Mott Insulators, No-Double-Occupancy, and Non-Abelian Superconductivity

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SU(4) dynamical symmetry is shown to imply a no-double-occupancy constraint on the minimal symmetry description of antiferromagnetism and d-wave superconductivity. This implies a maximum doping fraction of $\frac{1}{2}$ for cuprates and provides a microscopic critique of the projected SO(5) model. We propose that SU(4) superconductors are representative of a class of compounds that we term non-abelian superconductors. We further suggest that non-abelian superconductors may exist having SU(4) symmetry and therefore cuprate-like dynamics, but without d-wave hybridization.

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Suppression of double occupancy on sites in the copper oxide planes is critical in explaining why cuprate systems are antiferromagnetic Mott insulators at half filling and become superconductors through hole doping. The symmetric Zhang SO(5) model predicts no charge gap at half filling. To recover Mott insulator phases at half-filling in the Zhang model it is normal to impose a no-double-occupancy rule by Gutzwiller projection. This breaks SO(5) symmetry, but lattice calculations and schematic arguments suggest that many SO(5) features might survive in such a projected SO(5) model.

We have proposed a unified description of high temperature superconductivity and antiferromagnetism based on a $U(4)$ ⊃ SU(4) dynamical symmetry that has analytical solutions in three symmetry limits $\mathbb{Z}_2 \mathbb{R} \mathbb{R}$. The SO(4) limit of the SU(4) model corresponds to an antiferromagnetic phase, the SU(2) limit to a d-wave superconducting phase, and the SO(5) limit to a critical symmetry interpolating between the antiferromagnetic and superconducting phases.

Although the methodology of the SU(4) model differs substantially from that of the Zhang model, its SO(5) limit represents the Zhang SO(5) algebra subject to constraints implied by embedding SO(5) in the larger algebra SU(4). In this Letter we address the physical understanding of why SU(4) should play a crucial role in high temperature superconductivity, how no-double-occupancy and Mott insulator properties lie at the basis of this understanding, and provide a microscopic understanding of the projected SO(5) model.

The $U(4) \supset SU(4)$ model has 16 symmetry generators:

\[
p_{12}^+ = \sum_k g(k) c_{k+i}^\dagger c_{k-i}^\dagger, \quad p_{12} = \sum_k g^*(k) c_{k-i} c_{k+i}^\dagger,
\]

\[
g_{ij}^+ = \sum_k g(k) c_{k+Q_i}^\dagger c_{k-Q_j}^\dagger, \quad g_{ij} = (g_{ij})^+, \quad Q_{ij} = \sum_k c_{k+Q_i}^\dagger c_{k-Q_j}, \quad S_{ij} = \sum_k c_{k+Q_i}^\dagger c_{k-Q_j} - \frac{1}{2} \Omega_{ij},
\]

where $c_{k,i}^\dagger$ creates an electron of momentum $k$ and spin projection $i, j = 1$ or $2 \equiv \uparrow$ or $\downarrow$. $Q = (\pi, \pi, \pi)$ is an AF ordering vector, $\Omega/2$ is the electron-pair degeneracy, and $g(k)$ is the d-wave form factor

\[
g(k) = (\cos k_x - \cos k_y) \approx \text{sgn}(\cos k_x - \cos k_y). \quad (2)
\]

By forming new linear combinations, $\mathbf{g}$ may be replaced by operators having more direct physical meaning:

\[
Q_+ = Q_{11} + Q_{22} = \sum_k (c_{k+Q_i}^\dagger c_{k-i} + c_{k-Q_i}^\dagger c_{k+i}),
\]

\[
\bar{S} = \left( \frac{S_{12} + S_{21}}{2}, \frac{-S_{12} - S_{21}}{2}, \frac{S_{11} - S_{22}}{2} \right)
\]

\[
\bar{Q} = \left( \frac{Q_{12} + Q_{21}}{2}, \frac{-Q_{12} - Q_{21}}{2}, \frac{Q_{11} - Q_{22}}{2} \right)
\]

\[
\pi^+ = \left( \frac{Q_{11} - Q_{22}}{2}, \frac{Q_{11} + Q_{22}}{2}, \frac{-Q_{11} + Q_{22}}{2} \right)
\]

where $Q_+$ is associated with charge density waves, $\bar{S}$ is the spin operator, $\bar{Q}$ is the staggered magnetization, $D^\dagger$ ($D$) is the creation (annihilation) operator of spin-singlet d-wave pairs, $\pi^+ (\pi)$ are associated with spin-triplet pairs, and $2M = n - \Omega$ is related to the number (charge) operator $n$. The representation space of the $SU(4)$ model is built by the coherent $D$ and $\pi$ pairs:

\[
|n_\uparrow n_\downarrow n_\uparrow n_\downarrow\rangle = (\pi\uparrow^\dagger)^{n_\uparrow} (\pi\downarrow^\dagger)^{n_\downarrow} (D_1^\dagger)^{n_1} |0\rangle. \quad (4)
\]

The operator $Q_+$ commutes with all generators and will be ignored in this discussion. Thus the most general effective Hamiltonian in the symmetry-dictated truncated space is a linear combination of all scalar products constructed from the remaining 15 $SU(4)$ generators. Assuming only one and two-body interactions:

\[
H = \hat{n}\varepsilon - v n^2 - G_0 D^\dagger D - G_1 \pi^\dagger \pi - \chi \bar{Q} \cdot \bar{Q} + g \bar{S} \cdot \bar{S}, \quad (5)
\]

where $\varepsilon, v, G_0, G_1, \chi$, and $g$ define effective microscopic strengths of single-particle and interaction terms.
The operator set (12) is closed under $U(4) \supset U(1) \times SU(4)$ symmetry (hereafter termed $SU(4)$) only if the approximation in (2) holds. The physics implied in this approximation becomes more transparent if we transform (1) to coordinate space (using the exact form of Eq. (2)):

$$p_{12}^{\dagger} = \sum_i c_{r,i}^{\dagger} c_{r,i}$$

$$q_{ij}^{\dagger} = \sum_i (-)^r c_{r,i}^{\dagger} c_{r,j}$$

$$Q_{ij} = \sum_i (-)^r c_{r,i}^{\dagger} c_{r,j}$$

where $c_{r,i}^{\dagger}$ ($c_{r,i}$) creates (annihilates) an electron of spin $i$ located at $r$ and $c_{r,i}^{\dagger}$ ($c_{r,i}$) creates (annihilates) an electron of spin $i$ at the four neighboring sites, $r \pm a$ and $r \pm b$, with equal probabilities ($a$ and $b$ are lattice constants in $x$ and $y$ directions, respectively),

$$c_{r,i}^{\dagger} = \frac{1}{2} \left( c_{r+a,i}^{\dagger} + c_{r-a,i}^{\dagger} - c_{r+b,i}^{\dagger} - c_{r-b,i}^{\dagger} \right).$$

The factor $(-)^r$ in Eq. (12) is $(-)^{n_x + n_y}$ and $(n_x, n_y)$ are the coordinates of a lattice site on the copper oxide plane, $r = n_x a + n_y b$, which is positive for even sites ($n_x + n_y$ is even) and negative for the odd sites ($n_x + n_y = odd$). This factor originates from the assumption $e^{iQ^{\dagger} r} \approx (-)^r$ and implies Mott insulator properties: the electrons are localized at lattice sites with small overlap between orbitals of electrons on neighboring lattice sites.

From the coordinate representation (6) we see that spin-singlet and spin-triplet pairs are formed by holes on adjacent sites. Fig. 1 illustrates the spatial structure of a hole pair: if one hole is at $r$, the other hole occupies the four adjacent sites ($r \pm a$ and $r \pm b$) with equal probability. The summation over $r$ in the pair creation (annihilation) operators indicates that such pairs are highly coherent. It also can be seen that

$$\hat{n} = \hat{n}^{(e)} + \hat{n}^{(o)}$$

$$S_{ij} = S_{ij}^{(e)} + S_{ij}^{(o)}$$

with $\hat{n}^{(e)}$ ($\hat{n}^{(o)}$) and $S_{ij}^{(e)}$ ($S_{ij}^{(o)}$) the total electron number and spin operators at even (odd) sites, respectively:

$$\hat{n}^{(e)} = \sum_{i,r=even} c_{r,i}^{\dagger} c_{r,i}$$

$$S_{ij}^{(e)} = \sum_{r=even} c_{r,i}^{\dagger} c_{r,j}$$

Thus $Q_+$ and $\hat{Q}$ represent the differences in total charge and spin between even and odd sites, respectively.

However, (10) does not close under commutation unless

$$\{c_{r,i}^{\dagger}, c_{r,j}^{\dagger}\} = \delta_{r,r} \delta_{ij} \quad \{c_{r,i}, c_{r,j}\} = 0$$

(that is, $c_{r,i}^{\dagger}$ ($c_{r,i}$) is a basis for particles occupying sites adjacent to $r$). This separates lattice sites into categories $A$ and $B$: if $r$ is even $A$ sites (with operators $c_{r,i}^{\dagger}$ ($c_{r,i}$)), $r$ is odd are the $B$ sites (operators $c_{r,i}^{\dagger}$ ($c_{r,i}$)), or vice versa. Then (12) permits (10) to be written as

$$p_{12}^{\dagger} = \sum_{r \in A} \left( c_{r,i}^{\dagger} c_{r,i}^{\dagger} - c_{r,i}^{\dagger} c_{r,i} \right)$$

$$q_{ij}^{\dagger} = \pm \sum_{r \in A} \left( c_{r,i}^{\dagger} c_{r,j}^{\dagger} + c_{r,j}^{\dagger} c_{r,i}^{\dagger} \right)$$

$$S_{ij} = \sum_{r \in A} \left( c_{r,i}^{\dagger} c_{r,j} - c_{r,j}^{\dagger} c_{r,i} \right)$$

$$\hat{Q}_{ij} = \pm \sum_{r \in A} \left( c_{r,i}^{\dagger} c_{r,j} + c_{r,j}^{\dagger} c_{r,i} \right)$$

$$p_{12} = (p_{12}^{\dagger})^{\dagger} = (q_{ij}^{\dagger})^{\dagger}$$

with $\hat{Q}_{ij} \equiv Q_{ij} + \frac{t}{4} \delta_{ij}$, where the $\pm$ sign is $(-)$ if $A$ is chosen to be even (odd) sites. (Whether $A$ sites are taken to be even or odd is a labeling choice and does not influence the physics.) Then by explicit commutation the operators (13) close an $SU(4)$ algebra. But by Eq. (11),

$$\{c_{r,i}^{\dagger}, c_{r,j}^{\dagger}\} = \delta_{r,r} \delta_{ij} + \frac{1}{4} \sum_{t} g(t) \delta_{r,r+t}$$

with

$$g(t) = +1$$

$$g(t) = -1$$

and (12) is generally not satisfied unless the second term on the right side of (14) can be ignored. This term vanishes if a constraint is imposed that whenever there is an

\[\text{FIG. 1: (Color online) A schematic hole pair. Fuzzy balls are sites where electron holes form a pair: one hole at } r, \text{ the other with equal probability (1/4) at the four neighboring sites } (r \pm a \text{ and } r \pm b). \text{ Balls connected by bright lines are sites where the presence of a hole would imply double occupancy.}\]
electron pair $c_{r,i}^\dagger c_{r,j}^\dagger$ at $r$ (see Fig. 1), no pair is permitted at $r' = r + t$, leaving nothing to be annihilated by $c_{r,i}$. This is a no-double-occupancy constraint because without it there is a finite amplitude for double site occupancy. For instance, if one pair is at $r' = r + 2a$ and a second pair at $r$, the probability is $\frac{1}{2}$ for two electrons to be located at $r + a$ (see Fig. 1). We conclude that closure of the $SU(4)$ algebra is a direct consequence of no double occupancy in the copper oxide conducting plane.

Additional insight follows from observing that the validity of $[12]$ actually follows from the more general requirement that no pairs overlap, a consistency condition ensuring that the pair space and the pairing correlations be well defined, is sufficient to satisfy $[14]$. The no-pair-overlap constraint implies naturally that if a pair is centered at $r$, no pair may be located at $r' = r + t$ with $t$ given in $[15]$, and thus Eq. $[12]$ holds.

For an $N$-dimensional basis the minimum closed algebra is $SO(2N)$ if all bilinear particle–hole and pair operators are taken as generators. The simplest basis for cuprates may be regarded as 4-dimensional since electrons can exist only in four basic states, on $A$-sites or $B$-sites, with spin up or down. Thus, absent further constraints, the minimum Lie algebra for the set of generators that can describe high $T_c$ superconductivity and antiferromagnetism simultaneously in a cuprate system is $SO(8)$ and not $SU(4)$. The 28 generators of $SO(8)$ are the 16 operators in $[18]$ plus the 12 operators

$$
\begin{align*}
\hat{p}_{12}^\dagger & = \sum_{r \in A} \left( c_{r,i}^\dagger c_{r,j}^\dagger - c_{r,j}^\dagger c_{r,i}^\dagger \right) \\
\hat{q}_{12}^\dagger & = \pm \sum_{r \in A} \left( c_{r,i}^\dagger c_{r,j}^\dagger + c_{r,j}^\dagger c_{r,i}^\dagger \right) \\
\hat{S}_{ij} & = \sum_{r \in A} \left( c_{r,i}^\dagger c_{r,j} - c_{r,j} c_{r,i}^\dagger \right) \\
\hat{Q}_{ij} & = \pm \sum_{r \in A} \left( c_{r,i}^\dagger c_{r,j} + c_{r,j} c_{r,i}^\dagger \right) \\
\hat{p}_{12} & = (\hat{p}_{12}^\dagger)^\dagger, \quad \hat{q}_{12} = (\hat{q}_{12}^\dagger)^\dagger
\end{align*}
$$

(± depends on the even–odd choice for $A$ sites; see $[13]$).

Equation $[16]$ contains two kinds of new (spin-singlet) pairs created by $\hat{p}_{12}^\dagger$ and $\hat{q}_{12}^\dagger$, which may be termed $S$ and $S^*$ pairs, respectively. In both the two electrons (holes) occupy the same site, with equal probability to appear anywhere in the lattice coherently. The $S^*$ pairs differ from $S$ pairs in their phases. The operators $\hat{S}_{ij}$ are the hopping operators with and without spin flip, and $\hat{Q}_{ij}$ is the staggering of the hopping. These operators change $D$ and $p$ pairs into $S$ and $S^*$, or vice versa.

The $SO(8)$ algebra reduces to $SU(4)$ if the $S$ and $S^*$ pairs may be neglected, which occurs if we assume on-site Coulomb repulsion pushing the $S$ and $S^*$ pairs to sufficiently high energy. Thus, restriction to no double occupancy effectively allows the operators in Eq. $[16]$ to be ignored and reduces $SO(8)$ to the subalgebra $SU(4)$.

Therefore, the minimal Lie algebra that can describe antiferromagnetism and $d$-wave superconductivity in a cuprate system is in general $SO(8)$, but under the constraint of no double occupancy the symmetry effectively reduces to $SU(4)$. The assumption of an $SU(4)$ symmetry in a cuprate system automatically implies the imposition of a no-double-occupancy constraint on the general $SO(8)$ symmetry in the copper–oxygen planes.

It is likely that the hopping operator $\hat{S}_{ij}$ in Eq. $[16]$ is the source of the most important $SU(4)$ symmetry breaking terms. It breaks $SU(4)$ but is a generator of $SO(8)$, so this perturbation may be taken into account by an extension from $SU(4)$ to $SO(8)$. However, we may expect the no-double-occupancy rule and thus the $SU(4)$ symmetry to be a good initial approximation.

The implicit $SU(4)$ occupancy constraint dictates an upper limit for the doping fraction in $SU(4)$-conserving states. Fig. 2 illustrates the spatial distribution when the number of hole pairs is maximal. By counting, the maximum number of holes is $\Omega = \Omega_c/4$, where $\Omega_c$ is the total number of lattice sites. Thus the largest doping fraction preserving $SU(4)$ symmetry is $P_f = \Omega_c/(\Omega_c - 1)$. The empirical maximum doping fraction $(0.23 \sim 0.27)$ for cuprate superconductivity may then be interpreted as a direct consequence of $SU(4)$ symmetry.

The preceding discussion implies that: (1) The physical origin of cuprate $SU(4)$ symmetry is proximity of antiferromagnetism and $d$-wave pairing, coupled with suppression of double occupancy by on-site Coulomb repulsion. (2) Two important facts in cuprates, that normal states are Mott insulators and that superconductivity exists only in a narrow doping range ($P < 0.27$), are direct consequences of an $SU(4)$ dynamical symmetry.

Superconductivity in cuprates is a specific example of what we shall term non-abelian superconductivity, which
differs from conventional superconductivity in the richness of pair structure for condensed states and in the appearance of competing sources of long-range order. The key issues for $SU(4)$ non-abelian superconductivity are that coherent pairs are formed by holes on adjacent sites so that both singlet and triplet states contribute, and that alternative long-range order (anti-ferromagnetism) enters on an equal footing with superconductivity.

In contrast to BCS superconductivity, which is described by a single dynamical symmetry chain, having only abelian subgroups ($SU(2) \supset U(1)$), the minimal symmetry consistent with cuprate data is $SU(4)$, which has a much richer structure (three dynamical symmetries having non-abelian subgroups and differing fundamentally in their properties). We propose that the differences in observational characteristics for these two types of superconductivity originate in this difference in dynamical symmetry structure and in non-abelian superconductivity resulting from electron–electron interactions instead of electron–phonon interactions.

The primal role of $SU(4)$ symmetry in non-abelian cuprate superconductivity suggests that any pairing structure leading to the $SU(4)$ algebra entails dynamics similar to that of cuprates. Therefore, $d$-wave symmetry of the pairs need not be critical to non-abelian superconductivity in general and $SU(4)$ superconductivity in particular. Pairs with any internal symmetry (extended $s$-wave, $p$-wave, mixed symmetry, . . .) could exhibit $SU(4)$ superconductivity if the no-double-occupancy constraint is valid and correlations can form adjacent-site pairs. Generally, $c_{r,i}^\dagger c_{r+t,i}^\dagger$ may be defined as

$$c_{r,i}^\dagger = \sum_t g(t) c_{r+t,i}^\dagger, \quad \sum_t |g(t)|^2 = 1 \quad (17)$$

where $t$ is a few finite lattice displacements of $r$ and $g(t)$ is the form factor. Different forms of $g(t)$ reflect different internal symmetries of the pairs, but they all satisfy the condition under no double occupancy and thus preserve the $SU(4)$ algebra and the general Hamiltonians implied by its dynamical symmetry chains. The structure of the $d$-wave pairs is only a special case of (17) with $t = \pm a, \pm b$ and $g(\pm a) = \frac{1}{2}$ and $g(\pm b) = -\frac{1}{2}$.

In summary, we have shown that $SU(4)$ is the minimal symmetry accommodating superconductivity, anti-ferromagnetism, and a no-double-occupancy constraint in cuprate systems, and that $SU(4)$ symmetry implies a maximum doping fraction of $\frac{1}{4}$ in the cuprates, by symmetry alone. Because the Zhang $SO(5)$ algebra is a subalgebra of $SU(4)$, these results indicate that closure of the Zhang algebra also implies no double occupancy. Why then does the $SO(5)$ model require Gutzwiller projection? The work presented here suggests that the projection requirement arises from assumptions inconsistent with the underlying $SO(5)$ algebra in the Zhang effective Lagrangian formulation, where five of the $SU(4)$ generators ($D^I, D, \bar{Q}$) are treated as order parameters forming a superspin vector. Thus one cannot apply algebraic constraints to them through the commutators. This is most easily seen if not only the $SO(5)$ generators but also the elements of the Zhang superspin vector are treated as operators rather than order parameters, thereby enlarging the algebra to $SU(4)$. Within the $SU(4)$ framework, there is no need for projection. As demonstrated in Refs. 6, 7, within the parent $SU(4)$ group anti-ferromagnetism and superconductivity are described by different dynamical symmetries ($SO(4)$ and $SU(2)$, respectively), and $SO(5)$ is a critical dynamical symmetry that interpolates between $SO(4)$ and $SU(2)$. In the $SU(4)$ model it is the $SO(4)$ symmetry, not the $SO(5)$ symmetry, that naturally describes undoped states, and the spectrum for unbroken $SO(4)$ dynamical symmetry is intrinsically anti-ferromagnetic with gapped charge excitations.

Our results imply some important consequences of attributing cuprate superconductor behavior to an $SU(4)$ algebra that follow directly from symmetry, independent of details: (1) Normal states are anti-ferromagnetic Mott insulators. (2) Hole doping of normal compounds leads first to $SO(5)$ fluctuations in both anti-ferromagnetic and superconducting order (implying phases that may exhibit spin glass or stripe character), and then to $SU(4)$ non-abelian superconductivity. (3) $SU(4)$ superconductivity is strongly suppressed for doping fractions exceeding $\frac{1}{4}$. (4) Symmetry breaking resulting from violation of the no-double-occupancy constraint may be described by a parent $SO(8)$ algebra where terms that break $SU(4)$ may still respect $SO(8)$ symmetry. (5) $SU(4)$ symmetry, not $d$-wave pairing per se, is the ultimate cause of cuprate behavior, implying that systems could exist having non-$d$ pairing but cuprate-like dynamics. The first three consequences are postdictions in strong accord with existing data. The fourth is a prediction that may be tested through detailed applications of the $SU(4)$ model to data. The final prediction may be tested by searching experimentally for compounds having pairing structures other than $d_{x^2-y^2}$ that satisfy the $SU(4)$ algebra.

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