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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 tunnelling interactions. Some predictions can be made.

The problem with the spin gap [1] is that there are too many right ways to understand it within the interlayer theory [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.

(i) The most obvious is spinon pairing. We have realized all along that the normal state has charge–spin separation, so why did we not expect two pairings, one for spin and the second for charge?

(ii) Also obvious is that 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.

(iii) 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 [3] model is not a complete theory, but can be used to calculate $\chi(T)$, 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, with little or no tendency towards superconductivity or to exhibit antiferromagnetism, once it is metallic—that is, 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 [4] Fermi liquid symmetry $(\mathrm{U}(2))^Z = (U(1) \times \mathrm{SU}(2))^Z$, 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 article shows that this description includes, but is not confined 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.

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Our theory [7] 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, namely, 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,

$$\psi^*_{\hat{k}}(r) \simeq s^+_{\hat{k}}(r)\,\mathrm{e}^{\mathrm{i}\theta_{\hat{k}}(r)}.$$

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 at which the interplane interactions come into play.

Spinons in 2D are paired but gapless. What the nonexistence 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 intact the crucial fact of Fermi or Luttinger liquids: 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', that is, the spinons which used to have a free-electron-like linear spectrum

$$v_s\big(k - k_F\big) \qquad \text{or} \qquad v_s \sin\left(\frac{\pi}{2}\,\frac{(k-k_F)}{k_F}\right)$$

to open a gap and have energies

$$E^2 = \Delta^2(\hat{k}) + v_s^2\big(k - k_F\big)^2. \tag{1}$$

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 $-k = -k,\ -\sigma$ and $k = k,\ \sigma$)

$$s^+_k = s_{-k} \qquad s_k = s^+_{-k}$$

so that the Hamiltonian for free spinons may be written

$$v_s\big(k - k_F\big)\Big(s^+_k s^+_{-k} + s_{-k} s_k\Big) \tag{2}$$

just as well as it can 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 [6]. It is natural that spinons are more easily paired in the underdoped region, because the spinon velocity becomes progressively lower (J smaller) as we approach the Mott insulator; therefore the density of states is higher, χ_{pair} larger, on the underdoped side.

Finally, let me make one last remark of a synthetic, rather than analytical, nature. As I have already said, the basic description of either 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 and k_y. There is only one source of such interactions, namely the interlayer tunnelling

$$\mathcal{H}_{IL} = \sum_{k,\sigma,i,j} t_\perp(k) c^+_{ki\sigma} c_{kj\sigma} \tag{3}$$

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

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

and superexchange

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

(in both, $k' \simeq k$) which represent exchange of charge and spin, respectively, between two layers. The empirical (and theoretical) fact that coherent single-particle hopping does not occur in the cuprates leaves these as the two second-order terms which can lead to coherent interactions—such as those we are seeking—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.

Equation (5) does not involve any charge exchange between planes and 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. Equation (4) only conserves the total charge of the two planes and hence is not a true spinon operator at all. Nevertheless, 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 [1], neither does it 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 $t_\perp$. These systems are very like Mott insulators in one of three spatial dimensions and they exhibit superexchange in that dimension, but they retain no Mott character in the two dimensions of the planes.

It is an unpublished conjecture of Baskaran that λ_S/λ_J increases as we approach the insulating phase, namely, as α, the Fermi surface exponent, increases. This may be one other reason why underdoped materials exhibit the spin gap.

Now, finally, let us tackle 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 anything better than a rough guide. These assumptions are the following. (i) The Schrieffer pairing condition, namely, 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 quasi-coherent matrix element; our picture of the kind of process involved is that a transition to a high-energy state intervenes between two low-energy states which are connected by two—and only two—single-particle tunnelling processes, $k_a \to k_b$ and $-k_b \to -k_a$. It is perhaps best to think of the pairing as always k, $-k$ but with the centre of mass momentum thermally fluctuating. (ii) More orthodox but more serious, we neglect $|v_c - v_s|$ and treat c^+_k as though it were an eigenoperation; that is

$$\mathcal{H}_K = \sum_k \epsilon_k n_k. \tag{6}$$

Actually we use the Nambu–PWA form

$$\mathcal{H}_K(k) = \epsilon_k\big(n_k + n_{-k} - 1\big) = \epsilon_k \tau_{3k}.$$

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

$$\mathcal{H} = \sum_k \mathcal{H}_k$$

$$\mathcal{H}_k = \mathcal{H}_K(k) + \lambda_j c^+_{k1} c^+_{-k1} c_{-k2} c_{k2} + 1 \leftrightarrow 2 + \lambda_S c^+_{k1} c^+_{-k2} c^+_{-k1} c_{k2}$$

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

$$Z = 16\cosh^4\left(\frac{\beta\epsilon_k}{2}\right) + 2\left[\cosh\left(\beta\lambda_J\right) - 1\right]$$

(because with the added '-1' $n = 2$ states are at 0 energy).

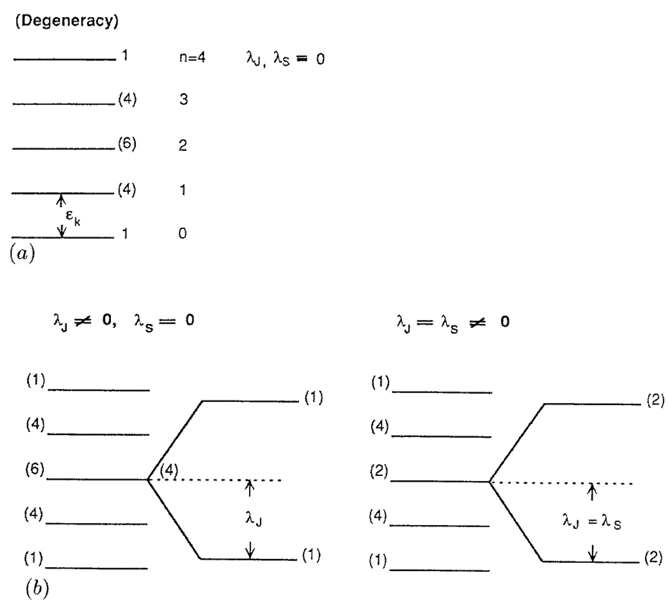

Figure 1. (*a*) Free-particle levels. (*b*) Levels with interactions, showing the diagonalization of the effective Hamiltonian.

χ for this case is

$$\chi = \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{\cosh^2 \beta\epsilon/2}{\cosh^4(\beta\epsilon/2) + \frac{1}{8}[\cosh(\beta J) - 1]}.$$

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 $\frac{1}{8}$ by $\frac{1}{4}$. This is the curve for susceptibility that I show in figure 2 and it is not a bad fit to susceptibility data.

However, 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'—that is, only the $n = 2$ states are connected to each other within the k manifold. However, in some real sense these are states with the spinons paired but with no holon pairing—no charge

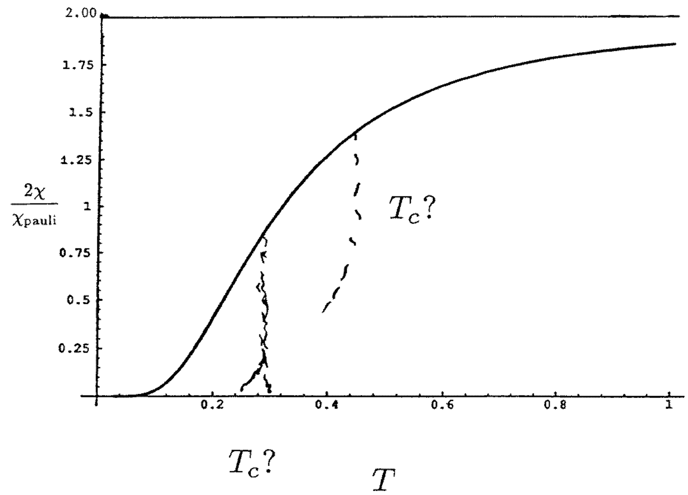

Figure 2. The susceptibility–temperature curve.

pairing—at all, even though nominally different layers are connected. I think it is more nearly valid to describe the correct state by re-writing $\mathcal{H}_j + \mathcal{H}_s$ as

$$\left(\mathcal{H}_J + \mathcal{H}_S\right)_k \simeq c^+_{ke} c^+_{-ke} c_{-ke} c_{ke}$$

where $c^+_{ke} = (c_{k1} + c_{k2})/\sqrt{2}$. That is, the spin-gap state is a state in which spinons belonging to the *even* linear combinations are paired, the *odd* unpaired. This has a strong relationship to the Keimer neutron selection rule observed for the superconducting state [8]. 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 assumptions of a Fermi rather than a 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. However, at low T, Δ_{SG} will not vary with T. This has been a very preliminary account of this work, which is emphatically in progress.

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