The “Spin Gap” in Cuprate Superconductors

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**Abstract**

We discuss some generalities about the spin gap in cuprate superconductors and in detail, how it arises from the interlayer picture. It can be thought of as spinon (uncharged) pairing, which occurs independently at each point of the 2D Fermi surface because of the momentum selection rule on interlayer superexchange and pair tunneling interactions. Some predictions can be made.
The problem with the Spin Gap \textsuperscript{1} is that there are too many right ways to understand it within the interlayer theory \textsuperscript{2} not too few: when one realizes what is going on it seems all too obvious in several ways that one should have known all along.

(1) The most obvious: spinon pairing. We have realized all along that the normal state has charge-spin separation, so why didn’t we expect two pairings, one for spin and the second for charge?

(2) Also obvious: there is no phase transition, hardly even a crossover. So the gap opens without change of symmetry or condensation. It must be not a self-consistent mean field but a property of the separate Fermi surface excitations.

(3) Finally, when one looks at the interlayer theory, and takes it seriously, one realizes that the phenomenon jumps out at you and is a trivial consequence of the interlayer interaction. The Strong-Anderson \textsuperscript{3} model is not a complete theory, but can be used to calculate with: \( \chi(T) \), for instance.

Let me start, then, in the inverse of chronological order and try to make the synthetic argument first. We start from the fact that every experimental, computational, and theoretical bit of evidence we have supports the dogma that the 2D interacting electron gas in the cuprates is a liquid of Fermions with a Fermi surface, and with little or no tendency to superconductivity or to exhibit antiferromagnetism, once it is metallic—i.e., there is no clear indication of “antiferromagnetic spin fluctuations”, as relatively soft bosonic modes, in the isolated plane. Rather, in the plane the magnetic interaction modifies the elementary excitation spectrum as it does in the ferromagnetic case. The symmetry of this state is the Haldane-Houghton \textsuperscript{4} Fermi liquid symmetry \( (U(2))^Z = (U(1) \times SU(2))^Z \), one of “Z” for each point on the Fermi surface. This large symmetry is the general description of a liquid of Fermions with a Fermi surface, which is necessarily a surface in \( k \)-space on which the Fermion lifetime becomes infinitely long in the limit as one approaches the surface, hence particles at the surface are conserved. Every point on the Fermi surface is independent, and charge and spin are separately conserved. The reference shows that this description includes, but is not confirmed to, the Landau Fermi liquid. For the Fermi liquid, \( U(2) \) applies: the
two spin components are uncoupled; but the basic symmetry is spin and charge separately conserved, in the general case.

Our theory postulates that in fact the $U(2)$ is broken into $U(1) \times SU(2)$ with the charge and spin excitations having different Fermi velocities and the charge also having anomalous dimension, i.e., the charge bosons are a Luttinger liquid; but this does not change the symmetry argument. What is little realized is that the spin excitations are always describable as spinons, even for free electrons,

$$\psi_k^*(r) \simeq s_k^+(r)e^{i\theta_k(r)}$$

The spin part is always a spinon, the charge is a bosonized Luttinger liquid. This, then, is our high-temperature, high energy state above temperatures and energies where the interplane interactions come into play.

Spinons in 2D are paired but gapless. What the non-existence of a phase transition when we lower $T$ to the interplanar scale tells us is that the spin gap state has the same symmetry. It must leave the crucial fact of Fermi or Luttinger liquids intact: the independence of different Fermi surface points. Then all that can happen is that the spectrum at each point changes, and the simplest way for that to happen is for the spinon to acquire a “mass”, i.e.,

the spinons which used to have a free electron like linear spectrum

$$v_s(k - k_F) \text{ or } v_s\sin\frac{\pi(k - k_F)}{2k_F}$$

open a gap and have energies

$$E^2 = \Delta^2(\hat{k}) + v_s^2(k - k_F)^2.$$

(1)

This is possible because of the peculiar nature of spinons, that they are BCS quasi-particle like even in the normal state (as shown long ago by Rokshar [5]). That is, they are semions, or Majorana Fermions, which have no true antiparticles (we use the convention $-k = -k, -\sigma$ $k = k, \sigma$)

$$s_k^+ = s_{-k} \quad s_k = s_{-k}^+$$
so that the Hamiltonian for free spinons may be written

\[ v_s(k - k_F) (s_k^+ s_{-k}^- + s_{-k}^+ s_k^-) \tag{2} \]

just as well as in terms of \( s_k^+ s_k^- \) and it is not a symmetry change to add a term

\[ \Delta_k s_k^+ s_{-k}^- \]

Spinons are always effectively paired. (Strong and Talstra [3]) It is natural that spinons are more easily paired in the underdoped regime, because the spinon velocity becomes progressively lower (\( J_1 \) smaller) as we go toward the Mott insulator; therefore the density of states is higher, \( \chi_{\text{pair}} \) larger, on the underdoped side.

Finally, let me make one last remark of a synthetic, rather than analytic, nature. As I have already said the basic description either of a Fermi or a Luttinger liquid is the independence of different Fermi surface points. If we are to go smoothly from a two-dimensional electron liquid to a gapped state without change of symmetry—without introducing any new correlations—we must do so without coupling the different Fermi surface points, that is we need interactions which conserve two dimensional momenta \( k_x \), \( k_y \). There is only one source of such interactions, namely the interlayer tunneling.

\[ \mathcal{H}_{IL} = \sum_{k, \sigma, i, j} t_{\perp}(k) \, c_{k \sigma i}^+ \, c_{k \sigma j} \tag{3} \]

which, in second order, leads to two types of interlayer coupling:

Pair tunneling

\[ \mathcal{H}_{PT} = \lambda_J(k) \sum_{(ij), k, k'} c_{k \uparrow i}^+ \, c_{-k' \downarrow j}^+ \, c_{-k' \downarrow j} \, c_{k \uparrow i} \tag{4} \]

and superexchange

\[ \mathcal{H}_{SE} = \lambda_S(k) \sum_{(ij), k, k'} c_{k \uparrow i}^+ \, c_{-k' \downarrow j}^+ \, c_{k' \downarrow j} \, c_{k \uparrow i} \tag{5} \]

(In both, \( k' \approx k \)) which represent exchange of charge and spin, respectively, between two layers. The empirical (and theoretical) fact that coherent single-particle hopping does not take place in the cuprates leaves these as the two second-order terms which can lead to coherent interactions—such as we are looking for—between two layers.
It is important to recognize that (4) and (5) have one extra conservation relative to conventional interactions. This seems to be very difficult for many theorists to grasp.

(5) does not involve any charge exchange between planes hence can be thought of as an exchange of a spinon pair, if one likes, but as we shall see it is formally unnecessary to write it in terms of spinons. (4) only conserves total charge of the two planes, hence is not a true spinon operator at all. Nonetheless we find that (4) and (5) together can be described in a sense as pairing spinon states [7]

This superexchange interaction does not much resemble that used by Millis and Monien,\textsuperscript{1} and it does not have anything to do with the “J” of the \( t-J \) model. Superexchange occurs as a result of frustrated kinetic energy, and the kinetic energy which is frustrated in the cuprate layer compounds is only the \( c \)-axis kinetic energy \( t_{\perp} \). They are very like Mott insulators in one of 3 spatial dimensions: and they exhibit superexchange in that dimension. But they retain no Mott character in the 2 dimensions of the planes.

It is an unpublished conjecture of Baskaran that \( \lambda_s/\lambda_J \) increases as we approach the insulating phase, i.e., as “\( \alpha \)”, the Fermi surface exponent, increases. This may be one other reason why underdoped materials show the spin gap.

Now, finally, let us do the calculational problem. At this point we have to stop talking in generalities and make some rather severe assumptions in order to make progress. They seem innocuous, and are quite standard in conventional BCS theory, but here we have no particular reason to believe that they will serve as better than a rough guide. These assumptions are: (1) the Schrieffer pairing condition, i.e., we use only the BCS reduced interaction \(-k' = -k\). This is justified at high enough \( T \) by the fact that a given state \( k \) can only pair with one other \(-k'\) to give a quasicoherent matrix element; our picture of the kind of process involved is that a transition into a high-energy state intervenes between two low-energy states which are connected by two—and only two—single-particle tunneling processes, \( k_a \rightarrow k_b; -k_b \rightarrow -k_a \). It is perhaps best to think of the pairing as always \( k, -k \) but with center of mass momentum thermally fluctuating. (2) More orthodox but more serious: We neglect \( |v_c - v_s| \) and treat \( c_k^\dagger \) as though it were an eigenoperation, i.e.
\[ H_K = \sum_k \epsilon_k n_k \]  

(6)

Actually we use the Nambu-PWA form

\[ H_K(k) = \epsilon_k(n_k + n_{-k} - 1) = \epsilon_k \tau_{3k} . \]

Now we have a straightforward Hamiltonian which is trivially diagonalized, because it separates into separate Hamiltonians for every \( k \).

\[ H = \sum_k H_k \]

\[ H_k = H_K(k) + \lambda_j c_{k1}^+ c_{-k1}^+ c_{-k2} c_{k2} + 1 \leftrightarrow 2 + \lambda_S c_{k1}^+ c_{-k2}^+ c_{-k1} c_{k2} \]

(Here we use the convention \( k = k \uparrow -k = -k \downarrow \)). The first attempt was made by Strong and Anderson neglecting \( \lambda_s \) and this leads to a beautiful spin gap. The \( KE \) spectrum of the 4 fermions \( 1,2, k, -k \) has \( 16 = 2^4 \) states which are grouped into 5 sets, \( n_{\text{tot}} = 0, 1, 2, 3, 4 \). (See Fig. 1) Of these only the \( n = 2 \) states are affected by the interactions, and of these 2 will be split off by \( H_J \) and 2 by \( H_S \). In either case, these gaps are completely \( T \)-independent and are simply manifested as the individual states drop out:

\[ Z = 16 \cosh^2 \beta \epsilon_k/2 + 2 (\cosh \beta \lambda_j - 1) \]

(because with the added “-1” \( n = 2 \) states are at 0 energy.

\( \chi \) for this case is

\[ \chi = \int_{-\infty}^{\infty} d\epsilon \frac{\cosh^2 \beta \epsilon/2}{\cosh^4 \beta \frac{\epsilon}{2} + \frac{1}{4} (\cosh \beta J - 1)} \]

A second calculation may be carried out with both terms, \( \lambda_J \simeq \lambda_S \) and the result is to split out two levels rather than one and to replace \( 1/8 \) with \( 1/4 \). This is the curve for susceptibility I show in Fig. 3 and it is not a bad fit to susceptibility data.

But actually I am not totally convinced that this is the right formalism, although it may be the right arithmetic. The reason it works seems clearly to me to be that we have picked a form for the pairing Hamiltonian that connects states which are “neutral” — i.e., only the
$n = 2$ states are connected to each other within the $k$ manifold. But in some real sense these are states with the spinons paired but with no holon pairing—no charge pairing—at all, even though nominally different layers are connected. I think it is more nearly valid to describe the correct state by rewriting $\mathcal{H}_j + \mathcal{H}_s$ as

$$(\mathcal{H}_j + \mathcal{H}_s)_k \simeq c_{ke}^+ c_{-ke}^+ c_{-ke} c_{ke}$$

where $c_{ke}^+ = \frac{c_{k1} + c_{k2}}{\sqrt{2}}$. That is, the spin-gap state is a state in which spinons belonging to the even linear combination are paired, the odd unpaired. This has a strong relationship to the Keimer neutron selection rule observed for the superconducting state. Keimer has begun neutron investigations on spin-gap material, but his results are completely preliminary. I anticipate that he will see peaks at energies corresponding to the spin gap and that they will satisfy his even $\leftrightarrow$ odd sum rule, which results from this pairing.

One consequence of the assumption of Fermi rather than Luttinger liquid is the $T$-independence of the spin gap. Actually, the broadening of single-particle states $\propto kT$ will damp out the spin gap when $KT > \Delta_{SG}$, as seems to be observed. But at low $T$, $\Delta_{SG}$ will not vary with $T$.

This has been a very preliminary account of this work, which is emphatically in progress. I have benefitted from discussions with many people, especially Steve Strong, but also T.V. Ramakrishnan, S. Sarker, G. Baskaran, D. Clarke; S-D. Liang helped me with the integral.
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