A suggested 4×4 structure in underdoped cuprate superconductors: a Wigner supersolid.

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A wave function is proposed for the "4×4" inhomogeneous structures observed on cuprate superconductors. It is based on the Gutzwiller-RVB technique proposed in recent papers, and consists of a Wigner solid of hole pairs embedded in a sea of d-wave spin singlet pairs. Arguments are given that the nodal quasiparticles may remain unscattered and even superconducting on such a structure.

A number of recent STM experiments on underdoped cuprate superconductors have shown evidence of structure with a Bravais lattice close to $4a \times 4a$ in the CuO_2 planes. A possibly similar structure has been observed in vortex cores in BSSCO, with a fractionally larger lattice constant; and we also call attention to the often-noticed anomalies of T_c and other parameters in LSCO at a doping of $x = \frac{1}{8}$, which to my knowledge have never been satisfactorily explained, and may be caused by the same structure. Both the tunnelling spectrum and the $\frac{1}{8}$ structure seem often to indicate that there is superconductivity at low temperatures in materials with these structures.

I propose here a microscopic description of these phases that is not inconsistent with their arising at low doping levels in an RVB superconductor-Mott insulator system. I am suggesting that they are in essence a two-dimensional crystal of singlet d-wave pairs of holes, commensurate in many cases with the underlying lattice, and existing within a background of a d-wave RVB of singlet pairs. (Which latter is our model of the electronic nature of the pseudogap state in these materials.) Our model differs in essential ways from those of Chen *et al.* [1] and Lee *et al.* [2], but has in common that we all propose a crystal of holes. The model of Lee *et al.* explicitly rejects hole pairs in favor of individual holes, but seems to us to fail to explain why the structure appears when the material is still superconducting and still exhibits quasiparticle nodes–clearly the pairs are a reality, in spite of the Coulomb repulsion between the two holes. It also loses the feature of explaining the "$\frac{1}{8}$" phenomenon and of why the doping level at which these observations occur is never as low as $\frac{1}{16}$. The model of Chen *et al.* is based on a proposed symmetry between antiferromagnetism and d-wave superconductivity which many consider problematic, and sees the crystal as a "Wigner crystal", which to my mind implies an insulating state. I should note that in a number of numerical simulations on underdoped multi-leg ladders (White and Scalalpino [3]), 4×4 squares centered on a hole pair in a single plaquette are observed as one of a number of inhomogeneous states.

In some recent papers [4, 5] the author and collaborators have returned to the early insight [6] that the ground state of the CuO_2 planes in the cuprate superconductors can be modelled as a Gutzwiller projection of a d-wave BCS superconducting state. Our point of view is to construct an effective Hamiltonian that operates only within the manifold of "lower Hubbard band" states – in first approximation, the "t-J" Hamiltonian – and then to recognize that the eigenstates of such a Hamiltonian must be general Gutzwiller projected states. We treat the states before projection by a Hartree-Fock-BCS approximation, that is we find variationally the best product of one-electron functions possible. As in Hartree-Fock, the mean field equations which arise from the variational procedure also specify the quasiparticle excitations and their energies – that is, there is effectively a Koopman's theorem for this system.

In studying point-contact tunneling with this technique [5] we found it useful to use a formulation of the ground state wave-function which to our knowledge was first given by Laughlin [7]:

$$|\Psi\rangle = \exp(iS)\hat{P}_G \times [Z]^{n_{pairs}} \times |\Phi_{BCS}\rangle, \qquad (1)$$

where n_{pairs} is the number of hole pairs.

Here, the Gutzwiller projector

$$\hat{P}_G = \frac{1}{2}\prod_i [1 - n_{i,\uparrow}n_{i,\downarrow}] \qquad (2)$$

is a projector that removes all doubly-occupied sites but otherwise leaves amplitude and phase relations unaltered in the d-wave BCS wave function $|\Phi_{BCS}\rangle$. The product in Eq. 2 is over all sites. The BCS function is that appropriate to the Fermi level for $1 - x$ electrons, where x is the doping fraction. $|\Psi\rangle$ is assumed to be determined variationally as in Ref. [4]. Finally, the canonical transformation $\exp(-iS)$ transforms the true Hamiltonian into the projected form of the t-J Hamiltonian, and correspondingly its inverse transforms the projected wave function into the true one.

Laughlin's innovation [7] was to make explicit the "fugacity factor" Z raised to the number of hole pairs, which is necessary to adjust the populations of the electron states on a given site. It is easily calculated that in a uniform state $Z = 2x/(1 + x)$, with x the doping fraction. In Refs. [3, 4, 6] this population adjustment is done by fiat. In Ref. [5] the Z factors were, further, incorporated into the BCS function, which modifies the definition of quasiparticle excitations in such a way as to give good agreement with tunneling measurements, but we emphasize that the wave function assumed there is

just Eq. 1. This variant of the wave function makes clear that Z plays the role of a Bose condensate amplitude – though we should emphasize that our theory does not involve assuming a "holon condensate."

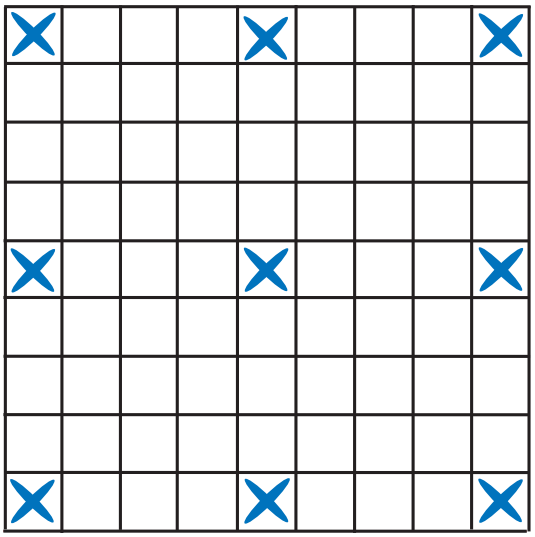

FIG. 1: Proposed 4×4 structure. Plaquets with crosses are nominal sites of hole pairs. The structure may also be thought of as "columnar" valence bond structure commensurate with hole-pair "liquid crystal".

What is being proposed here is that we approximate the wave function for a density wave or Wigner-like crystal as described above not primarily by changing the BCS function in Eq. 1 but by requiring the fugacity Z to vary from site to site. Its logarithm is the chemical potential for holes and thus must track the Madelung potential of the superlattice. The average fugacity is arranged to lead to the correct doping level overall, but (for instance) Z may be taken to have one value, Z_1, on the central four sites of a 4×4 square plaquette, and another, smaller value Z_2 on the remaining 12 sites (or, if desired, one may specify still a third value for the corners.) Then the hole density will be a maximum on the central plaquette, and will be small in the intermediate regions. The contrast in Z values cannot in the end be very great, because Z_{max} will likely not be greater than the value at optimal T_c , about $\frac{1}{3}$ (see Fig. 1).

The gap equations Eqs. 1 and 2 which result from variation of $|\Psi\rangle$ are, in the renormalized mean-field theory approximation of Ref. [4],

$$\Delta(\mathbf{k}) = J(2-Z)^2 \sum_{\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{E(\mathbf{k}')} \tag{3}$$

$$\xi(\mathbf{k}) = Z\epsilon(\mathbf{k}) + J(2-Z)^2 \sum_{\mathbf{k}'} \gamma(\mathbf{k}) \frac{\xi(\mathbf{k}')}{E(\mathbf{k}')}, \tag{4}$$

Here, $\gamma(\mathbf{k}) = \cos(k_x - k'_x) + \cos(k_y - k'_y)$ and

$$E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2} \tag{5}$$

is the standard BCS expression. The important thing to note is that the true kinetic energy $\epsilon(\mathbf{k})$ is renormalized relatively by a factor $Z/(2-Z)^2$ relative to J. The underdoped regime is defined by $Zt \ll 4J$, so that over most of the region near the Fermi surface, $E(\mathbf{k})$ is relatively weakly dependent on Z. Thus to a zeroth-order approximation the gap equations Eq. 3 are not affected by periodic spatial variation of Z, justifying our basic *ansatz* that the function before projection may be assumed not much changed. This signals the important fact that the CDW lives in an RVB background, not in a conventional band or in an antiferromagnetically (or even spin-glass) ordered state. The fact that $\frac{1}{8}^{\text{th}}$ of a hole relative to the Mott-Hubbard insulator corresponds to a unit cell of 16 sites does not add up in conventional band theory.

Of course, the periodic variation of Z will cause Bragg scattering of the quasiparticles, which can be represented by dividing the spectrum up into 16 sub-bands and describing the perturbation as a matrix in band indices which opens Bragg-scattering gaps at the subzone boundaries. I don't feel that Fermi surface nesting plays much of a role here. Treating the resulting self-consistency problem accurately is beyond the patience or ability of the present author to solve directly. But there are a number of insights one can recognize. First, there will only be one of these subbands which contains the nodal quasiparticles, and the lowest part of the spectrum around the nodes will be relatively little scattered, since the density of final states goes to zero as E^2 at low E. The experimental observation that the nodes survive and are coherent in the density-wave state is thus confirmed. Second, we can expect the spectrum near the antinodes to be severely broken up into rather flat "optical" bands, because both the gap and the underlying kinetic energy are rather flat in this neighborhood. The superfluid stiffness coming from these portions of the zone will be severely reduced by this scattering, and these excitations may move diffusively rather than coherently.

Either from this insight, or on general principles, we can expect that the superfluid stiffness ρ_s, which in the pure case is known to be proportional to Z, will be reduced more by the low values of Z between the peaks than by the higher value at the peaks, and since T_c is proportional to superfluid stiffness [4], T_c will be degraded. The nodal quasiparticles, which are responsible for the temperature dependence of ρ_s, are little changed.

It remains to discuss the motivation for this structure. It is obviously the long-range Coulomb interaction that furnishes the energy gain, and the stiffness of the hole wave function which opposes the deformation. We can suppose that Z is unlikely to exceed its value for optimal doping of 20%, about 0.33, on the central plaquette, so that the decrease on the periphery is not severe – I estimate 0.2 or so, or $x = 0.1$.

The energy gain is something like the Madelung energy of the charge distribution of the "liquid crystal" which will be of the order of the square of the charge contrast divided by the lattice constant (and corrected by the dielectric constant). Thus it scales as

$$E_{coulomb} \propto (\delta Z)^2 \times 1/d \tag{6}$$

where d is the superlattice constant.

The excess kinetic energy, on the other hand, will contain a gradient squared which is proportional to $(\delta Z/d)^2$. Clearly there is some d large enough so that the Coulomb energy gain wins. It is necessary that $d^2 = 2/x$. Otherwise, the Madelung estimate is not correct, and we would have to include the Coulomb repulsion of the extra pairs. Numerical estimates show that it is reasonable that the opposite variations of Coulomb and kinetic energy would match for $d = 4a$.

The above is not a complete theory. In particular, we have not calculated the energetics explicitly. But it is based on an explicit wave function, so that numerical calculations can be carried out when desired. It does have the advantage that it leads to an explicitly superconducting state closely related to the uniform state which explains many of the properties of the superconductors. There are several further questions which remain.

First, we need a reason why the lattice constant seems often to be slightly larger than 4.0, according to Fourier transforms of the tunnelling current. The only real-space images of the microscopic structure (Davis [8]) show however that the structure is made up of domains which are not continuously connected. The packing of such a granular structure will not be perfect and will have a smaller average wave number. We can speculate that commensurability with the lattice favors a definite hole density – $\frac{1}{8}$, we suppose – and that the grain boudaries adjust the net charge. Thus the deviation from $4a$ provides suggestive evidence for, rather than against, the lattice of hole pairs.

A second puzzle can be resolved in much the same way. The vortex core state at optimal doping exhibits a similar modulation, albeit with a lattice constant even larger than the previous one – about $4.5a$ is quoted. In the vortex core the superfluid stiffness is reduced by the large supercurrent. I expect the amplitude stiffness to gradients of Z and the phase stiffness which causes supercurrents to be the same, and if one is reduced the other will be, and again the Coulomb energy will be favored relatively to the kinetic energy. But here we expect the doping to be farther from $\frac{1}{8}$ and the grains to be even smaller, hence the larger deviation from 4.0.

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