Weak-coupling theory of high-temperature superconductivity in the antiferromagnetically correlated copper oxides

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We show that the retarded interaction between quasiparticles on a two dimensional square lattice induced by the exchange of antiferromagnetic paramagnons leads uniquely to a transition to a superconducting state with $d_{x^2-y^2}$ symmetry. We find that the effective quasiparticle interaction responsible for superconductivity possesses considerable structure in both momentum and frequency space, and show, by explicit calculations, that if one wishes to obtain quantitatively meaningful results it is essential to allow for that structure in solving the full integral equations that determine the superconducting transition temperature and the superconducting properties. With a spin-excitation spectrum and a quasiparticle-paramagnon coupling determined by fits to normal-state experiments, we obtain high transition temperatures and energy-gap behaviors comparable to those measured for $YBa_2Cu_3O_7$, $YBa_2Cu_3O_{6.63}$, and $La_{1.85}Sr_{0.15}CuO_4$.

I. INTRODUCTION

During the six years that have elapsed since the discovery of high-temperature superconductivity in copper oxide compounds,[1] it has become increasingly clear that the normal-state properties of the copper oxides are qualitatively different from those of the normal Fermi liquid found in the "low-temperature superconductors" while their superconducting properties can be understood qualitatively using a BCS approach.[2] Attention has therefore focused on understanding the physical origin of the novel properties of the planar excitations in the normal state in the expectation that these would provide an essential clue to the appearance of high-temperature superconductivity. It has been argued that it is the strong antiferromagnetic correlations of the nearly localized Cu^{2+} d orbitals (deduced from NMR experiments) that are chiefly responsible for the unusual properties of the normal state,[3] while in a preliminary communication we have shown that in a weak-coupling approximation, the retarded interaction between quasiparticles on a two-dimensional (2D) square lattice induced by the exchange of spin-fluctuation excitations leads uniquely to a transition to a superconducting state with $d_{x^2-y^2}$ symmetry.[4] With a spectrum of spin excitations determined by fits to NMR experiments, and physically reasonable values of their coupling to quasiparticles, we found high transition temperatures and energy-gap behaviors comparable to those measured for $YBa_2Cu_3O_7$, $YBa_2Cu_3O_{6.63}$, and $La_{1.85}Sr_{0.15}CuO_4$. We present here a detailed account of those calculations. We consider the sensitivity of our results to the parameters used to describe the spin excitations, compare our results with calculations by other authors, and discuss some of the remaining steps required in the development of a self-consistent theory of the properties of the normal and superconducting states.

The NMR experiments on the normal state used to determine the spin-excitation spectrum show that a single, nearly localized, Cu^{2+} spin component is responsible for the measured Knight shifts and spin-lattice relaxation times of ^{63}Cu and ^{17}O nuclei in planar sites of 1-2-3, 2-1-4, and 1-2-4 ($YBa_2Cu_3O_8$) systems, as well as for ^{89}Y nuclei located between CuO planes in 1-2-3 and 1-2-4 systems.[5] A quantitative fit to these experiments may be obtained with a phenomenological theory in which the imaginary part of the planar spin-spin correlation function $\chi''(\mathbf{q},\omega)$ is sharply peaked at $\mathbf{Q}=[\pm(\pi/a),\pm(\pi/a)]$ in the Brillouin zone, with the dominant magnetic excitations being temperature-dependent low-frequency antiferromagnetic paramagnons with a characteristic energy ω_{SF}, which is always less than k_BT.[6,7] These results led to the proposal that both the charge and spin properties of the normal state could be explained by regarding it as a nearly antiferromagnetic Fermi liquid of coupled quasiparticles and antiferromagnetic paramagnons.[3] Because the spin fluctuations are peaked at the commensurate wave vector $\mathbf{Q}$, while the quasiparticle Fermi surface is incommensurate, the resulting quasiparticle self energy $\Sigma(\mathbf{p},\omega,T)$ is sensitive to the position of the quasiparticle on or near the Fermi surface (quasiparticles capable of coupling to $\mathbf{Q}$ will clearly have their properties modified considerably more than those which do not), and to ω and T through the dependence of $\chi(\mathbf{q},\omega)$ on the latter quantities.

Thus far a complete self-consistent calculation of the resulting quasiparticle spectrum has not been carried out. However, in weak-coupling calculations using the Millis, Monien, and Pines (MMP) form for $\chi(\mathbf{q},\omega)$ (Ref. 8) and the random-phase approximation (RPA) result[9] or a form based on the self-consistent renormalization approach,[10] and taking the Fermi surface to be nearly circular, all authors find that the Fermi-surface-averaged imaginary part of the self-energy takes the form

$$\langle \mathrm{Im}\,\Sigma(\mathbf{p},\omega,T)\rangle \sim \mathrm{Max}(\omega,T) \ ,$$

in agreement with resistivity and optical experiments and in striking contrast to the Fermi-liquid value, $\mathrm{Im}\,\Sigma(\mathbf{p},\omega,T)\sim\omega^2+\pi^2T^2$. Millis has carried out an approximate analytic calculation of the imaginary part of the quasiparticle self-energy for this model,[11] for very low frequencies (and temperatures), he finds Fermi-liquid behavior characterized by an energy scale, which is small compared to the Fermi-liquid result, while for larger frequencies (and temperatures) he finds a Fermi-surface-averaged self-energy of the above form, in agreement with the preliminary results of numerical calculations that have been carried out by one of us.[12]

Some of the main facts that a theory of high-temperature superconductivity in the antiferromagnetically correlated copper oxide metals must explain are as follows.

(i) The transition to a superconducting state at remarkably high temperatures in the presence of strong Coulomb correlations between the electronic charges and strong antiferromagnetic correlations between the electronic spins.

(ii) A striking correlation between the magnetic properties of the cuprates and their transition temperatures T_c. In the $YBa_2Cu_3O_{7-\delta}$ (1-2-3) materials, the highest transition temperatures ($T_c\sim 93$ K) occur at $\delta=0$; at this concentration, the antiferromagnetic correlations measured in NMR experiments are comparatively modest $[(\xi/a)\le 2.5$, where ξ is the temperature-dependent antiferromagnetic correlation length and the 2D lattice constant].[6] As δ increases, the magnitude of the AF correlations increases, while T_c decreases, so that for $\delta\cong 0.37$, one finds $T_c\sim 60$ K, and $\xi/a\le 4$.[7] For the Sr-doped 2-1-4 materials $La_{2-x}Sr_xO_4$, the maximum T_c (~ 40 K), is found for $x=0.15$; at this concentration the phenomenological fit to NMR experiments on ^{63}Cu and ^{17}O nuclei yields a value of $(\xi/a)_{\max}$, while is considerably larger $[(\xi/a)\le 7]$ than found for $YBa_2Cu_3O_{6.63}$;[7] for lower values of x, T_c decreases and $(\xi/a)_{\max}$ increases.[13]

(iii) NMR measurements of the Knight shift and the spin-lattice relaxation times in $YBa_2Cu_3O_7$, which show that these are decidedly not those of a conventional s-wave BCS superconductor. Thus experiment shows (i) there is no Hebel-Slichter peak in either the ^{63}Cu or ^{17}O relaxation rate in the vicinity of T_c;[14,15] (ii) a very rapid falloff of the uniform susceptibility $\chi_0(T)$ below T_c; (iii) a low-temperature Knight shift for the chain sites, which vary linearly with T at low temperatures.[16] [Note that the present experimental uncertainty in the corresponding planar Knight shift measured by Barrett *et al.*[16] is sufficiently large that at low temperatures both a linear variation with T of $\chi_0(T)$ and an exponential variation with T are consistent with the data]; (iv) a very rapid falloff of the ^{63}Cu and ^{17}O relaxation rates for temperatures between T_c and $T_c/2$, followed by nearly T^3 behavior for temperatures $T_c/5\le T\le T_c/2$; and (v) a quite remarkable anisotropy in the measured ^{63}Cu spin-lattice relaxation rates $^{63}W(T)$. Found originally by Barrett *et al.*,[17] and confirmed by Takigawa, Smith, and Hults[18] and Martindale *et al.*,[19] the ratio of the relaxation rates for fields in the CuO plane and perpendicular to it, $[^{63}W_a(T)/^{63}W_c(T)]$, displays an initial rapid drop below T_c of some 20% (from its temperature-independent value above T_c) followed by a gradual increase, until at low temperatures it is some 30% above its normal-state value. We demonstrate below how spin-fluctuation-induced superconductivity makes possible high superconducting transition temperatures in a strongly correlated electron system, and show how it can account for the initial rapid falloff with decreasing temperature of the spin susceptibility $\chi_0(T)$ and the spin-lattice relaxation rates, which signal an energy gap that opens up very rapidly, reaching a maximum magnitude that is large compared to the weak-coupling BCS result.[20] We find that with a physically reasonable Fermi-liquid correction, the temperature dependence of our calculated $\chi_0(T)$ agrees with experiment, while the T^3 behavior in the spin-lattice relaxation rate is just what is to be expected in a temperature regime in which scattering of quasiparticles between the nodes plays a dominant role.[20] Model calculations by Bulut and Scalapino,[21] by Lu,[22], and by Thelen, Lu, and Pines,[22] show how the change in anisotropy of the spin-lattice relaxation rates is, perhaps uniquely, explicable by the interplay of antiferromagnetic correlations and d-wave pairing.

We find that the effective quasiparticle interaction responsible for spin-fluctuation superconductivity possesses considerable structure in that it is both momentum and frequency dependent. We show, by example, that if one wishes to obtain quantitatively meaningful results, it is essential to allow for that structure in solving the full integral equations that determine the superconducting transition temperature and superconducting properties.

The plan of the paper is the following. In Sec. II we set forth our model Hamiltonian, and present the results of our weak-coupling calculations. We discuss these results in Sec. III. In Sec. IV we consider the merits of some commonly used approximations in which some or all effects of the structure in momentum space are neglected, while in Sec. V we examine the role of impurity scattering. Section VI contains our conclusions.

II. WEAK-COUPLING CALCULATION

We follow Anderson[23] and use a one-band description of the planar excitations of a 2D square lattice; however, instead of introducing spinons and holons, we assume the planar excitations form a nearly antiferromagnetic Fermi liquid made up of quasiparticles coupled to spin fluctuations. In our model, the results of experiments on the normal state are used to fix the fundamental quantities that enter the spectrum of spin excitations and their coupling to quasiparticles. Our basic Hamiltonian is thus

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{\rm int} , \quad (1a)$$

where

$$\mathcal{H}_0=\sum_{\mathbf{q},\sigma} \varepsilon_{\mathbf{q}}\psi^\dagger_{\mathbf{q},\sigma}\psi_{\mathbf{q},\sigma} \quad (1b)$$

describes the quasiparticle excitations of energy $\varepsilon_{\mathbf{q}}$, which in the nearest-neighbor tight-binding approximation may be written as

$$\varepsilon_{\mathbf{q}}=-2t[\cos(q_x a)+\cos(q_y a)] . \quad (1c)$$

$\mathcal{H}_{\rm int}$ describes the interaction between the planar quasiparticle excitations and the spin fluctuations. We write it as

$$\mathcal{H}_{\rm int}=\frac{1}{\Omega}\sum_{\mathbf{q}} \bar{g}(\mathbf{q})\mathbf{s}(\mathbf{q})\cdot\mathbf{S}(-\mathbf{q}) , \quad (1d)$$

where

$$\mathbf{s}(\mathbf{q})=\tfrac{1}{2}\sum_{\alpha,\beta,\mathbf{k}} \psi^\dagger_{\mathbf{k}+\mathbf{q},\alpha}\sigma_{\alpha\beta}\psi_{\mathbf{k},\beta} \quad (1e)$$

and $\mathbf{S}$ is the spin-fluctuation operator whose properties are determined by the spin-spin correlation function $\chi_{ij}(\mathbf{q},\omega)=\delta_{ij}\chi(\mathbf{q},\omega)$.

We take the quasiparticle bandwidth $B\equiv 8t$ to be 2 eV, and require that $\chi(\mathbf{q},\omega)$ be such as to provide a quantitative fit to NMR experiments. We choose to use the low-frequency form of $\chi(\mathbf{q},\omega)$ determined by NMR, because as yet neutron-scattering experiments have not produced a consensus on the behavior of $\chi(\mathbf{q},\omega)$ in the frequency range 1–50 meV. We thus adopt the form of $\chi(\mathbf{q},\omega)$ proposed by MMP, which has been shown to provide a quantitative fit to the NMR experiments involving ^{63}Cu, ^{17}O, and where appropriate, ^{89}Y, in the copper oxide superconductors:

$$\chi(\mathbf{q},\omega)=\frac{\chi_{\mathbf{Q}}}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2-i\dfrac{\omega}{\omega_{\rm SF}}}, \quad q_x>0,\ q_y>0 , \quad (2)$$

where $\chi_{\mathbf{Q}}$ is the static spin susceptibility at wave vector $\mathbf{Q}=(\pi/a,\pi/a)$. In the normal state, $\chi_{\mathbf{Q}}\equiv\chi_0(\xi/a)^2\beta^{1/2}$, where χ_0 is the experimentally measured long-wavelength spin susceptibility, which is in general temperature dependent, ξ is a temperature-dependent antiferromagnetic correlation length $\beta\approx\pi^2$. With this form of $\chi(\mathbf{q},\omega)$ there are no well-defined low-frequency magnetic excitations, but rather one has a relaxational mode, the paramagnon, whose energy is given by

$$\omega_{\rm SF}=\frac{\Gamma}{\beta^{1/2}\pi\left[\dfrac{\xi}{a}\right]^2} , \quad (3)$$

where $\Gamma\approx 0.4$ eV plays the role of a magnetic Fermi energy. The fits to numerous NMR experiments[6,7] yield the values shown in Table I for $\xi(T_c)$ and $\omega_{\rm SF}(T_c)$. Since those experiments also suggest that the antiferromagnetic correlations become frozen in the superconducting state, the parameters Γ, ξ, $\omega_{\rm SF}$, and $\chi_{\mathbf{Q}}$ are taken to be constants below T_c.

As noted in the Introduction, the normal-state properties of this model Hamiltonian have been considered by a number of authors,[8–11] who find that in suitable approximations, the imaginary part of the quasiparticle self-energy takes the form $\langle {\rm Im}\,\Sigma(\mathbf{p},\omega,T)\rangle\sim{\rm Max}(\omega,T)$, in qualitative agreement with resistivity and optical experiments, and in contrast to the usual Fermi-liquid properties. The normal state is thus being viewed as a nearly antiferromagnetic Fermi liquid whose properties, as a result of the strong correlations [evident in $\xi(T_c)$], are decidedly unconventional. In the case of $YBa_2Cu_3O_7$, the spin susceptibility χ_0, which enters into Eq. (2), is independent of temperature, and, with a coupling constant $\bar{g}(\mathbf{q})$, which is temperature and wave vector independent, one obtains a normal-state resistivity, which is linear in T. For $YBa_2Cu_3O_{6.63}$ and $La_{1.85}Sr_{0.15}CuO_4$ the uniform spin susceptibility is markedly temperature dependent. We find that in order to obtain a linear resistivity, $\bar{g}(r)$ must be temperature dependent. A convenient form for large r is $\bar{g}(r)\propto(-1)^{(n_x+n_y)}\{\exp[-r/l(T)]/r\}$, $\mathbf{r}=(n_x a,n_y a)$, where $l(T)$ is chosen in such a way that the product of $\chi_0(T)$ and a temperature-dependent effective coupling

TABLE I. Input spin excitation and calculated pairing parameters for cuprate superconductors.

Superconductor	$YBa_2Cu_3O_7$	$YBa_2Cu_3O_{6.63}$	$La_{1.85}Sr_{0.15}CuO_4$
$\chi_0(T_c)$ (states/eV)	2.62	0.75	1.20
$\dfrac{\xi(T_c)}{a}$	2.5	4.1	6.5
$\omega_{\rm SF}(T_c)$ (K)	90	35	10
$\lambda(T_c)$ $(T_c\propto e^{-1/\lambda(T_c)})$	0.477	0.373	0.331
$\dfrac{\Delta_{\max}(0)}{k_B T_c}$	2.9	3.4	4.3
x $\left[\dfrac{\Delta_{\max}(T)}{\Delta_{\max}(0)_{T\to T_c}}\propto\left[\dfrac{T}{T_c}-1\right]^x\right]$	0.45	0.33	0.30

$$\bar{g}^2_{\text{eff}}(T) \equiv \frac{\sum_{\mathbf{q}} \bar{g}^2(\mathbf{q})\chi(\mathbf{q},\omega\to 0)}{\sum_{\mathbf{q}} \chi(\mathbf{q},\omega\to 0)} \tag{4}$$

is nearly independent of T. We find that $l(T)$ varies from ~ 3 (~ 2.1) lattice spacings at $T=60°$ K to ~ 1.5 (~ 1.7) lattice spacing at $T=250°$ K for the $YBa_2Cu_3O_{6.63}$ ($La_{1.85}Sr_{0.15}CuO_4$) compound.

In examining the possible transition to the superconducting state, we consider the irreducible representations of the gap allowed by the symmetry group D_4 of the square lattice. Since the equation determining the critical temperature T_c is linear, one may decompose the gap function into its irreducible components: they then decouple and have simple symmetry properties under D_4. It is then only necessary to know the gap function in the first octant of the Brillouin zone (BZ), i.e., for $k_x, k_y > 0$, $k_x > k_y$. If $\{\Phi_i\}_{i=1,\dots,8}$ are the group transformations that map any wave vector in the BZ onto the first octant, then in the weak-coupling limit, the linearized gap equation for T_c takes the form

$$\Delta(\mathbf{k}) = -g^2_{\text{eff}}(T)\int_0^{\pi/a}\frac{a\,dk'_x}{2\pi}\int_0^{k'_x}\frac{a\,dk'_y}{2\pi}\sum_{i=1}^{8}\left[\text{Re}\chi(\mathbf{k}-\Phi_i\mathbf{k}',\varepsilon_{\mathbf{k}'}-\mu)\frac{\tanh\left[\dfrac{\varepsilon_{\mathbf{k}'}-\mu}{2k_BT}\right]}{\varepsilon_{\mathbf{k}'}-\mu} + 2\int_0^\infty \frac{d\omega}{\pi}\coth\left[\frac{\omega}{2k_BT}\right]\text{Im}\chi(\mathbf{k}-\Phi_i\mathbf{k}',\omega) \times \frac{(\varepsilon_{\mathbf{k}'}-\mu)^2-\omega^2+\delta^2}{[(\varepsilon_{\mathbf{k}'}-\mu)^2-\omega^2+\delta^2]^2+4\omega^2\delta^2}\right]\Delta(\Phi_i\mathbf{k}') , \tag{5a}$$

$$\Delta(\mathbf{k}) = \frac{g^2_{\text{eff}}(T)}{3}\int_0^{\pi/a}\frac{a\,dk'_x}{2\pi}\int_0^{k'_x}\frac{a\,dk'_y}{2\pi}\sum_{i=1}^{8}\left[\text{Re}\chi(\mathbf{k}-\Phi_i\mathbf{k}',\varepsilon_{\mathbf{k}'}-\mu)\frac{\tanh\left[\dfrac{\varepsilon_{\mathbf{k}'}-\mu}{2k_BT}\right]}{\varepsilon_{\mathbf{k}'-\mu}} + 2\int_0^\infty \frac{d\omega}{\pi}\coth\left[\frac{\omega}{2k_BT}\right]\text{Im}\chi(\mathbf{k}-\Phi_i\mathbf{k}',\omega) \times \frac{(\varepsilon_{\mathbf{k}'}-\mu)^2-\omega^2+\delta^2}{[(\varepsilon_{\mathbf{k}'}-\mu)^2-\omega^2+\delta^2]^2+4\omega^2\delta^2}\right]\Delta(\Phi_i\mathbf{k}') . \tag{5b}$$

The upper line is for singlet (repulsive interaction) and the lower one for triplet pairing (attractive interaction). δ^2 is a broadening parameter ($\sim$ lifetime) necessary to make the second term well defined. It turns out that even for small values of δ^2 that term is small compared to the first one. We will therefore not consider it in what follows. As we shall demonstrate, when the frequency dependence of the susceptibility is taken into account, the interaction is cut off when $\varepsilon_{\mathbf{k}'}-\mu \geq \omega_{\text{SF}}(\xi^2/a^2) \equiv \Gamma/\pi^2$. The effective coupling constant is $g^2_{\text{eff}}(T) = \frac{3}{8}\bar{g}^2_{\text{eff}}(T)$. The latter equation is purely a convention. A factor $\frac{1}{4}$ comes from our definition of the interaction $\mathcal{H}_{\text{int}}$ Eq. (1) in terms of the spin density. We chose to absorb another factor of $\frac{1}{2}$ from $[\tanh(\varepsilon_{\mathbf{k}'}-\mu/2k_BT_c)]/[2(\varepsilon_{\mathbf{k}'}-\mu)]$ in the definition of the coupling constant and the factor of 3 comes from the trace over the susceptibility tensor.

To understand why the particular interaction in Eq. (5) leads uniquely to a gap with $d_{x^2-y^2}$ symmetry, it is best to write the gap equation without restriction on $\mathbf{k}$ and $\mathbf{k}'$. In the singlet channel, dropping the second term, Eq. (5) reads

$$\Delta(\mathbf{k}) = -g^2_{\text{eff}}(T)\int_{\text{BZ}}\frac{a^2d^2k'}{(2\pi)^2}\text{Re}\chi(\mathbf{k}-\mathbf{k}',\varepsilon_{\mathbf{k}'}-\mu) \times \frac{\tanh\left[\dfrac{\varepsilon_{\mathbf{k}'}-\mu}{2k_BT}\right]}{\varepsilon_{\mathbf{k}'}-\mu}\Delta(\mathbf{k}') . \tag{6}$$

Since the overall interaction in Eq. (6) is repulsive, if the gap does not have nodes, i.e., always has the same sign, it follows that the two sides of Eq. (6) have opposite signs and thus the gap must be zero. To get a nontrivial solution, one can easily convince oneself that the symmetry of the gap must be such that for the wave vectors $\mathbf{k}$ and $\mathbf{k}'$ that make the most contribution to the integral in Eq. (6), $\Delta(\mathbf{k})$ and $\Delta(\mathbf{k}')$ must have opposite sign. Since the frequency dependence of the susceptibility cuts off the interaction when $\varepsilon-\mu \geq (\Gamma/\pi^2)$, $\mathbf{k}$ and $\mathbf{k}'$ must be very near the Fermi surface (i.e., not more than an energy

Γ/π^2 away from E_F). Since the susceptibility $\chi(\mathbf{q},\omega)$ is sharply peaked at $[\pm(\pi/a),\pm(\pi/a)]$, values of $\mathbf{k}$ and $\mathbf{k}'$ such that $[k_x-k_x'\pm(\pi/a)]^2+[k_y-k_y'\pm(\pi/a)]^2$ is minimum make the largest contribution to the integral. These three conditions, which are illustrated in Fig. 1, thus combine to rule out d_{xy} pairing and produce a gap function that takes the form

$$\Delta(\mathbf{k})=\Delta_0(\mathbf{k})[\cos(k_x a)-\cos(k_y a)] \ . \qquad (7)$$

Another singlet state that has been proposed is the extended s wave, for which $\Delta(\mathbf{k})=\Delta_0(\mathbf{k})[\cos(k_x a)+\cos(k_y a)]$. A little thought shows that as soon as one is away from a nested Fermi surface, the wave vectors $\mathbf{k}$ and $\mathbf{k}'$ shown in Fig. 1 lie in regions in which the gap function has the same sign, so that this pairing will not work. In the triplet channel the sign of the interaction is changed and since the gap does have nodes, the wave vectors $\mathbf{k}$ and $\mathbf{k}'$ that satisfy the above two conditions must then be such that $\Delta(\mathbf{k})$ and $\Delta(\mathbf{k}')$ have the same sign. For the p-wave gap $\Delta(\mathbf{k})$, which involves any linear combination of $\sin(k_x a)$ and $\sin(k_y a)$, this is not possible for spin fluctuations of an antiferromagnetically correlated Fermi liquid. If however, as in ^{3}He, the spin correlations are primarily ferromagnetic, the dominant contribution to the quasiparticle interaction will come from low momentum transfers, and the triplet pairing condition is easily met. From now on, we will only consider singlet pairing.

Because of the structure of the quasiparticle spectrum and the gap $\Delta(\mathbf{k})$, it is convenient to write the integral equation (5) for $\Delta_0(\mathbf{k})$ in terms of the new dimensionless variables ε and θ:

$$k_x a=\arccos[-\varepsilon-(1-|\varepsilon|)\cos(\theta)], \quad -1\le\varepsilon\le 1 \ ,$$
$$k_y a=\arccos[-\varepsilon+(1-|\varepsilon|)\cos(\theta)], \quad 0\le\theta\le\frac{\pi}{2} \ . \qquad (8)$$

We neglect the θ dependence of Δ_0, and write Eq. (5) as a one-dimensional integral equation in the variable ε:

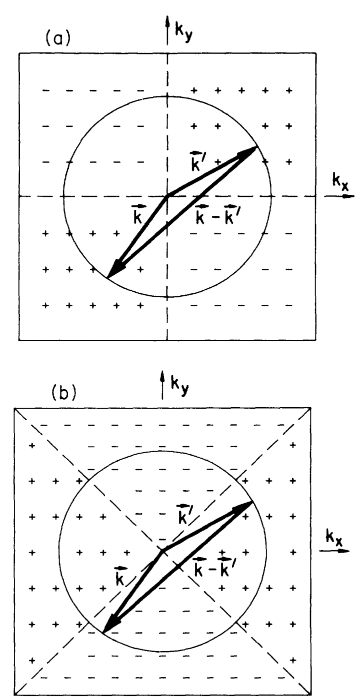

FIG. 1. Quasiparticle pairing and gap symmetries for d-wave pairing. The dotted lines indicate the location of the nodes of the gap, while the regions where the gap function is positive or negative are denoted by $(+,-)$. Quasiparticles whose momentum lies near the Fermi surface such that $[k_x-k_x'+(\pi/a)]^2+[k_y-k_y'+(\pi/a)]^2$ is a minimum are shown: (a) illustrates the gap function $\Delta_{xy}(\mathbf{k})=\Delta_0(\mathbf{k})\sin(k_x a)\sin(k_y a)$ for d_{xy} symmetry; (b) illustrates the gap function $\Delta_{x^2-y^2}(\mathbf{k})=\Delta_0(\mathbf{k})[\cos(k_x a)-\cos(k_y a)]$. Note that for d_{xy} pairing, both momenta lie in regions where the gap has the same sign, while for $d_{x^2-y^2}$ pairing, the regions are such that the gap has opposite sign.

$$\bar{\Delta}(\varepsilon)=\frac{g_{\rm eff}^2(T)}{B\pi^2}\int_{-1}^{+1}d\varepsilon'\,V(\varepsilon,\varepsilon')\frac{\tanh\left[\dfrac{B(\varepsilon'-\mu')}{4k_BT}\right]}{(\varepsilon'-\mu')}\bar{\Delta}(\varepsilon') \ , \qquad (9)$$

where

$$V(\varepsilon,\varepsilon')\equiv-\int_0^{\pi/2}d\theta\int_0^{\pi/2}d\theta'\frac{\cos(\theta')\sum_{i=1}^{8}(-1)^{\Phi_i}\mathrm{Re}\chi\left[\mathbf{k}(\varepsilon,\theta)-\Phi_i\mathbf{k}'(\varepsilon',\theta'),\frac{B}{2}(\varepsilon'-\mu')\right]}{[(1+|\varepsilon'|)^2-(1-|\varepsilon'|)^2\cos^2(\theta')]^{1/2}}$$

and $\bar{\Delta}(\varepsilon)\equiv\Delta_0(\varepsilon)(1-|\varepsilon|)$. $(-1)^{\Phi_i}$ denotes the parity of the gap under the transformation Φ_i, B is the bandwidth $\mu\equiv(B/2)\mu'$ and the quasiparticle energy $\varepsilon_{\mathbf{k}}=(B/2)\varepsilon$. The above approximation amounts to expanding Δ_0 in powers of $\cos(k_x a)+\cos(k_y a)$ and solving Eq. (5) exactly in that subspace. Because of the considerable structure of the effective interaction, a very fine mesh in the ε variable is needed. Since the solution of the ensuing 164 coupled equations is computationally expensive, we have not explored various chemical potentials: μ was set to 0.25 eV [a representative value, corresponding to $N(0)=0.568$ eV^{-1}] for the three compounds and its temperature dependence was neglected throughout. We obtain an identical result with $\mu\rightarrow-\mu$ provided we make the substitution $\varepsilon\rightarrow-\varepsilon$.

The dependence of the effective interaction $V(\varepsilon,\varepsilon')$ on the respective energies of the pairing quasiparticles is illustrated in Fig. 2, where we see that the characteristic energy scale on which the spin-fluctuation-induced interaction is effective is $\sim\Gamma/\pi^2$, where Γ, the magnetic Fermi energy, is ~ 0.4 eV.

Below T_c the full gap equation is obtained from Eq. (5) by changing $\varepsilon_{\mathbf{k}}-\mu$ everywhere to the quasiparticle energy in the superconducting state $E_{\mathbf{k}}\equiv[(\varepsilon_{\mathbf{k}}-\mu)^2+\Delta^2(\mathbf{k})]^{1/2}$. Dropping the term containing the imaginary part of the susceptibility one thus has

$$\Delta(\mathbf{k})=-g_{\text{eff}}^2(T)\int_0^{\pi/a}\frac{a\,dk_x'}{2\pi}\int_0^{k_x'}\frac{a\,dk_y'}{2\pi}\sum_{i=1}^{8}\left[\text{Re}\chi(\mathbf{k}-\Phi_i\mathbf{k}',E_{\mathbf{k}'})\frac{\tanh\left[\dfrac{E_{\mathbf{k}'}}{2k_BT}\right]}{E_{\mathbf{k}'}}\right]\Delta(\Phi_i\mathbf{k}') . \tag{10}$$

An important feature of Eq. (10) is that, because of retardation effects, the effective interaction in the superconducting state now depends on the gap via $E_{\mathbf{k}}$. We again change variables according to Eq. (8) and neglect the θ dependence of Δ_0. Equation (10) is then written as

$$\bar{\Delta}(\varepsilon)=\frac{g_{\text{eff}}^2(T)}{B\pi^2}\int_{-1}^{+1}d\varepsilon' K(\varepsilon,\varepsilon')\bar{\Delta}(\varepsilon') , \tag{11a}$$

$$K(\varepsilon,\varepsilon')=-\int_0^{\pi/2}d\theta\int_0^{\pi/2}d\theta'\frac{\cos(\theta')\sum_{i=1}^{8}(-1)^{\Phi_i}\text{Re}\chi\left[\mathbf{k}(\varepsilon,\theta)-\Phi_i\mathbf{k}'(\varepsilon',\theta'),\frac{B}{2}E'(\varepsilon',\theta')\right]}{[(1+|\varepsilon'|)^2-(1-|\varepsilon'|)^2\cos^2(\theta')]^{1/2}}\frac{\tanh\left[\dfrac{BE'(\varepsilon',\theta')}{4k_BT}\right]}{E'(\varepsilon',\theta')} , \tag{11b}$$

where $E'(\varepsilon',\theta')=\{(\varepsilon'-\mu')^2+[(4/B)\bar{\Delta}(\varepsilon')\cos(\theta')]^2\}^{1/2}$, $\bar{\Delta}(\varepsilon)\equiv\Delta_0(\varepsilon)(1-|\varepsilon|)$, and $(-1)^{\Phi_i}$ denotes the parity of the gap under the transformation Φ_i. Our principal results are displayed in Figs. 3, 4, 5, and 6, and in Table I, and we comment on them briefly.

(i) As shown in Fig. 3, our numerical solution for T_c is well approximated by

$$T_c=\alpha\hbar\omega_{\text{SF}}(T_c)\frac{\xi^2(T_c)}{a^2}\exp\left[-\frac{1}{\lambda(T_c)}\right]$$
$$\equiv\alpha\frac{\Gamma(T_c)}{\pi^2}\exp\left[-\frac{1}{\lambda(T_c)}\right] , \tag{12}$$

where the dimensionless effective coupling constant

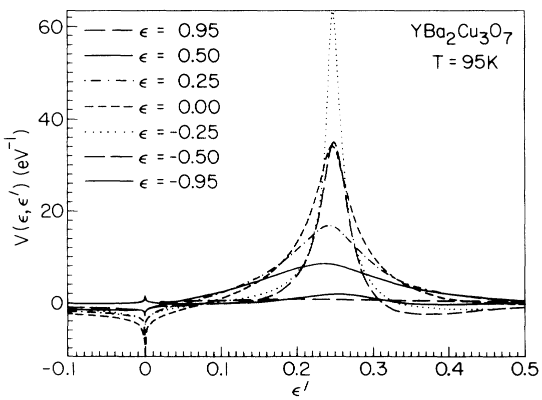

FIG. 2. Structure of the retarded interaction $V(\varepsilon,\varepsilon')$ between quasiparticles. For a quasiparticle on the Fermi surface $\varepsilon_{\mathbf{k}'}=0.25$ eV and $\varepsilon'=0.25$, the maximum interaction occurs with quasiparticles of energy $\varepsilon_{\mathbf{k}}=-0.25$ eV, $\varepsilon=-0.25$, which are coupled to ε' by $\mathbf{Q}=[\pm(\pi/a),\pm(\pi/a)]$. However, since the pairing quasiparticles must both lie near the Fermi surface, with $\varepsilon\approx\varepsilon'\approx 0.25$, we see that it is spin fluctuations involving momentum transfers comparatively far from $[\pm(\pi/a),\pm(\pi/a)]$, which play the dominant role in producing superconductivity.

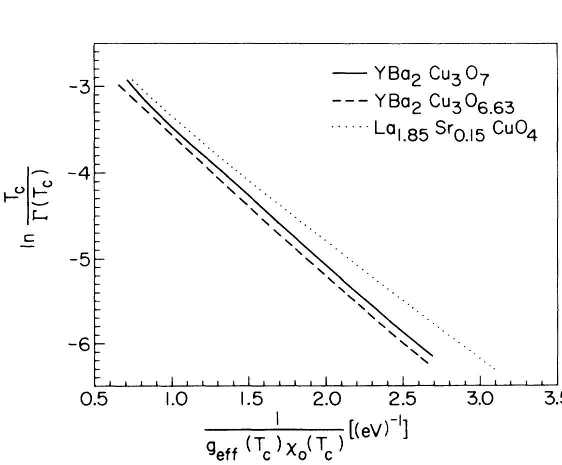

FIG. 3. Plot of the relationship $T_c=\alpha[\Gamma(T_c)]/\pi^2\exp\{-1/[\eta g_{\text{eff}}^2(T_c)\chi_0(T_c)N(0)]\}$. α and η are material-dependent constants that are found to be ($\alpha=1.66$, $\eta=1.07$) for $YBa_2Cu_3O_7$ ($\alpha=1.49$, $\eta=1.07$) for $YBa_2Cu_3O_{6.63}$, and ($\alpha=1.51$, $\eta=1.21$) for $La_{1.85}Sr_{0.15}CuO_4$.

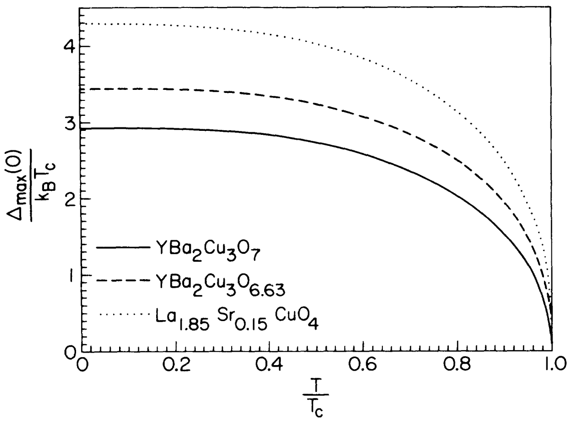

FIG. 4. The temperature dependence of the maximum value of the energy gap for the three high-T_c compounds $YBa_2Cu_3O_7$ ($T_c=95°$ K), $YBa_2Cu_3O_{6.63}$ ($T_c=60°$ K), and $La_{1.85}Sr_{0.15}CuO_4$ ($T_c=40°$ K).

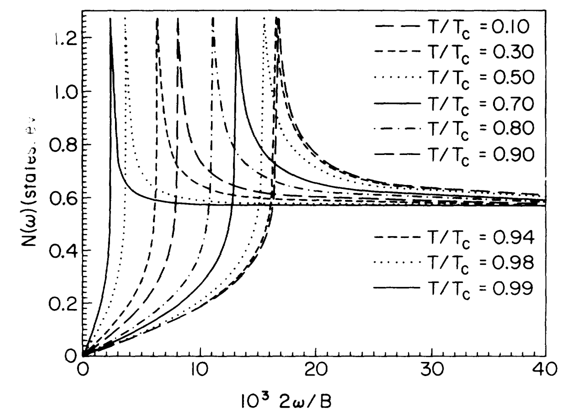

FIG. 5. The density of states for the d-wave gap $\Delta_{x^2-y^2}(\mathbf{k})$ as a function of the variable $2\omega/B$, where $B=2$ eV is the bandwidth, at various values of T/T_c for $YBa_2Cu_3O_7$. Note the linear behavior in frequency for small ω and the logarithmic divergence in two dimensions.

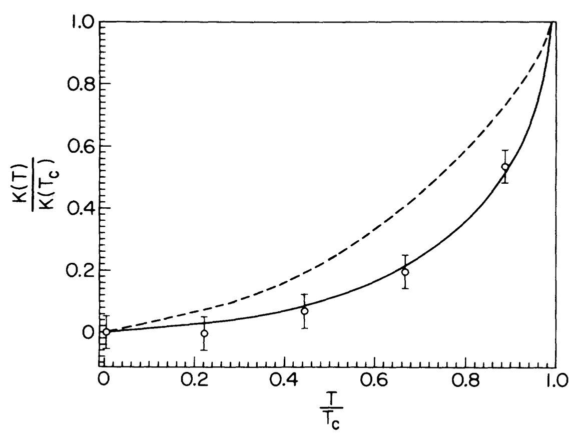

FIG. 6. Knight shift for planar Cu sites in the superconducting state. The dashed line is the bare value, the full line includes the Fermi-liquid correction and $F_0^a=-0.6$. The dots are the experimental values of Barrett *et al.* (Ref. 16).

$\lambda(T_c)=\eta g_{\rm eff}^2(T_c)\chi_0(T_c)N(0)$ varies from 0.48 to 0.33 depending on the compound, and α and η are material constants of order unity. Because momentum transfers far from $\mathbf{Q}=(\pi/a,\pi/a)$ play a significant role, the formula for T_c does not involve the antiferromagnetic correlation length ξ.

(ii) As shown in Fig. 4, even though the coupling is intermediate to weak, below T_c the energy gap opens up very rapidly, reaching a maximum magnitude large compared to the weak-coupling BCS result,[24] in good qualitative agreement with experiment.[16]

(iii) Lower values of T_c are accompanied by larger values of the gap ratio $[\Delta_{\rm max}(0)]/(k_BT_c)$.

(iv) The coupling constants $g_{\rm eff}^2(T_c)$ inferred from λ appear to be in the range required to explain the anomalous resistivity and optical properties of the normal state.

(v) As displayed in Fig. 6, with a physically reasonable Fermi-liquid correction,[25] $F_0^a=-0.6$, the temperature dependence of our calculated planar spin susceptibility agrees with experiment.[16]

(vi) As shown in Fig. 7 for $YBa_2Cu_3O_7$, a susceptibility peaked at the incommensurate wave vector

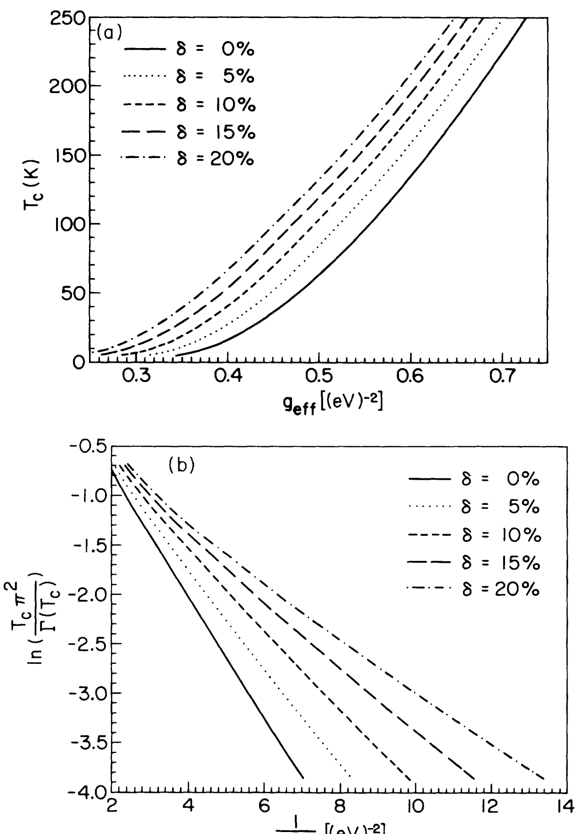

FIG. 7. Effect of incommensurate antiferromagnetic correlations on T_c: (a) shows a plot of T_c vs $g_{\rm eff}$ for various choices of the incommensurate parameter δ defined in the text; (b) shows a plot of log $[(T_c\pi^2)/\Gamma]$ vs $1/g_{\rm eff}^2$ to demonstrate that the incommensuration mainly affects the dimensionless coupling constant λ.

$Q_{inc}=[(\pi/a)(1-\delta),\pi/a]$ and its equivalents in the first Brillouin zone yields higher values of T_c via an increased dimensionless coupling constant λ. For reasonable values of δ, say less than 0.6, the $d_{x^2-y^2}$ gap is still the only possible symmetry. It should be clear from Fig. 1 that the symmetry of the gap becomes d_{xy} as $\delta\rightarrow 1$.

III. DISCUSSION OF THE RESULTS

A striking feature of the present calculation is that even though strong-coupling effects are left out, the gap ratio $[\Delta_{max}(0)]/(k_BT_c)$ is quite large indeed. A plot of the gap ratio versus T_c for the model interaction considered in this paper with the parameters appropriate for $YBa_2Cu_3O_7$ is shown in Fig. 8. Part of this effect can be attributed to the symmetry of the gap. It has been shown by one of us[24] that a separable BCS-like interaction producing a gap with $d_{x^2-y^2}$ symmetry yields a gap ratio $[\Delta_{max}(0)]/(k_BT_c)$ of 2.135, independent of the coupling in the weak-coupling limit. We clearly see that the gap ratio calculated here depends on T_c and thus on the dimensionless coupling constant λ, and that it becomes very large as $T_c\rightarrow 0$. The present calculation leads to a large gap ratio because it includes an anisotropy in both variables θ (because of the $d_{x^2-y^2}$ symmetry) and ϵ (because of the momentum and frequency dependence of the susceptibility); the simple model calculation,[24] which led to $[\Delta\max(0)]/(k_BT_c)=2.135$, only considered the anisotropy in the angular variable θ. However, this is not the whole story, since as we will see below our careful treatment of retardation effects in the superconducting state has an effect on the gap ratio as well.

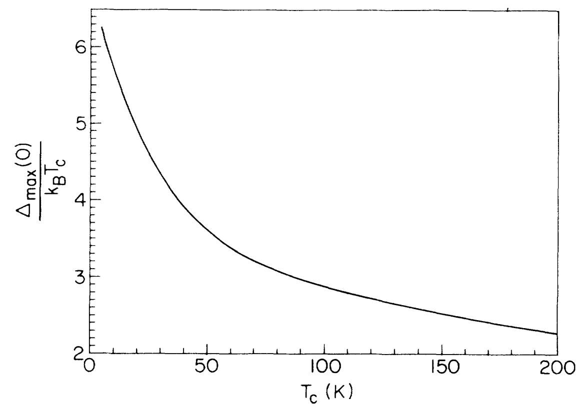

FIG. 8. Calculated values of the maximum value of the energy-gap ratio $[\Delta_{max}(0)]/(k_BT_c)$ as a function of T_c, using the spin-fluctuation spectrum appropriate for $YBa_2Cu_3O_7$.

Another important feature of our results is the very rapid variation of the gap near the critical temperature T_c. We can attribute this to the retardation effects in the superconducting state, since the effective interaction becomes gap dependent below T_c as was noted after Eq. (10). It is easy to demonstrate this point explicitly by calculating the gap in the superconducting state with a gap-independent interaction according to the following equation:

$$\Delta(\mathbf{k})=-g_{\rm eff}^2(T)\int_0^{\pi/a}\frac{adk_x'}{2\pi}\int_0^{k_x'}\frac{adk_y'}{2\pi}\sum_{i=1}^{8}\left[\mathrm{Re}\chi(\mathbf{k}-\Phi_i\mathbf{k}',\varepsilon_{\mathbf{k}'}-\mu)\frac{\tanh\left[\frac{E_{\mathbf{k}'}}{2k_BT}\right]}{E_{\mathbf{k}'}}\right]\Delta(\Phi_i\mathbf{k}')\ . \tag{13}$$

Notice that we have changed $E_{\mathbf{k}'}$ to $\varepsilon_{\mathbf{k}'}-\mu$ in the susceptibility compared with the true equation below T_c, Eq. (10). Figure 9 shows plots of the gaps $\Delta_{max}(T)$ and scaled gaps $[\Delta_{max}(T)]/[\Delta_{max}(0)]$ obtained from Eqs. (10) and (13) for $YBa_2Cu_3O_7$. Figure 9(a) shows that the retardation effects lead to a reduction of the gap, and hence of the gap ratio. This occurs because retardation reduces the effective interaction. The real part of the susceptibility is maximum at zero frequency; i.e. $\mathrm{Re}\chi(\mathbf{k}-\Phi_i\mathbf{k}',\varepsilon_{\mathbf{k}'}-\mu)$ is largest when the quasiparticle is on the Fermi surface $\varepsilon_{\mathbf{k}'}=\mu$. When the spectrum develops a gap, the zero-frequency part of the susceptibility is only available at the nodes of the gap, leading to a decrease of the effective interaction. As can be seen in Fig. 9(b), the feedback effect of the opening up of the gap on the effective interaction is responsible for the rapid variation of $\Delta_{max}(T)$ near T_c.

As was noted in the previous section, our BCS-like formula for the critical temperature, Eq. (12), does not involve the antiferromagnetic correlation length ξ. To clarify this we calculated the critical temperature for $YBa_2Cu_3O_7$ for different values of the correlation length, according to $\xi^2\rightarrow\kappa\xi^2$, keeping all the other quantities constant. A plot of T_c versus κ is shown on Fig. 10. As long as the correlation length is large enough, T_c is nearly independent of κ. As pointed out by Millis,[11] this is due to the fact that spin excitations of wave vector more than ξ^{-1} away from $\mathbf{Q}=(\pi/a,\pi/a)$ make a significant contribution to the effective interaction. However, one gets into trouble when the correlation length becomes of order unity; the critical temperature then begins to drop sharply. This can be understood as a result of the projection onto a d-wave harmonic of a function that is now only weakly momentum dependent.[25]

IV. COMPARISON WITH OTHER CALCULATIONS

It is instructive to compare the present calculations, in which the low frequency and momentum dependence of the effective interaction plays a significant role, with ear-

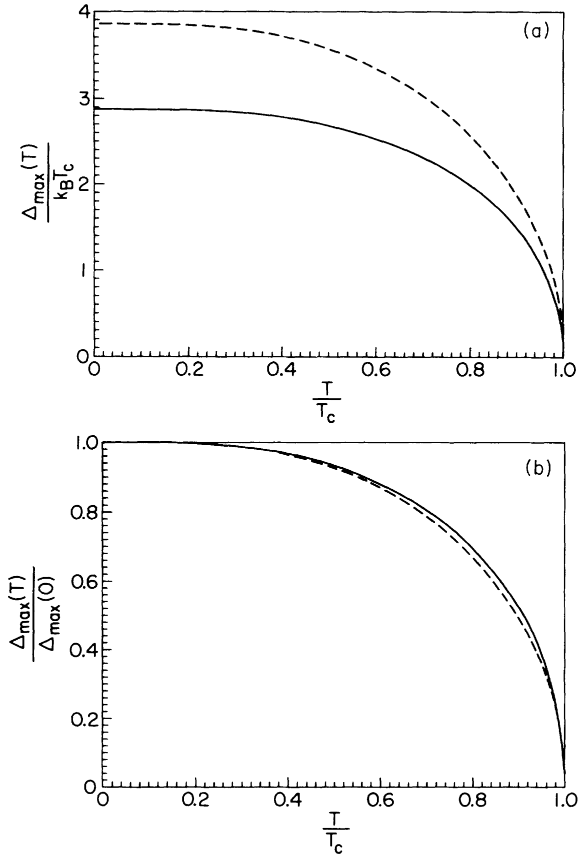

FIG. 9. Result of calculations that make evident the influence of retardation on $\Delta_{max}(T)$; (a) $\Delta_{max}(T)$ calculated without retardation (dashed line) and with retardation (full line); (b) the corresponding calculated gap ratios $[\Delta_{max}(T)]/[\Delta_{max}(0)]$.

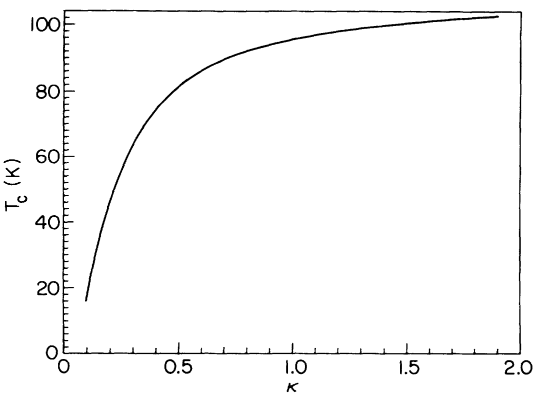

FIG. 10. Calculated dependence of T_c on the correlation length ξ. The spin-fluctuation spectrum is that of $YBa_2Cu_3O_7$. The scaling parameter κ is defined in the text.

lier calculations in which certain simplifying approximations have been made. We first discuss the approach of Millis,[11] which is related to earlier calculations of Millis, Sachdev, and Varma,[26] and which employs approximations borrowed from phonon-induced superconductivity. For the latter systems, the characteristic energy scale of phonons ω_D, is much smaller than the Fermi energy E_F, and only electronic states near the Fermi surface are important (i.e., in a region of relative size ω_D/E_F). It is then argued that one may put both momenta in the effective interaction on the Fermi surface and integrate the electron propagators over the magnitude of the electron momentum. The resulting equations then involve Fermi-surface quantities only. Since our characteristic energy scale is also much smaller than the bandwidth, i.e., the prefactor in the T_c formula $\Gamma/\pi^2 \sim 40$ meV, it has been argued by Millis[11] that a similar type of approximation should hold for our spin-fluctuation mechanism, in that such an approach should yield results that are logarithmically accurate (i.e., one should be able to get the dimensionless coupling constant λ right, while perhaps missing out on the prefactor in the expression for T_c). The physical arguments being plausible, it is worth comparing this approach to the one we have been following. We carry out the comparison for the calculation of T_c, using the spin-fluctuation spectrum appropriate to $YBa_2Cu_3O_7$.

The weak-coupling linearized gap equation in momentum and Matsubara space for singlet pairing is

$$\Delta(\mathbf{k},i\omega_n) = -2g_{\text{eff}}^2(T)\int_0^{\pi/a}\frac{a\,dk_x'}{2\pi}\int_0^{k_x'}\frac{a\,dk_y'}{2\pi}k_BT\sum_{\Omega_n}\sum_{i=1}^{8}(-1)^{\Phi_i}\frac{\chi(\mathbf{k}-\Phi_i\mathbf{k}',i\omega_n-i\Omega_n)}{\Omega_n^2+(\varepsilon_{\mathbf{k}'}-\mu)^2}\Delta(\mathbf{k}',i\Omega_n)\ . \tag{14}$$

As before, $\{\Phi_i\}_{i=1,\ldots,8}$ are the transformations that map any wave vector $\mathbf{k}'$ in the Brillouin zone onto the first octant and $(-1)^{\Phi_i}$ is the parity of the gap under Φ_i, i.e., $\Delta(\Phi_i\mathbf{k},i\omega_n)=(-1)^{\Phi_i}\Delta(\mathbf{k},i\omega_n)$. The factor $2g_{\text{eff}}^2$ comes from our definition of the coupling constant: the factor $\frac{1}{2}$ from $\{\tanh[(\varepsilon_{\mathbf{k}}-\mu/2k_BT)]\}/[2(\varepsilon_{\mathbf{k}}-\mu)]$ was absorbed in the definition of g_{eff}^2.

For the sake of comparison, we also transform the equation using the energy and angle variables introduced in Eq. (8) with a corresponding transformation from k_x', k_y' to ε', θ'. One then has $\varepsilon_{\mathbf{k}'}-\mu=(B/2)(\varepsilon'-\mu')$, where $\mu=(B/2)\mu'$, $B=8t$ is the bandwidth. The Jacobian of the transformation is

$$J(\varepsilon',\theta')=\frac{2}{[(1+|\varepsilon'|)^2-(1-|\varepsilon'|)^2\cos^2(\theta')]^{1/2}}\ .$$

The gap with $d_{x^2-y^2}$ symmetry is then transformed to $\Delta(\mathbf{k},i\omega_n)\equiv\Delta_0(\mathbf{k},i\omega_n)[\cos(k_x)-\cos(k_y)] \rightarrow -2\Delta_0(\varepsilon,\theta,i\omega_n)(1-|\varepsilon|)\cos(\theta)$. In the new variables the gap equation becomes

$$\Delta_0(\varepsilon,\theta,i\omega_n)(1-|\varepsilon|)\cos(\theta)=-\frac{2g_{\rm eff}^2(T)}{4\pi^2}\int_{-1}^{1}d\varepsilon'\int_0^{\pi/2}d\theta' k_B T\sum_{\Omega_n}\sum_{i=1}^{8}(-1)^{\Phi_i}\frac{\chi[\mathbf{k}(\varepsilon,\theta)-\Phi_i\mathbf{k}'(\varepsilon',\theta'),i\omega_n-i\Omega_n]}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}\times\frac{2\Delta_0(\varepsilon',\theta',i\Omega_n)(1-|\varepsilon'|)\cos(\theta')}{[(1+|\varepsilon'|)^2-(1-|\varepsilon'|)^2\cos^2(\theta')]^{1/2}} . \quad (15)$$

What is actually done in the electron phonon problem is to set ε and ε' equal to μ' everywhere, except in

$$\frac{1}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2} .$$

The latter is replaced by its average over the energy interval $[-\infty,\infty]$. The argument is that this quantity is sharply peaked near the Fermi surface and thus its average is mostly determined by the relevant energy scales $E_F\pm\omega_D$ $[E_F\pm(\Gamma/\pi^2)$ in our case]. On the other hand it is argued that the other terms in the equation are weakly momentum dependent in this energy range and can be approximated by their values on the Fermi surface.

Thus

$$\frac{1}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}\rightarrow\int_{-\infty}^{\infty}\frac{d\varepsilon'}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}=\frac{2\pi}{B|\Omega_n|} , \quad (16)$$

and one obtains

$$\Delta_0(\mu',\theta,i\omega_n)\cos(\theta)=-\frac{2g_{\rm eff}^2(T)}{\pi^2 B}\int_0^{\pi/2}d\theta'\pi k_B T\sum_{\Omega_n}\sum_{i=1}^{8}(-1)^{\Phi_i}\frac{1}{|\Omega_n|}\chi[\mathbf{k}(\mu',\theta)-\Phi_i\mathbf{k}'(\mu',\theta'),i\omega_n-i\Omega_n]\times\frac{\Delta_0(\mu',\theta',i\Omega_n)\cos(\theta')}{[(1+|\mu'|)^2-(1-|\mu'|)^2\cos^2(\theta')]^{1/2}} . \quad (17)$$

When the frequency dependence of the gap can be ignored, $i\omega_n$ can be analytically continued to $\omega+i\delta$ after the sum over Ω_n is performed, and ω is set to zero. In the present case, working in the Matsubara frequency representation, $i\omega_n$ is set to $\pi k_B T$. From now on we drop the index μ' of Δ_0 and we define $\overline{\Delta_0}(\theta)\equiv\Delta_0(\theta)\cos(\theta)$.

One thus has the weak-coupling gap equation

$$\overline{\Delta_0}(\theta)=\frac{g_{\rm eff}^2(T)}{\pi^2 B}\int_0^{\pi/2}d\theta' V_{\rm eff}(\theta,\theta')\overline{\Delta_0}(\theta') , \quad (18a)$$

where

$$V_{\rm eff}(\theta,\theta')=-2\pi k_B T\sum_{\Omega_n}\sum_{i=1}^{8}\frac{(-1)^{\Phi_i}\chi[\mathbf{k}(\mu',\theta)-\Phi_i\mathbf{k}'(\mu',\theta'),i\pi k_B T-i\Omega_n]}{|\Omega_n|[(1+|\mu'|)^2-(1-|\mu'|)^2\cos^2(\theta')]^{1/2}} . \quad (18b)$$

We have solved equations (18a) and (18b) numerically for the transition temperature; the results are displayed in Fig. 11, where they are compared to the transition temperatures obtained from the more complete calculation embodied in Eq. (9). With the Millis approximation a BCS-like fit to T_c similar to Eq. (12) is possible and one has

$$T_c=\alpha\frac{\Gamma}{\pi^2}\exp\left[-\frac{1}{\eta g_{\rm eff}^2 N(0)\chi_0}\right] ,\alpha=2.65,\quad \eta=0.57 . \quad (19)$$

On comparing those results to those we obtained with the full gap equation ($\alpha=1.66$, $\eta=1.07$), we see that the Millis approximation leads to a significant underestimate of the dimensionless coupling constant $\lambda=\eta g_{\rm eff}^2 N(0)\chi_0$, the magnitude of the kernel in the integral equation, which measures the effectiveness of the spin-fluctuation-

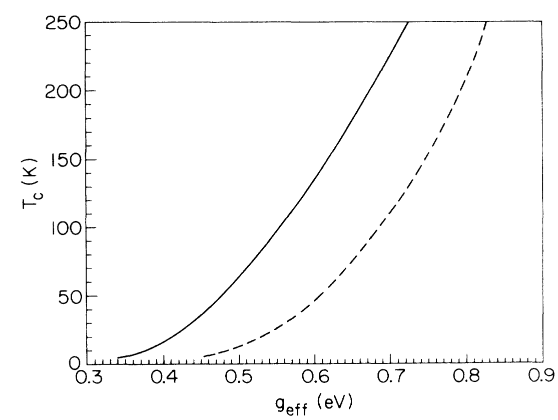

FIG. 11. Comparison of T_c calculated in the Millis approximation (dashed line) with that obtained by the authors using the full momentum and frequency dependence of the effective quasiparticle interaction (full line).

induced interaction in bringing about superconductivity.

To understand the physical origin of this underestimate we examine the steps leading to Eqs. (18a) and (18b) one by one. In our calculation, the fashion in which $V(\varepsilon,\varepsilon')$ decreases away from the Fermi surface is determined both by the frequency and momentum dependence of the susceptibility. It is not straightforward to determine precisely how much is due to the momentum dependence alone. We have explicitly checked that changing $V(\varepsilon,\varepsilon')$ for energies further than Γ/π^2 away from the Fermi surface does not influence the value of T_c at all. It is then true that only a comparatively thin shell around the Fermi surface actually matters. However, when one replaces

$$\frac{1}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}$$

by its average over the energy interval $[-\infty,\infty]$ one gets a contribution from energies that should have no influence on T_c. Clearly that approximation has an influence on the result. The question is, does it influence the dimensionless coupling constant λ or the prefactor $\alpha(\Gamma/\pi^2)$? To answer this, we carry out the average over a finite interval

$$\frac{1}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}\rightarrow\int_{-\Lambda+\mu'}^{\Lambda+\mu'}\frac{d\varepsilon'}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}=\frac{4\pi}{B|\Omega_n|}\arctan\left[\frac{\Lambda B}{2|\Omega_n|}\right]. \tag{20}$$

Plots of $\log[(T_c\pi^2/\Gamma)]$ versus $1/[g_{\rm eff}^2N(0)\chi_0]$ for various choices of Λ are shown in Fig. 12. Since the curves are parallel we conclude that the approximation of replacing

$$\frac{1}{\Omega_n^2+\left[\frac{B}{2}(\varepsilon'-\mu')\right]^2}$$

by its average over the energy interval $[-\infty,\infty]$ only affects the cutoff. It should lead to the overestimate of the latter, since the integral over the infinite interval is obviously larger than that over the finite-energy range that actually matters in the calculation of T_c. In fact, by fitting the curves of Fig. 12 to the formula $T_c=\alpha(\Gamma/\pi^2)\exp\{-1/[\eta g_{\rm eff}^2N(0)\chi_0]\}$, one sees that α goes from 1.80 to 2.55 as Λ increases from 0.25 to 2.0 eV, while η does not change within the accuracy of the fit. Thus one is led to suspect that it is the approximation made in putting both momenta $\mathbf{k}$ and $\mathbf{k}'$ on the Fermi surface in the expression for the susceptibility in Eq. (14), which is invalid.

One can easily convince oneself that for $\mathbf{k}$ in the first octant of the Brillouin zone ($k_x,k_y>0$ and $k_x>k_y$), the momenta $\mathbf{k}'$ that make a large contribution to the integral are such that $k_x'=-k_y$ and $k_y'=-k_x$, since then $\mathbf{k}-\mathbf{k}'\|(\pi/a,\pi/a)$. Then, for the lowest Matsubara frequency $i\nu_l=0$, $\chi(\mathbf{k}-\mathbf{k}',0)$ is given by

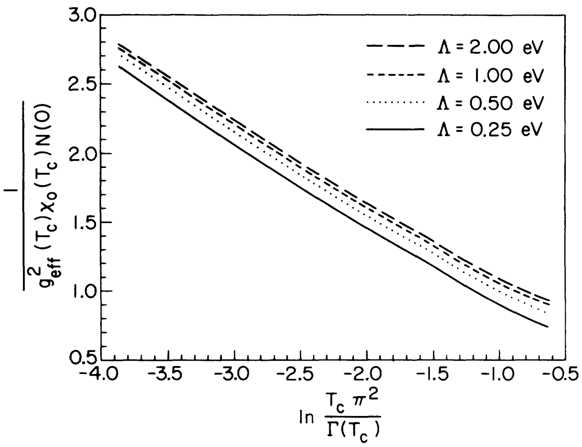

FIG. 12. Calculated dependence of T_c on the cutoff parameter Λ [cf. Eq. (20)].

$$\chi(\mathbf{k}-\mathbf{k}',0)\big|_{\substack{k_x'=-k_y\\ k_y'=-k_x}}=\frac{\chi_Q}{1+2\xi^2[k_x+k_y-(\pi/a)]^2}. \tag{21}$$

To make it easier to visualize what is going on, we parametrize $\mathbf{k}$ as in Eq. (8), and look at the variation of χ for a fixed angle θ as ε goes from 0 to 1. A plot of $\mathbf{k}$ and $\mathbf{k}'$ for ε and ε' equal to 0 and 1 is given in Fig. 13 (notice that $\varepsilon=0$ corresponds to perfect nesting), while the variation of $\chi(\mathbf{k}-\mathbf{k}',0)$ between those extremes is shown in Fig. 14 for $\theta=(\pi/2)-0.01$ at $T=100°$ K. The Fermi level and the relevant energy range for superconductivity are indicated by dotted lines. One then sees from Fig. 14 that the important spin fluctuations for superconductivity are those with momenta far away from $(\pi/a,\pi/a)$, while in that region of momentum space the susceptibility falls off very rapidly (by nearly a factor 2), making it impossible to put both quasiparticle momenta on the Fermi surface in the gap equation (14). If one seeks a quanti-

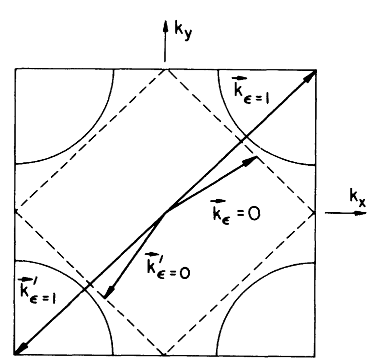

FIG. 13. Quasiparticle wave vectors $\mathbf{k}$ and $\mathbf{k}'$ whose difference is parallel to $\mathbf{Q}$, for two different choices of the dimensionless energy parameter ε. For $\varepsilon=0$, the interaction between the quasiparticles is maximum ($\mathbf{k}-\mathbf{k}'=\mathbf{Q}$), while for $\varepsilon=1$, one has $\mathbf{k}-\mathbf{k}'=0$.

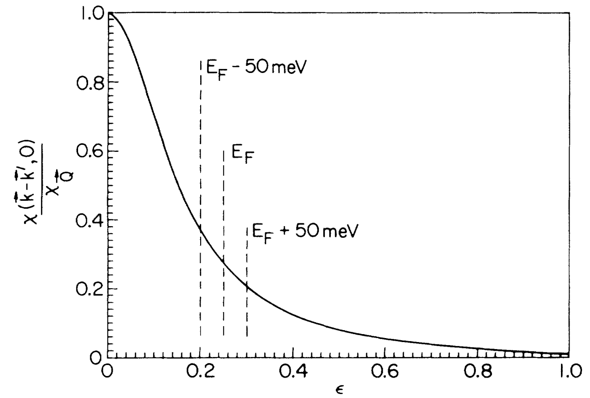

FIG. 14. Reduced interactive susceptibility $[\chi(\mathbf{k}-\mathbf{k}',0)]/\chi_{\mathbf{Q}}$, as a function of the parameter ε as explained in the text. Quasiparticles lying within 50 meV of the Fermi surface are seen to sample quite different values of $\chi(\mathbf{k}-\mathbf{k}',0)$.

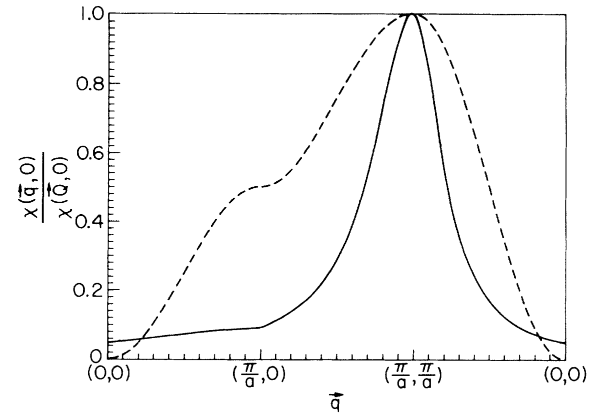

FIG. 15. Comparison of $\chi_0(\mathbf{q})=J_0+J_1[\cos(q_x a)+\cos(q_y a)]$ with the $\chi_0(\mathbf{q})$ calculated using the MMP expression Eq. (2) and taking $\xi=a$. The ratio $J_0/J_1=0.5$ displayed here is the maximum ratio that yields a susceptibility that is positive over the entire Brillouin zone.

tative answer, one therefore has no choice but to allow for the full momentum dependence of the interaction, as we have done in our treatment of Eq. (9).

Another approach to spin-fluctuation superconductivity has involved solving model problems in which the model interaction is separable,[27]

$$\chi(\mathbf{q},\omega)=\chi_0(\mathbf{q})f(\omega)\ , \tag{22a}$$

and $\chi_0(\mathbf{q})$ is further approximated by expressions of the form[27]

$$\chi_0(\mathbf{q})=J_0+J_1[\cos(q_x a)+\cos(q_y a)]\ . \tag{22b}$$

To obtain a rough estimate of the validity of approximations of this kind, we compare this form of the static susceptibility with the MMP expression calculated for a short correlation length $\xi\cong a$. As may be seen in Fig. 15, using an expression of the form (22b) leads to a momentum dependence of $\chi_0(\mathbf{q})$ that is even weaker than that obtained with the MMP form with $\xi\cong a$. Since we have already shown that for such short correlation lengths antiferromagnetic spin fluctuations are ineffective in bringing about superconductivity, it follows that model calculations based on simple expressions of the form (22b) cannot be expected to yield high transition temperatures, and will lead to unrealistic estimates of spin-fluctuation superconductivity for systems in which there are strong antiferromagnetic correlations between electron spins.

V. ROLE OF IMPURITIES

For d-wave pairing, it is well known that the Anderson theorem[28] does not apply, so that the elastic scattering of quasiparticles by nonmagnetic, i.e., scalar impurities, gives rise to significant pair-breaking effects, and so reduces T_c. In this section, we examine, in the weak-coupling approximation, the importance of such pair breaking for our $d_{x^2-y^2}$ pairing state, and compare our results with those obtained by Abrikosov and Gor'kov[29] for the influence of nonmagnetic impurities on conventional s-wave superconductors. We then discuss briefly the role played by the inelastic scattering of quasiparticles by spin fluctuations, a pair-breaking effect that is considerably more important for good samples of the copper oxide superconductors.

Scalar impurity scattering acts to change the quasiparticle propagators that enter the gap equation, Eq. (9). We describe the effect of impurities by a Lorentzian broadening of the one-particle spectral function. The retarded Green's function is thus

$$G_R(\mathbf{p},\omega)=\frac{1}{\omega-(\varepsilon_{\mathrm{p}}-\mu)+\dfrac{i}{2\tau}} \tag{23}$$

and we parametrize the quasiparticle lifetime according to

$$\frac{1}{2\tau}=\gamma k_B T_{c0}\ , \tag{24}$$

where T_{c0} is the transition temperature of the pure material. The gap equation (6) in the presence of nonmagnetic impurities is thus

$$\Delta(\mathbf{k})=-g_{\mathrm{eff}}^2(T)\int_{\mathrm{BZ}}\frac{a^2d^2k'}{(2\pi)^2}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\mathrm{Re}\chi(\mathbf{k}-\mathbf{k}',\omega)\tanh\left[\frac{\omega}{2k_BT}\right]\mathrm{Re}G_R(-\mathbf{k}',-\omega)\mathrm{Im}G_R(\mathbf{k}',\omega)\Delta(\mathbf{k}')\ . \tag{25}$$

This gap equation can be solved numerically after the change of variables according to Eq. (8) is performed; our results are given in Fig. 16, where they are compared with the Abrikosov-Gor'kov results for the influence of scalar impurities on an s-wave superconductor, which, for the case of d-wave pairing, can be shown to apply for a separable potential.[24]

We see that for intermediate to large values of γ, pair breaking is considerably less effective than a simple calculation based on the Abrikosov-Gor'kov formula would have led one to believe. The physical origin of this difference is again to be found in the structure of the effective spin-fluctuation-induced interaction. When that structure is ignored, as in our example of a simple calculation using a separable potential approach,[24] impurity scattering appears to play a far more significant pair-breaking role than it does for a realistic quasiparticle interaction. For the realistic case we see that impurities tend to destroy superconductivity altogether only when $\hbar/\tau \sim \Delta_{max}(0)$, a physically reasonable result, since this is the condition for scattering to influence appreciably the possibility of pair formation.

Experiment shows that for good samples, the normal-state quasiparticle lifetime as measured in both resistivity and optical experiments is temperature dependent and large compared to that produced by impurity scattering; thus one has

$$\frac{1}{2\tau} = \gamma k_B T \gg \left[\frac{1}{\tau}\right]_{imp},$$

where $\gamma \le 1$. In the description of the normal state as a nearly antiferromagnetic Fermi liquid, the physical origin of this lifetime is the quasielastic scattering of quasiparticles against low-frequency spin fluctuations. How then to take this scattering into account? Because these same spin fluctuations are here assumed to be the physical origin of the superconductivity, the effective quasiparticle interaction will not be modified by this scattering; it will only act to modify the single-particle propagators that enter the gap equation. That modification will, however, be far from simple since, as we have noted earlier, because the quasiparticle Fermi surface is incommensurate while the spin-fluctuation excitation spectrum to which these couple is peaked about the commensurate wave vector **Q**, the quasiparticle self-energy varies appreciably over the Fermi surface. We therefore expect that using Eq. (24), with $\gamma \sim 1$ to deal with the pair-breaking effect of quasielastic spin-fluctuation scattering may well lead to an underestimate of their importance. What is required is a strong-coupling self-consistent solution of the Eliashberg equations for the spin-fluctuation model considered here.

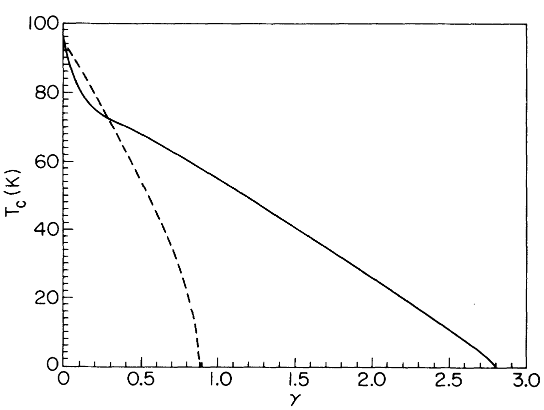

FIG. 16. Comparison of the results of our calculations for the influence of elastic impurity scattering on T_c, a calculation in which the momentum dependence of the spin-fluctuation-induced interaction is taken into account, with those obtained using the Abrikosov-Gor'kov formula.

Even in the absence of detailed calculations, it is clear that the quasielastic scattering of quasiparticles is sufficiently large in the copper oxide superconductors that it reduces T_c appreciably from the value T_{c0}, as it would have were the scattering not present. Since such quasielastic scattering becomes markedly reduced in the superconducting state (the experiments of Bonn *et al.*[30] suggest that this reduction follows closely the corresponding reduction in spin-lattice relaxation times), it is highly plausible that at low temperatures its influence on the gap will be small. Consequently, as is well known, the measured gap ratios $[\Delta_{max}(0)]/(k_B T_c)$ are larger than the intrinsic ratio $[\Delta_{max}(0)]/(k_B T_{c0})$, which would occur in the absence of the reduction of T_c by pair-breaking effects, and which we calculate here in the weak-coupling limit.

Finally, we note that since the structure of the effective interaction between quasiparticles influences the way in which impurities (or quasielastic scattering) act to reduce T_c, we do not expect the critical temperatures to be a universal function of $1/\tau T_c$, even in the weak-coupling limit.

VI. CONCLUSION

In this paper we have demonstrated that spin fluctuations represent a highly attractive mechanism for high-temperature superconductivity. When compared to the conventional low-temperature BCS superconductors, the superconducting state we obtain possesses a number of unconventional properties, most if not all of which are in qualitative agreement with experiment. Our pairing state possesses the $d_{x^2-y^2}$ symmetry, and so provides a natural explanation for the unconventional NMR properties (no Hebel-Slichter peak,[14,15] an overall T^3 behavior,[14] and a temperature-dependent anisotropy in the spin-lattice relaxation rates[17–19]). Our calculated maximum energy gap opens up quite rapidly below T_c, in agreement with NMR, optical, and high-resolution electron energy loss spectroscopy (HREELS) experiments, while the maximum gap ratio $[\Delta_{max}(0)]/(k_B T_c)$ is intrinsically large, in qualitative agreement with experiment. There is an emerging consensus[31,32] that at low temperatures, the temperature dependence of $\rho_n(T)/\rho$, as measured by many techniques, takes the form $[\rho_n(T)]/\rho = a + bT^2$. Gross *et al.*[33] and Prohammer and Carbotte[34] have argued that this result, which is incompatible with the conventional

BCS theory, will follow from a combination of d-wave pairing and impurity scattering, in which case, as Annett *et al.*[31] have pointed out, the coefficient of the T^2 term will be sample dependent.

We have also shown that in systems such as the one studied in this paper, in which the effective quasiparticle exhibits considerable structure, there is no substitute for doing calculations that take the full structure of the interaction into account. Specifically, we find that the structure of the spin-fluctuation-induced interaction (i) makes possible larger transition temperatures, (ii) leads to larger gap ratios, and (iii) renders elastic impurity scattering far less effective as a pair-breaking mechanism.

In several examples in Sec. IV, we have demonstrated explicitly how disregarding structure leads one to seriously underestimate the effectiveness of spin-fluctuation-induced interactions in bringing about superconductivity. This leads us to propose a theorem for superconducting and superfluid systems: if the proposed interaction possesses structure, that structure *must* be allowed for by solving the full integral equations, which determine the superconducting transition temperature and superconducting properties. Since spin fluctuations are prime candidates for the superconductivity of the heavy electron systems and for the superfluidity of ^{3}He, it will be interesting to test our proposed theorem for these systems.

In our calculations we have allowed for some feedback effects on the gap equation; we have, however, assumed that the effective interaction between quasiparticles in the superconducting state is little changed from its value at T_c. In the absence of a microscopic theory of the spin-excitation spectrum, it is difficult to estimate how significant such feedback effects will be.

The problem of the nature of the superconducting state in two dimensions in the presence of antiferromagnetic correlations that we have studied here is interesting in its own right. However, the superconductivity in high-T_c compounds is three dimensional. Interplanar coupling in some form will establish the true 3D coherence of the order parameter. Since the interplanar coupling is weak, we believe that the in-plane symmetry will remain $d_{x^2-y^2}$, and that the superconducting properties will be close to those calculated here.

There is not yet sufficient experimental evidence on the spin-fluctuation-excitation spectrum of the BSCCO family of materials to enable one to carry out calculations for this system that are comparable to the results presented here for the 1-2-3 and 2-1-4 systems. The recent results of Li, Huang, and Lieber,[35] who use HREELS techniques to study the behavior of very well characterized thin films suggest that the energy-gap behavior in these materials is close to that found for 1-2-3 systems: a gap that opens up very rapidly below T_c and reaches a maximum $\Delta_{max}(0) \sim 3k_B T_c$.

We have also not discussed here the behavior of the chain quasiparticles in the normal state, their transition to superconductivity, and their properties in the superconducting state. NMR experiments[36] show that the chain quasiparticles behave quite differently from their planar counterparts; for example, the spin-lattice relaxation rate follows a Korringa law, so that there is no evidence for antiferromagnetic correlations among the chain quasiparticle spins. It appears likely that superconductivity in the chains is induced by the planar excitations (T_c is the same), in which case the chain pairing state must also be d wave. That could explain the linear temperature dependence of the low-temperature Knight shift observed by Barrett *et al.*,[16] while the assumed very weak coupling between chains and planes would explain the quite different magnitude and temperature dependence of $\Delta_{max}(T)$ found for the chain quasiparticles.

The present calculations, however, represent only a first step toward the development of a consistent theory of superconductivity in the copper oxides. For example, before a quantitative comparison with experiment for the transition temperature, gap properties, etc., can be made, it is important to incorporate lifetime effects and to carry out the self-consistent calculation of the chemical potential that is needed as well for normal-state properties. While we find it is possible to obtain large energy gaps in a weak-coupling approximation, the role of strong-coupling corrections needs to be explored. We note that to the extent that the Migdal approximation is valid, it suffices to solve the Eliashberg equations for our model Hamiltonian, Eq. (1); we have obtained solutions to these equations for the model Hamiltonian, Eq. (1), and will report our results in a subsequent paper.[37]

Although we can now demonstrate through the explicit solutions of the Eliashberg equations that high-temperature superconductivity emerges from the model Hamiltonian Eq. (1) for physically realistic values of coupling constants and spin-excitation spectra, there remains the further question of deriving this model Hamiltonian from first principles. For example, while it is clear that the very strong Coulomb correlations play a significant role in almost localizing the Cu^+ spins and determining the spin-fluctuation spectrum, it remains to be seen whether these can influence the system behavior in other ways.

In conclusion, we emphasize the importance of verifying experimentally our prediction of a $d_{x^2-y^2}$ pairing state, and of exploring the consequences of such pairing on all aspects of the superconducting state.

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