Exact Realization of SO(5) Symmetry in Extended Hubbard Models

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Zhang recently conjectured an approximate SO(5) symmetry relating antiferromagnetic and superconducting states in high-T_c cuprates. Here, an exact SO(5) symmetry is implemented in a generalized Hubbard model (with long-range interactions) on a lattice. The possible relation to a more realistic extended Hubbard Hamiltonian is discussed. [S0031-9007(98)05904-3]

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S. C. Zhang [1,2] recently conjectured that high-T_c cuprate compounds possess an approximate SO(5) symmetry. His theory aims to explain the proximity of superconducting (SC) and antiferromagnetic (AF) phases in the phase diagram, and to account for the low-energy excitations as approximate SO(5) Goldstone modes. Antiferromagnetism and superconductivity are unified in one grand order parameter field $(m^x, m^y, m^z, \mathrm{Re}\,\Psi, \mathrm{Im}\,\Psi)$, behaving as a five-component vector, where the first three elements are Cartesian components of the staggered magnetization and Ψ is a spin-singlet SC order parameter. (Here "$\mathrm{Re}\,\Psi$" $\equiv \frac{1}{2}(\Psi + \Psi^\dagger)$, etc.) In this picture, small symmetry-breaking terms drive the system in a "superspin flop" between antiferromagnetism and superconductivity, just as, in a magnet with approximate SO(3) symmetry, competing spin-space anisotropies and external field can drive a "spin-flop" transition between magnetic order along the z axis and in the xy plane [1].

The SO(5) theory, while positing an intimate relationship between SC and AF order, does not imply that the pairing mechanism is AF fluctuations [3,4]. Rather, it quantifies the notion (also relevant to superfluid ^{3}He) that there need not be a sharp difference between interactions mediated by magnetic and "charge" (number) fluctuations. I pass over Zhang's specific mechanism (whereby the system accommodates doping by switching from the AF state to a symmetry-related SC state which has a different particle number), for SO(5) symmetry can be valid even if another sort of perturbation is found responsible for the symmetry breaking and the AF-SC transition.

The 41 meV mode observed in spin-flip neutron scattering on $YBa_2Cu_3O_7$ [5] is interpreted as a Goldstone mode of SO(5) with a gap due to the symmetry-violating terms, analogous to the anisotropy gap in a spin-wave branch of the unixial magnet [1]. These excitations are created by "$\hat{\pi}^\dagger$" operators [6] [SO(5) generators that mix magnetic and SC components] [7]. They are charged bosons with the quantum numbers of "preformed" Cooper pairs, and presumably carry the current in the "normal" metal [1]; it has been speculated [9] that this explains the linear temperature dependence of the normal-state resistivity.

To the extent that SO(5)-violating terms are small (as in Zhang's phase diagram "A" [1]), relations between AF and SC quantities are obviously predicted. For example, the Néel temperature T_N on one side should equal the SC T_c on the other side (the real ratio is 5:1 in $YBa_2Cu_3O_7$). Furthermore, when converted into the proper units, the tensors of superfluid density and AF spin stiffness should be equal, as should the order-parameter lengths (staggered moment and SC gap magnitude, respectively) and the interlayer couplings (interlayer superexchange and intrinsic Josephson coupling, respectively. An order-of-magnitude equality of the interlayer couplings is indeed expected in the interlayer tunneling picture [10]. Finally, the SO(5) Ginzburg-Landau theory predicts that vortices have magnetic cores [1,11]; conversely, in analogy to the Bloch wall in the SO(3) magnet, it suggests that magnetic domain walls contain SC stripes, as proposed for other reasons by Emery and Kivelson [12].

Microscopic SO(5) symmetry.—In this paper, using elementary notations, I implement a literal SO(5) symmetry in a one-band lattice model, construct a Hamiltonian with exact SO(5) symmetry, and finally consider whether a realistic Hamiltonian of an extended Hubbard form might approximate an SO(5) symmetric Hamiltonian. Take a lattice with N sites (using periodic boundary conditions). Creation operators for the orbitals on site $\mathbf{x}$ are $c^\dagger_\sigma(\mathbf{x})$ for $\sigma = \uparrow, \downarrow$. Let $\mathbf{Q}$ be the ordering wave vector of some two-sublattice AF state, so that $e^{i\mathbf{Q}\cdot\mathbf{x}} = \pm 1$ at every site. The usual staggered-magnetization components are

$$m_z^{(c)}(\mathbf{x}) \equiv \frac{1}{2} e^{i\mathbf{Q}\cdot\mathbf{x}}[c^\dagger_\uparrow(\mathbf{x})c_\uparrow(\mathbf{x}) - c^\dagger_\downarrow(\mathbf{x})c_\downarrow(\mathbf{x})],$$
$$m_+^{(c)}(\mathbf{x}) \equiv e^{i\mathbf{Q}\cdot\mathbf{x}}[c^\dagger_\uparrow(\mathbf{x})c_\downarrow(\mathbf{x})], \quad (1)$$

and $m_-^{(c)}(\mathbf{x}) \equiv m_+^{(c)}(\mathbf{x})^\dagger$. The SC order parameter operator has the general form $\Psi(\mathbf{x}) = \sum_{\mathbf{r},\mathbf{r}'} \psi(\mathbf{r},\mathbf{r}')c_\downarrow(\mathbf{x}+\mathbf{r})c_\uparrow(\mathbf{x}+\mathbf{r}')$ [which allows different spatial symmetries depending on the form of the coefficients $\psi(\mathbf{r},\mathbf{r}')$]. We seek a continuous, unitary operation that turns a component of $\mathbf{m}(\mathbf{x})$ into one of $\Psi(\mathbf{x})$, i.e., turns creation into annihilation operators: Clearly, it must be some form of Bogoliubov transformation.

Indeed, a *discrete* SO(3) symmetry of this sort is already known for the negative-U Hubbard

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model [13], for which the appropriate SC order parameter is $\Psi(\mathbf{x}) = c_\downarrow(\mathbf{x})c_\uparrow(\mathbf{x})$. One maps $c_\downarrow(\mathbf{x}) \to e^{i\mathbf{Q}\cdot\mathbf{x}}c_\downarrow(\mathbf{x})^\dagger$ [leaving $c_\uparrow(\mathbf{x})$ alone] which implies $[\Psi(\mathbf{x})^\dagger, \Psi(\mathbf{x}), e^{i\mathbf{Q}\cdot\mathbf{x}}n(\mathbf{x})] \to [m_+(\mathbf{x}), m_-(\mathbf{x}), m_z(\mathbf{x})]$; here $n(\mathbf{x}) \equiv c^\dagger_\uparrow(\mathbf{x})c_\uparrow(\mathbf{x}) + c^\dagger_\downarrow(\mathbf{x})c_\downarrow(\mathbf{x})$. The only change induced in the Hubbard Hamiltonian is $U \to -U$; thus a hidden SO(3) symmetry relates SC order (Ψ) and charge-density-wave order $[e^{i\mathbf{Q}\cdot\mathbf{x}}n(\mathbf{x})]$ in the limit of large negative U.

To write the exact SO(5) symmetry transparently, and to ensure it in the order parameters and Hamiltonians, I use the duality [14] between the "c" operators and an alternate set of canonically commuting operators,

$$d_{\mathbf{k}+\mathbf{Q},\sigma} \equiv \eta_\mathbf{k} c_{\mathbf{k}\sigma} \tag{2}$$

(with $|\eta_\mathbf{k}| \equiv 1$). In real space, Eq. (2) states

$$d_\sigma(\mathbf{x}) = e^{-i\mathbf{Q}\cdot\mathbf{x}} \sum_\mathbf{r} \varphi(\mathbf{r}) c_\sigma(\mathbf{x} + \mathbf{r}), \tag{3}$$

where $\eta_\mathbf{k} \equiv \sum_\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}}\varphi(\mathbf{r})$. To make the symmetry (5b) work, we will need the important condition

$$\eta_{\mathbf{k}+\mathbf{Q}} = -\eta_\mathbf{k} \tag{4}$$

for all $\mathbf{k}$, which in real space states that $\varphi(\mathbf{r}) = 0$ for "even" $\mathbf{r}$ (vectors connecting sites in the same sublattice). Equation (4) implies $\{c^\dagger_\sigma(\mathbf{x}), d_{\sigma'}(\mathbf{x}')\} = 0$ if $\mathbf{x}$ and $\mathbf{x}'$ are on the same sublattice (e.g., $\mathbf{x} = \mathbf{x}'$) [15].

Then the proposed symmetry operation is just

$$c'_\sigma(\mathbf{x}) = \cos(\theta/2)c_\sigma(\mathbf{x}) + \sin(\theta/2)d^\dagger_{-\sigma}(\mathbf{x}), \tag{5a}$$

$$d'_\sigma(\mathbf{x}) = -\sin(\theta/2)c^\dagger_{-\sigma}(\mathbf{x}) + \cos(\theta/2)d_\sigma(\mathbf{x}). \tag{5b}$$

The symmetry (5b) is generated by $\frac{1}{2}(\hat\pi + \hat\pi^\dagger)$, where $\hat\pi = i\sum_\mathbf{x}[c_\downarrow(\mathbf{x})d_\uparrow(\mathbf{x}) - d_\downarrow(\mathbf{x})c_\uparrow(\mathbf{x})]$. To transform wave functions, it is useful to know that the vacuum $|0\rangle$ transforms to $\prod_\mathbf{k}[\cos(\theta/2) + \eta_\mathbf{k}\sin(\theta/2)c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}+\mathbf{Q},\downarrow}]|0\rangle$.

So that it will map exactly under (5b), the SO(5) staggered magnetization must be defined as

$$\mathbf{m}(\mathbf{x}) = \frac{1}{2}[\mathbf{m}^{(c)}(\mathbf{x}) - \mathbf{m}^{(d)}(\mathbf{x})], \tag{6}$$

where $\mathbf{m}^{(d)}$ is (1) with "c" $\to$ "d". Note this gives a sensible result for the Néel state: If $\mathbf{m}^{(c)}(\mathbf{x})$ is up, then $\mathbf{m}^{(d)}(\mathbf{x})$ is down (since the d "orbital" on site $\mathbf{x}$ is a linear combination of c orbitals from the opposite sublattice).

The SC order parameter is

$$\Psi(\mathbf{x}) \equiv e^{i\mathbf{Q}\cdot\mathbf{x}}\frac{1}{2}[c_\downarrow(\mathbf{x})d_\uparrow(\mathbf{x}) + d_\downarrow(\mathbf{x})c_\uparrow(\mathbf{x})]. \tag{7}$$

Then

$$m'_z(\mathbf{x}) = \cos\theta\, m_z(\mathbf{x}) + \sin\theta\, \mathrm{Re}\,\Psi(\mathbf{x}), \tag{8a}$$

$$\mathrm{Re}\,\Psi'(\mathbf{x}) = \cos\theta\, \mathrm{Re}\,\Psi(\mathbf{x}) - \sin\theta\, m_z(\mathbf{x}), \tag{8b}$$

while the other three components are invariant. The SO(5) rotation of the Néel state with $\theta = \pi/2$ gives

$$2^{-N/2}\prod_\mathbf{k}(1 + \eta_\mathbf{k} c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow})|0\rangle. \tag{9}$$

This BCS state has no remnant of Fermi surface ($\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle \equiv 1/2$ throughout reciprocal space).

One could construct a total of six such rotations, each of which mixes one of the three components of $\mathbf{m}(\mathbf{x})$ with one of the two components of $\Psi(\mathbf{x})$. The other five could all be obtained by combining (5b) with the usual SO(3) rotations acting on the spin labels of c and d operators, plus the usual SO(2) $\equiv$ U(1) gauge symmetry changing their complex phases. [Zhang has discussed the algebra of SO(5) generators [1,2].]

For the square lattice, we must have $\mathbf{Q} = (\pi, \pi)$ so the hopping term (12) will be SO(5) invariant. This leaves much freedom to $\eta_\mathbf{k}$ [16], but the simplest choice is

$$\eta_\mathbf{k} \equiv \mathrm{sgn}(\cos k_x - \cos k_y). \tag{10}$$

This has inversion symmetry $\varphi(\mathbf{r}) = \varphi(-\mathbf{r})$ in real space, i.e., $\eta_{-\mathbf{k}} = \eta_\mathbf{k}$ [17]. Equation (10) is inspired by the original and approximate SO(5) symmetry [1], which had the same form but with coefficients $\eta_\mathbf{k} \to \cos k_x - \cos k_y$. Kohno [2] discovered independently the exact version (10). Comparison with (9) shows that (10) is essentially the Cooper pair wave function and has $d_{x^2-y^2}$ pairing symmetry, consistent with strong experimental evidence in the cuprates [18]. Interestingly, one other simple, inversion-symmetric choice would also satisfy condition (4): $\eta_\mathbf{k} \equiv \mathrm{sgn}(\cos k_x + \cos k_y)$. That variant of SO(5), which entails "extended s-wave" pairing, appears free from internal contradictions (contrary to a suggestion in Ref. [1]).

The coefficients in (3) [Fourier transform of (10)] are $\varphi(x,y) = 4/[\pi^2(x^2 - y^2)]$ for $x + y$ odd, zero for $x + y$ even. A possibly useful one-dimensional toy realization of SO(5) symmetry is given by $Q = \pi$ and $\eta_k \equiv \mathrm{sgn}(\cos k)$, which gives $\varphi(r) = 2(-1)^{(r-1)/2}/(\pi r)$ for r odd, zero for r even.

Microscopic Hamiltonian.—Next I will produce an artificial generalization of the Hubbard Hamiltonian which has exact SO(5) symmetry. The basic Hubbard model with particle/hole symmetry can be written as

$$\mathcal{H}_{\rm Hubb} = \mathcal{H}_{\rm hop} + U\sum_\mathbf{x}\frac{1}{2}[n(\mathbf{x}) - 1]^2, \tag{11}$$

$$\mathcal{H}_{\rm hop} = (-t)\sum_{\mathbf{x}\sigma}\sum_\mathbf{u} c^\dagger_\sigma(\mathbf{x})c_\sigma(\mathbf{x} + \mathbf{u}) = \sum_{\mathbf{k}\sigma}\epsilon_\mathbf{k} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}, \tag{12}$$

with $\mathbf{u}$ running over nearest neighbors, and $\epsilon_\mathbf{k} = (-t)(\cos k_x + \cos k_y)$.

The minimal Hamiltonian that includes the terms in (11) is simply the SO(5) symmetrization of (11). The hopping term $\mathcal{H}_{\rm hop}$ is already invariant under all of the SO(5) rotations [such as (8b)], *provided* that $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_\mathbf{k}$. That is true in any bipartite lattice, if and only if $\mathbf{Q}$ describes the original Néel state with opposite spin orientations on nearest-neighbor sites.

However, SO(5) symmetrization turns the number operator $n(\mathbf{x})$ into something quite different,

$n^s(\mathbf{x}) \equiv \frac{1}{2}[n(\mathbf{x}) - n^{(d)}(\mathbf{x})]$. [I take the obvious definition $n^{(d)}(\mathbf{x}) \equiv d^\dagger_\downarrow(\mathbf{x}) d_\downarrow(\mathbf{x}) + d^\dagger_\uparrow(\mathbf{x}) d_\uparrow(\mathbf{x})$.] In contrast to the usual number operator, $\sum_\mathbf{x} n^s(\mathbf{x}) \equiv 0$. The $n^{(d)}(\mathbf{x})$ operator includes terms $|\varphi(\mathbf{r})|^2 n(\mathbf{x} + \mathbf{r})$, all on the opposite sublattice from $\mathbf{x}$ and largest for nearest neighbors, $|\mathbf{r}| = 1$, as well as long-range hopping between sites of the same sublattice. Thus the SO(5)-symmetrized Hubbard model has a modified interaction term:

$$\mathcal{H}^s = \mathcal{H}_{\text{hop}} + U^s \sum_\mathbf{x} [n^s(\mathbf{x})]^2. \tag{13}$$

When we expand $n^s(\mathbf{x})^2$, we get a variety of terms, which include interactions and hoppings (with diminishing coefficients) to arbitrarily large distances [16]. In particular, many terms implement *two* hops, all sites involved being on the same sublattice.

What is the ground state of (13)? If $U^s/t \to 0$, at half-filling, it is the Fermi sea which manifestly possesses SO(5) symmetry. The $t/U^s \to 0$ limit of (13)—assuming half-filling—is more relevant and more challenging. If, say, we take $(n_\uparrow, n_\downarrow) \equiv (1,0)$ on all even sites, then $(n^{(d)}_\uparrow, n^{(d)}_\downarrow) \equiv (1,0)$ on all odd sites (recall that d states are concocted from c states on the opposite sublattice). This ferromagnetically aligned even sublattice has total spin $N/4$ which could point in any direction; similarly, the odd sublattice can be oriented in an independent direction, and any state of this type can have $n(\mathbf{x}) \equiv n^{(d)}(\mathbf{x}) \equiv 1$, thus giving $[n^s(\mathbf{x})]^2 \equiv 0$ in (13). The two sublattice moments can be added to make a total angular momentum l taking any value $\{0, 1, \ldots, N/2\}$. Further, as Ref. [2] pointed out, via $\hat{\pi}$ and $\hat{\pi}^\dagger$ operators, as well as familiar spin-space rotations, each angular momentum is part of an SO(5) multiplet with a total degeneracy [19] $(l + 1)(l + 2)(2l + 3)/6$. This includes states with particle numbers differing from N by multiples of ± 2. The total degeneracy of this family of states is thus $(N + 2)(N + 4)^2(N + 6)/192$, small compared to 2^N in the ordinary Hubbard model (11) with $t = 0$; however, conceivably this family does not exhaust the ground states.

A small t value splits these states in second-order perturbation theory. Within the subspace in which each sublattice is aligned ferromagnetic, the excitation energies and matrix elements are proportional to those in the ordinary Hubbard model. Therefore, I claim the Néel state is in fact one of the $t \ll U^s$ ground states—and so is (9), the SO(5) rotation of the Néel state, since $\mathcal{H}$ has SO(5) symmetry. Thus I conjecture the $t \ll U^s$ ground state has SO(5) *broken symmetry*.

Group theory could be used to enumerate additional allowed terms in the Hamiltonian as in [2]; in particular, a bilinear coupling of the order parameter on neighboring sites [SO(5) symmetrization of the exchange interaction]. However, I have avoided this SO(5) t-J model analog. It could be derived from the SO(5) Hubbard-model analog in the fashion I just outlined; as usual, this is valid only in the limit $t \ll U^s$ (hence $|J| \sim t^2/U^s \ll 1$).

Comparison to an extended Hubbard model.—I now discuss how one might search for approximate SO(5) symmetry in some Hubbard-like model, such as

$$\mathcal{H}_{\text{ext}} = \mathcal{H}_{\text{Hubb}} + \frac{1}{2} V \sum_{\mathbf{xu}} n(\mathbf{x}) n(\mathbf{x} + \mathbf{u}), \tag{14}$$

with a Coulomb repulsion between nearest-neighbor sites (of course, $V > 0$ in the real cuprates [20]).

The aim is to find the point(s) in the parameter space of $\mathcal{H}_{\text{ext}}$ which make it closest to (13): Can the parameters U, V, and t' of (14) be related to U^s in (13)? First, the U term is crudely guessed simply by retaining only the terms from (13) of exactly this form. They come not only from $n(\mathbf{x})^2$ but also from expanding $n^{(d)}(\mathbf{x})^2$. The result is $U = \frac{1}{2} U^s [1 + \sum_\mathbf{r} |\varphi(\mathbf{r})|^4] = \frac{1}{2}(1 + \frac{1}{9}) U^s$.

Next, we estimate V in the same fashion, from the nearest-neighbor term in $n(\mathbf{x}) n^{(d)}(\mathbf{x})$, obtaining $V \approx -U^s |\varphi(\mathbf{u})|^2 \simeq -0.16$, where $\mathbf{u}$ is a nearest neighbor. Here the SO(5) symmetry demands an *attractive* nearest-neighbor electron interaction, which is understandable: In the $U \to \infty$ limit, only singly occupied states could occur in a ground state, so only the AF states could be ground states. The SC state has a certain density of doubly occupied and vacant sites, so an additional term is needed to equalize its energy with that of the AF state. Any pairing interaction might play the same role.

Finally, second-neighbor hopping (which would break the electron/hole symmetry) *does not* appear in (13). In fact, any single-electron hopping within the same sublattice would violate SO(5) symmetry and get annihilated by the SO(5) symmetrization [21].

Very recently, an extended Hubbard model was simulated using a new interaction with double hoppings [22], $\sum_\mathbf{x} K(\mathbf{x})^2$, where $K(\mathbf{x}) = \sum_{\sigma\mathbf{u}} c^\dagger_\sigma(\mathbf{x}) c_\sigma(\mathbf{x} + \mathbf{u}) +$ h.c. There are two suggestions that this model may realize SO(5) approximately: (i) It has terms with the same form as the largest terms (after those previously mentioned) of $n(\mathbf{x}) n^d(\mathbf{x})$ and $[n^d(\mathbf{x})]^2$ in (13); (ii) it seems to have a continuous AF/SC transition [22].

Of course, even at the SO(5) multicritical point in Zhang's picture, the *microscopic* Hamiltonian might have no visible SO(5) symmetry; just as at the spin-flop point of an anisotropic magnet, a cancellation of terms favoring competing types of order might suffice, with the symmetry emerging only at long wavelengths [1]. But if that length scale is much larger than the numerically tractable system size for Hubbard models, then direct numerical calculations on finite lattices (such as [23]) are too small to address the order-parameter symmetry.

Even if that length scale is comparable to system size, the spatial decay of ground-state correlations is usually inconclusive as a test of order. Yet it is possible that, already at small system size, the (excited) eigenstates show a well-defined structure characteristic of a particular symmetry;

this provided the convincing evidence for long-range order in the spin-$\frac{1}{2}$ triangular lattice AF [24]. (Reference [19] has sought SO(5) symmetry in this fashion in exact diagonalizations of the t-J model.) I suggest identifying an SO(5) multiplet numerically in a model with manifest SO(5) symmetry, and then following its evolution while the Hamiltonian is adiabatically modified to a more realistic model such as (14).

In conclusion, I have identified inklings of SO(5) symmetry in popular existing models and exhibited the form an exact SO(5) symmetry could take in one- or two-dimensional lattice models. The SO(5) symmetry in microscopic models is promising as a spur to the comparison or unification of competing models of high-T_c superconductivity, and to improved understanding of extended Hubbard models.

However, I have not addressed the murkier issue of its application to the cuprates. Of the objections mounted so far to a possible SO(5) relationship between the actual AF and SC phases, one seems to be really inescapable: the Fermi surface [8]. If the SC metal shows a sharp drop in electron occupation along a certain surface in reciprocal space, as found in angle-resolved photoemission experiments [25], then [see (2)] its AF image under SO(5) has a similar surface (shifted by $\mathbf{Q}$). Apparently, this AF must be a spin-density-wave metal [26]. But the real AF phase of the cuprates looks more like a Mott insulator [4], and its AF correlations are well modeled using nearest-neighbor exchange [27].

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