group [55, 56], which find that either singlet or triplet pairs could be favored energetically depending on the detailed interactions. However, NMR data now indicate that the FeAs pairing gap has singlet spin character [21–23]. Therefore, we shall assume the observed gaps to be dominantly singlet, as for cuprates.

d. Two-dimensional physics

Another potential difference between FeAs compounds and cuprates concerns whether the physics responsible for SC is dominated by two-dimensional $a-b$ plane physics. For the cuprates this assumption is a relatively good approximation. In the iron arsenide compounds the situation is less clear. The present evidence suggests that for some FeAs superconductors the SC is rather two-dimensional, but for others the superconductivity depends significantly on properties in the $c$-axis direction.

e. On-site coulomb repulsion

In the cuprates the large on-site Coulomb repulsion strongly suppresses double occupancy and leads to a Mott insulator normal state. In Ref. [1] we demonstrated that non-double occupancy for pairs in the real space is a sufficient condition to guarantee that the minimal closed
algebra is $SU(4)$, independent of detailed microscopic considerations such as the orbital or spin symmetry of the gap and the associated structure of the pairs.

The situation in the FeAs compounds is less clear. A variety of calculations and arguments suggest that $U$ must lie in an intermediate range between no correlations and the strong on-site repulsion observed for the cuprates: if $U$ were too large the parent states would develop a charge gap and be good insulators; if it were too small the parent states would be good metals. That they are in fact found to be poor metals suggests an intermediate range of $U$. The presence experimentally of the spin density wave state discussed below also implies a correlated metal, suggesting a non-trivial $U$.

Various calculations indicate that the on-site repulsion on the Fe atoms is approximately half of that observed for Cu atoms in the cuprates, and the normal states for the iron arsenides are observed to be AF metals, not AF Mott insulators. However, these metals are poor metals and various considerations suggest that the FeAs normal states may generally be near a Mott transition. For example, an analysis based on density functional and dynamical mean field theory [57] concludes that a realistic on-site Coulomb repulsion $U \approx 4$ eV would be sufficient to open a Mott gap for a single band at the Fermi surface, but not for the five Fe bands expected to be near the Fermi surface in FeAs undoped compounds. Instead these calculations give a correlated metal structure but with poor charge transport properties (a scattering rate at the Fermi level corresponding to $0.4$ eV at $T = 116$ K). However, a small increase of the on-site repulsion to $U \approx 4.5$ eV in these same calculations begins to open a semiconductor-like gap even at room temperature and Ref. [57] suggests that these compounds are near the metal–insulator transition.

f. Nearest neighbor or next nearest neighbor pairing
Because the arsenic atoms are out of the Fe plane, general arguments imply that next nearest neighbor (NNN) interactions can compete or even exceed nearest neighbor (NN) interactions, raising the question of whether possible bond-wise pairs (pairs with particles on different lattice sites) involve NN or NNN. Calculations indicate that for low enough values of the Hubbard repulsion $U$ the NN pairing dominates the NNN pairing, but for increasing values of $U$ it is found that NNN pairing begins to compete more favorably with NN [56].

g. Differences in antiferromagnetism
Neutron scattering measurements indicate that for both cuprates and pnictides antiferromagnetism is important and in close proximity to the superconductivity in the phase diagram. However, the nature of the antiferromagnetism is different in the two cases. The schematic spin structure associated with the undoped FeAs compounds that is consistent with neutron scattering results is illustrated in the bottom portion of Fig. 1. This structure corresponds to alternating spins in one direction but stripes with spins all aligned with each other in the orthogonal direction [58, 59]. This is in contrast to the antiferromagnetism of the cuprate parent compounds illustrated in the upper portion of Fig. 1, where in either the horizontal or vertical direction the spins alternate. It is with respect to such a magnetic structure that we must add or remove electrons to make FeAs superconductors, if we adopt the point of view that the magnetism and superconductivity are closely related and that the latter develops out of the former with doping.

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3 Similarities and differences

We shall now make a case that the similarities observed for cuprate and Fe-based SC suggest that a minimal description of either involves the same $SU(4)$ Lie algebra, and that this algebra is sufficient to ensure a unified picture of the most general properties observed for these superconductors. Further, we shall argue that the differences between the two classes of superconductors do not change the algebraic structure of a minimal model and thus do not change the most fundamental properties of these superconductors, but rather influence the theory only parametrically. Thus, we shall propose a unification in the emergent degrees of freedom that can exist for cuprate and FeAs superconductors, even if the microscopic structure and the pairing gap symmetry are different in the two cases.

4 A minimal closed set of operators
Let us use the phenomenology of the Fe-based super-
The presence of strongly competing AF and SC ensures that Fe-based superconductors correspond to a non-abelian symmetry as discussed in Ref. [1], but the relevant non-abelian algebra need not be the SU(4) cuprate algebra. The question of the minimal closed algebra for the iron arsenides turns on whether the pairing that can produce the superconductivity involves both on-site pairs (two particles on the same lattice site) and bondwise pairs (two particles on different lattice sites). If we make the simplest model and restrict attention to a single kind of nearest neighbor or next nearest neighbor bondwise pairs (two particles on different lattice sites), the on-site repulsion could be sufficiently strong to make it energetically unfavorable either to form on-site collective pairs or to have double site occupancy by unpaired particles, in which case the symmetry is SU(4) and in addition the material would be expected to be insulating. This is representative of the situation in the cuprates. But one could also have a situation where the same-site repulsion strongly disfavors on-site pairs over bondwise pairs, but does not forbid some charge transport by the unpaired particles in the normal state. The resulting material would again be described by SU(4), but now is expected to be a metal (or poor metal). This situation is representative of the FeAs compounds.

Although a few models involving on-site pairs have been proposed for the iron arsenides, numerical calculations such as those of Refs. [55, 56] indicate that the dominant pairing channels involve nearest neighbor or next nearest neighbor bondwise pairing. We take this as microscopic evidence that a minimal description of FeAs high temperature superconductors involves dominantly bondwise pairing for physically reasonable ranges of the on-site repulsion U and thus corresponds to an SU(4)
the fermion operators have acquired a band index \( b \) and a pairing formfactor. These operators are equivalent to a set of operators: electrons that can form coherent pairs with momentum \( \mathbf{k} \). The preceding general arguments suggest that the non-abelian superconductivity that is in fact isomorphic (described by the same \( SU(4) \) algebra) to the nonabelian superconductivity of the cuprates. This isomorphism and corresponding similarity of the Fe-based and cuprate phenomenologies suggests two unique opportunities. (1) If the algebra associated with the minimal set of Fe-based operators closes under commutation then both cuprate and Fe-based superconductivity can be described by \( SU(4) \) symmetry, thus providing a unified description of these two types of superconductivity, irrespective of differences at a microscopic level. (2) Requiring the algebra to close implies a set of non-linear equations on the operators that, coupled with data, can be used to constrain their microscopic form. In particular, these relations can be used to predict the allowed orbital symmetries of the pair gap by requiring consistency of those gaps with the observed magnetic structure. In the following we shall implement these ideas quantitatively.

5 Extension of \( SU(4) \) to multiband pairing

The preceding general arguments suggest that the non-abelian superconductivity found in the iron arsenides corresponds to an \( SU(4) \) symmetry. To implement this idea quantitatively, we must extend the \( SU(4) \) formalism developed for the cuprates under the simplifying assumption of a single band near the Fermi surface to the case where multiple bands may lie near the Fermi surface within the Brillouin zone. With the preceding discussion and Refs. [2–4] as a guide, we introduce the following set of operators:

\[
p = \sum_{k} g(k) C_{\alpha_k \alpha_{-k} b}^\dagger C_{\alpha_{-k} b}^\dagger, \quad p = (p)^\dagger \tag{1a}
\]

\[
q = \sum_{k} g(k) C_{\alpha_k + Q, \alpha_{-k} b}^\dagger C_{\alpha_{-k} b}^\dagger, \quad q = (q)^\dagger \tag{1b}
\]

\[
Q_{ij} = \sum_{k} g(k) C_{\alpha_k + Q, \alpha_{-k} b}^\dagger C_{\alpha_{-k} b'}^\dagger, \quad Q_{ij} = (Q_{ij})^\dagger \tag{1c}
\]

\[
S_{ij} = \sum_{k} g(k) C_{\alpha_k + Q, \alpha_{-k} b}^\dagger C_{\alpha_{-k} b'}^\dagger - \frac{1}{2} \Omega \delta_{ij} \tag{1d}
\]

where \( g(k) \) is the amplitude to have a \( b \)-band electron with momentum \( k \), \( C_{\alpha_k b}^\dagger \) creates a fermion of momentum \( k \) and spin projection \( \alpha \), \( \delta \) is 1 or 2 = \( \uparrow \) or \( \downarrow \) in band \( b \). \( Q \) is an AF ordering vector, \( \Omega \) is the effective lattice degeneracy, which is the maximum allowed number of doped electrons that can form coherent \( SU(4) \) pairs, and \( g(k) \) is a pairing formfactor. These operators are equivalent to the \( SU(4) \) generators defined in Refs. [2–4] except that the fermion operators have acquired a band index \( b \), with the number of bands included in the sum determined by the physics of the particular problem being addressed. If we define effective one-band creation and annihilation operators through

\[
a_{k b}^\dagger = \sum_{\alpha} g_{\alpha_k b} C_{\alpha_k b}^\dagger, \quad a_{k b} = (a_{k b}^\dagger)^\dagger \sum_{\alpha} |g_{\alpha_k b}|^2 = 1 \tag{2}
\]

then Eq. (1) may we written as:

\[
p_{ij}^\dagger = \sum_{k} g(k) a_{k b}^\dagger (a_{-k b}^\dagger)^\dagger, \quad p = (p_{ij}^\dagger)^\dagger \tag{3a}
\]

\[
q_{ij}^\dagger = \sum_{k} g(k) a_{k + Q, b}^\dagger (a_{-k, b'}^\dagger)^\dagger, \quad q = (q_{ij}^\dagger)^\dagger \tag{3b}
\]

\[
Q_{ij} = \sum_{k} a_{k + Q, b_i}^\dagger a_{k, b_j}, \quad S_{ij} = \sum_{k} a_{k, b_i}^\dagger a_{k, b_j} - \frac{1}{2} \Omega \delta_{ij} \tag{3c}
\]

which is now exactly the form of the \( SU(4) \) symmetry.

If these conditions are met, the operators defined in Eq. (1) close a Lie algebra isomorphic to the \( SU(4) \) algebra describing cuprate superconductivity. By defining new operators that are linear combinations of the operators (1), we may restrict attention to the \( SU(4) \) subalgebra that is generated by 15 operators corresponding physically to singlet pairing, triplet pairing, antiferromagnetism, spin and charge [1–4].

Let’s illustrate these ideas more graphically for two bands, with the argument easily generalized to more bands. Simple possibilities for forming \( SU(4) \) pairs are illustrated schematically in Fig. 2 for nearest neighbor pairs and Fig. 3 for next nearest neighbor pairs, where
now we concentrate on spin-singlet pairs and where we have assumed that the vacuum to which we add pairs is the stripe-AF magnetic state found in neutron scattering experiments. In this picture we see that the multiband pairs are formed in a manner similar to the case for SU(4) in the single-band cuprates, but now each individual pair in the coherent sum over the lattice is more complex in structure because the electrons in the bondwise pair are distributed over more than one orbit on each site. Figures 2 and 3 are of course just cartoons illustrating the coherent multiband pairs defined precisely in Eq. (1).

Thus, as long as the pairs entering the formalism as basis states may be viewed as strongly collective, multiband pairing in the presence of antiferromagnetism may be treated formally in the same way as single-band pairing in the presence of antiferromagnetism. Of course the pairs may have a richer internal structure in the multiband case and experiments sensitive to single-particle degrees of freedom like ARPES may probe that structure. However, at the level of emergent collective degrees of freedom and their corresponding physical consequences, the important point is that the collective pairs—whatever their detailed internal structure—close an algebra when commuted with other physically relevant operators in the system. If that is the case, then the overall physics of the problem is strongly constrained by the corresponding (generally nonabelian) algebra and one has a theoretical formalism constructed specifically to deal with the common general features of a class of superconductors.

The philosophy that underlies this approach rests on the assumption that a set of emergent strongly-correlated electron phenomena observed to occur with some systematic phenomenology over a range of compounds can be best understood by first identifying the features common to all occurrences and viewing the differences as perturbations around the unifying features. This approach can fail if there are no common recurring collective modes across a class of compounds, or if the recurring collective modes are strongly perturbed from compound to compound. However, there is abundant empirical evidence in the cuprates that this approach is a physically reasonable starting point, and in the FeAs compounds we believe that the evidence is also strong enough to justify a focus on the unifying emergent properties across compounds as a more reasonable starting point than one focusing on the differences at the microscopic level.

6 Pair formfactors and closed algebras

Let us now consider in more detail the closure conditions (4). The first requirement \( g(\mathbf{k}) = g(-\mathbf{k}) \) is almost always satisfied by physically reasonable formfactors. As discussed in Ref. [1], the condition \( |g(\mathbf{k})| = 1 \) necessary to close the algebra in momentum space may be interpreted as an occupation constraint on the full formfactor without this condition in the real space. Specifically, for cuprates the \( d \)-wave formfactor \( g(\mathbf{k}) = \cos k_x - \cos k_y \) must be approximated by \( \text{sgn} (\cos k_x - \sin k_y) \) to close the algebra in momentum space. However, if the operators are Fourier transformed to the real space retaining the full formfactor (that is, \( \cos k_x - \cos k_y \)) the SU(4) algebra closes but only if the lattice is restricted to no double pair occupancy. This indicates that \( |g(\mathbf{k})| = 1 \) is not an approximation but rather is a physically necessary momentum-space corollary to no double occupancy (by pairs) for the collective wavefunction in the real space. Therefore, we shall assume that closure of the SU(4) algebra requires no double site occupancy by pairs and the condition

\[
g(\mathbf{k} + \mathbf{Q}) = \pm g(\mathbf{k})
\]

applied to the full formfactor (without the condition \( |g(\mathbf{k})| = 1 \)), which will imply a set of real-space occupancy constraints imposed by the algebra that depends on the exact form of \( g(\mathbf{k}) \).

7 Unified SU(4) model

Since Fe-based SC is observed to occur with many features similar to that for cuprate SC, the simplest assumption is that the operator set (1) describes the minimal collective degrees of freedom consistent with iron arsenide phenomenology. But this, coupled with our provisional assumption of suppressed double site occupancy by pairs, means that the minimal algebra consistent with FeAs phenomenology is SU(4), just as for the cuprates. Furthermore, with this assumption Eq. (5) provides immediate constraints on the permissible form of \( g(\mathbf{k}) \) for Fe-based compounds. In Table 1 we apply these constraints to some gap symmetries that have been proposed for Fe-based superconductors, indicating whether the SU(4) algebra can be closed for each assumption, and for reference we carry out the same procedure for the cuprates (without regard to whether each symmetry has been proposed seriously for cuprates). Some of the formfactors considered in Table 1 are illustrated in
be the symmetry cannot orbital symmetry of the pair gap for Fe-based compounds based superconductors requires that the corresponding cuprates, and maximum doping fraction $P_f$ for allowed FeAs symmetries.

| $g(k)$ | Fe-based | Cuprate | $P_f$ |
|--------|----------|---------|-------|
| $s_{x^2+y^2} = \cos k_x + \cos k_y$ | No | Yes | – |
| $d_{x^2-y^2} = \cos k_x - \cos k_y$ | No | Yes | – |
| $s_{x^2+y^2} = \cos k_x \cos k_y$ | Yes | Yes | 1/3 |
| $d_{x^2-y^2} = \sin k_x \sin k_y$ | Yes | Yes | 1/3 |
| $s_{x^2+y^2} \pm d_{x^2-y^2}$ | Yes | Yes | 2/3 |
| $s_{x^2+y^2} \pm id_{x^2-y^2}$ | No | Yes | – |

It is easily verified that $k \rightarrow k + Q$ interconverts the $s_{x^2+y^2}$ and $d_{x^2-y^2}$ formfactors, which implies that while neither separately can close the $SU(4)$ algebra because they cannot satisfy Eq. (5), the linear combination

$$g(k) = g(s_{x^2+y^2}) \pm g(d_{x^2-y^2})$$

which is proportional to $\cos k_x$ or $\cos k_y$, does close the algebra. On the other hand, the time-reversal breaking linear combination

$$g(k) = g(s_{x^2+y^2}) + ig(d_{x^2-y^2})$$

proposed in Ref. [60] as a possible FeAs gap symmetry is seen from Table 1 to be compatible with cuprate antiferromagnetism but not with FeAs antiferromagnetism.

There is a further constraint that can be placed on the orbital formfactor. The coherent pair states corresponding to allowed formfactors in Table 1 have a structure $D^f = \sum_{r=(x,y)} c^f_{r1} c^f_{r1}^\dagger$ (with $D^f \equiv p^f$) in the real space, where $c^f_{r1}$ is the electron creation operator $c^f_{r1}$ in the coordinate representation. The $c^f_{r1}$ for $s_{x^2+y^2} \pm d_{x^2-y^2}$ pairs are formed from nearest-neighbors:

$$c^f_{r1} = 2^{-1/2} (c^f_{(x+a,y)}) + c^f_{(x-a,y)})$$

and for $\cos k_x \cos k_y$ or $\sin k_x \sin k_y$ pairs are formed from next-nearest neighbors:

$$c^f_{r1} = \frac{1}{2} (c^f_{(x+a,y+b)}) + c^f_{(x-a,y-b)})$$

with $(\pm)$ corresponding to $\cos k_x \cos k_y$ and $(-)$ to $\sin k_x \sin k_y$. These are illustrated in Fig. 5.

From Table 1 we conclude that $s_{x^2+y^2}$ and $d_{x^2-y^2}$ do not lead to a closed $SU(4)$ algebra, but symmetries such as $s_{x^2+y^2}$ and $d_{x^2-y^2}$ can. Thus, we predict that neither $s_{x^2+y^2}$ nor $d_{x^2-y^2}$ can be correct orbital symmetries for the Fe-based superconductors because they are fundamentally incompatible with the observed magnetic structure. Hence a unified $SU(4)$ model of cuprate and Fe-based superconductors requires that the corresponding orbital symmetry of the pair gap for Fe-based compounds cannot be the symmetry $d_{x^2-y^2}$ found for the cuprates. More generally, one can see from Table 1 that the more symmetric antiferromagnetism of the cuprates is compatible with many possible pairing formfactors (though most appear to not be realized physically), but the asymmetric AF of the iron arsenides places much stronger constraints on a compatible pairing structure.
a lattice occupancy restriction associated with each of these pair structures. By counting the maximum number of pairs that can be placed on the lattice without overlap, as illustrated in Fig. 6, the largest doping fraction consistent with SU(4) symmetry is found to be \( P_f = 2/3 \) for \( \cos k_x \) and \( P_f = 1/3 \) for \( \cos k_x \cos k_y \) or \( \sin k_x \sin k_y \). These are summarized in the last column of Table 1. Current data suggest that the superconductivity does not extend much beyond \( P_f = 1/3 \). Even allowing for some uncertainty in how many doped particles end up in the coherent pairs, this strongly favors \( \cos k_x \cos k_y \) or \( \sin k_x \sin k_y \) among the allowed orbital symmetries for iron arsenides in Table 1.

![Fig. 6 Schematic count of maximum pair density consistent with SU(4) symmetry assuming electron-doped material with a singlet \( \cos k_x \cos k_y \) pair gap formfactor. For this segment of the lattice, no additional pairs of this structure can be added without causing a finite amplitude for double site occupancy by pairs, which would break SU(4) symmetry. By counting of occupied and unoccupied sites, the maximum fraction of lattice sites that can be occupied by \( \cos k_x \cos k_y \) pairs without double occupancy is 1/3. The realistic wavefunction will be a superposition of such configurations, each with a maximum pair occupancy of 1/3. The spatial pair structure and maximum doping for \( \sin k_x \sin k_y \) is the same as for \( \cos k_x \cos k_y \), since they differ only in phases [see Eq. (7)].](image)

### 8 Magnetism and superconductivity

The preceding discussion assumes implicitly that there is a sufficiently intimate relationship between antiferromagnetism and superconductivity in cuprate and FeAs superconductors that the observed magnetic structure can be used to constrain the form of the pairing interaction leading to the superconductivity. There is significant empirical evidence to suggest this. For example, recent ARPES measurements in the underdoped pnictides by Xu et al. [61] provide strong support for a picture very similar to the one proposed theoretically in this paper.

However, it is by no means uniformly agreed (particularly in FeAs compounds) that superconductivity and magnetism are so strongly related and that the SC state develops directly from doping the AF state. Thus, we may invert the preceding discussion to provide a test of this hypothesis: failure of the constraint predictions implied by Table 1 would be strong evidence that AF and SC are not sufficiently related in iron arsenides that one constrains the form of the other. Conversely, verification of these predictions would support the SU(4) unification hypothesis for cuprate and FeAs superconductivity proposed here, which would imply that magnetism and superconductivity are inextricably linked in high temperature superconductors.

### 9 Singlet and triplet pairing

NMR measurements suggest singlet charge carriers for the FeAs superconductors [21–23]. As discussed above, consistency requires both singlet and triplet pairs in the truncated SU(4) subspace and non-abelian superconductivity can accommodate either as charge carriers. Which is realized depends on the effective interaction, which can be determined empirically and could differ between Fe-based and cuprate superconductors. For cuprates the effective interaction is well determined and indicates that singlet pair correlation is substantially larger than triplet pair correlation [5, 6]. Because the singlet pairing energy scale is much larger than the triplet pairing energy scale for cuprate superconductors, we may expect that scattering at finite temperature is larger for triplet pairs and that charge transport in the superconducting state is dominated by coherent singlet pairs, as observed. The understanding of iron arsenides is incomplete at this point and the effective interaction is not as well established as for cuprates, but the evidence that superconductivity in the iron arsenides is also singlet in character suggests that similar considerations apply for FeAs superconductivity.

### 10 Spatial inhomogeneity

For the cuprates and (to a lesser degree) FeAs superconductors there is evidence for a relatively universal phase diagram, but also evidence for a variety of spatial inhomogeneity, particularly in the underdoped region. As we have shown for the cuprates [10], the coherent-state solutions for SU(4) have the natural property that in underdoped compounds (and only in underdoped compounds) there are many nearly degenerate ground states having different ratios of pairing correlation to antiferromagnetic correlation. Thus, the underdoped region is extremely sensitive to external perturbation and a realistic wavefunction may be expected to be a superposition of components respecting SU(4) symmetry but having
different expectation values for pairing gaps and staggered magnetization. (Mathematically, the wavefunction has components corresponding to the same irreducible representations of SU(4), but to different irreducible representations with respect to its SU(2) pairing subgroups.) This has two important consequences:

(1) It can produce a partially-gapped state above the superconducting transition temperature in which there are significant correlations corresponding to phase fluctuations modulated by competing AF and SC order, but small expectation values for static order.

(2) This nearly-degenerate superposition of trial ground states will exhibit a high degree of complexity (extreme susceptibility to external perturbations) in the underdoped region.

The first consequence leads to a quantitative description of the pseudogap state (for which there is strong evidence in the cuprates and growing evidence in FeAs compounds; see Refs. [61–65], for example); the second implies that – in the underdoped region only – a rich variety of spatial inhomogeneity can be induced by small background perturbations, and that the nature of that inhomogeneity will depend sensitively on the electronic and structural properties of individual compounds.

Thus, the natural tendency to complexity exhibited by the SU(4) solutions in the underdoped region, and the dependence of that complexity on the detailed structure of individual compounds, provide a possible explanation for differences in pseudogap behavior and spatial inhomogeneity among different cuprates and pnictides. Since the solution exhibits this complexity yet remains SU(4)-symmetric in this emergent state, it can account for rich variety in inhomogeneity within the (seemingly contradictory) context of a global phase diagram.

12 Multiband, momentum-dependent SU(4)

As we have seen, by introducing the effective creation and annihilation operators defined in Eq. (2) the SU(4) model can be reduced to its original form in which momentum-dependent effects have been averaged over. This is a reasonably good approximation for the cuprates where one deals with effectively single-band physics and a gap that is nodal but a Fermi surface that is topologically connected. In the iron arsenides the Fermi surface is more complex, with disconnected sheets in different regions of the Brillouin zone. This implies that averaging over k may miss qualitatively important physics for measurements that resolve momentum. In Ref. [7] we extended the SU(4) model to include explicit k dependence for a single band. We may generalize this SU(4)k model to include multiple bands and gaps in the following way.

Since the pairing formfactor g(k) remains uncertain in the iron arsenides and in the most general case might even differ from compound to compound, we take it initially as unknown, to be determined by measurements. We then generalize the k-dependent SU(4) formalism of Ref. [7] by introducing momentum-dependent coupling strengths G_{kk'}^{i} for pairing and χ_{kk'} for antiferromagnetism through

\[ G_{kk'}^{i} = G^{0}_{i} g_{k} g_{k'} \], \[ χ_{kk'} = χ^{0}_{i} g_{k} g_{k'} \]  

(8)

where \( g_{k} \equiv |g(k)| \) and \( G^{0}_{i} \) and \( χ^{0}_{i} \) are parameters that are independent of momentum but may depend on doping and temperature. This expression for \( χ_{kk'} \) is identical to that of Eq. (14) of Ref. [7] but the expression for \( G_{kk'}^{i} \) generalizes Eq. (13) of Ref. [7], in anticipation of a richer pairing structure because of the multiband physics that we expect to be important in the FeAs compounds.

We may now develop the formalism in a manner parallel to that described in Refs. [2–4, 7]. One obtains a set
of gap equations that generalize the BCS gap equations. Introducing a doping parameter \( x \) and defining a critical doping \( x_q \) by

\[
x_q = \sqrt{\frac{\chi - G_0}{\chi - G_1}}
\]  

(9)

where \( G_1 = G_0 \hat{g}^2 \), \( \chi = \chi_0 \hat{g}^2 \), and \( \hat{g} \) is an averaged \( g \), the solutions of the gap equations for temperature \( T = 0 \) and momentum \( \mathbf{k} \) if \( x \leq x_q \) are found to be

\[
\Delta_0(k) = \frac{\Omega}{2G_0} \frac{g(k)}{\hat{g}} \sqrt{x(x_q^3 - x)}
\]

(10a)

\[
\Delta_1(k) = \frac{\Omega}{2} \frac{g(k)}{\hat{g}} \sqrt{x(x_q^3 - x)}
\]

(10b)

\[
\Delta_2(k) = \frac{\Omega}{2} \frac{g(k)}{\hat{g}} \sqrt{x(x_q^3 - x)(x_q^3 - x)}
\]

(10c)

\[
\lambda'_k = -\frac{\Omega}{2} \frac{g(k)}{\hat{g}} (\chi - G_1)x_q(1 - x_qx) + G_1x
\]

(10d)

and the corresponding solutions for \( x > x_q \) are

\[
\Delta_0(k) = \Delta_1(k) = 0
\]

(11a)

\[
\Delta_0(k) = \frac{\Omega}{2} \frac{g(k)}{\hat{g}} \sqrt{1 - x^2}
\]

(11b)

\[
\lambda'_k = -\frac{\Omega}{2} \frac{g(k)}{\hat{g}} G_0x
\]

(11c)

Physically, \( \Delta_0 \) and \( \Delta_1 \) correspond to correlation energies for singlet and triplet pairing, respectively, \( \Delta_2 \) corresponds to correlation energy in the pseudogap state that is fluctuating AF in nature, and \( \lambda' \) denotes the chemical potential.

These solutions may then be used to determine other physically important quantities using the methods described inRefs. [1–10]. For example, the superconducting transition temperature \( T_c \) is

\[
T_c(k) = G_0 \frac{g(k)}{\hat{g}} \frac{R_x}{4k_B \tanh x}
\]

(12)

where the parameter \( R \) is of order one and defined in Ref. [7], and because of the AF interaction there are pseudogap correlations that extend from \( T_c \) up to a pseudogap temperature:

\[
T^*(k) = \chi \frac{g(k)}{\hat{g}} \frac{R(1 - x^2)}{4k_B}
\]

(13)

The pseudogap states lying between \( T_c \) and \( T^* \) are correlated by AF and pairing, but are not expected to have large static order parameters because of the fluctuations discussed in the earlier section on spatial inhomogeneity. Physically these states may be interpreted in terms of competing AF and SC correlations, but in a paired basis. Thus, they unify the preformed pair and competing order pictures for pseudogap states.

Eqs. (8)–(13) define a \( k \)-dependent \( SU(4) \) model that can accommodate multiband physics. They are appropriate for comparison with experimental data that can resolve \( k \). If one averages these expressions over all momenta \( k \) near the Fermi surface then the averaged factors \( \langle g(k) / \hat{g} \rangle \rightarrow 1 \) and Eqs. (8)–(13) reduce to the equations of the original \( SU(4) \) model. These are appropriate for comparison with experimental quantities that do not resolve \( k \).

### 13 Multiple pairing gaps in the FeAs compounds

The gap equations and their solutions given in the preceding section represent a general formalism applicable for systems in which the pairing involves multiple bands and the possibility of multiple pairing gaps within the Brillouin zone. Let us now apply this formalism specifically to an analysis of the iron superconductors.

We have argued that consistency of pairing with observed antiferromagnetic structure strongly constrains the permissible forms of the pairing formfactor \( g(k) \) and that the forms most consistent with the observed properties of the FeAs compounds are \( g(k) = \cos k_x \cos k_y \) or \( g(k) = \sin k_x \sin k_y \). Let us first consider the \( \cos k_x \cos k_y \) case. Restricting attention for purposes of illustration to doping \( x \) less than the critical value \( x_q \), we obtain from Eq. (10) a singlet pairing gap

\[
\Delta_0(k) = \Delta_0 \cos k_x \cos k_y, \quad \Delta_0 \equiv \frac{G_0 \Omega}{2g} \sqrt{x(x_q^3 - x)}
\]

(14)

ARPES measurements of Ref. [24] find evidence for a total of four sheets of Fermi surface within the Brillouin zone. To illustrate ideas in a transparent way, let us introduce a simple model in which we assume the four pockets of Fermi surface (labeled \( \alpha, \beta, \gamma, \) and \( \delta \)) to be spheres centered at the appropriate momentum, with the radii \( k_\alpha, k_\beta, k_\gamma, \) and \( k_\delta \) of the spheres determined by fits to the ARPES data. We illustrate in Fig. 7. Then from Eq. (14) the pairing gaps on the four sheets of Fermi surface are given by

\[
\Delta_i \equiv \Delta_i(k_i, \theta_i) = \Delta_0 \cos(k_i \cos \theta_i) \cos(k_i \sin \theta_i)
\]

(15)

where \( i = \alpha, \beta, \gamma, \delta \) labels the Fermi surface sheets and the polar angles \( \theta_i \) are centered at the \( \Gamma \) and \( M \) points of the Brillouin zone (see Fig. 7). Writing this out explicitly for the four cases we obtain the results given in Table 2 for the gaps on the four pockets of Fermi surface.

A fit of the parameters \( \Delta_0 \) and the \( k_i \) to the data of Ref. [24] gives the description of the pairing gaps illustrated in Figs. 8–10, where in Fig. 8 the circles indicate data with associated uncertainties given by the error
Fig. 7  Spherical approximations to the Fermi surfaces. The four Fermi surface pockets, two around the \( \Gamma \) point and two around the \( X \) point are approximated by circles.

**Table 2**  Pairing gaps on four sheets of the idealized Fermi surface.

| Label | Fermi surface | Pairing gap |
|-------|---------------|-------------|
| \( \Delta_\alpha \) | \( k_x^2 + k_y^2 = k_\alpha^2 \) | \( \Delta_0 \cos(k_x \cos \theta_\alpha \cos(k_y \sin \theta_\alpha) \) |
| \( \Delta_\beta \) | \( k_x^2 + k_y^2 = k_\beta^2 \) | \( \Delta_0 \cos(k_x \cos \theta_\beta \cos(k_y \sin \theta_\beta) \) |
| \( \Delta_\gamma \) | \( k_x^2 + k_y^2 = k_\gamma^2 \) | \( \Delta_0 \cos(k_x \cos \theta_\gamma \cos(k_y \sin \theta_\gamma) \) |
| \( \Delta_\delta \) | \( k_x^2 + k_y^2 = k_\delta^2 \) | \( \Delta_0 \cos(k_x \cos \theta_\delta \cos(k_y \sin \theta_\delta) \) |

Fig. 8  Pairing gaps on four sheets of the Fermi surface. Note that \( \Delta_\gamma \) is displaced by 5 meV for plotting purposes. Circles are data from Ref. [24] and dashed lines are theoretical using Eq. (14). Parameters \( \Delta_0 = 13.5 \) meV, \( k_x/\pi = 0.135 \), \( k_y/\pi = 0.370 \), \( k_\alpha/\pi = 0.141 \), and \( k_\delta/\pi = 0.181 \) were determined by fitting to the data.

bars and the dashed lines represent the gaps calculated from Eq. (15). Thus we see that the ARPES measurements of Ref. [24] are at least approximately consistent with the \( \cos k_x \cos k_y \) pairing gap formfactor deduced in the present paper by requiring self-consistency of antiferromagnetism and superconductivity within an \( SU(4) \) symmetry.

The \( \sin k_x \sin k_y \) formfactor that would also be compatible with the antiferromagnetism according to Table 1 would on the other hand not be compatible with the data displayed in Fig. 8, since it would imply nodes on the Fermi surfaces (compare Figs. 4 and 9) not observed in the data. We conclude that consistency of the observed antiferromagnetism with the superconductivity in the FeAs compounds is possible with either \( \cos k_x \cos k_y \) or \( \sin k_x \sin k_y \) pairing formfactors, but requiring in addition consistency with the ARPES data of Ref. [24] restricts to the \( \cos k_x \cos k_y \) choice.

Fig. 9  Fermi surfaces \( \alpha, \beta, \gamma, \) and \( \delta \) superposed on contours of the pairing formfactor \( |\cos k_x \cos k_y| \). Gap nodes are indicated by dashed lines.

Fig. 10  Pairing gaps on four sheets of the Fermi surface versus \( |\cos k_x \cos k_y| \). Data from Ref. [24] and the squares and rectangles indicate theoretical values for gaps on the four sheets deduced from Fig. 9. The same parameters as for Fig. 8 were used.

14  Top-down approach to superconductivity

The approach advocated in this paper may be termed “top-down”: The appropriate theory for describing the superconductivity is inferred from the global properties exhibited by the physical interacting system, rather than from the underlying atomic and crystal structure of the
non-interacting system (which we shall term “bottom-up” approaches). This is not the most common approach to this problem, but it is a powerful one. It is closely related to the philosophy advocated in emergent theories of complex systems where it is argued that the appropriate building block for a theoretical understanding of complex systems are the ones actually observed to occur, and that these should be considered just as fundamental as more “microscopic” building blocks.

Practically, the top-down approach may be on firmer ground than bottom-up approaches because it is constrained more directly by data. However, it is not phenomenological since it is based on an exact many-body solution within a truncated space. Therefore, comparing a top-down analysis with data constrains the validity of proposed bottom-up models. A specific example is afforded by the analysis associated with Table 1, where neutron scattering data were shown to restrict severely the collective pairing structures that can be consistent with the observed competing antiferromagnetism. Our dynamical symmetry approach thus unifies cuprate and FeAs superconductivity in a coherent picture that demonstrates how the Cooper instability originates from a single theoretical framework in these diverse systems. That the interaction responsible for exploiting the Cooper instability is different in BCS superconductors and cuprates superconductors, and could be different yet again in FeAs superconductors is of secondary importance. Seen at the level of abstraction implied by the non-abelian superconductor hypothesis, these are all the same superconductors, all made possible by a Cooper instability that morphs into more complex behavior but persists in clearly identifiable form even in the presence of competing degrees of freedom like antiferromagnetism, and that leads to a phenomenology with many common features, even when enabled by physically very different weakly attractive interactions [9].

Finally, if our identification of FeAs superconductivity as the second example of non-abelian superconductivity is valid, there may be experimental lessons to be learned. The dynamical symmetry framework presented here unifies cuprate and iron arsenide superconductivity. It is then instructive to recall that both the discovery of cuprate superconductivity and that of FeAs superconductivity were surprising when viewed from standard perspectives. The reason for that surprise lies largely in what we now realize is a too-narrow view of the microscopic conditions under which superconductivity could arise. This suggests that one should search for new examples of non-abelian superconductivity guided not only by microscopic considerations but also by general principles of where we might expect the Cooper instability in the presence of emergent collective degrees of freedom.

The cuprate and iron arsenide data suggest that any region having magnetism competing with a pairing interaction (which might be mediated by a variety of possible microscopic interactions) is fertile ground for such a search, but this is not necessarily the only possibility. Any strongly collective mode that can compete with pairing for available strength within a relevant Hilbert space could lead to non-abelian superconductivity and the attendant complex behavior exemplified by cuprate and FeAs superconductors, with the non-abelian algebra not necessarily SU(4) in that case but with the basic ideas qualitatively similar to those discussed here.

15 Conclusions

We have presented evidence that the new Fe-based high-temperature superconductors represent the second example (after the cuprates) of the non-abelian superconductors proposed in an earlier paper. These superconductors differ from normal ones because the non-abelian properties exhibited by commuting their minimal sets of physical operators imply non-linear constraints for collective degrees of freedom interacting with the superconductivity. The identification of non-abelian superconductivity in these two classes of compounds permits a unified model of cuprate and Fe-based superconductors to be constructed based on an SU(4) group (and subgroups) generated by emergent degrees of freedom.

The requirement that the SU(4) algebra both close under commutation and be consistent with the magnetic structure inferred from neutron scattering experiments permits constraints to be placed on orbital symmetries for the pairing gap in FeAs compounds. We find that neither $s_{x^2+y^2}$ nor $d_{x^2-y^2}$ symmetries appear compatible with the neutron scattering data but $s_{x^2+y^2}$ could be, and comparing the predicted gaps with ARPES data restricts the choice uniquely to $d_{x^2-y^2}$ (that is, cos $k_x$ cos $k_y$). Thus, we reach the quite interesting conclusion that a unified SU(4) model of FeAs and cuprate high temperature superconductivity is possible, but consistency with neutron scattering and ARPES data requires that the pairing in the two cases corresponds to different orbital formfactors at the microscopic level.

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