An SU(4) Approach to High-Temperature Superconductivity and Antiferromagnetism

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(March 24, 2022)

We present an SU(4) model of high-$T_c$ superconductivity. One dynamical symmetry of this model corresponds to the previously proposed SO(5) model for unification of superconductivity and antiferromagnetism, but there are two additional dynamical symmetries: SO(4), associated with antiferromagnetic order and SU(2), associated with a D-wave pairing condensate. These provide a 3-phase microscopic model of high-$T_c$ superconductivity and permit a clear understanding of the role played by the SO(5) symmetry.

There are strong arguments that the mechanism for high-temperature superconductivity (SC) is not BCS S-wave pairing. The interaction leading to the formation of the singlet pairs appears not to be the traditional lattice phonon mechanism underlying the BCS theory but a collective electronic interaction. The pairing gap has nodes in the $k_x-k_y$ plane suggestive of D-wave hybridization in the 2-particle wavefunctions, and SC in the cuprates seems to be closely related to the antiferromagnetic (AF) insulator properties of their normal states. Furthermore, the formation of Cooper pairs and their condensation in high-$T_c$ states may be distinct, with pair formation at a higher temperature scale than the formation of the SC state. This is reminiscent of grand unified theories in particle physics, where a hierarchy of symmetry breakings is implied by a Lie group structure that is broken spontaneously (and explicitly) on different temperature scales. Such observations argue for a theory that is based on symmetries describing pairing more sophisticated than BCS and that can unify phases such as AF order and SC in the same theory.

Dynamical symmetries having many of these characteristics have been developed extensively in nuclear structure physics. There it has proven fruitful to ask the following questions: what are the relevant low-lying collective degrees of freedom, what are the microscopic operators that create and annihilate these modes, and what is the commutator algebra that they obey? It has been shown that dynamical symmetries having the representation structure described in Ref. 3 are realized to remarkably high accuracy in the spectrum and the wavefunctions of large-scale numerical calculations.

Recently, S. C. Zhang and others have applied related ideas to high-temperature SC. In order to unify AF and SC order parameters, Zhang assembled these into a 5-dimensional vector order parameter and constructed an SO(5) group that rotates AF order into SC order. In this paper we proceed differently by closing a minimal fermion algebra containing D-wave pairs of singlet spin (D-pairs) and triplet spin ($\pi$-pairs), charge, and spin operators. Nevertheless, we shall recover an SO(5) subgroup of a more general U(4) symmetry.

Thus, the recent discussion of Zhang’s SO(5) symmetry applies directly to our results, but we extend this discussion in three ways: (1) The SO(5) subgroup is embedded in a larger fermion algebra that constrains the SO(5) subgroup. (2) The SU(4) highest symmetry has subgroups in addition to SO(5) that may be relevant for AF and SC phases, and that aid in interpreting the SO(5) symmetry. (3) We implement an exact dynamical symmetry using Casimir invariants of group chains and a corresponding collective subspace of low dimensionality.

Let us introduce bilinear fermion generators:

$$p_{12} = \sum_k g(k)c_{k\uparrow}c_{-k\downarrow} \quad p_{12}^* = \sum_k g^*(k)c_{-k\downarrow}c_{k\uparrow}$$

$$q_{ij} = \sum_k g(k)c_{k+Q_i}c_{-k-j} \quad q_{ij} = (q_{ij}^*)^\dagger$$

$$Q_{ij} = \sum_k c_{k+Q_i}c_{k,j} \quad S_{ij} = \sum_k c_{k,i}c_{k,j} - \frac{1}{2}\Omega \delta_{ij}$$

where $c_{k,i}^\dagger$ creates a fermion of momentum $k$ and spin projection $i, j = 1 \text{ or } 2 = \uparrow \text{ or } \downarrow$. $Q = (\pi, \pi, \pi)$ is an AF ordering vector, $\Omega$ is the lattice degeneracy, and $g(k) = \text{sgn}(\cos k_x - \cos k_y)$ with $g(k + Q) = -g(k)$ and $|g(k)| = 1$ (see Refs. 4, 5). The operator set (1) is closed under commutation, generating a U(4) Lie algebra with 3 dynamical symmetry chains:

$$\supset \text{SO}(4) \times \text{U}(1) \supset \text{SU}(2)_\pi \times \text{U}(1)$$

$$\text{U}(4) \supset \text{SU}(4) \supset \text{SO}(5) \supset \text{SU}(2)_\pi \times \text{U}(1)$$

that end in the subgroup $\text{SU}(2)_\pi \times \text{U}(1)$ representing spin and charge conservation. The physical interpretation is aided by rewriting the generators of the U(4) algebra as

$$Q_+ = Q_{11} + Q_{22} = \sum_k (c_{k+Q}^\dagger c_k + c_k^\dagger c_{k+Q})$$

$$\vec{S} = \left( \frac{S_{12} + S_{21}}{2}, -i \frac{S_{12} - S_{21}}{2}, \frac{S_{11} - S_{22}}{2} \right)$$
\[
\hat{Q} = \left( \frac{Q_{12} + Q_{12}}{2}, -i \frac{Q_{12} - Q_{21}}{2}, \frac{Q_{11} - Q_{22}}{2} \right)
\]
\[
\hat{\pi} = \left( \frac{1}{2} (q_{11} + q_{22}), \frac{1}{2} (q_{11} + q_{22}), -\frac{1}{2} (q_{11} + q_{22}) \right)
\]
\[
\tilde{\pi} = (\tilde{\pi})^\dagger \quad D^\dagger = p_{12}^\dagger \quad D = p_{12} \quad M = \frac{1}{2} (n - \Omega)
\]

where \(Q_+\) generates charge density waves, \(\tilde{S}\) is the spin operator, \(\tilde{Q}\) is the staggered magnetization, and \(\tilde{\pi}, \tilde{\pi}^\dagger\) are the triplet D-wave pairs (Ref. [3]), the operators \(D^\dagger, D\) are associated with singlet D-wave pairs, \(n\) is the electron number operator, and \(M\) is the charge phase. As we justify below, \(SU(2)_p\) is associated with superconductivity, \(SO(4)\) with AF order, and \(SO(5)\) with a “spin-glass” phase.

The group \(SU(4)\) has a Casimir operator
\[
C_{su(4)} = \tilde{\pi}^\dagger \cdot \tilde{\pi} + D^\dagger D + \tilde{S} \cdot \tilde{S} + \tilde{\pi} \cdot \tilde{Q} + M (M - 4)
\]
(4)

and the irreps may be labeled by 3 quantum numbers, \((\sigma_1, \sigma_2, \sigma_3)\). We choose a model collective subspace
\[
| \Omega \rangle \equiv | n_d n_d n_d n_d \rangle = (\pi_1 \uparrow)^{n_\uparrow} (\pi_1 \downarrow)^{n_\downarrow} (\pi_2 \uparrow)^{n_\uparrow} (\pi_2 \downarrow)^{n_\downarrow} (D \uparrow)^{n_\uparrow} (D \downarrow)^{n_\downarrow} |0 \rangle
\]
(5)

which is associated with irreps of the form \((\sigma_1, \sigma_2, \sigma_3) = (\Omega, 0, 0)\). The corresponding expectation value of the \(SU(4)\) Casimir is a constant, \(C_{su(4)} = \Omega(\Omega + 4)\).

The full space is of dimension \(2^\Omega\), but the collective subspace is much smaller, scaling as \(\sim \Omega^4\).

\[
\text{Dim} \left( \frac{1}{2}, 0, 0 \right) = \frac{1}{4} \left( \Omega^2 + 1 \right) \left( \Omega^2 + 2 \right)^2 \left( \Omega^2 + 3 \right)
\]
(6)

This corresponds to truncation by a factor \(10^5\) for \(\Omega \sim 100\). For small lattices we may enumerate all states of the collective subspace, yielding a simple model where observables can be calculated analytically.

The charge density wave operator
\[
Q_+ = \sum_k \left( c_{k+Q_1} c_{k-}^\dagger + c_{k+Q_2} c_{k-}^\dagger \right) = \sum_{rj} (-)^r n_{rj}
\]
(7)

(where \(n_{rj}\) is the number operator for electrons on site \(r\) with spin \(j\)) generates the \(U(1)\) factor in \(U(4) \to U(1) \times SU(4)\) and commutes with all generators. Thus \(\langle \Omega | Q_+ | \Omega \rangle = 0 \) and charge-density waves are excluded from the present collective subspace.

An \(SU(4)\) model Hamiltonian can be constructed from a linear combination of Casimir operators for all subgroups: \(H = A_0 + \sum_{Gi} A_{Gi} C_{Gi}\), where \(A_0\) and \(A_{Gi}\) are parameters and the Casimir operators \(C_{Gi}\) are

\[
C_{so(5)} = \tilde{\pi} \cdot \tilde{\pi} + \tilde{S} \cdot \tilde{S}, \quad C_{so(4)} = \tilde{Q} \cdot \tilde{Q} + \tilde{S} \cdot \tilde{S}
\]
\[
C_{su(2)_p} = D^\dagger D + M (M - 1), \quad C_{su(2)_s} = \tilde{S} \cdot \tilde{S}
\]
\[
C_{U(1)} = M^2 \quad \text{and} \quad M^2
\]
(8)

For conserved electron number the terms in \(M\) and \(M^2\) in Eq. [8] are constant. Since \(\langle C_{su(4)} \rangle\) is a constant, by using Eq. [4] we can eliminate the \(\pi^\dagger \cdot \pi\) term and by renormalizing the interaction strengths the \(SU(4)\) Hamiltonian can be written
\[
H = H_0 - G (1 - p) D^\dagger D + p \tilde{Q} \cdot \tilde{Q} + \kappa \tilde{S} \cdot \tilde{S}
\]
(9)

with \((1 - p)G = C_{su(4)}^{(0)}, pG = \chi_{\text{eff}}\) and \(\kappa\) as the effective interaction strengths, and \(0 \leq p \leq 1\). The term \(H_0\) is a quadratic function of \(n\) and may be parameterized as \(H_0 = \epsilon_{\text{eff}} n + \nu_{\text{eff}} n(n - 1)/2\), where \(\epsilon_{\text{eff}}\) and \(\nu_{\text{eff}}\) are the effective single-electron energy and the average two-body interaction in zero-order approximation, respectively.

In the full \(SU(4)\) symmetry, D-wave pairing, antiferromagnetism, and \(\pi\) collective modes enter on an equal footing. The system has formed local \(SU(4)\) pairs, which fixes the length of vectors \([SU(4)\) Casimir] but not their direction. Physically, the system is paired with \(SU(4)\) symmetry but is neither superconducting nor antiferromagnetic since the energy difference in those directions are small on a scale set by the temperature. Neither AF nor SC order parameters have finite expectation values but a sum of their squares \([SU(4)\) Casimir] does.

At this “unification” level, there is no distinction among these degrees of freedom, just as in the Standard Electroweak Theory the electromagnetic and weak interactions are unified above the intermediate vector boson mass. The full symmetry should hold while the temperature of the system is sufficiently high that anisotropic fluctuations in the directions associated with these collective degrees of freedom are negligible, but not so high that thermal fluctuations destroy the local \(SU(4)\) pairs. However, \(SU(4)\) symmetry is broken to its subgroups at lower temperature, leading to 3 dynamical symmetry chains with eigenstates labeled by the length of the \(SU(4)\) vectors, but with orientations no longer isotropic in the full \(SU(4)\) space. These low-temperature degrees of freedom may be interpreted as follows.

The three dynamical symmetry limits \(SU(2), SO(4)\) and \(SO(5)\), correspond to the choices \(p = 0, 1, 1/2\), respectively, in Eq. [9]. The Hamiltonian, eigenfunctions, energy spectrum and the corresponding quantum numbers of these symmetry limits are listed in Table I (where we introduce a doping parameter \(x\) that is related to particle number and lattice degeneracy through \(x = 1 - n/\Omega\)). The pairing gap \(\Delta\) and the staggered magnetization \(Q\),
\[
\Delta = \langle D^\dagger D \rangle^{1/2}, \quad Q = \langle \tilde{Q} \cdot \tilde{Q} \rangle^{1/2},
\]
(10)

may be used to characterize the states in these symmetry limits. As we shall see, each limit represents a different possible low-energy phase of the \(SU(4)\) system.

(1) The dynamical symmetry chain \(SU(4) \supset SU(2)_s \supset SU(2)_p \times SU(2)\) corresponds to SC order and is the \(p = 0\) symmetry limit of Eq. [3]. The seniority quantum number \(v\) is the number of particles that do not form D-pairs. The ground state has \(v = 0\), implying
that all electrons are singlet-paired. In addition, there exists a large pairing gap \( \Delta = \frac{1}{2} \Omega(1 - x^2)^{1/2} \), and \( Q = 0 \). Thus we propose that this state is a D-pair condensate, associated with the SC phase of the cuprates.

(2) The chain \( SU(4) \supset SO(4) \supset SU(2)_s \) corresponds to long-range AF order. This is the symmetry limit of Eq. (9) when \( p = 1 \). The \( SO(4) \) subgroup is locally isomorphic to \( SU(2)_F \times SU(2)_G \) generated by

\[
\vec{F} = \frac{1}{2} (\vec{S} + \vec{Q}), \quad \vec{G} = \frac{1}{2} (\vec{S} - \vec{Q}),
\]

(11)

where \( \vec{F} \) and \( \vec{G} \) are the total spin of electrons at even sites and odd sites, respectively. Therefore, the \( SO(4) \) Casimir operator can be expressed as

\[
C_{so(4)} = 2(\vec{F}^2 + \vec{G}^2).
\]

(12)

The \( SO(4) \) representations can be labeled by the spin-like quantum numbers \( (F = n/2, G = n/2) \) and are of dimension \( (w + 1)^2 \). The ground state corresponds to \( \omega = N \) and \( S = 0 \), and has \( n/2 \) spin-up electrons on the even sites \( (F = N/2) \) and \( n/2 \) electrons on odd sites with spin down \( (G = N/2) \), or vice versa. Thus it has maximal staggered magnetization

\[
Q = \frac{1}{2} \Omega(1 - x) = \frac{1}{2} n
\]

(13)

and a large energy gap due to the correlation energy \( \vec{Q} \vec{Q} \) that inhibits electronic excitation, suggesting magnetic insulator properties at half filling. In addition, the pairing gap \( \Delta = \frac{1}{2} \Omega(x(1-x))^{1/2} \) is small (zero at half filling). Thus we propose that these states are associated with an AF phase of the cuprates.

(3) The dynamical symmetry chain \( SU(4) \supset SO(5) \supset SU(2)_s \times U(1) \) corresponds to a phase with spin-glass character. This symmetry limit appears when \( p = 1/2 \) in Eq. (9) and has unusual behavior. At half filling, \( x = 0 \), the ground state is highly degenerate with respect to the number of \( \pi \)-pairs \( \lambda \), and mixing different numbers of \( \pi \)-pairs costs no energy. The \( \pi \)-pairs must be responsible for the antiferromagnetism in this phase, since only \( \pi \)-pairs carry spins. Thus the ground state in this symmetry limit has large-amplitude fluctuation in the AF order and we propose that this symmetry limit may be associated with a spin-glass phase of the cuprates.

Away from the symmetry limits there are no exact solutions but the ground state properties can be studied easily using the coherent state method. This is discussed in a separate paper, but we quote one result of that study here to reinforce our point concerning the interpretation of the \( SO(5) \) symmetry. In Fig. 1, energy surfaces for the ground states for various particle number \( n \) or doping \( x \) are plotted as a function of a quantity \( \beta \), which is related directly to the AF order parameter (see figure caption). Three plots are associated with the symmetry limits discussed above \( (p = 0, 1, 1/2) \) and one corresponds to a situation with a slight \( SO(5) \) symmetry breaking \( (p = 0.52) \).

The energy minimum lies at \( \beta = 0 \) for all the \( n \)’s (or \( x \)’s) for the \( SU(2) \) (Fig. 1a), and at \( \beta = [(1 - x)/4]^{1/2} \) for the \( SO(4) \) limit (Fig. 1b). In Fig. 1c, there is a broad range of doping in which the \( SO(5) \) energy surface is almost flat in the parameter \( \beta \), implying large excursions in the AF order. Therefore, the \( SO(5) \) symmetry may be interpreted as a phase having much of the character of a spin glass for a range of particle numbers. Notice in Fig. 1d that as doping varies the \( SO(5) \) Hamiltonian with slight symmetry breaking interpolates between AF order at half filling and SC order at smaller filling. Thus \( SO(5) \) acts as a kind of doorway between \( SU(2)_p \) and \( SO(4) \) symmetries and this gives a precise meaning to the assertion that the \( SO(5) \) symmetry rotates the AF and SC order parameters into each other.

Our \( SU(4) \) model and Zhang’s \( SO(5) \) model have the same building blocks [the operator set (3)]. The essential difference is that we implement the full quantum dynamics (commutator algebra) of these operators exactly, while in Ref. [1], the dynamics is implemented in an approximate manner: a subset of 10 of the operators acts as a rotation on the remaining 5 operators \( \{D^1, D, \vec{Q}\} \), which are treated phenomenologically as 5 independent components of a vector.

The embedding of \( SO(5) \) in our larger algebra has various physical consequences that do not appear if the \( SO(5) \) subgroup is considered in isolation. We list three:

(1) A phase transition from AF to SC at zero temperature and controlled by the doping emerges naturally, whereas in the \( SO(5) \) model a symmetry-breaking term proportional to a chemical potential has to be introduced by hand.

(2) The present results suggest that the \( SO(5) \) subgroup is the appropriate description of the underdoped regime, but that the AF phases at half filling and the optimally doped superconductors are more simply described by our \( SO(4) \) and \( SU(2)_p \) symmetries, respectively.

(3) As we shall discuss in a separate paper, the present \( SU(4) \) theory leads naturally to the appearance of a pseudogap in the underdoped region, which occurs above the SC transition temperature \( T_c \) and merges with \( T_c \) near the optimal doping point.

The temperature dependence of the phase diagram requires thermodynamic calculations that are in progress and will be presented separately. However, we may use the preceding discussion to construct the qualitative phase diagram illustrated in Fig. 2. First, \( H_0 \) in the Hamiltonian may be regarded as the energy scale for the \( U(4) \rightarrow U(1) \times SU(4) \) symmetry, representing a fermion system in which electrons are all paired but with no distinction among the D-pairs and \( \pi \)-pairs. We may expect this symmetry to hold while the thermal energy is less than \( H_0 \). When the system is cooled, the pairing and AF correlations \( [H - H_0, \text{see Eq. (3)}] \) become important, \( SU(4) \) breaks to its subgroups, and different low-
temperature phases will appear depending on the competition between $D^\dagger D$ and $\vec{Q} \cdot \vec{Q}$ interactions as a function of doping concentrations. From the preceding discussion, at zero temperature we expect the $SO(4)$ AF phase to dominate at half filling, the $SU(2)_p$ SC phase to be favored at larger doping, and the intermediate doping region to be described naturally by the $SO(5)$ spin-glass phase that interpolates between SC and AF behavior with doping. Thus, $SU(4)$ symmetry implies the schematic phase diagram of Fig. 2, independent of detailed calculations.

In summary, an $SU(4)$ model of High-$T_c$ SC has been proposed that contains three phases: A SC phase identified with the $SU(2)_p$ dynamical symmetry, an AF phase identified with the $SO(4)$ dynamical symmetry, and an $SO(5)$ phase extremely soft against AF fluctuations over a substantial doping fraction that we term (loosely) a spin-glass phase. Realistic systems may mix these sub-symmetries while retaining an approximate $SU(4)$ symmetry. Zero-temperature phase transitions are shown to be driven by the competition between the D-wave pairing and the staggered magnetization $\vec{Q}$, as controlled microscopically by the hole-doping concentration. As we shall discuss in detail separately, this model leads naturally to the appearance of pseudogaps in the underdoped regime. Thus, we propose that high $T_c$ behavior of the cuprates results from a $U(4)$ symmetry realized dynamically, and because this symmetry is microscopic its physical interpretation is accessible to calculation. This provides a possible understanding of the cuprate phase diagram and substantial insight concerning recent $SO(5)$ theories of D-wave superconductivity.

We thank Eugene Demler, Pengcheng Dai, and Ted Barnes for useful discussions. L. A. Wu was supported in part by the National Natural Science Foundation of China. C.-L. Wu is supported by the National Science Council of ROC.

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FIG. 1. Coherent state energy surfaces for Eq. (9). The staggered magnetization $Q$ is related to $\beta$ by $\langle Q \rangle = 2\Omega \beta_0 (n/2\Omega - \beta_0^2)^{1/2}$, where $\beta_0$ is the value of $\beta$ at the stable point, so $\beta$ measures the AF order.

FIG. 2. Schematic phase diagram for $U(4)$ symmetry based on Fig. 1d. The $H_0$ in Eq. (9) is expressed in terms of hole doping $x$ with $x = 1 - n/\Omega$; $\epsilon_{eff} = \epsilon_{eff} \Omega$, and $\nu_{eff} = \nu_{eff} \Omega^2/2$. 
| Limit | State | Hamiltonian | Ground State Energy | Excitation Energy | Pair Number | Pair Number | Pair Number | Pair Number |
|-------|-------|-------------|---------------------|------------------|-------------|-------------|-------------|-------------|
| SU(2) | $|\psi_{SU(2)}\rangle$ | $H = H_0 + \kappa_{\text{eff}} \vec{S} \cdot \vec{S}$ | $E_{\text{g.s.}} = H_0$ | $\Delta E = \nu \kappa_{\text{eff}} \Omega + \kappa_{\text{so4}} S(S+1)$ | $N = n/2$ | $x = 1 - n/\Omega$ | $\kappa_{\text{so4}} = \kappa_{\text{eff}} + \chi_{\text{eff}}$ | - |
| SO(4) | $|\psi_{SO(4)}\rangle = |N,v,S,m_S\rangle$ | $H = H_0 + \kappa_{\text{eff}} \vec{S} \cdot \vec{S}$ | $E_{\text{g.s.}} = H_0 - \frac{1}{4} \kappa_{\text{so4}} \Omega^2 (1 - x^2)$ | $\Delta E = \mu \chi_{\text{eff}} (1 - x) \Omega + \kappa_{\text{so4}} S(S+1)$ | $w = N - \mu$ | - | - |
| SO(5) | $|\psi_{SO(5)}\rangle = |\tau,S,m_S\rangle$ | $H = H_0 + \kappa_{\text{eff}} \vec{S} \cdot \vec{S}$ | $E_{\text{g.s.}} = H_0 - \frac{1}{4} \chi_{\text{eff}} \Omega^2 (1 - x^2)$ | $\Delta E = \lambda \chi_{\text{eff}} (1 - x) \Omega + \kappa_{\text{so4}} S(S+1)$ | $\Omega/2 - \tau = N - \lambda$ | $\lambda$ | $\lambda$ | - |
Energy vs. AF Order ($\beta$)

(a) $p = 0$
SU(2)

(b) $p = 1$
SO(4)

(c) $p = 0.5$
SO(5)

(d) $p = 0.52$
SO(5)

$n/W = 1.0$
\[ H_0 = \epsilon_{\text{eff}} (1-x)_{\text{eff}} V (\xi X) \]

\[ H = e^{(1-x)_{\text{eff}} V (\xi X)} + v (1-x)_{\text{eff}}^{2} \]