The SO(5) Theory as a Critical Dynamical Symmetry

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We use generalized coherent states to analyze the SO(5) theory of high-temperature superconductivity and antiferromagnetism. We demonstrate that the SO(5) symmetry can be embedded in a larger algebra that allows it to be interpreted as a critical dynamical symmetry interpolating between antiferromagnetic and superconducting phases. This dynamical interpretation suggests that SO(5) defines a phase with the character of a spin-glass for a significant range of doping.

Data for cuprate high-temperature superconductivity (SC) suggests D-wave singlet pairing and that SC in these systems is closely related to the antiferromagnetic (AF) insulator properties of the undoped compounds. Zhang et al (1) proposed to unify AF and SC states by assembling their order parameters into a 5-dimensional vector and constructing an SO(5) group that rotates AF order into D-wave SC order. Recently (2), we introduced a U(4) model of high-temperature SC and AF order having SO(5) as a subgroup. In this paper we use coherent states (1) to analyze this subgroup and provide a dynamical interpretation of SO(5) and the order parameters that it rotates. The resulting energy surfaces suggest that SO(5) is a critical dynamical symmetry interpolating between AF and SC phases that is extremely soft against AF fluctuations. Thus, we shall propose that the Zhang SO(5) theory corresponds to a spin-glass phase that can serve as a doorway between AF and SC order.

Gilmore (3) and Perelomov (4) (see also earlier work by Klauder (5)), demonstrated that Glauber coherent states (1) for the electromagnetic field could be generalized to coherent states for an arbitrary Lie group. These states can be analyzed in terms of their geometry, which is in one-to-one correspondence with the coset space. However, it is often simpler to view them as Hartree–Fock–Bogoliubov (HFB) variational states constrained by the dynamical symmetry. The symmetry-constrained HFB coherent state method is discussed in Refs. (1) (6) (7) (8). It may be viewed as a type of mean-field approximation to the underlying many-body problem that is particularly useful in the present context because it leads to easily visualized energy surfaces. This provides a natural connection to spontaneously broken symmetries and effective Lagrangian field theories.

Let us begin with a group structure. We introduce 16 bilinear fermion operators:

\[ p_{ij} = \sum_k g(k)c_{k \uparrow}^\dagger c_{k \downarrow} \]
\[ q_{ij} = \sum_k g(k)c_{k \uparrow}^\dagger c_{k \downarrow} + c_{k \downarrow}^\dagger c_{k \uparrow} \]

where \( c_{k \uparrow}^\dagger \) creates a fermion of momentum \( k \) and spin projection \( i \), \( j = 1 \) or \( 2 \) = \( \uparrow \) or \( \downarrow \), \( Q = (\pi, \pi, \pi) \) is an AF ordering vector, \( \Omega \) is the lattice degeneracy, and following Refs. (2) (3) we define \( g(k) = \text{sgn}(\cos k_x - \cos k_y) \) with \( g(k + Q) = -g(k) \) and \( |g(k)| = 1 \).

Under commutation the operator set (1) closes a U(4) algebra corresponding to the group structure

\[ \supset \text{SO}(4) \times \text{U}(1) \supset \text{SU}(2)_x \times \text{U}(1) \]

\[ U(4) \supset \text{SU}(4) \supset \text{SO}(5) \supset \text{SU}(2)_x \times \text{U}(1) \]

where we require subgroup chains to end in \( \text{SU}(2)_x \times \text{U}(1) \) representing spin and charge conservation. In Ref. (1) we discuss the representation structure of (2) and show that the SO(4) subgroup is associated with AF and the SU(2)_p subgroup with D-wave SC; in this paper, we justify interpreting the SO(5) subgroup as a critical dynamical symmetry leading to a “spin glass” phase (SG).

It is convenient to take as the generators of U(4) \( \rightarrow U(1) \times SU(4) \) the combinations

\[ Q_+ = Q_{11} + Q_{22} = \sum_k (c_{k \uparrow}^\dagger c_{k \uparrow} + c_{k \uparrow}^\dagger c_{k \downarrow}) \]
\[ \bar{S} = \left( \frac{S_{12} + S_{21}}{2}, -i \frac{S_{12} - S_{21}}{2}, \frac{S_{11} - S_{22}}{2} \right) \]
\[ \bar{Q} = \left( \frac{Q_{12} + Q_{21}}{2}, -i \frac{Q_{12} - Q_{21}}{2}, \frac{Q_{11} - Q_{22}}{2} \right) \]
\[ \pi = \left( \frac{i q_{11} - q_{22}}{2}, \frac{q_{11} + q_{22}}{2}, -i \frac{q_{12} + q_{21}}{2} \right) \]
\[ \bar{\pi} = (\pi^\dagger) \]

where \( Q_+ \) generates the U(1) factor and is associated with charge density waves, \( \bar{S} \) is the spin operator, \( \bar{Q} \) is the staggered magnetization, the operators \( \pi, \bar{\pi} \) are those of Ref. (1), the operators \( \pi^\dagger, D \) are associated with D-wave pairs, and \( M = \frac{1}{2}(n - \Omega) \) is the charge operator.
To facilitate comparison with the \(SO(5)\) symmetry the \(SO(6) \sim SU(4)\) generators may be expressed as

\[
L_{ab} = \begin{pmatrix}
0 & 0 & \pi x_+ & \pi y_+ & \pi z_+ & iD_-
\end{pmatrix}
\begin{pmatrix}
D_+ & 0 & -Q_x & -Q_y & -Q_z & S_x
\end{pmatrix} = \begin{pmatrix}
0 & -Q_x & -Q_y & -Q_z & S_x & 0
\end{pmatrix}
\]

(4)

\[
D_\pm = \frac{1}{2}(D \pm D^\dagger) \quad \pi_{i\pm} = \frac{1}{2}(\pi_i \pm \pi_i^\dagger)
\]

(5)

with \(L_{ab} = -L_{ba}\) and with commutation relations

\[
[L_{ab},L_{cd}] = i(\delta_{ac}L_{bd} - \delta_{ad}L_{bc} - \delta_{bc}L_{ad} + \delta_{bd}L_{ac}).
\]

(6)

The coherent state method requires a faithful matrix representation of \(SU(4)\). Explicit multiplication verifies that the following mapping preserves the algebra of \([\mathfrak{g}]:\)

\[
p_{12} \mapsto \begin{pmatrix}
0 & i\sigma_y \\
0 & 0
\end{pmatrix}, \quad q_{12} \mapsto \begin{pmatrix}
0 & \sigma_x \\
0 & 0
\end{pmatrix}, \quad q_{11} \mapsto \begin{pmatrix}
0 & I + \sigma_z \\
0 & 0
\end{pmatrix}, \quad q_{22} \mapsto \begin{pmatrix}
0 & I - \sigma_z \\
0 & 0
\end{pmatrix},
\]

\[
S_{12} \mapsto \begin{pmatrix}
\sigma_+ & 0 \\
0 & -\sigma_-
\end{pmatrix}, \quad S_{21} \mapsto \begin{pmatrix}
\sigma_- & 0 \\
0 & -\sigma_+
\end{pmatrix},
\]

\[
Q_{11} \mapsto \begin{pmatrix}
\sigma_+ & 0 \\
0 & \sigma_-
\end{pmatrix}, \quad Q_{12} \mapsto \begin{pmatrix}
\sigma_- & 0 \\
0 & \sigma_+
\end{pmatrix},
\]

\[
Q_{21} \mapsto \begin{pmatrix}
0 & -I \\
0 & 0
\end{pmatrix}, \quad N - \Omega = S_{11} + S_{22} \mapsto \begin{pmatrix}
0 & 0 \\
0 & 0
\end{pmatrix}
\]

(7)

where \(\sigma_i\) are Pauli matrices, \(\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)\) and \(I\) is a unit matrix. The Casimir operator of \(SU(4) \simeq SO(6)\) is

\[
C_{su(4)} = \pi_{1\dagger}\pi + D_{1\dagger}D + \tilde{S}_{1\dagger}\tilde{S} + \tilde{Q}_{1\dagger}\tilde{Q} + M(M - 4)
\]

(8)

and the irreps may be labeled by the \(SO(6)\) quantum numbers, \((\sigma_1, \sigma_2, \sigma_3)\). We take as a Hilbert space

\[
|S\rangle = |n_x n_y n_z n_d\rangle = (\pi_{1\dagger})^{n_x} (\pi_{y\dagger})^{n_y} (\pi_{z\dagger})^{n_z} (D_{1\dagger})^{n_d}|0\rangle
\]

(9)

which is a collective subspace associated with \(SO(6)\) irreps of the form \((\sigma_1, \sigma_2, \sigma_3) = (\frac{M}{2}, 0, 0)\).

Utilizing the methods of Ref. [13], the coset space is \(SU(4)/SO(4) \times U(1)\), where the \(SO(4)\) subgroup is generated by \(\tilde{Q}\) and \(\tilde{S}\) and \(U(1)\) is generated by the charge operator \(M\). The coherent state may be written as

\[
|\psi\rangle = \exp(\eta_{00}p_{1d}^\dagger + \eta_{10}q_{12}^\dagger - h. c.) |0\rangle \equiv T |0\rangle
\]

(10)

where the real parameters \(\eta_{00}\) and \(\eta_{10}\) are symmetry-constrained variational parameters. Since they weight the elementary excitation operators \(p_{12}\) and \(q_{12}\) in Eq. (11), they represent collective state parameters for a subspace truncated under the \(SU(4)\) symmetry. The most general coherent state corresponds to a 4-dimensional, complex, compact manifold parameterized by 8 real variables. The reduction of the coherent state parameters to only two in Eq. (11) follows from requiring spin and time reversal symmetries for the most general wavefunction.

From the coset representation expressed in the 4-dimensional matrix representation \([\mathfrak{g}]\), the transformation \(T\) can be written as

\[
T = \begin{pmatrix}
Y_1 & X \\
-\bar{X}^\dagger & Y_2
\end{pmatrix}, \quad X \equiv \begin{pmatrix}
0 & \alpha + \beta \\
-(\alpha - \beta) & 0
\end{pmatrix}
\]

(11)

where \(Y_1\) and \(Y_2\) are determined by the requirement that \(T\) be unitary and \(\alpha\) and \(\beta\) are variational parameters related to \(\eta_{00}\) and \(\eta_{10}\) in Eq. (10) (see Ref. [13]). Introducing \(v_+ \equiv \alpha + \beta\) and \(v_- \equiv \alpha - \beta\), and \(n_+ = (1 - v_+)^{1/2}\) and \(n_- = (1 - v_-)^{1/2}\), the matrices can be written as:

\[
X = \begin{pmatrix}
0 & v_+ \\
-v_- & 0
\end{pmatrix}, \quad Y_1 = \begin{pmatrix}
u_+ & 0 \\
0 & u_-
\end{pmatrix}, \quad Y_2 = \begin{pmatrix}
u_- & 0 \\
0 & u_+
\end{pmatrix}
\]

We may also introduce the gap parameters \(\Delta_+ \equiv u_+v_+\) and \(\Delta_- \equiv u_-v_-\).

One can regard Eq. (10) as a Bogoliubov type transformation, which, through the operator \(T\), transforms the bare vacuum state \(|0\rangle\) to a quasiparticle vacuum state \(|\psi\rangle\). Likewise, the basic fermion operators \(c^\dagger, c\) can be transformed to quasifermion operators \(a^\dagger, a\) through

\[
T \begin{pmatrix}
c \\
[c^\dagger]
\end{pmatrix} T^{-1} \rightarrow \begin{pmatrix}
a \\
a^\dagger
\end{pmatrix}
\]

(12)

Using the transformation \([\mathfrak{g}]\), one can express any one-body operator in the quasiparticle space \([\mathfrak{g}^\prime]\). In this way, many results known in HFB theory can be applied directly in the present case. Generally,

\[
\hat{O} = \sum_{i,j} O^{(22)}_{i,j} a_i a_j + \sum_{i,j} [O^{(11)}_{i,j} - O^{(22)}_{i,j}] a_i^\dagger a_j + O^{(12)}_{i,j} a_i a_j + O^{(21)}_{i,j} a_i^\dagger a_j,
\]

(13)

with the \(O^{\prime}\)s determined by the transformation properties of the operator \(\hat{O}\) (see Appendix E of Ref. [13]).

The expectation value for an operator \(\hat{O}\) in the coherent state representation is given by \(\langle \hat{O} \rangle = \text{Tr}(\hat{O}^{(22)})\) and for a 2-body operator \(\hat{O}^{(2)}\),

\[
\langle \hat{O}^{(2)} \rangle = \text{Tr}(\hat{O}^{(12)}) \text{Tr}(\hat{O}^{(22)}) + \text{Tr}(\hat{O}^{(11)} \hat{O}^{(22)}) + \text{Tr}(\hat{O}^{(22)} \hat{O}^{(11)}).
\]

(14)

Utilizing \([\mathfrak{g}]\) and \([\mathfrak{g}^\prime]\), the expectation value of the particle number in the coherent state is

\[
n \equiv \langle \hat{N} \rangle = 2\Omega(\alpha^2 + \beta^2) = \Omega(v_+^2 + v_-^2).
\]

(15)
From Eq. (13), the squares of $\alpha$ and $\beta$ are constrained by the equation of a circle having radius $\sqrt{n/2\Omega}$. Thus, for fixed particle number $n$ we may evaluate matrix elements in terms of a single variational parameter, say $\beta$, which may be related to standard order parameters by comparing matrix elements. For example, the $z$ component of the staggered magnetization is given by

$$\langle Q_z \rangle = 2\Omega\beta(n/2\Omega) - \beta^2)^{1/2} = \frac{1}{2}\Omega(v_+^2 - v_-^2).$$  \hspace{1cm} (16)$$

Let us consider a simple $SO(5)$ Hamiltonian given by $H_5 \sim C_{so(5)}$ where the Casimir for $SO(5)$ is

$$C_{so(5)} = \#^i : \pi + S \cdot S + M(M - 3).$$  \hspace{1cm} (17)$$

We evaluate the $SO(5)$ ground-state energy surface by taking the expectation value of $H_5$ in the coherent state $|\Omega\rangle$. The expectation value of the $SO(5)$ Casimir operator may be written as [see Eq. (8)]

$$\langle C_5 \rangle = \langle C_{su(4)} \rangle - \langle D^1 D \rangle - \langle \vec{Q} \cdot \vec{Q} \rangle + (n - \Omega)/2$$  \hspace{1cm} (18)$$

where $\langle C_{su(4)} \rangle = \frac{\Omega(\Omega + 4)}{2}$. From (11), (12), and (14),

$$\langle D^1 D \rangle = \frac{1}{2}\Omega^2(\Delta_+ + \Delta_-)^2 + \frac{1}{2}\Omega(v_+^4 + v_-^4),$$  \hspace{1cm} (19)$$

$$\langle \vec{Q} \cdot \vec{Q} \rangle = \frac{1}{2}\Omega^2(v_+^2 - v_-^2)^2 + \frac{1}{2}\Omega(\Delta_+^2 + \Delta_-^2 + (u_+v_- - u_-v_+)^2),$$  \hspace{1cm} (20)$$

and the energy surface follows from Eqs. (17)–(20).

Eq. (13) is an expectation value of a Hamiltonian that can be parameterized more generally as

$$H = -G_0(1 - p)D^1 D + p\vec{Q} \cdot \vec{Q},$$  \hspace{1cm} (21)$$

with $G_0 > 0$ and $0 \leq p \leq 1$. Then $p = \frac{1}{2}$ corresponds to $SO(5)$ symmetry, while the extreme values 0 and 1 correspond to $SU(2)$ and $SO(4)$ symmetries, respectively (see Ref. [8]). Other values of $p$ respect $SU(4)$ symmetry but break the $SO(5)$, $SO(4)$, and $SU(2)$ subgroups. In Fig. 1 we illustrate the classical ground-state energy $\langle H \rangle$ as a function of the order parameter $\beta$ for different lattice occupation fractions with $p = 0, \frac{1}{2}$ and 1.

For $p = 0$ [$SU(2)$ limit], the minimum energy occurs at $\langle \beta \rangle = 0$ for all values of $n$, indicating SC order. For $p = 1$ [$SO(4)$ limit], the opposite situation occurs: $\langle \beta \rangle = 0$ is an unstable point and an infinitesimal fluctuation will drive the system to the energy minima at finite $\langle \beta \rangle$ (and thus finite $\langle Q_z \rangle$), causing a transition to AF order. From Fig. 1b, the $SO(5)$ dynamical symmetry is seen to have extremely interesting behavior: For $n$ near $\Omega$ (half filling), the system has an energy surface almost flat for broad ranges of $\beta$, corresponding to large-amplitude fluctuations in AF order. We conclude that the $SO(5)$ symmetry represents a phase having much of the character of a spin glass for a range of doping fractions.

Under exact $SO(5)$ symmetry, AF and SC states are degenerate at half filling and there is no classical barrier between them (the $n/\Omega = 1$ curve of Fig. 1b). To see clearly how the $SO(5)$ interpolates between AF and SC states as particle number varies, let us perturb slightly away from the $SO(5)$ limit of $p = 1/2$. In Fig. 2a, results for $p = 0.52$ are shown. We denote the value of $\langle \beta \rangle$ minimizing $\langle H \rangle$ as $\langle \beta \rangle_0$. For small values of $n$ the stable point is $\langle \beta \rangle_0 = 0$. This corresponds to SC order. If $n$ is near $\Omega$ (half filling), $\langle \beta \rangle_0 \simeq \pm 0.5$; this corresponds to AF order. For intermediate values of $n$ there is a substantial region in which the system has an energy surface almost flat for broad ranges of $\langle \beta \rangle$, implying the presence of large-amplitude fluctuations in AF order. The corresponding variation of the AF order parameter $\langle Q_z \rangle$ with $n$ for several values of $p$ is summarized in Fig. 2b.

Thus, as particle number varies the $SO(5)$ symmetry, or slightly perturbed $SO(5)$ symmetry, interpolates between AF order at half filling and SC order at smaller filling, with the intermediate regime acting like a spin glass. Because for exact $SO(5)$ symmetry there is no barrier at half filling between AF and SC states, one can fluctuate into the other at zero cost in energy. Only when $SO(5)$ is broken does the energy surface interpolate between AF and SC order as doping is varied (compare the surfaces for $p = 1/2$ and $p = 0.52$). From Ref. [11] and the present paper we conclude that the underdoped portion of the cuprate phase diagram is described by a Hamiltonian that conserves $SU(4)$ but breaks (explicitly and weakly) $SO(5)$ symmetry in a direction favoring AF order over SC order. Thus, we propose that the underdoped regime is associated with a conserved $SU(4)$ but weakly broken $SO(5)$ symmetry. Likewise, optimally doped superconductors and AF insulators are associated with the symmetries $SU(4) \supset SU(2)$ and $SU(4) \supset SO(4)$ respectively, or small perturbations around them.

Dynamical symmetries that interpolate between other dynamical symmetries have been termed critical dynamical symmetries [11]. Thus, $SO(5)$ is a critical dynamical symmetry. Such symmetries are well known in nuclear structure [18,24,34], and the $SO(5)$ critical dynamical symmetry discussed here has many formal similarities with the $SO(7)$ critical dynamical symmetry of the (nuclear) Fermion Dynamical Symmetry Model [18]. The condition for realization of the $SO(5)$ phase is that the strength of $Q \cdot Q$ equals that of $D^1 D$ in the Hamiltonian; This is similar to the $SO(7)$ nuclear critical dynamical symmetry, which is realized when there is an overall $SO(8)$ symmetry and the pairing and quadrupole interaction terms are equal in the Hamiltonian [34].

Finally, let us revisit a critical conclusion of Ref. [4] in light of the present discussion. In the $SU(4)$ model, the $SO(5)$ subgroup defines only one possible dynamical symmetry. The AF phase near half filling and the SC phase near optimal doping of the $SU(4)$ model are associated, not with the $SO(5)$ subgroup, but with $SU(2)$ and $SO(4)$ subgroups, respectively. The $SO(5)$ subgroup (identical to the Zhang $SO(5)$ but embedded in a larger
group structure) defines a phase interpolating between the SU(2) and SO(4) phases and characterized by large AF and SC fluctuations. Thus, in the SU(4) model the relationship of the AF phase near half filling and the SC phase near optimal doping is not constrained by the SO(5) subgroup, and SO(5) should be viewed as the appropriate symmetry for the underdoped compounds.

To conclude, we have proposed separately that high \( T_c \) behavior of the cuprates results from a \( U(4) \) symmetry realized dynamically in terms of 3 subgroup chains. One of those subgroups is the SO(5) subgroup discussed extensively by S. C. Zhang [1]. In this paper, we have used SU(4) coherent states to analyze the SO(5) energy surface. We interpret the Zhang SO(5) as a critical dynamical symmetry that interpolates between AF and D-wave SC order as doping is varied, and have noted similarities with analogous critical dynamical symmetries from nuclear structure physics. This permits the SO(5) symmetry to be understood dynamically as a critical phase that for a range of doping has an energy surface extremely soft against AF fluctuations and therefore having much of the character of a spin glass. Thus, we propose that slightly broken SO(5) is the symmetry of the underdoped regime, but that AF and optimally doped SC compounds are described by different subgroups of SU(4).

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Energy

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

(b) $p=1/2$
SO(5)

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