# Theory of the spin gap in high-temperature superconductors

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We analyze pairing in two-dimensional spin liquids. We argue that interplane pairing enhanced by magnetic correlations is the most plausible explanation of the spin-gap phenomenon observed in underdoped cuprates. The details of the pairing theory depend on the in-plane antiferromagnetic correlations. We consider two models:  $2p_F$  correlations induced by a strong gauge-field interaction and undamped spin waves. We estimate the pairing temperature  $T_s$  and the angular dependence of the gap function and discuss physical consequences.

## I. INTRODUCTION

Many high- $T_c$  materials exhibit anomalous temperature dependence of the bulk magnetic susceptibility,  $\chi$ , in a range of temperatures above  $T_c$ , suggesting that a spin pseudogap opens above the superconducting transition temperature.<sup>1</sup> To define more precisely what we mean by spin pseudogap consider the susceptibility data for YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> shown as the curve labeled "248" in Fig. 1. (The data points shown in Fig. 1 were obtained from the susceptibility reported in Refs. 2, 3 as discussed in Ref. 4) There are clearly two regimes, separated by a scale  $T_s \approx 200$  K. For  $T > T_s$ ,  $\chi \cong A + BT$  with A,B > 0. For  $T < T_s$ ,  $\chi(T)$  drops more rapidly; indeed a straight line fit to  $\chi(T)$  for  $T_c < T < T_s$  ( $T_c = 80$  K is the superconducting transition temperature for this compound) would yield a *negative*  $\chi$  at T=0. A negative  $\chi(0)$  is impos-

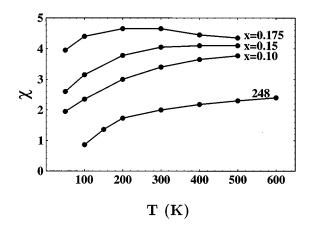


FIG. 1. Susceptibility of several high- $T_c$  materials: one-plane  $La_{2-x}Sr_xCuO_4$  with varying doping x which, as we shall argue, does not show spin-gap behavior and bilayer YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> (248) which does show it. Susceptibility is measured in the units of  $\mu_B^2$  eV per Cu atom.

sible; therefore the negative extrapolation implies that even for  $T > T_c$  (but  $T < T_s$ ) there is a gap for spin excitations. The origin of this "spin" gap is the main focus of this paper.

The properties of high-temperature superconducting materials are anomalous, and many different theories have been proposed to describe them. However, no general consensus has emerged. The origin of spin gap has been discussed by many authors<sup>1,5–8,4,9–11</sup> but these treatments are not completely satisfactory because, as we shall argue below, they are based on models which do not agree with all available data. We believe that any theory of the spin gap should have the following ingredients:

- (i) At least some of the magnetic response is Pauli-like, i.e., it comes from a particle-hole continuum of spin-1/2 fermions.
- (ii) Formation of the spin gap involves pairing instability of these fermions.
- (iii) This pairing is *not* a superconducting pairing, i.e., does not produce a Meissner effect or paraconductivity.

These assumptions imply that paired fermions are neutral and that any theory of the spin gap must involve the phenomenon of spin-charge separation; we use the gauge theory formalism to describe this.

Points (i)–(iii) do not completely specify the model. There are two additional issues.

- (iv) It is widely believed that there are strong antiferromagnetic spin fluctuations in high- $T_c$  materials. In the body of the paper we summarize the evidence for the existence of antiferromagnetic spin fluctuations, outline the different theories proposed to describe them, and give the implications for our calculations.
- (v) We believe that bilayer structure of YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> is important for the formation of the spin gap because it leads to interplane pairing. Whether the spin gap ex-

ists in single-plane materials such as  $La_{2-x}Sr_xCuO_4$ , in which interplane coupling is geometrically frustrated, is controversial.<sup>4,9</sup> Certainly, the evidence for it is weaker (see Fig. 1). Our theoretical results imply that spin-gap effects are greatly enhanced in bilayer or multilayer systems.

The outline of the paper is as follows. In Sec. II, we review the relevant experimental data and show that it implies points (i)-(v) above. In Sec. III we formulate the theoretical model and identify two different scenarios. In Secs. IV and V we present the solutions for the different scenarios. Section V contains a comparison of results to data and a conclusion.

## II. DATA

(i) Particle-hole continuum: We begin with the evidence that at least some of the magnetic response in spin-gap systems such as YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> comes from a particle-hole continuum of spin-1/2 fermions. A phenomenological argument is that there is little doubt that such a continuum describes the magnetic properties of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>. The uniform susceptibility of this compound has magnitude slightly larger than predicted by band theory and has very weak temperature dependence (as expected for a Fermi liquid).<sup>12</sup> The oxygen NMR relaxation rate  $1/{}^{17}T_1T$  is temperature independent (as expected in a Fermi liquid) and has magnitude slightly larger than predicted by the Korringa relation.<sup>13</sup> The copper relaxation rate  $1/^{63}T_1T$  increases as the temperature is decreased;<sup>14</sup> this has been argued to be due to antiferromagnetic correlations within a Fermi-liquid state.<sup>15</sup> Also, photoemission experiments<sup>16</sup> have observed a large Fermi surface in optimally doped YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>. The spin-gap compounds YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.6</sub> and YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> are produced by removing carriers from YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>; further, the physical properties seem to vary smoothly with doping. Therefore, it is natural to assume that the particle-hole continuum is also present in the spin-gap compounds.

An alternative point of view<sup>9</sup> is that the important spin excitations in underdoped compounds are weakly damped, gapped antiferromagnetic spin waves, with dispersion  $\omega^2 = c^2 k^2 + \Delta^2$ . However, theories in which the only magnetic excitations are spin waves with a gap are inconsistent with the  $\chi_s(T)$  data at high temperatures  $(T > T_s)$ , because at temperatures greater than the value of the zero-temperature gap  $\Delta_0$ , these theories predict<sup>17</sup>  $\chi_s = A + BT$  with A < 0 if  $\Delta_0 > 0$  and also predict for YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> a value for *B* larger, by a factor of 6, than is observed.<sup>18</sup> Another difficulty with the spin-wave-only model is that the kinematics of spin waves implies that the oxygen relaxation rate drops very rapidly with temperature. Indeed the theoretical prediction is  $1/[T_1T\chi_s] \sim T$  in contrast to the experimental result  $1/(T_1T_{\chi_s}) \approx \text{const.}^{18}$  Therefore there is little doubt that one must at least supplement the spin-wave model with a particle-hole continuum of fermions which controls at least the small-q spin response.<sup>19,20</sup> We note, however, that although the existence of such a particle-hole continuum would increase the constant part A of the uniform susceptibility and would add a constant contribution to the oxygen relaxation rate, it would not affect the slope B of the susceptibility if the interaction between spin waves and particlehole continuum is weak. There is as yet no model which describes all of the data. In any event, to understand the spin gap observed in  $\chi_s(T)$  one must understand how to open a gap in the spectrum of the fermions making up the particle-hole continuum.

(ii) Singlet pairing: In the absence of charge-density-wave order the only possibility for suppressing the spin response of fermions is to pair them into singlets. One example of such pairing is the BCS superconducting state. The pairing scale  $T_s \approx 200$  K is much less than any microscopic scale such as J or the bandwidth, so the pairing must be understood as a low-energy instability of the system.

(iii) Superconductivity: The data strongly suggest that the spin gap is not due to incipient superconducting pairing. There are three arguments; one is that the spin-gap scale  $T_s$ in YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> is approximately 200 K, far above the maximum  $T_c \approx 95$  K observed in any member of the Y-Ba-Cu-O family. The second is that superconducting fluctuations normally have a dramatic effect on the resistivity. In the layered materials the in-plane resistivity is expected to drop as T is decreased through the scale at which the fluctuations begin and to drop more and more rapidly as  $T_c$  is approached while the c-axis resistivity may increase or decrease depending on parameters of the material.<sup>21</sup> This behavior is not observed in  $YBa_2Cu_3O_{6.6}$  and in  $YBa_2Cu_4O_8$ . In these materials, there is some drop in  $\rho_{ab}$  as T is decreased through  $T_s$ , but then  $\rho_{ab}$ flattens out and depends only weakly on T near  $T_c$ .<sup>22,23</sup> The drop in  $\rho$  for  $T \sim T_s$  has been attributed,<sup>23</sup> in our view correctly, to changes in the inelastic scattering mechanism associated with the onset of the spin gap. The third argument is that although the c-axis resistivity does increase as T decreases below  $T_s$  in agreement with the predictions<sup>21</sup> for sufmaterials, anisotropic ficiently the observed magnetoresistance<sup>24</sup> is incompatible with superconducting fluctuations explanation because in a layered system the fluctuational superconductivity is strongly affected only by the fields perpendicular to the ab plane whereas the observed magnetoresistance was almost isotropic. It has been argued that the negative-U Hubbard model, in which the important physics is singlet pairing of conventional electrons, describes the spin-gap phenomena.<sup>8</sup> In our view the strong evidence for repulsive interactions and against paraconductivity renders this model irrelevant.

Of course, conventional superconductivity does produce a spin gap; thus  $T_s$  cannot be less than  $T_c$ . The interesting question is why, in some materials, it is much greater than  $T_c$ .

To summarize: the data imply the existence of a particlehole continuum of spin excitations and require that these excitations be paired into singlets in a way that does not produce superconductivity. This implies that "spin-charge separation" must occur. There are many scenarios of spincharge separation, all stemming from Anderson's original proposal.<sup>25</sup> We shall adopt the gauge theory approach.<sup>26,27</sup> We also note that unlike the conventional superconducting pairing of electrons, the pairing of chargeless fermions does not necessary imply the breaking of any symmetry, and so may result in a crossover, not in a genuine phase transition.<sup>5</sup>

(iv) Antiferromagnetism: A large literature has developed around the issue of antiferromagnetic correlations in high- $T_c$  materials. Many controversies remain unresolved, but it is

generally agreed that NMR  $T_1$  and  $T_2$  experiments imply the existence of strong, temperature dependent antiferromagnetic correlations. Specifically, for YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub>, the two Cu relaxation rates,  $1/T_1T$  and  $1/T_2$ , increase roughly as 1/T as T is decreased (for  $T > T_s$ ).<sup>28,29</sup> Generally, the NMR rates are given by

$$\frac{1}{T_1 T} = \lim_{\omega \to 0} \sum_q F_q \frac{\chi''(q,\omega)}{\omega}, \qquad (1)$$

$$\frac{1}{T_2} = \left[\sum_{q} \left[F_q \chi'(q,0)\right]^2\right]^{1/2},$$
(2)

where  $F_q$  is a form factor which is different for different nuclei.

The only tenable interpretation of the temperature dependence of the copper relaxation rate is that both real and imaginary parts of  $\chi(\mathbf{q})$  diverge at a particular wave vector Q, i.e., that there is an incipient magnetic instability. To prove this, suppose on the contrary that the T dependence of  $1/(T_1T)$  came from a wide range of momenta, so  $\chi(q,\omega)$  $=\phi(q)f(\omega,T)$ , with  $\phi(q)$  a temperature-independent function. For large frequencies,  $\omega \gg T$ ,  $f(\omega)$  should not depend on temperature, so in particular the imaginary part  $f''(\omega) = A_1 \omega^x$ , whereas at small frequencies,  $\omega \ll T$ ,  $f''(\omega)$ should be proportional to frequency,  $f''(\omega) = A_2 \omega$ . The proportionality coefficient  $A_2$  can be estimated by matching the low-frequency formula and the high-frequency formula at  $\omega \approx T$ , yielding  $A_2 = A_1 T^x$ . The NMR  $T_1$  data imply  $x \approx 0$ which via the Kramers-Kronig relation implies  $\chi'(q,\omega=0) \sim \ln T$ . This temperature dependence is too weak to account for the  $T_2$  data, so the hypothesis of a momentumindependent divergence of  $\chi$  must be rejected. It should be noted, however, that although neutron-scattering experiments detect antiferromagnetic fluctuations, neutron and NMR data are at present not quantitatively consistent.<sup>30,31</sup>

The proper theoretical model for the antiferromagnetic fluctuations is not clear. The two principal proposals are that the dominant antiferromagnetic excitations are weakly damped spin waves,<sup>9,17</sup> or are particle-hole pairs of an antiferromagnetically correlated fermion system.<sup>15</sup> The weakly damped spin-wave picture applies to the magnetic insulating parent compound and by continuity might be expected to apply to lightly doped but nonordered materials. The particle-hole picture presumably applies to the optimally doped materials which have been shown by photoemission to have large (Luttinger) Fermi surface] and by continuity might be expected to apply to somewhat underdoped materials. The crossover between these two regimes is an active area of research<sup>32</sup> but has not been understood in detail. We consider implications of both pictures for the pairing interaction.

The model of particle-hole pairs requires further discussion. We argued above on the basis of resistivity data that the fermions must be charge zero objects. An additional argument against conventional charge *e* Fermi liquid with anti-ferromagnetic correlations is that the magnetic properties of conventional Fermi liquid are incompatible with the  $T_1$ ,  $T_2$ , and  $\chi_s$  data.<sup>28,29,2,33</sup> The only known model of spin-1/2 charge 0 fermionic excitations ("spinons") which does not break time reversal or parity symmetry is the "spin liquid."

In a spin liquid, the gauge interaction between fermions affects the magnetic properties and has been shown to lead to a reasonable description of the spin dynamics of high- $T_c$  materials.<sup>34</sup> In the spin-wave picture a particle-hole continuum is also present; for the reasons given above we must assume that the underlying fermionic excitations are spinons. However, in this case the spin waves dominate the large q magnetic response.

(v) *Bilayers*: Our discussion so far has been focused on members of the Y-Ba family of high- $T_c$  materials. We believe that the magnetic dynamics of members of other families of high- $T_c$  materials are similar in all respects except for the existence of a spin gap *in a wide temperature range above*  $T_c$ . It is possible that, as some authors have argued,<sup>9</sup> La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> shows the beginning of spin-gap behavior for  $T\sim 60$  K, relatively near the superconducting  $T_c$ . However, to our knowledge only underdoped members of the Y-Ba family exhibit spin-gap behavior over a wide range of temperatures above  $T_c$ .

Consider first the  $\chi_s$  for La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> data presented in Fig. 1. These are obtained from bulk susceptibility data by subtracting core and van Vleck susceptibilities given in Ref. 36. Note that although there is a downturn in  $\chi_s(T)$  at T<100 K, extrapolated value of  $\lim_{T\to 0} \chi_s(T)$  is positive and relatively large. Although uncertainties in the value of the van Vleck susceptibility may exist, these are in our view by no means large enough to produce a  $\lim_{T\to 0} \chi_s(T) \leq 0$ . The oxygen<sup>30</sup> and copper<sup>30,37</sup>  $T_1$  relaxation data similarly show no sign of an extra downturn at a temperature  $T > T_c$  (although the rate of increase of the copper  $T_1^{-1}$  may slow for  $T \le 80$  K). Note that at  $T > T_s \approx T_c$ ,  $La_{2-x}Sr_xCuO_4$  does exhibit a  $\chi_s \approx A + BT$  regime as well as other properties difficult to describe in either a Fermi-liquid or a purely spinwave picture. We infer from this that the bilayer structure of the Y-Ba material is important only for raising  $T_s$  sufficiently far above  $T_c$  that spin-gap effects are easily observable.

There is, in fact, substantial evidence that the spin degrees of freedom in different planes of a bilayer are strongly coupled. Neutron-scattering measurements have essentially only detected spin fluctuations in which spins on adjacent CuO<sub>2</sub> layers are perfectly anticorrelated.<sup>31,38–40</sup> Moreover, the coupling between Cu spins on adjacent planes has been directly measured in a recent NMR  $T_2$  experiment in which the Cu nuclear spins in one plane of a bilayer were pumped and Cu nuclear spins in the other were measured.<sup>41</sup> This experiment determines the cross-relaxation time  $T_2^*$  which is given by expression<sup>42</sup>

$$\frac{1}{T_2^*} = \left[\sum_q \left[F_q \chi'_{12}(q,0)\right]^2\right]^{1/2}.$$
(3)

This expression is very similar to the expression (2) for inplane relaxation rate, except that instead of a single-plane susceptibility  $\chi'(q,0)$  it contains  $\chi'_{12}(q,0)$  which measures the response of spins on plane 1 to the magnetic field on plane 2.

We assume that electrons on adjacent planes in bilayer interact via the Hamiltonian

$$H_{\perp} = J_{\perp} \sum S_i^{(1)} S_i^{(2)} .$$
 (4)

If the interaction,  $J_{\perp}$  is weak then the between the planes susceptibility,  $\chi_{12}$ , may be calculated by perturbation theory<sup>43</sup> and is

$$\chi_{12}'(q,0) = J_{\perp} [\chi'(q,0)]^2.$$
<sup>(5)</sup>

Experimentally the ratio  $T_2/T_2^*$  grows from 0.14 at 200 K to 0.28 at 100 K. This increase reflects the temperature dependence of  $\chi'$ . If  $\chi'$  is divergent at some wave vector  $\mathbf{Q}$  as  $T \rightarrow 0$  and is given by a scaling form  $\chi' = T^{-\alpha} f(|q-Q|T^{-x})$  (where x and  $\alpha$  are scaling exponents) then from Eqs. (2), (3), and (5) it may be shown that  $T_2/T_2^* = cJ_{\perp}\chi'(0,Q)$  with c a constant of the order of unity.<sup>43</sup> Thus, the observed maximal ratio of  $T_2/T_2^* = 0.3$  implies that the interplane coupling is not negligible, but still may be treated via perturbation theory. In this paper we shall show that the effect of this interplane coupling on the fermions is large and in fact leads to the opening of a spin gap.

Equation (4) applies to Y-Ba-Cu-O and to the multilayer Bi-Sr-Ca-Cu-O compounds in which the Cu ion on one plane sits directly over the Cu ion in the next lower plane. It does not apply to  $La_{2-x}Sr_xCuO_4$  compounds in which the crystal structure is such that a Cu ion on plane is coupled equally to four Cu in each adjacent plane, so Eq. (4) would become

$$H_{\perp \prime} = \sum_{a,\langle ij\rangle} J_{ij}^{\perp} S_i^{(a)} S_j^{(a+1)} \,. \tag{6}$$

The crystal structure of  $La_{2-x}Sr_xCuO_4$  implies that  $J_{\perp}(q)$  vanishes at  $q = (\pi, \pi)$ , so the enhancement of interplane pairing by antiferromagnetic fluctuations is much less effective than in the Y-Ba-Cu-O or Bi-Sr-Ca-Cu-O systems.

#### III. MODEL

(i) Single plane. In Sec. II we showed that experiment implies that a theoretical treatment of spin-gap effects in high- $T_c$  superconductors should involve pairing of fermions in a spin liquid. In this subsection we describe the model we use for the spin liquid in one CuO<sub>2</sub> plane and discuss different pairing mechanisms.

The low-energy excitations of a spin liquid are S=1/2, charge 0 fermions,  $c^{\dagger}$ , near a Fermi line, and a bosonic gauge field, *a*. The action describing the spin liquid has been derived from more fundamental models of correlated electrons by assuming that spin-charge separation exists, i.e., that the electron field  $\psi^+$  may be written as the product of a spinless, charge *e* Bose field *b* and a S=1/2 charge 0 Fermi field  $c^+$ as  $\psi^+=c^+b$  and that the effect of the charge degrees of freedom on the spin degrees of freedom is small. These assumptions have been shown to be justified in the low doping, large spin degeneracy limit of the *t-J* model.<sup>26</sup> Whether these assumptions are theoretically justifiable in the physically relevant regime is still controversial. We shall assume that they are because we see no other way to explain the experimental data discussed in Sec. II.

The spin-liquid model is specified by the action

$$H = \sum_{p,\sigma} c^{\dagger}_{p\sigma} \boldsymbol{\epsilon}(p) + c_{p\sigma} + \sum_{p,k,\sigma} c^{\dagger}_{p+k/2,\sigma} \vec{a}_k \vec{v}(p) c_{p-k/2,\sigma} + \sum_{p_i} W c^{\dagger}_{p_1,\sigma} c_{p_2,\sigma} c^{\dagger}_{p_3,\sigma} c_{p_4,\sigma} \delta \left( \sum p_i \right) + \frac{1}{4g_0^2} f^2_{\mu\nu}.$$
(7)

Here, as usual,  $f_{\mu\nu} = \partial_{\mu}a_{\nu} - \partial_{\nu}a_{\mu}$ ,  $g_0$  is the bare fermiongauge-field interaction constant,  $\mathbf{v} = \partial \epsilon / \partial \mathbf{p}$ , W is a constant of short-range interaction, and  $\sigma = 1 \dots N$  is a spin index. In the physical case the spin degeneracy N=2. The gauge field modifies the properties of the fermions. These modifications have been studied in detail. The results we shall need are (i) the electron self-energy is<sup>44,45</sup>  $\Sigma(\epsilon) = \omega_0^{1/3} \epsilon^{2/3}$  (ii) the vertex  $\Gamma$ coupling the fermion spin to an external magnetic field of wave vector q becomes singular at  $|q| = 2p_F$ , while at all other wave vectors the vertex corrections are not singular.<sup>46</sup> Specifically,

$$\Gamma = \Gamma_0 \left(\frac{\omega_0}{\Lambda}\right)^{\sigma}.$$
(8)

Here  $\Lambda$  is the largest of  $v_F(|q|-2p_F)$ ,  $\omega^{2/3}$ ,  $T^{2/3}$ , and

$$\omega_0 = \left(\frac{1}{2\sqrt{3}}\right)^3 \frac{v_F^3 g_0^4}{\pi^2 p_0} \tag{9}$$

is the upper cutoff scale determined by the strength of the gauge-field fluctuations. By " $2p_F$ " we mean a wave vector **Q** which connects two points on the Fermi line with parallel tangents. For a circular Fermi line any vector **Q** of magnitude  $2p_F$  connects two such points. The exponent  $\sigma$  has been calculated only in the limits  $N \ge 1$  and  $N \ll 1$ ; by extrapolation of these results to the physical value N=2 we estimated<sup>46</sup> that  $1 \ge \sigma \ge 1/3$ .

The main effect of the self-energy renormalization is that the resulting inelastic-scattering rate  $\sim T^{2/3}$  is so strong that no nonsingular interaction can lead to a BCS pairing of spinons<sup>47</sup> (except via a first-order transition which is not observed); therefore any spinon-based theory of the spin gap must involve a singular interaction.

Two cases arise for the vertex renormalization. If  $\sigma < 1/3$ , the spin physics is not modified in an essential way. A T=0critical point separates a  $W < W_c$  phase with short-range spin correlations from a  $W > W_c$  phase with long-range order; the appearance of the anomalous exponent  $\sigma$  in the " $2p_F$ " vertex modifies the critical properties of the transition at  $W = W_c$ as discussed in detail in Ref. 34. However, if  $\sigma > 1/3$  then the  $0 \le W < W_c$  phase is anomalous, and exhibits a divergent " $2p_F$ " spin susceptibility and power-law spin correlations

$$\chi(\boldsymbol{\omega}, \mathbf{k}) = \sqrt{\frac{\omega_0 p_0}{v_F^3}} \frac{1}{\left[c_{\boldsymbol{\omega}} \left(\frac{|\boldsymbol{\omega}|}{\omega_0}\right)^{2\sigma - 2/3} + c_k \left(\frac{|\boldsymbol{k}| |\boldsymbol{v}_F}{\omega_0}\right)^{3\sigma - 1}\right]},\tag{10}$$

where  $c_{\omega}, c_k \sim 1$ . Here we use local momentum coordinates associated with the Fermi line, namely  $\mathbf{k} = \mathbf{Q} + \mathbf{e}_{\parallel} k_{\parallel}$  where  $\mathbf{Q}$ connects two points on the Fermi line with parallel tangents and  $\mathbf{e}_{\parallel}$  is the unit vector parallel to the Fermi velocity at these points. These coordinates are generalization of radial  $k_{\parallel} = |p| - 2p_F$  and angular coordinates for the case of a noncircular Fermi line. The experimental implications have been discussed elsewhere;<sup>34</sup> in particular, it has been shown that the choice  $\sigma = 3/4$  yields rough agreement with experimental data.

Having discussed the spin-liquid model we now consider possible pairing interactions. The short-range interaction W would lead to pairing in a Fermi liquid; however, as mentioned above, for a spin liquid the inelastic scattering due to the gauge-field suppresses any second-order pairing instability due to a nonsingular interaction. For this reason we believe the results obtained in Ref. 7 do not explain the spingap phenomena. Of course, a first-order transition would still be possible;<sup>47</sup> but there is no experimental evidence for this in high- $T_c$  materials. However, singular interactions exist. One involves the gauge field, but this interaction is repulsive in all channels for the model specified above and does not lead to pairing.<sup>26</sup> Another singular interaction comes from exchange of long-ranged spin fluctuations; these may arise either from proximity to a T=0 antiferromagnetic transition or because  $\sigma > 1/3$ .

There are three types of antiferromagnetic transitions, distinguished by the relation of the ordering wave vector, **Q**, to  $2p_F$ . If  $|\mathbf{Q}| > 2p_F$ , the fermion-fermion interaction mediated by spin fluctuations is, in fact, not singular for the fermions near the Fermi line. If  $|\mathbf{Q}|=2p_F$  and  $\sigma < 1/3$ , then the singularity of the interaction is too weak to overcome the pairbreaking effect of the gauge field. If  $Q < 2p_F$ , then one obtains a logarithmic divergence in the pairing amplitude. The theory of the pairing for  $Q < 2p_F$  case may be derived by the following arguments given in Ref. 10 but replacing the factor  $\chi^2(\omega,q)$  by the first power  $\chi(\omega,q)$  in Eq. (5) of Ref. 10. The steps leading to Eq. (8) of Ref. 10 yield a logarithmic divergence of the pairing kernel in the gap equation. However, we do not believe that the  $\mathbf{Q} < 2p_F$  case is relevant to high- $T_c$ materials because the predicted temperature dependence of the copper NMR  $T_2$  rate is too weak and because neutron scattering has only observed fluctuations peaked at wave vectors  $Q \ge 2p_F$ .<sup>31,38,40</sup>

If  $\sigma > 1/3$ , then the susceptibility is divergent at  $Q \rightarrow 2p_F$ ,  $(\omega,T) \rightarrow 0$ . However, as was shown in Ref. 46, the same physics implies that the fermion-fermion interaction is renormalized to zero (due to the renormalization in the Cooper channel), so the divergence in the susceptibility does not propagate into any other physical quantity.

(ii) *Two planes*: The theoretical discussion in the previous subsection and the experimental analysis of Sec. II implied that theories involving only a single CuO<sub>2</sub> plane could not explain the existence of a spin gap in a wide range of temperatures above  $T_c$ . In this subsection we extend the theory of the spin liquid to include interplane coupling. We assume that each plane is described by the Hamiltonian, Eq. (7), and that the only coupling between the planes is given by Eq. (4). In particular, terms of the form  $t_{\perp}c^{+(1)}c^{(2)}$ +H.c. are not allowed: there is no coherent hopping of spinons between planes. The assumption that there is no interplane hopping of spinons may be justified by extending the derivation<sup>26</sup> of the spin-liquid action H to the two-plane situation. In the microscopic model there is a between-planes electron hopping  $t_{\perp}^{el}$  which, it is reasonable to assume, is much less than the inplane hopping t. It emerges from the theoretical derivation

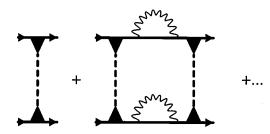


FIG. 2. Ladder sum leading to pairing of fermions on adjacent planes. Solid lines denote fermions propagators renormalized by the gauge field, dashed lines denote spin-spin interaction,  $J_{\perp}$ , between the planes and solid triangles denote vertices renormalized by the gauge field.

that one must have  $t_{\perp}^{\text{el}}$  greater than a critical value of order t in order to have coherent between-planes hopping of spinons. If there is no coherent hopping then the leading coupling term is Eq. (4).

We assume that  $J_{\perp}$  is sufficiently weak that it may be treated in perturbation theory. This assumption is justified by the cross-relaxation experiment of Stern *et al.*,<sup>41</sup> as previously discussed. The only effect we need consider the pairing interaction due to  $J_{\perp}$ . If  $Q < 2p_F$  then the relevant theory was given in Refs. 10 and 48. If  $Q = 2p_F$  and  $\sigma < 1/3$  the theory is very similar. As discussed above, we do not believe any of these starting points are consistent with experiment. We therefore study in Sec. IV the case  $\sigma > 1/3$ . In Sec. V we treat the case of undamped spin fluctuations.

# IV. GAP EQUATION: $\sigma > 1/3$

In this section we consider pairing due to the betweenplanes interaction, Eq. (4). In general, a pairing instability of a fermion system is signaled by a divergence of the series of particle-particle ladder diagrams as shown in Fig. 2.<sup>49</sup> In the present problem, the two lines correspond to fermions on different planes and the between planes interaction  $J_{\perp}$  is renormalized by the gauge interaction. This renormalization implies that the basic rung of the ladder is an effective pairing interaction

$$V(\omega,k) = J_{\perp} [\Gamma(\omega,k)]^2, \qquad (11)$$

where  $\Gamma$  is given in Eq. (8). Note the absence in Fig. 2 of gauge-field lines connecting fermions on one plane to fermions on the other plane. This absence follows from the assumption of no coherent fermion hopping between the planes and is the reason why the interaction is enhanced by the gauge field, rather than suppressed by it as is the in-plane interaction.

Because the interaction  $V(\omega,k)$  connects fermions on different planes it does not give rise to a fermion self-energy in the leading order of perturbation theory. Diagrams of higher order in  $J_{\perp}$  may be absorbed into the short-range interaction W between the fermions on each plane and its renormalization by gauge fields. We have previously shown that W is renormalized to zero by gauge fields, so these diagrams may be neglected. Therefore we may obtain the pairing effects of the interaction V from the ladder sum in Fig. 2. The analytic expression corresponding this diagram is, after integration over  $p_{\parallel}$ 

$$\Delta(p_{\perp}, \epsilon) = \frac{T}{4\pi} \frac{J_{\perp}a^2}{v_F}$$

$$\times \sum_{\omega} \int \frac{\Delta(p'_{\perp} + p_{\perp}, \epsilon + \omega)dp'_{\perp}}{\left[ \left(\frac{\omega}{\omega_0}\right)^{\sigma} + \left(\frac{v_F p_{\perp}^2}{p_0 \omega_0}\right)^{3\sigma/2} \right]^2 (\omega + \epsilon)^{2/3} \omega_0^{1/3}}$$
(12)

The integral on the right-hand side of this equation is infrared dominated and so may be evaluated by scaling (up to numerical factors). We also use the definition of  $\omega_0$ , Eq. (9), to eliminate the combination  $\omega_0/v_F$ . We find that  $T_s$  is given by

$$T_s = \beta \omega_0 (J_\perp a^2 g^2)^{3/(6\sigma - 2)}, \qquad (13)$$

where  $\beta$  is a numerical coefficient of the order of unity and  $g^2$  is renormalized fermion-gauge-field interaction constant. The value of  $g^2$  has been estimated from the temperature dependence of the resistivity,<sup>50</sup> and  $\omega_0$  from the band structure. Roughly,  $1/(a^2g^2) \sim 50$  meV and  $\omega_0 \sim 100$  meV.  $J_{\perp}$  can be estimated from the cross-relaxation experiment to be  $J_{\perp} \sim 5$  meV. In order for this  $T_c$  to be of a reasonable order of magnitude, one must have  $6\sigma - 2\approx 3$ , i.e.,  $\sigma \approx 5/6$ , because  $J_{\perp}$  is small. This value of  $\sigma$  would imply a  $1/T_1T \sim T^{-4/3}$ , a somewhat more rapid variation than is observed. The dependence of  $T_s$  on materials parameters is similar to the dependence of the Cu NMR relaxation rates;<sup>34</sup> also  $T_s$  is large when  $1/T_2$  and  $1/T_1T$  are large and conversely.

Although the divergent interaction exists at all points on the Fermi line, the amplitude varies with position,  $\theta$ . There are two effects: the gauge interaction energy scale  $\omega_0$  varies with  $\theta$  and also in a lattice one must consider processes involving momentum transfer  $\mathbf{q} + \mathbf{G}$  where  $\mathbf{G}$  is a reciprocallattice vector. For Fermi surfaces near half filling, there exists momenta **p** on the Fermi line for which both  $\mathbf{p}-\mathbf{q}$  and  $\mathbf{p}+\mathbf{q}+\mathbf{G}$  are on the Fermi line; near these points the interaction is particularly large. As discussed in Sec. VI of Ref. 46 we expect these effects to produce a substantial variation of the interaction in high- $T_c$  materials. Therefore we expect that as one lowers the temperature the gap first appears at the points  $\theta_{\rm max}$ at which  $\omega_0$  is maximal, so  $T_s = \beta \omega_0 (\theta_{\text{max}}) (J_\perp a^2 g^2)^{3/6\sigma - 2}$ . For T near  $T_s$  the gap function  $\Delta(\theta)$  will be very strongly peaked about  $\theta_{max}$ ; indeed from Eq. (12) we see that  $\Delta(\theta)$  decays away from  $\theta_{\text{max}}$  as  $|\theta - \theta_{\text{max}}|^{-6\sigma}$ . For T=0 the gap spreads over the whole Fermi surface but remains very anisotropic:

$$\Delta(\theta) \approx \beta \omega_0(\theta) (J_\perp a^2 g^2)^{3/6\sigma - 2}.$$
 (14)

Finally, we note that because the gap function is so strongly peaked at particular points on the Fermi line, the energy is not very sensitive to the symmetry of the gap. In single-plane models, the pairing tends to be d wave so that the two members of the Cooper pair can avoid each other. In the present model, the two members of the Cooper pair reside on different planes, so d-wave pairing becomes favorable only when tunneling between planes is included.<sup>51</sup>

## V. GAP EQUATION: SPIN WAVES

In this section we consider the implications for the formation of the spin gap of an alternative picture of the origin of the antiferromagnetic correlations. We suppose that there are weakly damped propagating spin waves **n** with dispersion  $\omega^2 = c^2 [(\vec{k} - \vec{Q})^2] + \delta^2$  and we ask how these lead to pairing. Here  $Q = (\pi, \pi)$ , *c* is the spin-wave velocity and  $\delta$  is the spin-wave gap. In the "quantum critical" regime relevant for high- $T_c$  superconductors,  $\delta = \alpha T$  with  $\alpha \approx 1$ . We assume that  $\Delta G = |Q| - 2p_F > 0$ , so the low-energy spin waves lie outside of the particle-hole continuum, and it is consistent to assume they are coupled to the fermions, but are undamped. The condition that the low-energy spin waves are outside the particle-hole continuum is (if  $c \leq v_F$ )

$$c\Delta G > T.$$
 (15)

In high- $T_c$  materials we estimate from the Fermi line observed in Ref. 52 that  $\Delta G \ge 0.1$  Å<sup>-1</sup>. In insulating La<sub>2</sub>CuO<sub>4</sub>, c=0.75 eV-Å;<sup>53</sup> the previously discussed fits to  $T_2/T_1T$  in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.6</sub> imply c=0.35 eV-Å.<sup>18</sup> Adopting the latter value we find that the condition for the validity of this assumption is  $T \le 0.035$  eV $\approx 400$  K. Thus the model may be adequate for discussion of spin-gap phenomena at  $T \sim 150$  K, but the relevance to the spin dynamics at room temperature or above is questionable.

The action describing the coupling of fermions to spin waves is

$$H_{t} = H + H_{sw},$$

$$H_{sw} = g \sum_{\omega,\epsilon,k,p} \vec{n}_{\omega,k} c^{\dagger}_{\epsilon+\omega,p+k} \vec{\sigma} c_{\epsilon,p}$$

$$+ \sum_{\omega,k} \frac{1}{2D(\omega,k)} \vec{n}_{\omega,k} \vec{n}_{-\omega,-k} + J_{\perp} \vec{n}^{(1)}_{\omega,k} \vec{n}^{(2)}_{-\omega,-k}.$$
(16)

Here *H* is the fermion-gauge-field action given in Eq. (7),  $\vec{n}$  describes the undamped spin fluctuation, and the spin-fluctuation propagator  $D(\omega,k)$  is

$$D(\omega,k) = \frac{u}{\omega^2 + (ck)^2 + \delta^2}$$
(17)

and u and  $\delta$  are parameters with the dimension of energy. As in the previous section, the interplane coupling leads to an effective pairing interaction  $V_{\text{eff}}$  given by

$$V_{\rm eff}(\omega,k) = \frac{(gu)^2 J_{\perp}}{[\omega^2 + (ck)^2 + \delta^2]^2}.$$
 (18)

In order to account for the Cu relaxation rate data, we must assume that for  $T > T_s$  the model is in the quantum critical regime in which  $\delta = \alpha T$ . Note that the momentum k is measured from the commensurate antiferromagnetic wave vector  $\mathbf{Q} = (\pi, \pi)$  and that  $V_{\text{eff}}$  is a very strongly peaked function of k. Thus,  $V_{\text{eff}}$  scatters a fermion of momentum **p** mostly to states with momentum very near  $\mathbf{p}+\mathbf{Q}$  and if Eq. (15) is satisfied and **p** is on the Fermi surface, these final states are far from the Fermi surface. This strong momentum dependence means that the gap equation decomposes into two equations, one expressing the gap at momentum near  $\mathbf{p}$ ,  $\Delta_{\epsilon}(p)$ , in terms of the Green function at momenta near  $\mathbf{p}+\mathbf{Q}$  and another one expressing the gap at momentum  $\mathbf{p}+\mathbf{Q}$ ,  $\Delta_{\epsilon}^{*}(p)$ , in terms of the Green function at momenta near p. Specifically,

$$\Delta_{\epsilon}(p) = \sum_{\omega,q} \frac{TV_{\text{eff}}(\omega,q)\Delta^*_{\epsilon+\omega}(p+q)}{\omega_0^{2/3}|\epsilon+\omega|^{4/3}+\tilde{\zeta}^2_{p+q}+[\Delta^*_{\epsilon+\omega}(p+q)]^2},$$
(19)

$$\Delta_{\boldsymbol{\epsilon}}^{*}(p) = \sum_{\boldsymbol{\omega},q} \frac{TV_{\text{eff}}(\boldsymbol{\omega},q)\Delta_{\boldsymbol{\epsilon}+\boldsymbol{\omega}}(p+q)}{\boldsymbol{\omega}_{0}^{2/3}|\boldsymbol{\epsilon}+\boldsymbol{\omega}|^{4/3} + \boldsymbol{\zeta}_{p+q}^{2} + [\Delta_{\boldsymbol{\epsilon}+\boldsymbol{\omega}}(p+q)]^{2}}.$$
(20)

Here  $\zeta_p$  is the fermion energy,  $\tilde{\zeta}_p = \zeta_{p+Q}$ ; for circular Fermi line  $\zeta_p = v_F(|\mathbf{p}| - p_F)$ . Because  $V_{\text{eff}}$  is a strongly peaked function of q, we may neglect the q in the denominator of (19). The magnitude of the denominator is then controlled by the magnitude of  $\zeta_{p+Q}$ . This depends on the position of p along the Fermi line. The minimal value of  $\zeta_{p+Q}$  is  $v_F\Delta G$  and the maximal value is of the order of  $\epsilon_F$ . Because  $\int V_{\text{eff}}(\omega,q)d^2q$ is a singular function of  $\omega$ , the frequency sum is dominated by  $\omega \sim max(T,\delta)$  and we expect that  $\delta \sim T$ , so by (15) we may also neglect the frequency and  $\Delta^*$  dependence of the fermionic denominator in (19). The first equation (19) then becomes a linear convolution equation; it can be combined with the second equation (19) giving an equation which contains only the gap function in the vicinity of the Fermi line

$$\Delta_{\epsilon}(p) = \frac{T}{\zeta_{p+Q}^2} \sum_{\omega,q} \frac{W_{\text{eff}}(\omega,q)\Delta_{\epsilon+\omega}(p+q)}{\omega_0^{2/3} |\epsilon+\omega|^{4/3} + \zeta_{p+q}^2 + \Delta_{\epsilon+\omega}^2(p+q)}$$
(21)

with the singular kernel

$$W_{\text{eff}}(\omega,q) = T \sum_{\eta,k} V_{\text{eff}}(\eta,k) V_{\text{eff}}(\omega-\eta,q-k). \quad (22)$$

In the gap equation (21) the assumption that p is on the Fermi surface means that the singularities in the fermion denominator must be also considered and compared to the singularities of the kernel  $W_{\text{eff}}$ . The fermion propagator depends sensitively only on the component of momentum normal to the Fermi surface and, as we show below,  $\Delta_{\epsilon}(p)$  also changes smoothly along the Fermi surface. We may therefore integrate over the component along the Fermi line,  $q_{\perp}$ , immediately, obtaining an equation similar to (21) but with  $q_{\perp}=0$  and a modified kernel

$$W_{\rm eff}(\omega, q_{\parallel}) = \frac{T(gu)^4 J_{\perp}^2}{16c^2} \sum_{\eta, k_{\parallel}} \frac{1}{\left[\eta^2 + (ck_{\parallel})^2 + \delta^2\right]^{3/2}} \times \frac{1}{\left[(\omega - \eta)^2 + (ck_{\parallel} - cq_{\parallel})^2 + \delta^2\right]^{3/2}}.$$
(23)

Two cases then arise. If

$$\frac{\delta}{c} < \frac{\max(\omega_0^{1/3} T^{2/3}, \Delta)}{\upsilon_F}, \qquad (24)$$

then the singularity in  $W_{\text{eff}}$  is dominant and we may perform the  $k_{\parallel}$  and  $q_{\parallel}$  integrals obtaining

$$\Delta_{\epsilon}(p) = \frac{T}{\zeta_{p+Q}^2} \sum_{\omega} \frac{W_{\text{eff}}(\omega) \Delta_{\epsilon+\omega}(p)}{\omega_0^{2/3} |\epsilon+\omega|^{4/3} + \zeta_p^2 + \Delta_{\epsilon+\omega}^2(p)}$$
(25)

with

$$W_{\rm eff}(\omega) = \frac{T(gu)^4 J_{\perp}^2}{16\pi^2 c^4} \sum_{\eta} \frac{1}{[\eta^2 + \delta^2]} \frac{1}{[(\omega - \eta)^2 + \delta^2]}.$$
(26)

However, if the condition (24) is not satisfied, then the singularity in the fermion denominator is dominant and we obtain

$$\Delta_{\epsilon}(p) = \frac{T}{\zeta_{p+Q}^2} \sum_{\omega} \frac{W_{\text{eff}}(\omega) \Delta_{\epsilon+\omega}(p)}{\sqrt{\omega_0^{2/3} |\epsilon+\omega|^{4/3} + \Delta_{\epsilon+\omega}^2(p)}}$$
(27)

with

$$W_{\text{eff}}(\omega) = \frac{T(gu)^4 J_{\perp}^2}{32 \,\pi c^3 v_F} \sum_{\eta} \int \frac{dk}{[\eta^2 + \delta^2 + k^2]^{3/2}} \times \frac{1}{[(\omega - \eta)^2 + \delta^2 + k^2]^{3/2}}.$$
 (28)

This system of equations may be solved to determine  $T_s$  and  $\Delta(T)$ . At low T, or for not too small c we expect Eq. (24) to be satisfied, so we shall consider in detail only Eqs. (25) and (26). The other case leads to very similar results.

To estimate  $T_s$  we linearize Eq. (25) and, because the sums are infrared dominated, take only the contribution from the lowest Matsubara frequency. We find

$$T_{s}(p_{\theta}) = \left[\frac{J_{\perp}(gu)^{2}}{4\pi^{5/3}c^{2}\zeta_{p_{\theta}} + \varrho\omega_{0}^{1/3}\alpha^{2}}\right]^{3/5}.$$
 (29)

Similarly, if the condition (24) is not satisfied we find from (27) and (28) the slightly different formula

$$T_{s}(p_{\theta}) = \left[\sqrt{3} \frac{J_{\perp}(gu)^{2}}{16\pi^{1/3}c^{3/2}v_{F}^{1/2}\zeta_{p_{\theta}}+Q\omega_{0}^{1/6}\alpha^{5/2}}\right]^{6/11}.$$
 (30)

As found in the previous section, the onset of the spin gap is angle dependent. It appears first at the angle  $\theta^*$ , for which  $\zeta_{p+Q}$  has a minimum, and as *T* is lowered spreads over the Fermi line. Because the interaction is more singular than in the case of the damped spin waves considered in the previous section,  $T_s$  goes as a smaller power of  $J_{\perp}$ . Roughly,  $\Delta$  is large for  $\theta_p$  such that  $T_s(p_{\theta}) > T$ , and drops rapidly for larger  $\theta$ . We denote the interval in which  $\Delta$  is large by  $(\theta^* + \theta_0, \theta^* - \theta_0)$ . We note that

$$\zeta_{p_{\theta}+Q} = \zeta_* + \epsilon_0 (\theta - \theta^*)^2, \qquad (31)$$

where  $\epsilon_0$  is an energy scale of the order of  $\epsilon_F$ . Thus, for T very near  $T_s$ ,  $\theta_0$  is given by

$$\theta_0 \sim \left(\frac{T_s - T}{T_s}\right)^{1/2} \left(\frac{\zeta_*}{\epsilon_0}\right)^{1/2}.$$
(32)

For T much less than  $T_s$ 

$$\theta_0 \sim \left(\frac{T_c}{T}\right)^{5/6} \left(\frac{\zeta_*}{\epsilon_0}\right)^{1/2}.$$
(33)

For  $|\theta - \theta^*| > \theta_0$ ,  $\Delta(\theta)$  is induced by the value of  $\Delta$  inside the interval  $(\theta^* + \theta_0, \theta^* - \theta_0)$ . From Eqs. (25) and (26) it can be seen that the kernel is so sharply peaked that

$$\Delta(\theta) \sim \Delta(\theta_0) \frac{\theta_0^4}{(\theta - \theta_0)^4}.$$
(34)

Finally, at T=0 one finds

$$\Delta(\theta) \sim \left[ \frac{J_{\perp}(gu)^2}{4 \pi c^2 \zeta_{p+Q} \omega_0^{1/3} \alpha^2} \right]^{3/5}.$$
 (35)

In words, because the interaction is so strongly peaked, the value of the T=0 gap is controlled by the energy,  $\zeta_{p+Q}$ , of the intermediate state of momentum p+Q.

# VI. CONCLUSION

We have argued that any theory of the spin gap observed in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6+x</sub> or YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub> must be based on a pairing instability of a Fermi sea of chargeless fermions (i.e., a spin liquid) in the presence of antiferromagnetic correlations. The large inelastic scattering found in the models of spin liquids leads to strong pair-breaking effects which can only be overcome by singular pairing interaction. The most plausible origin of this interaction is a between planes coupling enhanced by in-plane antiferromagnetic correlations. We considered two specific models: a spin liquid with  $2p_F$  over damped magnetic correlations induced by a gauge-field interaction and a spin liquid coexisting with weakly damped antiferromagnetic spin waves. (A third possible model, namely a spin liquid with magnetic correlations induced by tuning a fourfermion interaction, has been considered elsewhere<sup>10,47</sup>). The former model is clearly appropriate to optimally doped materials, where there is convincing photoemission evidence for a large Fermi line. We expect by continuity that it is also appropriate for dopings somewhat below optimal. Weakly damped spin waves exist in the insulating "parent compound" materials, and it has been proposed that low doping induces a gap (but no damping) in the spin-wave spectrum as well as a particle-hole continuum of spin excitations. This picture might be justified if there is a small Fermi line (i.e., "hole pockets"), but if there is a large (Luttinger) Fermi line the absence of spin-wave damping is difficult to justify. It is controversial which picture applies to the most extensively studied spin-gap compounds YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.7</sub> or YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub>. We analyzed both models, obtaining estimates for the onset temperature,  $T_s$ , of the spin gap and the angular dependence of the gap function.

In both models  $T_s$  scales as a power of the between planes coupling  $J_{\perp}$ , and the gap function is sharply peaked about particular regions of the Fermi line. In both models, pairing of spinons does not imply a true thermodynamic transition.<sup>26</sup>  $T_s$  is a crossover temperature and superconductivity sets in at a lower temperature  $T_c$  at which the charge carrying bosons condense.

In the overdamped case the physics is controlled by divergences in the fermion  $2p_F$  response function due to the singular gauge-field interaction. These divergencies are char-

acterized by an exponent  $\sigma$  which depends only on the fermion spin degeneracy *N* and by an energy scale  $\omega_0$  defined in Eq. (9) which varies substantially as one moves along the Fermi line. We found that  $T_s \propto \omega_0^{\max} J_{\perp}^{3/6\sigma-2} [\omega_0^{\max}]$  is the maximal value of  $\omega_0(\theta)$  on the Fermi line which occurs at  $\theta^*$ ]. At  $T \approx T_s$  the gap is very sharply peaked at  $\theta = \theta^*$ . As *T* is lowered the region where gap is appreciable grows and the T=0gap  $\Delta(\theta) \propto \omega_0(\theta) J_{\perp}^{3/6\sigma-2}$ . Evidently the result depends sensitively on the exponent  $\sigma$  which has been estimated to be in the range  $1 \ge \sigma \ge 1/3$ . Consistency with NMR for  $T \ge T_s$  requires that  $1 \ge \sigma \ge 2/3$ ; for this range of  $\sigma T_s$  is proportional to  $J_{\perp}$  to a power of order 1 and is of the correct order of magnitude, but the precise value depends on numerical coefficients which are not known.

For  $T_s \gtrsim T \gtrsim 0$ , the spin gap is appreciable over a part of the Fermi line, and suppresses the contribution of that part of the Fermi line to the uniform susceptibility and NMR relaxation rates. We see from Eqs. (9) and (14) that the gap is largest along the zone diagonal (where  $v_F$  is largest) and smallest at the zone corners where  $v_F$  becomes very small. All parts of the Fermi line make roughly equal contribution to the oxygen relaxation rate and uniform susceptibility (although the logarithmic divergence associated with the van Hove singularity may emphasize the corners to some extent), so we may roughly estimate the suppression of these quantities from the fraction of the Fermi line which is gapped. The copper relaxation rate is more complicated. It is dominated by the  $2p_F$  fluctuations which lead to

$$\frac{1}{T_1T} \sim \frac{\omega_0^{2\sigma-2/3}}{p_0^{1/3}}.$$

Thus the contribution to the Cu relaxation rate is largest where  $\omega_0$  is largest (i.e., along the zone diagonal) so one would expect that in this model the formation of the spin gap would suppress the Cu relaxation rate more strongly than the oxygen rate. However, the contributions of the ungapped portions of the Fermi line continue to grow as *T* is lowered, so the maximum in the Cu  $1/T_1T$  relaxation rate occurs at a  $T < T_s$  determined by the interplay between these two effects.

We now consider the underdamped case. The basic assumption is that there are two distinct types of spin excitations: propagating antiferromagnetic spin waves and particlehole continuum of spinon excitations. This picture has been derived<sup>20</sup> from a microscopic Hamiltonian using the assumption that the doping is so low that long-range magnetic order is present, and it is plausible that it may apply to lightly doped high- $T_c$  materials which lack long-range order if these materials do not have large (Luttinger) Fermi line but have instead hole pockets. An advantage of this picture is that large-q properties are dominated by spin waves, which explain in a natural way the strong T dependence of the Cu  $1/T_1T$  and  $1/T_2$  rates observed experimentally. The disadvantage of this picture is that the same spin waves would give a factor of 6 too large contribution to  $d\chi/dT$  at high temperatures so to account for the observed  $d\chi/dT$  one must assume that the particle-hole continuum leads to a large negative contribution to  $d\chi/dT$  which almost precisely cancels the spin-wave contribution.

We studied the pairing of fermions in the presence of the undamped spin waves. The pairing interaction is very

strongly peaked at the antiferromagnetic wave vector  $\mathbf{Q} = (\pi, \pi)$ , so the dominant process in the gap equation is a virtual scattering from a state p on a Fermi line to one at  $\mathbf{p} + \mathbf{Q}$  away from the Fermi line. We found that the resulting pairing interaction is very strong, the onset temperature  $T_s \propto J_{\perp}^{3/5}$ . As in the overdamped case, the gap has a strong angular dependence, it appears first at a particular point on the Fermi line and spreads over it as T is decreased. However in the underdamped case the angular dependence of the gap is controlled by the energy of the intermediate state,  $\zeta_{p+Q}$ . The pairing affects the particle-hole contribution to physical response functions but does not directly affect the spin-wave contribution. Thus, the copper relaxation rate is not significantly affected by the pairing, but the oxygen relaxation rate and uniform susceptibility are. The detailed temperature dependence is determined by the way in which the gap spreads over the Fermi line as the temperature is decreased, and this depends sensitively on the shape of the Fermi line and, in particular, on its curvature.

Our results provide a qualitative understanding of the doping dependence of the spin-gap phenomena observed in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6+x</sub>. Our basic assumption is that spin-charge separation occurs. The essential result is that the spin-gap scale  $T_s$  is correlated with the strength of the in-plane anti-ferromagnetic fluctuations. As doping increases away from the insulating state, the antiferromagnetic fluctuations decrease as does  $T_s$ . Further, if no other instability intervenes, the spin-charge separated system is believed to cross over to a Fermi-liquid regime for  $T \lesssim T_{\rm FL}$  with the crossover temperature  $T_{\rm FL}$  which grows with doping; true superconductivity can occur only at  $T_c \lesssim T_{\rm FL}$ .<sup>26</sup> When  $T_{\rm FL} \gtrsim T_s$ , the pairing of spinons becomes a conventional superconductivity transition; thus the spin-gap regime should not exist as sufficiently

high doping. Further, the infrared singularities which produced the between-planes pairing are cut off by the Fermiliquid crossover at a scale of order  $T_{\rm FL}$ , so the betweenplanes contribution to the pairing is rapidly suppressed as doping is increased beyond the point at which  $T_{\rm FL} \sim T_s$ .

The forgoing remarks apply to all scenarios of betweenplanes pairing. A more detailed discussion requires a model for in-plane spin fluctuations. It seems natural to assume that the undamped spin-wave model is relevant for very lightly doped materials,<sup>9,20,55</sup> while the over-damped model is more appropriate for the materials near optimal doping with the crossover occurring for doping near YBa2Cu3O6.7. Indeed one may show that the overdamped model is unstable at sufficiently small dopings.<sup>56</sup> This hypothesis leads to a natural explanation of the doping dependence of the relative magnitudes of the temperature  $T_{\text{max}}$  of the maximum in the Cu relaxation rate  $1/T_1T$  and  $T_s$  inferred from the uniform susceptibility. In very lightly doped materials,  $T_{\text{max}} \ll T_s$  [e.g., in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.5</sub> where  $T_s \sim 300$  K (Ref. 54) and strong antiferromagnetic fluctuations with no evident gap have been observed in neutron scattering<sup>39</sup>], as found in the calculations reported in Sec. V. However, for YBa2Cu4O8 and  $YBa_2Cu_3O_{6+x}$  with  $0.7 \le x \le 1$ ,  $T_{max} \sim T_s$ . This has no natural explanation in the "underdamped" model, but is expected in the overdamped model discussed in Sec. IV. In the spincharge separation model superconductivity occurs when the charge carriers condense; the transition temperature  $T_c = T_{\rm FI}$ and increases with doping. At some doping,  $\delta^*$ ,  $T_c$ ,  $T_{\rm FL}$  and  $T_{s}$  will coincide. At larger dopings a Fermi liquid is formed before pairing occurs, the pairing mechanism we have discussed becomes rapidly weaker and we expect  $T_c$  to decrease also. We identify  $\delta^*$  with the optimal doping.

- <sup>1</sup>T. M. Rice, *Proceedings of the ISSP Symposium on the Physics* and *Chemistry of Oxide Superconductors, Tokyo, 1991* (Springer-Verlag, Berlin, 1991).
- <sup>2</sup>H. Zimmermann, M. Mali, M. Bankay, and D. Brinkmann, Physica C **185–189**, 1145 (1991).
- <sup>3</sup>T. Nakano, M. Oda, C. Manako, N. Momono, Y. Miura, and M. Ido, Phys. Rev. B **45**, 1600 (1994).
- <sup>4</sup>A. J. Millis and H. Monien, Phys. Rev. Lett. **70**, 2810 (1993).
- <sup>5</sup>B. L. Altshuler and L. B. Ioffe, Solid State Commun. **82**, 253 (1992).
- <sup>6</sup>S. Sachdev, Phys. Rev. B **45**, 389 (1992).
- <sup>7</sup>T. Tanamoto, K. Kohno, and H. Fukuyama, J. Phys. Soc. Jpn. **61**, 1886 (1992).
- <sup>8</sup>M. Randeria, N. Trivedi, A. Moreo, and R. T. Scalettar, Phys. Rev. Lett. **69**, 2001 (1992).
- <sup>9</sup>A. V. Sokol and D. Pines, Phys. Rev. Lett. **71**, 2813 (1993); V. Barzykin, D. Pines, A. V. Sokol, and D. Thelen, Phys. Rev. B **49**, 1544 (1994).
- <sup>10</sup>L. B. Ioffe, A. I. Larkin, A. J. Millis, and B. L. Altshuler, JETP Lett. **59**, 67 (1994).
- <sup>11</sup>A. J. Millis, H. Monien, and L. B. Ioffe, J. Phys. Chem. Solids (to be published).
- <sup>12</sup>R. E. Walstedt, R. F. Bell, L. F. Schneemeyer, J. V. Waszczak, and G. P. Espinosa, Phys. Rev. B 45, 8074 (1992).

- <sup>13</sup>P. C. Hammel, M. Takigawa, R. H. Heffner, Z. Fisk, and K. C. Ott, Phys. Rev. Lett. **63**, 1992 (1989).
- <sup>14</sup>R. E. Walstedt, W. W. Warren, Jr., R. F. Bell, G. F. Brennert, G. P. Espinosa, R. J. Cava, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. B **38**, 9299 (1988).
- <sup>15</sup>A. J. Millis, H. Monien, and D. Pines, Phys. Rev. B 42, 167 (1990).
- <sup>16</sup>J. C. Campuzano, G. Jennings, M. Faiz, L. Beaulaigue, B. W. Veal, J. Z. Liu, A. P. Paulikas, K. Vandervorort, H. Claus, R. S. List, A. J. Arko, and R. J. Bartlett, Phys. Rev. Lett. **64**, 2308 (1990).
- <sup>17</sup>S. Sachdev and J. Ye, Phys. Rev. Lett. **65**, 2711 (1992); S. Sachdev, A. V. Chubukov, and J. Ye, Nucl. Phys. B **408**, 485 (1993).
- <sup>18</sup>A. J. Millis and H. Monien, Phys. Rev. B 50, 16 606 (1994).
- <sup>19</sup>A. J. Millis, Phys. Rev. Lett. **71**, 3614 (1993).
- <sup>20</sup>A. V. Chubukov and S. Sachdev, Phys. Rev. Lett. **71**, 3615 (1993).
- <sup>21</sup>L. B. Ioffe, A. I. Larkin, A. A. Varlamov, and L. Yu, Phys. Rev. B 47, 8936 (1993).
- <sup>22</sup>J. M. Harris, Y. F. Yan, and N. P. Ong, Phys. Rev. B **21**, 14 293 (1992); D. A. Brawner, Z. Z. Wang, and N. P. Ong, *ibid.* **40**, 9329 (1989).
- <sup>23</sup>B. Bucher, P. Steiner, J. Karpinski, E. Kaldis, and P. Wachter, Phys. Rev. Lett. **70**, 2012 (1993).

<sup>24</sup>Y. F. Yan, P. Matl, J. M. Harris, and N. P. Ong, *ibid.* **52**, 751 (1995).

- <sup>26</sup>L. B. Ioffe and A. I. Larkin, Phys. Rev. B **39**, 8988 (1989).
- <sup>27</sup>G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. 63, 973 (1987).
- <sup>28</sup>T. Machi, I. Tomeno, T. Miyatake, N. Koshizuka, S. Tanaka, T. Imai, and H. Yasuoka, Physica C **173**, 32 (1991).
- <sup>29</sup> Y. Itoh, H. Yasuoka, Y. Fujiwara, Y. Ueda, T. Machi, I. Tomeneo, K. Tai, N. Koshizuka, and S. Tanaka, J. Phys. Soc. Jpn. **61**, 1287 (1992).
- <sup>30</sup>R. E. Walstedt, B. S. Shastry, and S.-W. Cheong, Phys. Rev. Lett. 72, 3610 (1994).
- <sup>31</sup>J. Rossat-Mignon, L. P. Regnault, C. Vettier, P. Burlet, J. Y. Henry, and G. Lapertot, Physica B **169**, 58 (1991); J. Rossat-Mignon, L. P. Regnault, C. Vettier, P. Bourges, P. Burlet, J. Bossy, J. Y. Henry, and G. Lapertot, *ibid.* **180–181**, 383 (1992).
- <sup>32</sup>S. Sachdev, A. V. Chubukov, and A. V. Sokol, Phys. Rev. B 51, 14 874 (1995).
- <sup>33</sup>L. B. Ioffe and A. J. Millis, Phys. Rev. B **51**, 16151 (1995).
- <sup>34</sup>B. L. Altshuler, L. B. Ioffe, A. I. Larkin, and A. J. Millis, Phys. Rev. B **52**, 4607 (1995).
- <sup>35</sup>D. C. Johnston, J. Magn. Magn. Mater. **100**, 218 (1991).
- <sup>36</sup>T. Imai, Ph. D. thesis, University of Tokyo, 1991.
- <sup>37</sup>G. Shirane, J. Als-Nielsen, M. Nielsen, J. M. Tranquada, H. Chou, S. Shamoto, and M. Sato, Phys. Rev. B **41**, 6547 (1990).
- <sup>38</sup>J. M. Tranquada, Phys. Rev. B 46, 5561 (1992).

- <sup>39</sup>H. A. Mook, M. Yethirai, G. Aeppli, and T. Mason, Phys. Rev. Lett. **70**, 3490 (1993).
- <sup>40</sup>R. Stern, M. Mali, J. Roos, and D. Brinkman (unpublished).
- <sup>41</sup>H. Monien and T. M. Rice, Physica C 235-240, 1705 (1994).
- <sup>42</sup>A. J. Millis and H. Monien (unpublished).
- <sup>43</sup>M. Reizer, Phys. Rev. **40**, 11 571 (1989).
- <sup>44</sup>P. A. Lee, Phys. Rev. Lett. **63**, 680 (1989).
- <sup>45</sup>B. L. Altshuler, L. B. Ioffe, and A. J. Millis, Phys. Rev. B **50**, 14 048 (1994).
- <sup>46</sup>M. U. Ubbens and P. A. Lee, Phys. Rev. B 49, 6853 (1994).
- <sup>47</sup>M. U. Ubbens and P. A. Lee, Phys. Rev. B **50**, 438 (1994).
- <sup>48</sup>A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).
- <sup>49</sup>L. B. Ioffe and G. Kotliar, Phys. Rev. B **42**, 10 348 (1990).
- <sup>50</sup>K. Kuboki and P. A. Lee (unpublished).
- <sup>51</sup>Z. X. Shen and D. S. Dessau, Phys. Rep. **253**, 1 (1995).
- <sup>52</sup>T. E. Mason, G. Aeppli, and S. M. Hayden, Phys. Rev. Lett. **71**, 919 (1993); S. M. Hayden, G. Aeppli, and R. Osborn, *ibid.* **67** (1991).
- <sup>53</sup>H. Alloul, T. Ohno, and P. Mendels, Phys. Rev. Lett. **63**, 1700 (1989).
- <sup>54</sup>For a review see, e.g., P. A. Lee, in *High Temperature Superconductivity Proceedings*, edited by K. S. Bedell, D. Coffey, D. E. Meltzer, D. Pines, and J. R. Schreiffer (Addison-Wesley, Reading, MA, 1990), p. 96.
- <sup>55</sup>L. B. Ioffe and A. J. Millis (unpublished).

<sup>&</sup>lt;sup>25</sup> P. W. Anderson, Science **235**, 1196 (1987).