On an SO(5) unification attempt for the cuprates

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Zhang [1] in his paper 'A unified theory based on SO(5) symmetry of superconductivity and antiferromagnetism, Science **275** 1089 (97)' has argued that there exists an approximate global SO(5) symmetry in the low temperature phase of the high Tc cuprates. This suggestion contains a five component order parameter: three components correspond to a spin 1, charge zero particle-hole pair condensed at the center of mass momentum (π, π), corresponding to antiferromagnetic order in the vicinity of the Mott insulating state; while the last two components correspond to a spin singlet, charge $\pm 2e$ cooper pair of orbital symmetry $d_{x^2-y^2}$ condensed in the zero momentum state, corresponding to superconductivity in the doped Mott insulator. He identifies the operator

$$\pi = \sum (cosk_x - cosk_y) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}+\pi\uparrow} \tag{1}$$

as one of the generators which rotates the 5-vector between the spin and charge direction. The doping density apparently acts like a pseudo magnetic field for the order parameter.

For an exact SO(5) symmetry breaking scheme the generator π should annihilate the vacuum (as it will be a zero momentum Goldstone mode creation operator) or its spectral function should have a pole of finite residue at zero energy. However, if the pole has a finite but small energy, small compared to transition temperatures, one can claim an approximate symmetry. Such a state above the top of the two-particle continuum is referred to as an "antibound" state. Demler and Zhang [2] (DZ) claim that the spectral function of the π operator has a pole around 41 meV for the cuprate YBCO based on a fermi liquid t-matrix analysis, and identify the pole (*i.e.* the antibound state) with a resonance in neutron spectroscopy.

There are many criticisms which can be made of these ideas, from mathematical ones to contradictions of the model with experimental features of the cuprates, to deep general questions of physics. The latter are more conclusive and less arguable, but perhaps initially it is essential to demonstrate the implausibility of this work so we shall start at the simplest and work up. First let us list our objections:

1) (due to M. Greiter [3]) The Hubbard gap is ignored, the chemical potential misidentified and issues of projections are not discussed.

2) The model Hamiltonian omits a large term , t', which is experimentally observed and which displaces the resonance and possibly removes it.

3) The exchange terms in the Hamiltonian have little resemblance to the correct ones, and the antibound state from magnetic interactions disappears once this error is corrected.

4) The conventional Hubbard Hamiltonian omits longer range coulomb interactions, which are not important in the usual low energy physics but are very much so here. (We learned that Greiter also has brought up this point in his second comment [3]).

5) The antiferromagnetic and superconducting phases each derive from a more fundamental thermodynamic phase, the Mott insulator and the metal respectively. The Mott insulator and the metal can not be related to a quantum critical point, by Elitzur's theorem, since they differ by a local gauge symmetry. These phases hence have no locally stable, homogeneous intermediate phases, and can not be deformed continuously into each other, certainly not by an operator as simple as an SO(5) rotation.

We elaborate our points now. 1) Greiter has brought up the importance of the upper Hubbard band and the problems related to treating the chemical potential in a mean field fashion without invoking projections. We do not wish to go into the Greiter - Demler, Zhang [3,4] discussion on the issue of chemical potential. The following is our comment on the projection issue. The spectral function of the π operator will have a range from zero (the ground state) to an energy of the order of U. The average energy of the state created by π operator is unimportant. The issue is whether the spectral function has a low energy pole with finite residue, and if so, whether the π operator projected (renormalized) to this pole continues to be a generator obeying the old SO(5) algebra or not. The projected operator may be defined as

$$\pi_\alpha = P_\alpha \pi P_\alpha \tag{2}$$

where $P_\alpha = |\alpha><\alpha|$ is the projection operator; and the state $|\alpha>$ is the many body (N + 2)-particle state corresponding to the pole. Projections to subspaces can change the commutation relations. For example, in the case of the Mott insulator, the π operator projected to the lower Hubbard band creates only spin and hence it is incapable of rotating between the charge and spin sectors of SO(5).

2) The known fermi surfaces of cuprates are inconsistent with the bipartite model used by DZ, which contains only nearest neighbor hopping. The correct form of dispersion, as has also been noted by DZ, is

$$\epsilon_k = -2t(cosk_x + cosk_y) - 2t'(cos(k_x + k_y) + (cos(k_x - k_y)) \quad (3)$$

with t' of the order of $\frac{1}{2}$ t. The t' term does not commute with the operator π and spreads its spectrum [7] over 0.1 eV. Any resonance must be outside this range, presumably an antibound state above it. It is also easy to show that the spreading of the two particle spectrum at(π, π) reduces the already small antibinding energy [5] ($0.1J \approx 10$ to $15meV$). This is because the spin triplet antibinding state has a p-symmetry in the relative orbital co-ordinate forced by antisymmetry, and a p-wave bound state [6] (to be precise $p_x - p_y$ symmetry) does not effectively make use of short range attraction in view of the node at the origin.

That spreading of the two particle band (corresponding to relative motion) will destroy the two particle antibound state can be already inferred from DZ's results directly. A change of the center of mass momentum by only about $\frac{\pi}{50}$ is enough to remove the antibinding energy (figure 1 in DZ). This happens when the two particle band width is $\approx 0.1J$, comparable to the antibinding energy at (π, π). This is a consequence of the fact that in a tight binding situation nearest neighbor attraction will give a p-wave binding only when its strength is of the order of the band width.

3) The Hamiltonian (equation 1 of DZ) used by DZ includes a nearest neighbor exchange term in a Hubbard model. This is, rather confusingly, included in order to capture the higher order effects in $\frac{1}{U}$. The derivation of this exchange term (see PWA [9]) leads to the expression

$$J_{ij}(\mathbf{S}_i.\mathbf{S}_j - \frac{1}{4}n_i n_j) \quad (4)$$

not $\mathbf{S}_i.\mathbf{S}_j$ alone: hence there is no interaction (repulsion) between parallel spins at all. This means [8] the absence of an antibound state to leading order in J ;(*i.e.* absence of 41 meV resonance for YBCO within DZ's scheme. In fact, the correct Hamiltonian would also contain a ferromagnetic true exchange term (whose origin is potential rather than kinetic), and the net effective interaction between parallel spins on nearest neighbor sites would be attractive, thereby removing any antibinding tendency by magnetic interactions.

We also wish to point out that any induced magnetic exchange interaction between two electron spins will have the form,

$$J_{ij;kl} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} \sum_{\sigma'} c^{\dagger}_{k\sigma'} c_{l\sigma'} \quad (5)$$

in both metallic and insulating states, irrespective of the value of U, in view of the kinetic origin of the induced magnetic exchange interactions in tight binding systems like cuprates. When we specialize $J_{ij;kl}$ to two sites we recover equation (4).

4) While considering excited states, interactions that were not very effective at low energies may start playing a major role. There is a strong repulsive term which prevents a parallel spin two particle resonance at low energies: the unscreened part of the coulomb repulsion between pairs of particles on neighboring sites. This must be of the order of an eV. It is easy to show using the same t-matrix analysis that this term brings back the antibound state but at about 1000 meV and not 40 meV ! In most Hubbard model calculations this term is neglected, or taken care of through Hartree like approximations, because 'U' is so much larger, but of course it is always present and where one is discussing a resonance in the particle-particle channel it must be taken into account as a final state interaction.

Incidentally, these antibound states share a common origin with the two particle anti bound state in the singlet channel whose energy is of the order of onsite U; in the triplet channel it is of the order of the nearest neighbor V which is the major repulsion felt by parallel spins.

5) The presence of all of the above terms means simply that the delicate balance created by the artificially restricted model used in the SO(5) theory is, indeed, an artifact of model building and has little relation to physical reality. But there is a much deeper and more profound difficulty with theories of the cuprates based upon a quantum critical point. Of these, the most ambitious is the SO(5) hypothesis of Zhang , but others have been suggested (e.g. by Sachdev et al. [10])

The general idea is to propose that thermodynamic phases are characterized by an order parameter such as superconducting pair wave functions or an (anti)ferromagnetic moment. One imagines a critical point at T = 0, at which this order parameter changes continuously from one type to another (or ceases to exist) as some parameter - in the case of cuprates, the doping - is varied. One has then a multi-dimensional space of some sort, containing an order parameter vector of finite dimensionality and this vector rotates from one sector of this space to another at the critical point. The associated T = 0 quantum critical fluctuations spread its influence into a range of finite T and doping.

This picture does not take into account the basic physics of the two states. The antiferromagnet is a Mott insulator, and it is an antiferromagnet because it is a Mott insulator, not vice versa. Superexchange is a consequence of the insulating state (see PWA [11]). The insulating state has a large gap for charge fluctuations, and the antiferromagnetic order parameter forms in the subspace formed by bare spins.

The superconductor, on the other hand, forms in a metal, and is a property of low-energy quasiparticle-like excitations near a fermi surface. The fermi surface is meaningless in the insulator, but is crucial to the superconductor.

The dominant transition, then, is between metal and insulator, each being states described by an infinite dimensional order parameter [12]. The transition between these two states can not be continuous, and is not; the insulator has a discontinuity in chemical potential, $\mu = \frac{\delta F}{\delta n}$ and is therefore a cusp of the free energy. States

of intermediate doping cannot be homogeneous and are not. When doping is done by mobile charges (laser doping, or oxygen doping in $La_2CuO_{4+\delta}$) the system segregates. In summary, the order parameter characterizing antiferromagnetism and superconductivity relate to subspaces of Hilbert space which are algebraically inequivalent and can not be mapped on each other; thus neither can the order parameters themselves. There is no underlying quantum critical point expressing an essential continuity between the two phases.

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[1] Shou-Cheng Zhang, Science **275** 1089 (97)
[2] E. Demler and S.C. Zhang, Phys. Rev. Lett. **75** 4126 (95)
[3] M. Greiter, cond-mat/9705049 and cond-mat/9705282
[4] E. Demler and S.C. Zhang, cond-mat/9705191
[5] DZ get the energy of the π resonance E_π by adding this antibinding energy $E_b \approx 0.1J$ to the center of the two particle (π,π) band which is assumed to be around 0.2J above the ground state; $E_\pi \approx 2\mu + E_b = 0.2J + 0.1J \approx 40meV$.
[6] That the π operator creates a state that has a $p_x - p_y$ symmetry can easily be seen by rewriting π in terms of relative momenta as follows

$$\begin{aligned}\pi &= \sum (cosk_x - cosk_y) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}+\pi\uparrow} \\ &= \sum (sinq_x - sinq_y) c^\dagger_{\mathbf{q}+\frac{\pi}{2}\uparrow} c^\dagger_{-\mathbf{q}+\frac{\pi}{2}\uparrow}\end{aligned} \tag{6}$$

[7] Pauli blocking of the two particle states reduce this spread. However, a spread as little as 10 meV seems to be enough to remove the antibound state.
[8] It is easily seen that the term $\frac{J}{4} n_{i\uparrow} n_{j\uparrow}$ coming from the S_z components of $\mathbf{S}_i.\mathbf{S}_j$ which causes binding (see equation 3 of DZ) in leading order in J is canceled by our term $\frac{1}{4} n_i n_j$.
[9] P.W. Anderson, Phys. Rev. **115** 2 (59)
[10] S. Sachdev et al., Phys. Rev. **B51** 14874 (95)
[11] P.W. Anderson, Adv. Phys. **46** 3 (97)
[12] G. Baskaran and P.W. Anderson, Phys. Rev. **B 37** 580 (88); F.D.M. Haldane, in Perspectives in Many Particle Physics (Varenna Course CXXI), Ed. R. A. Broglia et al., North Holland (1994) page 5 - 29