Spin-fluctuation-induced superconductivity and normal-state properties of $YBa_2Cu_3O_7$

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We have carried out strong-coupling calculations using the Eliashberg formalism for $YBa_2Cu_3O_7$. We consider the influence of potential impurity scattering on T_c. We find that, as the strength of the impurity potential increases, the unitary limit is reached comparatively quickly. In this (unitary) limit, the influence of isotropic impurity scattering on T_c is relatively weak. We show, with the aid of a simple model to describe the disruption of the local magnetic order brought about by the substitution of Zn, that the latter has a strong influence on T_c. We consider the competition between antiferromagnetic and superconducting instabilities and find that, for our model parameters, the instability to a superconducting state always comes first. Next, we examine the sensitivity of our results for T_c to the details of the spin-fluctuation spectrum and hole concentration. When that spectrum is modified so that it is consistent with both NMR T_1 and T_2 measurements, a superconducting transition temperature of 90 K is obtained with a dimensionless coupling contant, $\lambda < \frac{1}{2}$. Strong-coupling calculations of the normal state, using these latter parameters and including vertex corrections, yield an in-plane resistivity which varies linearly with temperature, with a magnitude at 100 K of 20 $\mu\Omega$ cm, and, with minor changes in parameters, a frequency dependence of the optical conductivity in quantitative agreement with experiment for energies < 50 meV. With an interlayer hopping $t_\perp$ of 8 meV, the c-axis resistivity is found to be linear in temperature with a magnitude at 150 K of 2.5 mΩ cm.

I. INTRODUCTION

In previous papers we have described the results of extensive numerical calculations on the normal state and superconducting transition temperature for $YBa_2Cu_3O_7$ using a model of planar quasiparticles, obeying a dispersion relation determined by ARPES experiments, which are magnetically coupled to antiferromagnetic paramagnons, spin fluctuations whose spectrum is taken from fits to NMR experiments.[1,2] In Ref. 1, hereafter referred to as MBP, we described the results of weak-coupling calculations which demonstrated that the resulting spin-fluctuation-induced interaction between the quasiparticle would lead uniquely to a transition to a superconducting state with $d_{x^2-y^2}$ symmetry. We demonstrated the importance, in any quantitative calculation, of taking the full structure, in frequency and momentum space, of that interaction into account, showing, by example, that calculations in which that structure was ignored led to a significant underestimate (by factors of 3–5) of T_c, a result we called a "no free lunch theorem." In Ref. 2, hereafter referred to as MP I, we described the results of strong-coupling calculations, using the Eliashberg equations, which provide a "proof of concept" for spin-fluctuation-induced superconductivity and $d_{x^2-y^2}$ pairing in $YBa_2Cu_3O_7$. Thus we showed that while the lifetime effects neglected in a weak-coupling calculation reduce T_c dramatically, superconductivity at high temperatures is still possible for comparatively modest values of the quasiparticle–spin-fluctuation coupling constant and that the strong-coupling corrections contained in the Eliashberg equations do not alter the $d_{x^2-y^2}$ character of the pairing state. We demonstrated for $YBa_2Cu_3O_7$ a direct link between its anomalous magnetic, transport, and optical properties in the normal state and its high superconducting transition temperature. Thus we showed that for our model experiment-based Hamiltonian, the coupling constant g^2, which yields a transition temperature $T_c \sim 90$ K, is in the range required to provide a quantitative explanation of the measured normal-state resistivity and optical properties of the normal state. Put another way, we showed that the magnetic scattering of planar quasiparticles by the anomalous low-energy spin fluctuations[3] required to explain the NMR experiments on $YBa_2Cu_3O_7$ (Ref. 4) gives rise to measured anomalous charge transport and optical properties, while their resulting spin-fluctuation-induced interaction produces high-temperature superconductivity. We found from our numerical experiments that for a range of coupling constants this transition temperature could be written in a simple BCS-like strong-coupling form

$$T_c = \tilde{\Gamma} \exp\left[-\frac{1}{\lambda}\right], \tag{1}$$

where $\tilde{\Gamma}$ is a cutoff energy (~ 30 meV) for the effectiveness of the spin-fluctuation-induced interaction and the dimensionless coupling constant $\lambda \sim 0.8$ is proportional to the product of g and the calculated tunneling density of states per unit energy, $N(0)$.

In MP I we also presented the results of our strong-coupling calculations of the corrections to the quasiparticle self-energy which arise from their coupling to the spin fluctuations. We found that the normal state *is* a Fermi liquid in the sense that the single-particle Green's function has a set of well-defined poles at the quasiparticle excitation energy $\omega=E_{\mathbf{p}}$ as $T,\omega\rightarrow 0$, and that for the parameters used to characterize $YBa_2Cu_3O_7$ the residue of these poles at $T=90$ K was quite substantial ($0.4\leq Z_{\mathbf{p}_f}\leq 0.6$). However, the imaginary part of the quasiparticle self-energy, $\mathrm{Im}\Sigma(\mathbf{p}_f,\omega)$, turned out to be quite different from that of an ordinary Landau Fermi liquid. For frequencies smaller than the low-energy scale, ω_{SF}, which characterizes the spin-fluctuation spectrum, $\mathrm{Im}\Sigma(\mathbf{p}_f,\omega)$ goes like $\alpha T+\gamma\omega^2$, where α and γ are constants, while for frequencies large compared to ω_{SF} it becomes linear in ω for energies up to 0.25 eV. The magnitude of both the real and imaginary parts of the quasiparticle self-energy depends sensitively on its location with respect to the Fermi surface and its proximity to Van Hove singularities. We found that the very strong features of these quantities and of the tunneling density of states associated with Van Hove singularities calculated in first-order perturbation theory are largely washed out in the self-consistent Eliashberg results.

The physical origin of the remarkable normal and superconducting properties of this coupled system of quasiparticles and spin fluctuations is the novel magnetic low-energy scale ω_{SF} brought about by the strong commensurate antiferromagnetic correlations between the quasiparticles. Given the fact that apart from the presence of well-defined quasiparticle poles essentially no other property of the system is that of a normal Landau Fermi liquid, it seemed appropriate to distinguish such a novel state of matter from the usual Landau liquids found in normal superconductors. We therefore call such a system a *nearly antiferromagnetic Fermi liquid* (a term introduced some time ago by one of us[5]), and argued, in MP I, on the basis of the overall agreement between our theoretical calculations with experiment, that $YBa_2Cu_3O_7$ is a nearly antiferromagnetic Fermi liquid.

As in a normal Fermi liquid, the spin and charge properties of a nearly antiferromagnetic Fermi liquid are not separated; here, both are determined by the magnetically coupled quasiparticles. In MP I we gave a progress report on the extent to which a self-consistent description of the spin-fluctuation excitation spectrum could be obtained by combining the results of the Eliashberg calculations with a random-phase-approximation (RPA) calculation of the consequences of their spin-spin interaction. We found that if we took the magnetic response function to be $\chi(\mathbf{q},\omega)=\tilde{\chi}(\mathbf{q},\omega)/[1-J(\mathbf{q})\tilde{\chi}(\mathbf{q},\omega)]$, where $\tilde{\chi}(\mathbf{q},\omega)$ is the irreducible particle-hole susceptibility calculated (in the Eliashberg formalism) for quasiparticles coupled to the phenomenological spin excitation spectrum, $\chi_{\mathrm{MMP}}(\mathbf{q},\omega)$, which Millis, Monien, and Pines[3] (MMP) used to fit NMR experiments, we could find a $J(\mathbf{q})$ such that the output response function $\chi(\mathbf{q},\omega)$ was close to the input response function $\chi_{\mathrm{MMP}}(\mathbf{q},\omega)$.

At the conclusion of MP I, we emphasized that since our nearly antiferromagnetic Fermi-liquid approach predicts unambiguously that the superconducting state of $YBa_2Cu_3O_7$ must possess $d_{x^2-y^2}$ symmetry, experimental detection of that pairing state was a necessary condition for the description of $YBa_2Cu_3O_7$ as a nearly antiferromagnetic Fermi liquid to be correct. A number of recent experiments now provide strong support for this pairing state, including low-magnetic-field measurements of NMR relaxation rates in the superconducting state for ^{63}Cu and ^{17}O nuclei,[6] penetration depth measurements on a large pure single crystal,[7] high-quality thermal conductivity,[8] and microwave experiments.[9] Moreover, ARPES experiments[10] and the feature at $3\Delta_0$ seen in tunneling experiments[11] indicate that this pairing state may be found quite generally in the cuprates. Quite recently, Wollman *et al.*[12] have reported on results of superconducting quantum interference device (SQUID) experiments involving $YBa_2Cu_3O_7$ tunnel junctions which Leggett[13] and Sigrist and Rice[14] have shown independently can provide a direct test of the pairing state; they find that the evidence to data, based on five separate tunnel junctions, while favoring *d*-wave pairing (and tending to rule out *s*-wave pairing), is not yet decisive.

Encouraged by these experimental results, we have carried out a number of further strong-coupling calculations based on our model Hamiltonian of magnetically coupled quasiparticles and report on these here. Following a brief review of our nearly antiferromagnetic Fermi-liquid approach in Sec. II, in Sec. III we consider the sensitivity of our calculations of T_c to the presence of impurities. It is well known that Anderson's theorem[15] does not apply to *d*-wave superconductors, in that nonmagnetic impurity potential scattering is expected to reduce T_c. It is found experimentally that some impurities (notably Ni and Zn) are likely to be located at a planar copper site [Cu(2)], yet these influence the ^{63}Cu spin-lattice relaxation time and T_c in quite different ways. Thus Ishida *et al.*[16] find that Ni substitution essentially does not change $^{63}T_1$ while reducing T_c in comparatively modest fashion. Zn, on the other hand, goes in as a nonmagnetic impurity,[16,17] yet Zn substitution leads to a substantive reduction in both $^{63}T_1$ for copper atoms close to a Zn impurity and in T_c. We find in our strong-coupling Eliashberg calculations that, for nonmagnetic impurity potential scattering, as the strength of the impurity potential increases, the unitary limit is reached comparatively quickly. In this unitary limit, the influence of the impurity scattering on T_c is relatively weak. Rather surprisingly, a potential scattering model appears to describe what happens when Ni is substituted for the planar Cu sites. On the other hand, we show, with the aid of a simple model, that the substitution of Zn, a nonmagnetic closed-shell impurity, for planar copper sites disrupts local magnetic order and brings about a substantive reduction in T_c, with results in good qualitative agreement with experiment. To the extent that Anderson's theorem is applicable to the cuprates, the fact that Zn goes in as a nonmagnetic impurity, yet influences T_c, would, in itself, seem a strong argument against *s*-wave pairing and in favor of *d*-wave pairing.

In Sec. IV we consider the competition between the antiferromagnetic and superconducting instabilities. Because a nearly antiferromagnetic Fermi liquid is, by definition, not far from an antiferromagnetic instability, it is interesting to examine whether the spin-fluctuation-induced interaction can give rise to this instability. We find that for our input spin-fluctuation spectrum, even as $T\rightarrow 0$, one cannot find an instability to a spin-density wave in this model, and thus the instability to a superconducting state always comes first.

In Sec. V we examine the sensitivity of our results for T_c to the details of the hole concentration. We obtain a family of $T_c(g)$ curves for a number of hole concentrations and find that our results for each hole concentration can be fit by an expression of the form of Eq. (1). In Sec. VI we examine the sensitivity of T_c to details of the spin-fluctuation excitation spectrum. We find that when that spectrum is modified so that it is consistent with both the NMR measurements of the spin-lattice relaxation time[4] and the recent NMR measurements of T_2 by Imai *et al.*,[18] an expression of the form Eq. (1) still applies, but the prefactor which measures the cutoff energy for the effectiveness of the spin-fluctuation-induced interaction is increased to ~ 60 meV, while both the values of the coupling constant g^2 required to obtain $T_c=90$ K and the dimensionless coupling constant λ are considerably reduced, λ now being $\leq \frac{1}{2}$.

In Sec. VII we present the results of calculations of a class of vertex corrections to our previous calculations of the normal-state resistivity, the optical conductivity, and the irreducible particle-hole magnetic susceptibility. We find that while such corrections lead to modest quantitative changes in these quantities, they do not produce any qualitative changes in the system behavior. When these results are combined with the modification in the spin-fluctuation spectrum required by the recent NMR measurements of T_2 by Imai *et al.*,[18] we find, in a calculation in which all relevant parameters are fixed by other experiments (g^2 being fixed by the requirement that $T_c=90$ K), quantitative agreement between theory and experiment for both $\rho_{ab}(T)$ and $\sigma(\omega,T)$.

We present in Sec. VIII a brief discussion of quasiparticle properties and the low-frequency magnetic response, with particular attention to the difference between the results obtained using the nearly antiferromagnetic Fermi-liquid approach and those obtained using the Hubbard model. Section IX contains further discussion and our conclusions.

II. MODEL AND COMPUTATIONAL APPROACH

Our model Hamiltonian for the planar quasiparticles is given by

$$\mathcal{H}=\sum_{\mathbf{p},\sigma}\epsilon_{\mathbf{p}}\psi^{\dagger}_{\mathbf{p}\sigma}\psi_{\mathbf{p}\sigma}+\frac{\bar{g}}{2}\sum_{\mathbf{q},\mathbf{k},\alpha\beta}\psi^{\dagger}_{\mathbf{k}+\mathbf{q}\alpha}\psi_{\mathbf{k}\beta}\boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{S}(-\mathbf{q}) , \tag{2}$$

where

$$\epsilon_{\mathbf{p}}=-2t[\cos(p_x a)+\cos(p_y a)]-4t'\cos(p_x a)\cos(p_y a) \tag{3}$$

is the quasiparticle dispersion relation, with $t=0.25$ eV, $t'=-0.45t$, as suggested by Yu[19] and Si *et al.*[20] from fits to band theory and ARPES experiments, and a is the lattice constant. **S** is taken to be a spin-fluctuation operator whose properties are determined by the phenomenological spin-spin correlation function introduced by Millis, Monien, and Pines[3] to describe the low-frequency commensurate magnetic excitation spectrum, $\chi_{ij}(\mathbf{q},\omega)=\delta_{ij}\chi_{\mathrm{MMP}}(\mathbf{q},\omega)$, with

$$\chi_{\mathrm{MMP}}(\mathbf{q},\omega)=\frac{\chi_{\mathbf{Q}}}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2-i\omega/\omega_{\mathrm{SF}}} . \tag{4}$$

Here $\chi_{\mathbf{Q}}$ is the static spin susceptibility at wave vector $\mathbf{Q}=(\pi/a,\pi/a)$ and ξ is a temperature-dependent antiferromagnetic correlation length. With this form of $\chi(\mathbf{q},\omega)$, there are no well-defined low-frequency magnetic excitations; rather, one has a relaxational mode, the antiferromagnetic paramagnon, whose energy ω_{SF} defines the characteristic energy of the low-frequency magnetic response. The quantities $\chi_{\mathbf{Q}}$ and ω_{SF} may be related in turn to the experimentally measured long-wavelength spin susceptibility χ_0 and a magnetic Fermi energy Γ_{AF} by introducing a scale factor β,

$$\chi_{\mathbf{Q}}=\chi_0\beta^{1/2}(\xi/a)^2 , \tag{5a}$$

$$\omega_{\mathrm{SF}}=\frac{\Gamma_{\mathrm{SF}}}{\beta^{1/2}\pi(\xi/a)^2} . \tag{5b}$$

The fits by MMP (Ref. 3) to NMR experiments on $YBa_2Cu_3O_7$ yield $\xi(T_c)\sim 2.3a$, $\omega_{\mathrm{SF}}(T_c)\sim 7.7$ meV, and $\chi_{\mathbf{Q}}(T_c)=44$ states/eV, and, on taking $\chi_0=2.6$ states/eV, $\beta=\pi^2$, and $\Gamma_{\mathrm{AF}}\approx 0.4$ eV.

The two-dimensional (2D) Eliashberg equations[21] for the critical temperature of a single CuO plane in the Matsubara representation reduce, in the case of a spin-fluctuation-induced interaction between the quasiparticles, to

$$\Sigma(\mathbf{p},i\omega_n)=g^2\frac{k_BT}{N_{\mathbf{q}}^2}\sum_{\Omega_n}\sum_{\mathbf{q}}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)G(\mathbf{q},i\Omega_n) , \tag{6}$$

$$G(\mathbf{p},i\omega_n)=\frac{1}{i\omega_n-(\epsilon_{\mathbf{p}}-\mu)-\Sigma(\mathbf{p},i\omega_n)} , \tag{7}$$

$$\Phi(\mathbf{p},i\omega_n)=-g^2\frac{k_BT}{N_{\mathbf{q}}^2}\sum_{\Omega_n}\sum_{\mathbf{q}}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)G(\mathbf{q},i\Omega_n)\times G(-\mathbf{q},-i\Omega_n)\Phi(\mathbf{q},i\Omega_n) , \tag{8}$$

where $\Sigma(\mathbf{p},i\omega_n)$ is the self-energy, $G(\mathbf{p},i\omega_n)$ is the one-particle Green's function, $\Phi(\mathbf{p},i\omega_n)$ is the anomalous self-energy and is proportional to the order parameter, $\epsilon_{\mathbf{p}}$ is the bare quasiparticle spectrum [Eq. (3)], and μ is the chemical potential. $N_{\mathbf{q}}^2$ is the total number of momenta in the Brillouin zone, and $\omega_n=(2n+1)k_BT$, $n=-\infty,\ldots,=-1,0,1,\ldots,\infty$. For convenience, the coupling constant g^2 is chosen to be equal to $g^2=\frac{3}{4}\bar{g}^2$.

$\chi(\mathbf{q},i\nu_n)$ is related to the imaginary part of the response function, $\mathrm{Im}\chi_{MMP}(\mathbf{q},\omega)$ [Eq. (4)] via the spectral representation

$$\chi(\mathbf{q},i\nu_n)=-\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\frac{\mathrm{Im}\chi_{\mathrm{MMP}}(\mathbf{q},\omega)}{i\nu_n-\omega}\ . \tag{9}$$

To get $\chi(\mathbf{q},i\nu_n)$ to decay faster than $1/\nu_n$, we introduce a cutoff ω_0 and take $\mathrm{Im}\chi(\mathbf{q},\omega)=0$ for $\omega\geq\omega_0$. In the following we will adopt the value $\omega_0=0.4$ eV. The value of g^2 required to obtain a certain critical temperature is somewhat dependent on the cutoff [since $\chi(\mathbf{q},i\nu_n)$ is]. However, we will always choose the coupling constant so that T_c is the experimentally measured critical temperature. Under these conditions, provided $\omega_0\gg\omega_{\mathrm{SF}}$, we have checked by explicit calculations that the precise value of the cutoff does not influence low-frequency normal-state properties, such as the resistivity.

The equations are solved with a fast Fourier transform (FFT) algorithm on a 64×64 lattice, with a Matsubara frequency cutoff of ~3 times the bandwidth.[22] The critical temperature for the model is determined from Eq. (8), which is an eigenvalue equation for the vector $\Phi(\mathbf{p},i\omega_n)$. A nonzero solution for the order parameter can be found when the largest eigenvalue of the matrix

$$\mathcal{K}(\mathbf{p},i\omega_n;\mathbf{q},i\Omega_n)=-g^2\frac{k_BT}{N_{\mathbf{q}}^2}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)\times G(\mathbf{q},i\Omega_n)G(-\mathbf{q},-i\Omega_n)$$

is equal to 1. For the present model, a nontrivial solution can only be found for a d-wave gap $\Phi(\mathbf{p},i\omega_n)\propto\cos(p_xa)-\cos(p_ya)$. In MP I we found that for an assumed hole concentration of 0.25 and the above values for the spin-fluctuation spectrum and quasiparticle dispersion, with $g=1.36$ the superconducting transition occurs at 90 K. One interesting feature of our results is that we find the absolute value of the eigenvalue in the s-wave channel (it is negative) is larger in module than that in the $d_{x^2-y^2}$ channel. In other words, the spin-fluctuation-induced interaction is more repulsive for s-wave pairing than it is attractive for d-wave pairing. In the pure material, when the eigenvalue is 1 for d-wave pairing it is -1.54 for s-wave pairing.

III. INFLUENCE OF IMPURITY SCATTERING ON T_c

The Eliashberg equations for the critical temperature, Eqs. (6)–(8) in the presence of isotropic impurity scattering are

$$\Sigma(\mathbf{p},i\omega_n)=g^2\frac{k_BT}{N_{\mathbf{q}}^2}\sum_{\Omega_n}\sum_{\mathbf{q}}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)G(\mathbf{q},i\Omega_n)+\Sigma_{\mathrm{imp}}(i\omega_n)\ , \tag{10}$$

$$G(\mathbf{p},i\omega_n)=\frac{1}{i\omega_n-(\epsilon_{\mathbf{p}}-\mu)-\Sigma(\mathbf{p},i\omega_n)}\ , \tag{11}$$

$$\Phi(\mathbf{p},i\omega_n)=-g^2\frac{k_BT}{N_{\mathbf{q}}^2}\sum_{\Omega_n}\sum_{\mathbf{q}}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)G(\mathbf{q},i\Omega_n)\times G(-\mathbf{q},-i\Omega_n)\Phi(\mathbf{q},i\Omega_n)\ , \tag{12}$$

where $\Sigma_{\mathrm{imp}}(i\omega_n)$, the self-energy due to potential impurity scattering, is

$$\Sigma_{\mathrm{imp}}(i\omega_n)=n_i\frac{U^2}{N_{\mathbf{q}}^2}\sum_{\mathbf{q}}G(\mathbf{q},i\omega_n) \tag{13}$$

in the case of second-order Born scattering and

$$\Sigma_{\mathrm{imp}}(i\omega_n)=\frac{n_i(U^2/N_{\mathbf{q}}^2)\sum_{\mathbf{q}}G(\mathbf{q},i\omega_n)}{1-(U/N_{\mathbf{q}}^2)\sum_{\mathbf{q}}G(\mathbf{q},i\omega_n)} \tag{14}$$

when multiple scattering is taken into account. U is the strength of the impurity potential and n_i the impurity concentration.

The procedure used to solve Eqs. (10)–(12) is a straightforward extension of that used in the absence of impurity scattering. The results of our calculations of the effect of impurity scattering on T_c are shown in Figs. 1–3. Three features are immediately apparent. First, the Born-approximation calculation of the influence of impurities on T_c overestimates that influence. Second, one reaches the unitary limit with comparatively modest strength U of the impurity scattering. Third, the influence of impurity scattering on T_c is surprisingly modest. At 1% impurity concentration, potential scattering in the unitary limit reduces T_c by only 5 K, while a 10% impurity concentration still leaves us with a

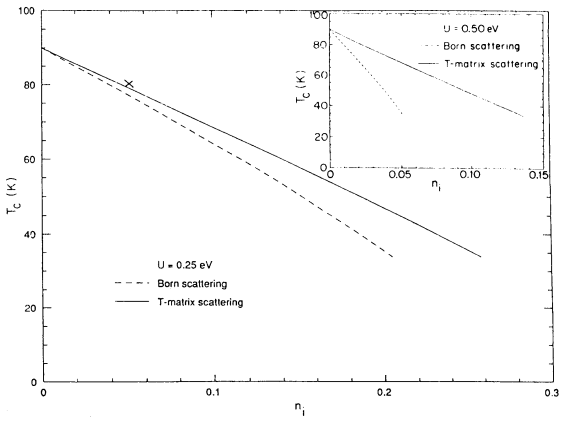

FIG. 1. Results of a strong-coupling calculation of the change in T_c brought about by potential impurity scattering U of strength 0.25 eV, calculated in the Born approximation and taking multiple scattering into account (T-matrix approximation); n_i is the impurity density, and the calculations are carried out for parameters which yield $T_c=90$ K in the absence of impurities. The experimental result obtained by Ishida *et al.* (Ref. 16) for the suppression of T_c by 5% Ni impurities is denoted by a cross ($\times$). As may be seen in the inset, for $U=0.5$ eV, the Born-approximation result leads to a significant overestimate of the influence of impurity potential scattering on T_c.

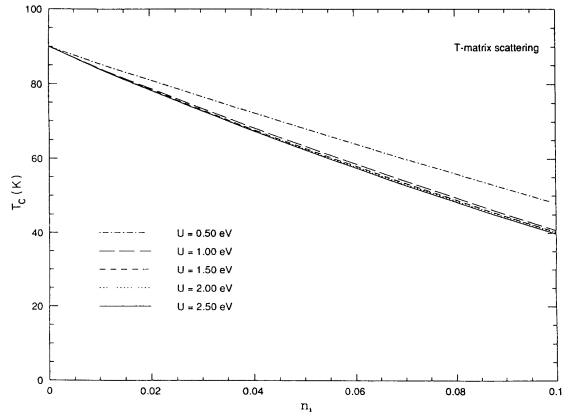

FIG. 2. Influence of impurity scattering on T_c, calculated in the unitarity limit, as a function of impurity density and scattering strength, for a 90-K superconductor with parameters appropriate to $YBa_2Cu_3O_7$.

superconducting transition temperature of 45 K. Figure 3 shows that the larger the value of T_{c0}, the transition temperature in the absence of impurities, the smaller is the reduction of T_c by impurity scattering.

This comparatively modest effect of impurity scattering on T_c for a d-wave superconductor is at first sight surprising. Its physical origin lies in the fact that we are considering a *strong-coupling* d-wave superconductor, in which the scattering of quasiparticles against spin fluctuations gives rise to a relatively large quasiparticle self-energy; as we have shown,[2] this reduces the transition temperature T_c considerably relative to the weak-coupling limit. If, therefore, the influence of impurities represents a comparatively modest add-on to this already substantial quasiparticle self-energy, then impurity potential scattering would not be expected to reduce T_c very much. To see whether this is the case, we calculated the influence of impurity scattering on the quasiparticle self-energy. $\mathrm{Im}\Sigma(\mathbf{p},\omega)$ for real frequencies is obtained by analytic continuation of $\Sigma(\mathbf{p},i\omega_n)$ using N-point Padé approximants.[23] Figure 4 shows the imaginary part of the quasiparticle self-energy in the presence of impurity scattering at two points on the Fermi surface and compares it with that of the pure material. We see that, as expected, impurity scattering provides only a modest, nearly isotropic, correction to the comparatively large value of $\mathrm{Im}\Sigma(\mathbf{p}_F^{(1)},\omega)$ which results from spin-fluctuation scattering. We note that because spin fluctuations are comparatively ineffective in influencing the quasiparticle energy at $\mathbf{p}_F^{(2)}=(0.371,0.371)\pi/a$, the percentage change in $\mathrm{Im}\Sigma(\mathbf{p}_F^{(2)},\omega)$ resulting from impurities is considerably larger for $\mathbf{p}_F^{(2)}$ than it is for $\mathbf{p}_F^{(1)}=(1,0.092)\pi/a$. Since, however, the energy gap vanishes along the diagonal, even a substantially altered quasiparticle spectrum at $\mathbf{p}_F^{(2)}$ will not be felt in the gap equation.

Another indication that nonmagnetic impurity scattering is a minor add-on to spin fluctuation comes from the concentration dependence of $\mathrm{Im}\Sigma$. For 1% nonmagnetic impurities, $\mathrm{Im}\Sigma$ changes (almost isotropically) by some 7 meV on the Fermi surface, while for 5% the corresponding change is only $\sim$21 meV.

We therefore conclude that in strong-coupling d-wave

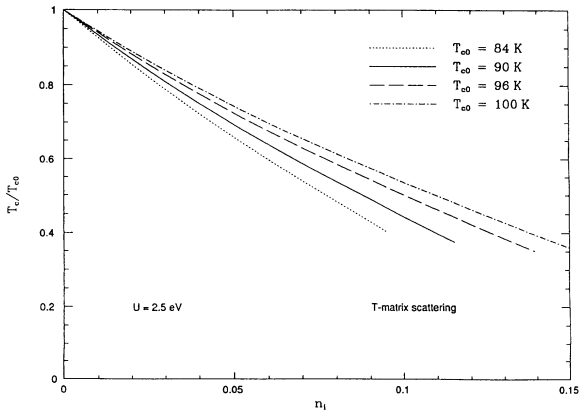

FIG. 3. Examination of the reduction in T_c brought about by impurity scattering at the unitary limit for various high-T_c superconductors, calculated with initial parameters similar to those used in studies of the changes in T_c with coupling constant for $YBa_2Cu_3O_7$.

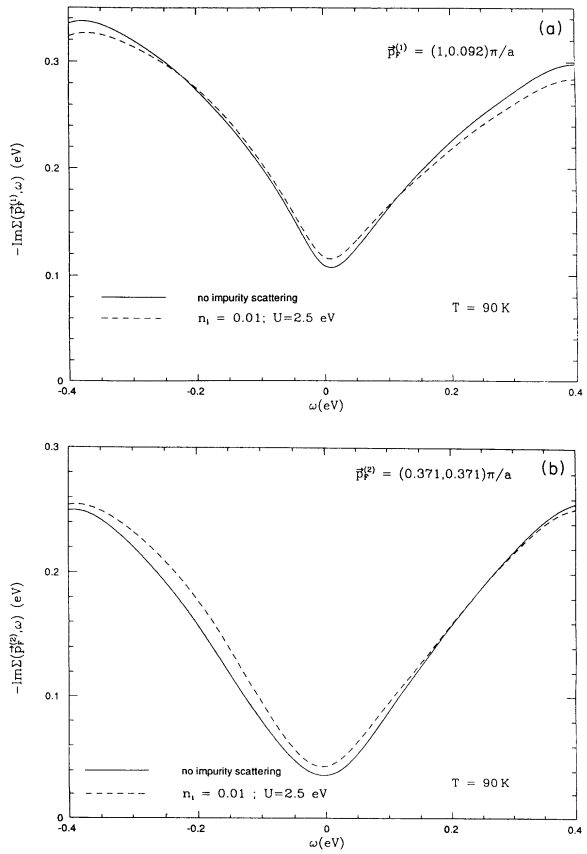

FIG. 4. Influence of impurity scattering on the imaginary part of the quasiparticle self-energy, calculated in the Eliashberg approximation with parameters appropriate to $YBa_2Cu_3O_7$ for two points on the Fermi surface: (a) at $\mathbf{p}_f^{(1)}=(1,0.092)(\pi/a)$ and (b) at $\mathbf{p}_f^{(2)}=(0.371,0.371)(\pi/a)$.

superconductors impurity potential scattering will, in general, lead to only a modest reduction in T_c and that for a given impurity concentration, the stronger the coupling g^2 between the quasiparticles and spin fluctuations, the weaker will be the influence of the impurities on T_c. Since larger T_{c0}'s are obtained with larger coupling constants g^2, which in turn imply larger quasiparticle self-energies, the results shown in Fig. 3 confirm the above explanation.

The problem of the influence of nonmagnetic potential impurity scattering on T_c is interesting in its own right, in that it nicely illustrates the effect on T_c played by self-energy corrections. However, it is found experimentally that a number of substitutional impurities are likely to be located at a planar copper site [Cu(2)] and thus have the potential of influencing the magnetic correlations between the planar quasiparticles in a significant way. Here it is useful to make a distinction between two kinds of such substitutional impurities: those like Ni, which although magnetic, do not alter the planar ^{63}Cu spin-lattice relaxation rate, and those like Zn, which do produce a significant change in $^{63}T_1$ (Ishida *et al.*[16]). We conjecture that impurities which do not alter $^{63}T_1$ may reasonably be assumed not to interfere with the local short-range magnetic order and hence do not expect any appreciable influence on the spin-fluctuation-induced interaction responsible for superconductivity; their influence is then primarily to alter the single-quasiparticle self-energy through potential scattering. Inspection of Fig. 1 thus suggests that the influence of the planar Ni impurities on T_c (and other properties) can be modeled by treating each impurity as giving rise to potential scattering of strength, $U \cong 0.25$ eV.

On the other hand, since a Zn impurity acts to change $^{63}T_1$ for Cu sites which are near it, it is necessary to take into account at the outset its influence on the local magnetic order. We model the introduction of Zn impurities and their effect on the spin excitation spectrum as follows. When a nonmagnetic atom is substituted for Cu^{2+}, we assume that it destroys magnetic correlations over a distance of the order of the correlation length ξ. We thus assume that in the presence of $N_{\rm Zn}$ impurities the spin-fluctuation operator in Eq. (1) is modulated by some function $h(\mathbf{x})$ that vanishes at the location of the Zn impurities:

$$\mathbf{S}(\mathbf{x}) \rightarrow \mathbf{S}(\mathbf{x}) h(\mathbf{x}) \ . \tag{15}$$

A function $h(\mathbf{x})$ that describes the destruction of the spin correlations over a range $\sim\xi$ is given by

$$h(\mathbf{x}) = \prod_{i=1}^{N_{\rm Zn}} \left[1 - \exp\left[-\frac{(\mathbf{x}-\mathbf{x}_i)^2}{2\xi^2} \right] \right] , \tag{16}$$

where $\mathbf{x}_i$, $i = 1, \ldots, N_{\rm Zn}$ denote the positions of the Zn atoms. The Eliashberg equations for the critical temperature [Eqs. (6)–(8)] in the presence of Zn substitution are

$$\Sigma(\mathbf{p}, i\omega_n) = g^2 \frac{k_B T}{N_{\mathbf{q}}^2} \sum_{\Omega_n} \sum_{\mathbf{q}} \chi_{\rm Zn}(\mathbf{p}-\mathbf{q}, i\omega_n - i\Omega_n) G(\mathbf{q}, i\Omega_n) \ , \tag{17}$$

$$G(\mathbf{p}, i\omega_n) = \frac{1}{i\omega_n - (\epsilon_{\mathbf{p}} - \mu) - \Sigma(\mathbf{p}, i\omega_n)} \ , \tag{18}$$

$$\Phi(\mathbf{p}, i\omega_n) = -g^2 \frac{k_B T}{N_{\mathbf{q}}^2} \sum_{\Omega_n} \sum_{\mathbf{q}} \chi_{\rm Zn}(\mathbf{p}-\mathbf{q}, i\omega_n - i\Omega_n) \times G(\mathbf{q}, i\Omega_n) G(-\mathbf{q}, -i\Omega_n) \times \Phi(\mathbf{q}, i\Omega_n) \ , \tag{19}$$

with

$$\chi_{\rm Zn}(\mathbf{x}-\mathbf{x}', i\nu_n) = \chi(\mathbf{x}-\mathbf{x}', i\nu_n) \overline{h(\mathbf{x}) h(\mathbf{x}')} \ , \tag{20}$$

where $\chi(\mathbf{x}, i\nu_n)$ is the spin-fluctuation propagator of the pure material and the overbar implies an average over the positions of the Zn atoms.

The computational approach is similar to that used so far. $N_{\rm Zn}$ Zn atoms are located at random on the 64×64 lattice, and the average $\overline{h(\mathbf{x}) h(\mathbf{x}')}$ is performed over 100 configurations of the Zn atoms. To ensure the numerical stability of the calculation of the largest eigenvalue of the kernel of Eq. (19) which determines the critical temperature, it is essential that $E(\mathbf{x}-\mathbf{x}') = \overline{h(\mathbf{x}) h(\mathbf{x}')}$ have the symmetry of the square lattice with high accuracy. Since, as noted earlier, the spin-fluctuation-induced interaction acts in both the s- and d-wave channels (and is in fact larger in module for the s-wave channel), the iterations have to preserve the orthogonality of the d- and s-wave gaps to a very high precision: Otherwise, a small admixture of s waves would tend to dominate after only a few iterations. Therefore, to ensure numerical stability, the function $E(\mathbf{x})$ is totally symmetrized

$$(E(x,y) \rightarrow [E(x,y) + E(-x,y) + E(x,-y) + E(-x,-y) + (x \leftrightarrow y)]/8)$$

after the average over the Zn configurations has been taken.

The results of our calculations are given in Fig. 5. There we see that the influence of the Zn impurities on

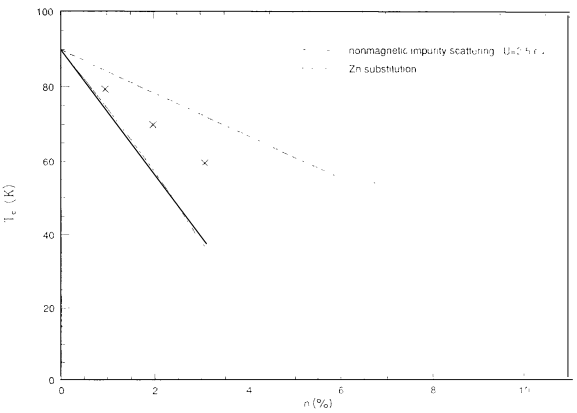

FIG. 5. Calculated influence of Zn impurities on T_c is compared with the experimental results of Ishida *et al.* (Ref. 16) [crosses ($\times$)] and with nonmagnetic impurity potential scattering, calculated in the unitary limit for an impurity potential of 2.5 eV.

T_c is considerably greater than that of nonmagnetic impurities, which act as simple potential scatterers. Because of computer memory constraints on the number of Matsubara frequencies, we are not able to carry out calculations below $T \sim 33$ K. However, a straightforward extrapolation of our results to lower temperatures suggests that $T_c \to 0$ for a Zn concentration in excess of $\sim 5\%$. Our results are somewhat sensitive to the width of the Gaussian expression [Eq. (16)] assumed for $h(\mathbf{x})$; for example, if the width is reduced from ξ^2 to $0.8\xi^2$, corresponding to assuming that Zn impurities cause less disruption of the planar magnetic correlations, we find it takes 0.4% Zn impurities to reduce T_c by 5 K, compared to the 0.34% Zn concentration which brings this about for ξ^2. This result also implies that the extent to which Zn impurities influence T_c depends on $\xi(T_c)$; quite generally, the larger the value of $\xi^2(T_c)$, the more disruptive (to T_c) will be the Zn impurities.

We have also indicated in Fig. 5 reports by several experimental groups concerning the influence of Zn impurities on T_c. The results shown there assume that *all* Zn impurities replace an atom on planar sites. The agreement between our theoretical results and experiment would seem satisfactory; as is perhaps evident, the solid line depicted there represents an upper limit on the influence of Zn impurities on T_c; to the extent that either the Zn atoms are less disruptive of planar quasiparticle magnetic correlations, or go, in part, to chain Cu sites, their influence on T_c may be expected to be less.

In the above calculations, we have not taken into account the fact that the planar Zn atoms, in addition to disrupting magnetic correlations, may also act as potential scatterers; to the extent the two effects are additive, one could add the two contributions shown, for example, in Fig. 5. In practice, we do not expect the effects to be additive; we hope to return to this topic at a later date.

While we have not yet carried out explicit calculations for the influence of Zn impurities on T_c for $YBa_2Cu_3O_{6.63}$, it appears likely from Fig. 5 that a concentration of Zn $\geq 3\%$ will be sufficient to destroy superconductivity. In making this estimate, we have first assumed that the shape of the T_c vs Zn concentration curve for this $T_c = 60$ K material will be similar to that of the $T_c = 90$ K sample; that would yield a "fatal" concentration of Zn of some 3.5%. Second, since it is known from fits to NMR experiments that $\xi(T_c) \cong 4a$ for $YBa_2Cu_3O_{6.63}$, it is quite likely that a somewhat smaller concentration of Zn impurities would destroy superconductivity for an $O_{6.63}$ sample.

IV. SUPERCONDUCTIVITY vs ANTIFERROMAGNETISM

It is natural to inquire how close one has come to a spin-density-wave (SDW) instability at the commensurate wave vector $(\pi/a, \pi/a)$ when our system becomes superconducting. For example, is it likely that with some small change in the parameters describing the spin-fluctuation spectrum, or the coupling constant g, that the system would, at a given hole density, rather become antiferromagnetic than superconducting? To study this, we

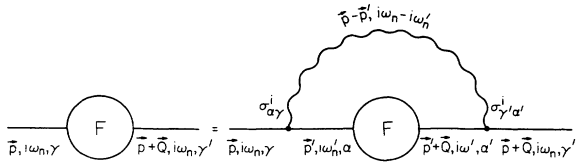

FIG. 6. Linearized equation for the anomalous propagator used to study spin-density-wave formation.

consider the time-ordered anomalous propagator which describes SDW formation,

$$F_{\gamma\gamma'}(\mathbf{p},\tau) = -\langle T_\tau\{\psi_\gamma(\mathbf{p},\tau)\psi^\dagger_{\gamma'}(\mathbf{p}+\mathbf{Q},0)\}\rangle , \tag{21}$$

where γ and γ' are spin indices. For a SDW the particle-hole pair must be in a triplet state for which the matrix of the components $F_{\gamma\gamma'}$ in spin space takes the form

$$\hat{F}(\mathbf{p},i\omega_n) = (\mathbf{d}\cdot\boldsymbol{\sigma})F^t(\mathbf{p},i\omega_n) . \tag{22}$$

It is then straightforward to show that the linearized equation for the anomalous propagator, depicted in Fig. 6, is given by

$$F^t(\mathbf{p},i\omega_n) = -\frac{g^2}{3}G(\mathbf{p},i\omega n)G(\mathbf{p}+\mathbf{Q},i\omega_n)\frac{k_BT}{N_{\mathbf{p}}^2} \times \sum_{\mathbf{p}'\omega_n}\chi(\mathbf{p}-\mathbf{p}',i\omega_n-i\omega_n')F^t(\mathbf{p}',i\omega_n') . \tag{23}$$

As was the case for the gap equation for the transition to the superconducting state, a nontrivial solution for $F^t(\mathbf{p},i\omega_n)$ can be obtained when the largest eigenvalue of the kernel

$$-\frac{g^2k_BT}{3N_{\mathbf{p}}^2}G(\mathbf{p},i\omega_n)G(\mathbf{p},+\mathbf{Q},i\omega_n)\chi(\mathbf{p}-\mathbf{p}',i\omega_n-i\omega_n') \tag{24}$$

is equal to 1. Figure 7 shows the largest eigenvalue of the

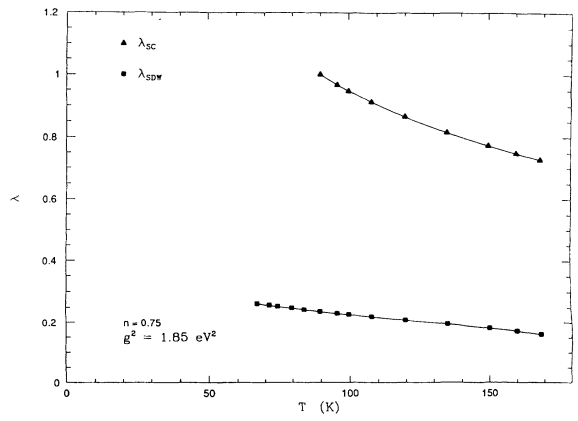

FIG. 7. Comparison of the temperature dependence of the largest eigenvalue λ_{SDW} for antiferromagnetic spin-density-wave formation with the corresponding eigenvalue λ_{SC} for the formation of the superconducting state.

kernel [Eq. (23)] and compares it with the largest eigenvalue of the superconducting kernel in Eq. (7). There one sees that the eigenvalue for SDW formation lies well below that for the superconducting transition and is considerably less than unity for all temperatures of interest.

V. SENSITIVITY OF T_c TO HOLE CONCENTRATION

In MP I we reported on our results for T_c of $YBa_2Cu_3O_7$ as a function of g^2 for a hole concentration of 0.25 using a particular choice of a spin-fluctuation spectrum which was consistent with both Knight-shift and T_1 measurements. It is instructive to explore the sensitivity of those results to the hole concentration n_h. Doing so requires the self-consistent determination of the chemical potential and single-particle Green's function in the normal state for each value of n_h under consideration. The resulting family of $T_c(g^2)$ curves for a number of hole concentrations is shown in Fig. 8. There one sees that as the hole concentration varies from 0.16 to 0.31, the coupling constant g required to get $T_c=90$ K varies from 1.29 to 1.48 eV. The similarity in shape of the $T_c(g^2)$ curves for varying hole concentration leads us to inquire whether our results can be fit with an algebraic expression of the form obtained in MP I [for calculations of $T_c(g^2)$ for $n_h=0.25$ and a quasiparticle spectrum specified by $t'=0$],

$$T_c=\alpha\frac{\Gamma_{AF}}{\pi^2}\exp\left[-\frac{1}{\eta N(0)g}\right]\equiv\alpha\frac{\Gamma_{AF}}{\pi^2}\exp\left[-\frac{1}{\lambda}\right], \quad (25)$$

where $N(0)$, the tunneling density of states for both spins at T_c, is the imaginary part of the full Green's function summed over all momenta. It was calculated from the single-particle Green's function, and we introduced a dimensionless coupling constant $\lambda\equiv\eta N(0)g$. We find that at each hole concentration a fit of the form of Eq. (25) can be obtained for the present case $t'\neq 0$ for values of g^2 such that 80 K $\leq T_c \leq$ 108 K; our results are given in Table I. We also find that $N(0)$ is reduced from its band-structure value by self-energy effects. [This trend is reflected in Tables I and II, where the smaller coupling constants yield a larger $N(0)$.]

A number of features of these results deserve comment. First, we note that the form of the strong-coupling expression does not appear to be sensitive to either n_h or t', although the particular values of α, η, and λ may vary. In fact, inspection of Table I shows that η is very nearly constant, while α scales very nearly with the electron concentration, $n_e=1-n_h$. Somewhat unexpectedly, the overall dimensionless coupling strength λ, required to bring about a 90-K transition, decreases as the hole concentration decreases.

As we have noted earlier, the form of our strong-coupling expression [Eq. (25)] agrees with that found by Hirsch and Scalapino,[24] who explored the role played by Van Hove singularities in enhancing T_c for low-dimensional systems; that led us to speculate, in MP I, that it might be a consequency of strong coupling plus a Van Hove singularity, since for $t'=0$ and $n_h=0.25$, one is *not* near a Van Hove singularity. Since, however, changing n_h by a factor of 2 seems to have no effect on

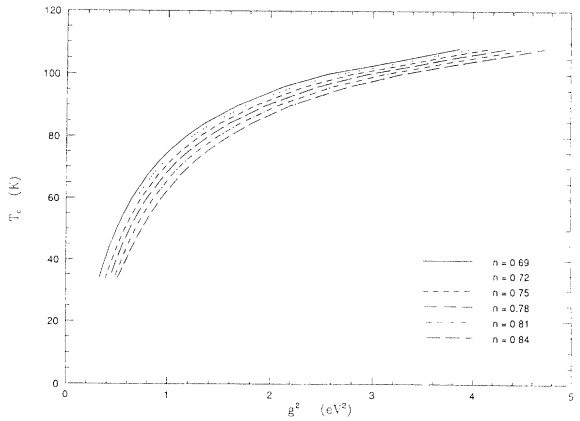

FIG. 8. Transition temperature T_c calculated in the strong-coupling Eliashberg approximation is shown as a function of coupling constant g^2 for electron concentrations n ranging from 0.69 to 0.84. In these calculations, the MMP spin-fluctuation spectrum is specified by the parameters $\omega_{SF}(T_c)=7.7$ meV, $\xi(T_c)/a=2.3$, and $\chi_Q(T_c)=44$ states/eV; the quasiparticle spectrum of the tight-binding form, with the nearest-neighbor hopping parameter $t=0.25$ eV, and the next-nearest-neighbor hopping parameter $t'=-0.45t$. The algebraic expression $T_c=(\alpha\Gamma_{AF}/\pi^2)\exp(-1/\eta N(0)g)$, with $0.70\leq\alpha(n_e)\leq 0.92$ and $0.326\geq\eta(n_e)\geq 0.315$, provides a quantitative fit to each curve.

TABLE I. Fit parameters and other quantities of interest which enter into the calculation of T_c as a function of hole concentration for spin-fluctuation parameters $\omega_{SF}(T_c)=7.7$ meV, $\chi_Q(T_c)=44$ states/eV, and $\xi(T_c)/a=2.3$, corresponding to $\Gamma_{AF}=0.4$ eV.

n_e	0.69	0.72	0.75	0.78	0.80	0.84
μ (eV)	−0.41	−0.39	−0.37	−0.34	−0.32	−0.29
$N(0)$ (states/eV)	1.83	1.73	1.63	1.53	1.44	1.36
g (eV)	1.29	1.32	1.36	1.40	1.44	1.48
η	0.326	0.326	0.325	0.323	0.319	0.315
λ	0.772	0.746	0.719	0.691	0.663	0.634
α	0.696	0.729	0.767	0.812	0.864	0.925
$\frac{\alpha\Gamma}{\pi^2}$ (meV)	28	30	31	33	35	37
$Z(\mathbf{p}^{(1)},\pi k_B T_c)$	5.58	5.63	5.68	5.73	5.78	5.83
$Z(\mathbf{p}^{(2)},\pi k_B T_c)$	2.54	2.60	2.66	2.74	2.82	2.91

the form of our result for T_c, we now conclude that it is more likely an intrinsic property of *any* strong-coupling calculation based on the present model Hamiltonian.

VI. SENSITIVITY OF T_c TO DETAILS OF THE SPIN-FLUCTUATION SPECTRUM

We now consider, for a fixed value of coupling constant g and electron concentration n_e, the extent to which T_c is sensitive to the choice of spin-fluctuation parameters ξ, ω_{SF}, and χ_Q or, what is equivalent, Γ_{AF}, ξ, and β [see Eq. (5)]. In Fig. 9 we plot the results of numerical experiments in which Γ_{AF}, ξ^2, and β are changed by a scale factor. We see in Fig. 9(a) that T_c increases as Γ_{AF} increases. The physical origin of that increase may be traced to the corresponding increase in ω_{SF}, which determines the range of energies over which the spin-fluctuation-induced interaction is effective. T_c is, in fact, very nearly linear in Γ_{AF}, as might have been anticipated from the form of our expression [Eq. (25)]; the comparatively small departure from linearity may be attributed to the relatively weak temperature dependence of $N(0)$. In Fig. 9(b) we present the results of keeping ω_{SF} and χ_Q fixed while changing the width in momentum space of the spin-fluctuation-induced interaction; thus, we let $\xi^2 \rightarrow \kappa\xi^2$, but vary both Γ_{AF} and χ_0 in such a way that both ω_{SF} and χ_Q are not changed. We see that the resulting variation of T_c with κ is quite similar to that found, namely, by changing the width in frequency space of the effective interaction, by varying Γ_{AF} (or ω_{SF}) alone. This demonstrates the importance of the momentum dependence of the interaction in determining T_c. In sharp contrast to the problem of phonon-induced superconductivity, in which only the frequency dependence of the phonon spectrum has to be taken into account, for spin-fluctuation-induced superconductivity the frequency *and* momentum dependence of the interaction have to be treated on an equal footing. This point was first made in MBP.

We next consider what happens when we change ξ^2, but keep both Γ and χ_0 fixed. Figure 9(c) shows that the influence of changes in ξ^2 alone is a comparatively subtle affair, with relatively small changes in T_c coming about for $1 \geq \xi/a \geq 5$ [recall that $\xi(T_c) \cong 2.3a$ for the canonical choice of MMP parameters], but a dramatic decrease in T_c occurs once $\xi < a$. There are two competing effects.

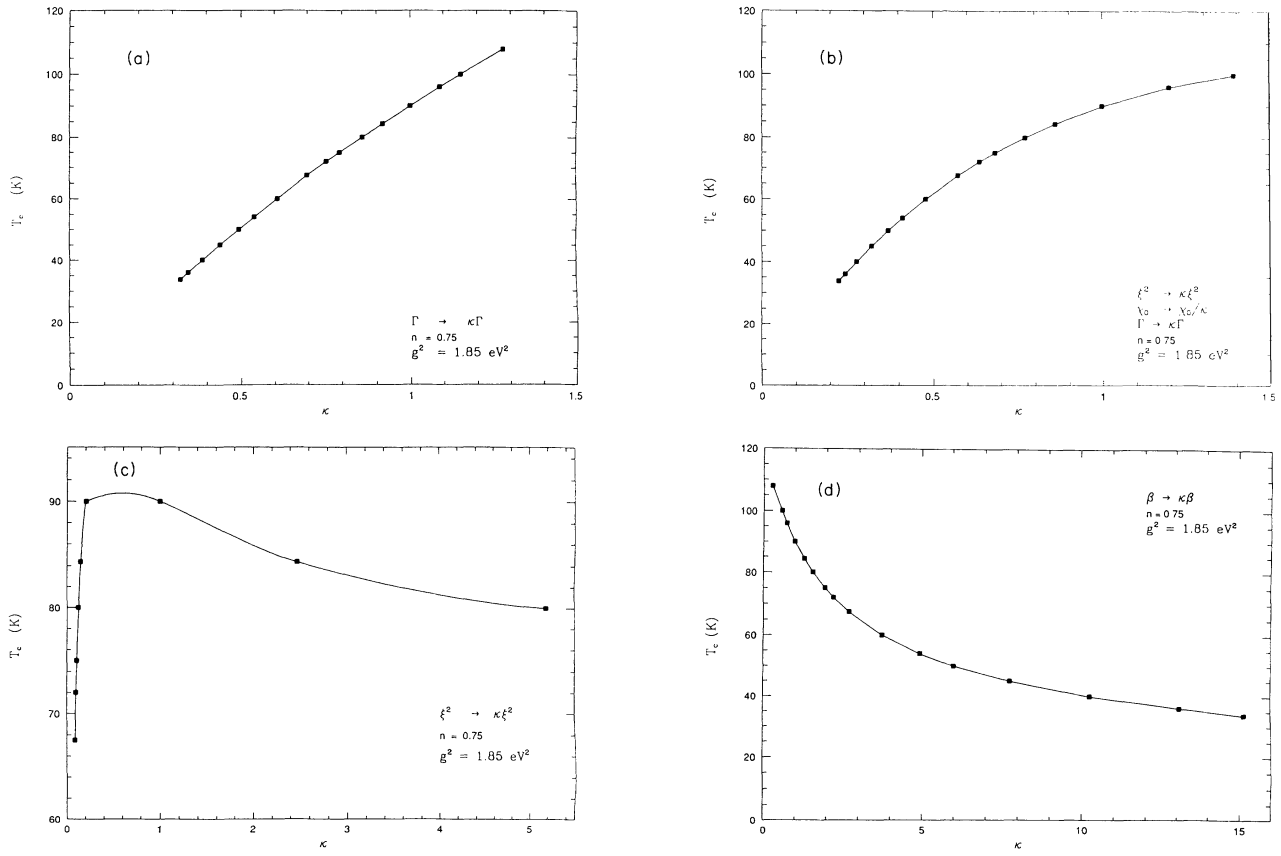

FIG. 9. Results of numerical experiments on the sensitivity of T_c to changes in the spin-fluctuation parameters Γ_{AF}, ξ, β, and χ_0, based on the quasiparticle and spin-fluctuation parameters given in the text and the caption for Fig. 8, and calculated for an electron density $n_e = 0.75$: (a) T_c as a function of $\kappa = \Gamma_{AF}/0.4$ eV; (b) T_c when ξ^2, χ_0, and Γ_{AF} are assumed changed in such a way that $\kappa \rightarrow \kappa\Gamma_{AF}$, while $\omega_{SF}(T_c)$ and $\chi_Q(T_c)$ remain constant; (c) T_c as a function of the scaling parameter κ for $\xi^2 \rightarrow \kappa\xi^2$, with other spin-fluctuation parameters unchanged; and (d) T_c as a function of $\kappa = \beta/\pi^2$, with other spin-fluctuation parameters unchanged.

By increasing ξ, one increases the projection of the interaction onto the $d_{x^2-y^2}$ state; this acts to increase T_c. However, one also lowers the spin-fluctuation energy ω_{SF} [see Eq. (5b)]; this gives rise to larger quasiparticle self-energies, and these in turn reduce T_c. By lowering ξ^2, one gets an increase in ω_{SF}, a decrease in the quasiparticle self-energies, and a potential increase in T_c; however, for $\xi \geq a$, this effect is dwarfed by the loss of the projection of the interaction onto the $d_{x^2-y^2}$ state. Taken together, these remarks explain the highly asymmetric nature of our results.

In Fig. 9(b) we see that increasing β reduces T_c substantially, essentially because the reduction in ω_{SF} has a greater negative consequence (through the altered frequency dependence of the effective interaction) than the positive consequence of the corresponding increase in χ_Q.

In practice, one cannot vary the MMP parameters independently, since for $YBa_2Cu_3O_7$, these are constrained by experimental measurements of both T_1 and T_2 for ^{63}Cu nuclei. These constraints take a simple form in the limit of long correlation lengths, $\xi/a \geq 2$. From the MMP fit to the measured values of T_1 for an external magnetic field perpendicular to the Cu-O plane, one finds that, at T_c (~ 90 K),

$$\frac{\chi_Q(T_c)[\xi^2(T_c)/a^2]}{\omega_{SF}(T_c)} = (3.0 \pm 0.3) \times 10^4 \text{ eV}^{-2} , \quad (26)$$

while Imai *et al.*[18] and Thelen and Pines[25] find from the measurements of T_2 by Imai *et al.*[18] that

$$\chi_Q(T)\omega_{SF}(T) = \frac{\chi_0 \Gamma_{AF}}{\pi} \cong 1.1 \pm 0.1 \quad (27)$$

for all $T > T_c$. For $\chi_0 \cong 2.6$ states/eV, the latter constraint requires that we increase Γ_{AF} by somewhat more than a factor of 3 to $\Gamma_{AF} = 1.3$ eV from the "canonical" MMP value $\Gamma_{AF} = 0.4$ eV. On combining Eq. (26) with Eqs. (5) and (2), we arrive at the equivalent constraints

$$\beta\xi^2(T_c)/a^2 = 170 \pm 20 . \quad (28a)$$

$$\chi_Q(T_c)[\xi(T_c)/a] = (173 \pm 20) \text{ states/eV} . \quad (28b)$$

We incorporate these constraints in our calculations in the following way. We begin by assuming that $\xi(T_c)$ is unchanged from the MMP value; thus, we choose $\xi = 2.3a$, obtaining $\omega_{SF}(T_c) = 14$ meV and $\chi_Q(T_c) = 75$ states/eV as the new parameters which characterize the MMP spectrum [Eq. (5)]. We then ask how well do we know $\xi(T_c)$? A lower limit on $\xi(T_c)$ is provided by the ratio of the ^{63}Cu and ^{17}O relaxation rates near T_c, which Barrett *et al.*[26] find to be ~ 20. As Millis and Monien have shown,[27] unless $(\xi/a) \geq 2$, there will be too much leakage of the antiferromagnetically enhanced $\chi''(\mathbf{q},\omega)$ onto the oxygen sites, producing a too small ratio of the nuclear relaxation rates. On the other hand, if one takes a markedly larger value of $\xi(T_c)$, one likely runs into conflict with the neutron-scattering experiments which suggest that at the energies at which experiments are carried out ($\omega \geq 20$ meV), $\xi \leq a$. We therefore conclude that the key spin-fluctuation parameters which determine T_c are given by

$$\xi(T_c) = (2.3 \pm 0.3)a , \quad (29a)$$

$$\omega_{SF}(T_c) = 14 \pm 2 \text{ meV} , \quad (29b)$$

$$\chi_Q(T_c) = (75 \mp 10) \text{ states/eV} . \quad (29c)$$

We now use the results [Eq. (29)] for the spin-fluctuation parameters to determine $T_c(g^2)$ for a range of electron concentrations, $0.69 \leq n_e \leq 0.84$. Our results, shown in Fig. 10, again suggest that a simple expression for T_c of the form of Eq. (25) likely exists; we find that it does, with the results shown in Table II. We see that compared to our previous choice of parameters, with the new set, the prefactor (the cutoff energy) is increased, while the values of g required to obtain $T_c = 90$ K are considerably reduced. As a result, we find that the dimensionless parameter which measures the overall effectiveness of the spin-fluctuation-induced interaction is now $\lambda \leq 0.5$. Thus we have gone from a hypothesized strong-coupling regime ($\lambda \sim 1$) to what is, in effect, an intermediate-coupling regime ($\lambda \leq 0.5$).

We have also explored, for our new parameters, the consequences of varying β and ξ^2 such that their product $\beta\xi^2$ is unchanged; our results are shown in Fig. 11. As the scaling parameter $\kappa = \beta/32$ is increased, the spin-fluctuation frequency ω_{SF} increases, which has a positive

TABLE II. Fit parameters and other quantities of interest which enter into the calculation of T_c as a function of hole concentration, for spin-fluctuation parameters $\omega_{SF}(T_c) = 14$ meV, $\chi_Q(T_c) = 75$ meV, and $\xi(T_c)/a = 2.3$, corresponding to $\Gamma_{AF} = 1.3$ eV.

n_e	0.69	0.72	0.75	0.78	0.80	0.84
μ (eV)	−0.40	−0.39	−0.37	−0.35	−0.33	−0.31
$N(0)$ (states/eV)	2.19	2.07	1.95	1.84	1.73	1.62
g (eV)	0.61	0.62	0.64	0.66	0.68	0.70
η	0.360	0.364	0.367	0.369	0.370	0.368
λ	0.481	0.470	0.457	0.445	0.432	0.418
α	0.470	0.494	0.524	0.558	0.594	0.644
$\tilde{\alpha}$	0.838	0.875	0.92	0.97	1.04	1.11
$\frac{\alpha\Gamma}{\pi^2}$ (meV)	62	65	69	74	78	85
$Z(\mathbf{p}^{(1)}, \pi k_B T_c)$	3.14	3.14	3.14	3.13	3.13	3.12
$Z(\mathbf{p}^{(2)}, \pi k_B T_c)$	1.54	1.57	1.59	1.62	1.66	1.70

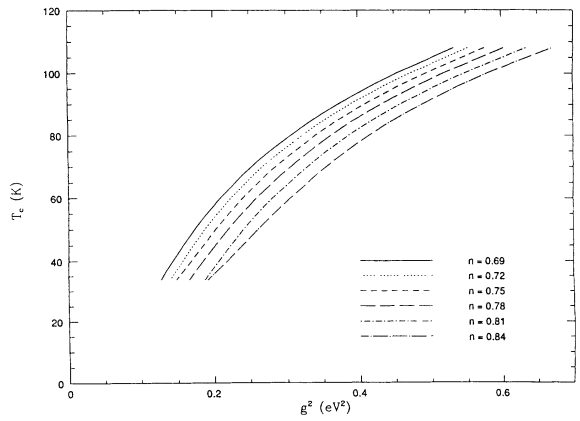

FIG. 10. Transition temperature T_c calculated in the strong-coupling Eliashberg approximation is shown as a function of the quasiparticle–spin-fluctuation coupling constant g^2 for electron concentrations ranging from 0.69 to 0.84. In these calculations, the MMP spin-fluctuation spectrum is specified by the parameters $\omega_{SF}(T_c)=14$ meV, $\xi(T_c)/a=2.3$, and $\chi_Q(T_c)=75$ states/eV.

effect on T_c. However, since the correlation length $\xi/a=2.3/\kappa^{1/2}$ decreases, the projection of the effective interaction onto the $d_{x^2-y^2}$ pairing state diminishes. A further negative effect on T_c is brought about by the decrease of the spin susceptibility at the commensurate wave vector χ_Q. When $\kappa>1$, these latter effects dominate and T_c goes down. On the other hand, when $\kappa<1$, the roles are reversed. The change in ω_{SF} (it decreases) has a negative effect on T_c, while the corresponding increase in ξ and χ_Q has a positive effect on the transition temperature. The negative effects dominate again, and T_c goes down. One sees from the plot the value $\beta=32$ is nearly the optimum one for this choice of coupling constant and hole doping.

Inspection of Tables I and II shows that, to first approximation, the prefactor, which reflects the cutoff energy for the effectiveness of the spin-fluctuation-induced interaction in bringing about superconductivity, scales with ω_{SF}. To see this, note that since in calculating Table I we have assumed that $\beta=\pi^2$, we may write the prefactor as

$$\frac{\alpha\Gamma_{AF}}{\pi^2}\equiv\tilde{\alpha}\omega_{SF}(T_c)[\xi^2(T_c)/a^2]\ , \tag{30}$$

where, for this example, $\tilde{\alpha}=\alpha$. If we adopt the form on the right-hand side of Eq. (30) for the cutoff, then the resulting values of $\tilde{\alpha}$, also given in Table II, are seen to be increased by some 21% over the corresponding results for α given in Table I. We conclude that in terms of the spin-fluctuation parameters and hole-density parameters used to obtain Table II, the expression

$$T_c\cong\{[\xi^2(T_c)/a^2]\omega_{SF}(T_c)(n_e/0.79)\}\times\exp\left[-\frac{1}{0.37N(0)g}\right] \tag{31}$$

provides a good starting point for understanding the results of our numerical calculations. From this point of view, the cutoff in frequency space is increased by a factor $\sim\xi^2$ from ω_{SF}. Since, according to Eq. (5), $\omega_{SF}\xi^2$ is independent of ξ^2, the prefactor possesses only a weak dependence on n_e, arising perhaps from the fact that as n_e increases, more quasiparticles can take advantage of the spin-fluctuation-induced interaction.

The approximate expression [Eq. (31)] also enables us to interpret the changes in T_c associated with the changes in spin-fluctuation parameters presented in Fig. 9(a)–9(d) and Fig. 11 in a simple way. In all five cases the primary cause in the changes in T_c is the change in the prefactor; the reader can easily verify that Eq. (31), under the assumption that the effective interaction λ is little influenced by changes in the spin-fluctuation parameters, provides a qualitative and, in some cases, quantitative measure of the influence of these quantities on T_c.

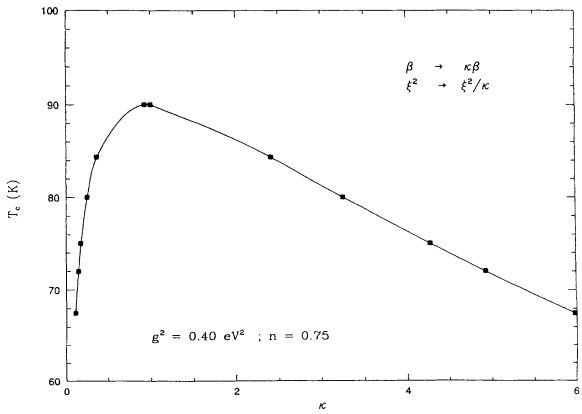

FIG. 11. Results of numerical experiments on the sensitivity of T_c to changes in the spin-fluctuation parameters β and ξ such that the product $\beta\xi^2$ is constant. In these calculations, $\kappa=\beta/32$, corresponding to spin-fluctuation parameters $\Gamma_{AF}=1.3$ eV, $\beta=32$, and $g^2=0.40$ eV^2; hence, $T_c=90$ K for $\kappa=1$.

VII. RESISTIVITY AND OPTICAL CONDUCTIVITY

The measured transport and optical properties of $YBa_2Cu_3O_7$ provide a stringent quantitative test of theories of the normal state of this system. Early weak-coupling calculations of $\rho(T)$ for a model Hamiltonian similar to that of Eq. (2) were carried out by Moriya, Takahashi, and Ueda,[28] who, independent of MMP, used a self-consistent renormalization (SCR) approach to obtain a spin-fluctuation spectrum similar to that proposed by MMP, and by Monien, Monthoux, and Pines,[29] while Arfi[30] carried out calculations of the frequency-dependent optical conductivity $\sigma(\omega,T)$ using the MMP spectral density and the memory function formalism. These results all led to qualitative agreement with experiment. As Moriya, Takahashi, and Ueda have emphasized,[28] an important test of the spin-fluctuation approach to the cuprates is to obtain a quantitative account of both the anomalous electrical resistivity *and* the high superconducting transition temperature using the same model Hamiltonian, i.e., using the same spin-fluctuation spec-

trum and coupling constant for both calculations. This criterion was met in the weak-coupling calculations of Moriya, Takahashi, and Ueda[28] and in our previous strong-coupling calculation, reported in MP I, where we found it possible to obtain good qualitative, but not quantitative, agreement with experiment for our calculation based on the original MMP spin-fluctuation parameters.

One possible reason for the failure of previous calculations to obtain quantitative agreement with experiment was the use of an incorrect spin-fluctuation spectrum; a second was the use of an incorrect quasiparticle spectrum, while a third was the neglect of vertex corrections in calculating the current-current correlation function which determines the in-plane resistivity and optical conductivity. In this section we remedy all these defects. Thus we use a spin-fluctuation spectrum [Eq. (29)] which is consistent with NMR measurements of both T_1 and T_2, a quasiparticle spectrum [Eq. (3)], and hole density $n_h=0.25$ which is consistent with ARPES experiments, and choose the coupling constant $g=0.64$ eV, since, as may be seen in Table II, this yields an "Eliashberg" transition temperature of 90 K. All parameters now being fixed, we proceed to calculate the resistivity.

The in-plane normal-state resistivity and optical conductivity are calculated from the current-current correlation function at zero momentum transfer, $R(i\nu_n)$, which is given by

$$R(i\nu_n)=-\frac{2k_BT}{N_{\mathbf{p}}^2}\sum_{\mathbf{p}}\sum_{\omega_n}\frac{\partial\epsilon_{\mathbf{p}}}{\partial p_x a}G(\mathbf{p},i\omega_n)G(\mathbf{p},i\omega_n+i\nu_n)\times\left[\frac{\partial\epsilon_{\mathbf{p}}}{\partial p_x a}+\Lambda(\mathbf{p},i\omega_n;i\nu_n)\right], \tag{32}$$

where the vertex function $\Lambda(\mathbf{p},i\omega_n;i\nu_n)$ satisfies the Bethe-Salpeter equation

$$\Lambda(\mathbf{p},i\omega_n;i\nu_n)=\frac{g^2k_BT}{N_{\mathbf{p}'}^2}\sum_{\mathbf{p}'}\sum_{\omega_n'}\chi(\mathbf{p}-\mathbf{p}',i\omega_n-i\omega_n')\times G(\mathbf{p}',i\omega_n')G(\mathbf{p}',i\omega_n'+i\nu_n)\times\left[\frac{\partial\epsilon_{\mathbf{p}'}}{\partial p_x' a}+\Lambda(\mathbf{p}',i\omega_n';i\nu_n)\right] \tag{33}$$

and $N_{\mathbf{p}}^2$ is the total number of points in the Brillouin zone. At the one-loop level, the vertex corrections consist of all ladder diagrams. The RPA-like diagrams do not contribute to the current-current correlation function when the interaction is spin dependent for the same reason that the Hartree diagram for the self-energy vanishes. The optical conductivity $\sigma(\omega)$ and electrical resistivity $\rho=1/\sigma(0)$ can be obtained from $R(i\nu_n)$ by analytic continuation to real frequencies using the method of Padé approximants.[23] One has

$$\sigma(\omega)=\frac{2e^2}{i\hbar^2c\omega}[R(\omega)-R(0)], \tag{34}$$

where c is the lattice constant along the z axis and the factor of 2 comes from the two CuO planes per unit cell.

The solution of Eq. (33) for the vertex is obtained as follows. For each value of ν_n, the term on the right-hand side of the equation is again a convolution and the iterative solution of Eq. (33) for each Matsubara frequency ν_n (with starting point $\Lambda=0$) can be obtained once again with the help of the fast Fourier transform. One first has to obtain the one-particle Green's function from Eqs. (6) and (7) and then solve the linear integral equation for the vertex function. To calculate $R(i\nu_n)$ for a system size of $64\times64\times256$ for about 50 Matsubara frequencies ν_n requires about 15 min of Cray Y-MP time.

As can be seen from Eq. (34), the real part of the optical conductivity is given by

$$\mathrm{Re}\sigma(\omega)\propto\frac{\mathrm{Im}R(\omega)}{\omega}. \tag{35}$$

At low frequencies, for a metal, one has

$$\underset{\omega\to0}{\mathrm{Im}}R(\omega)=A_R\frac{\omega}{\omega_R}, \tag{36}$$

where A_R is the amplitude and ω_R the characteristic frequency for the current-current correlation function. Vertex corrections contribute to both A_R and ω_R. It turns out that the ladder diagrams only modestly enhance the amplitude A_R (by a few percent) and, hence, the optical conductivity. However, their dominant effect is an increase in ω_R; namely, the function $R(i\nu_n)$ decays less rapidly as ν_n increases, leading to an overall decrease of the optical conductivity and a corresponding increase in the electrical resistivity by some 20%–25%.

Our results, which include the effect of vertex corrections on the in-plane normal-state resistivity, are shown in Fig. 12. As noted above, the coupling constant $g=0.64$ eV is chosen such that the Eliashberg transition temperature is 90 K. As may be seen, the agreement between our theoretical calculation and the experimental results of Ginsberg, Lee, and Stupp[31] is quite reasonable, since we do not distinguish between the a and b directions and thus ignore the possibility of a different Fermi

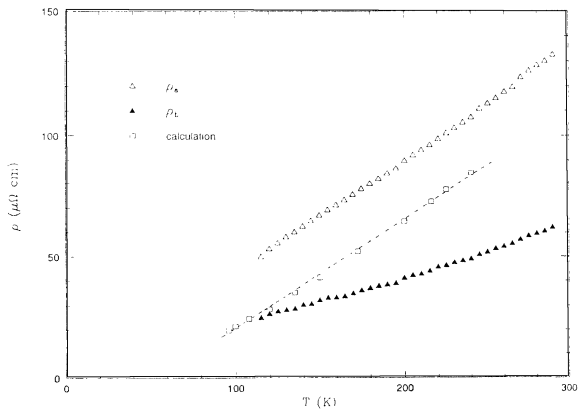

FIG. 12. Comparison of our calculated results for the "average" planar resistivity $\rho(T)$ with the experimental results of Ginsberg, Lee, and Stupp (Ref. 31).

velocity along these two directions. Since the resistivity must eventually, at low enough temperatures, cross over to a T^2 behavior characteristic of a Fermi liquid, we expect the negative intercept to be a generic feature of spin-fluctuation models. We have not yet established which parameters of the spin spectrum determine the magnitude of this intercept. It is worth mentioning that the slope and magnitude of $\rho(T)$ are relatively sensitive to the value of the spin-fluctuation frequency ω_{SF}. We found that, typically, a 10% change in ω_{SF} results in a 20% change in the slope of $\rho(T)$. Since we know ω_{SF} only to about 10% from NMR experiments, there is some uncertainty in the calculation of $\rho(T)$. Also, the small scatter in the calculated values of the resistivity reflects the difficulty in the analytic continuation problem since ω_R in Eq. (36) is rather low.

Our result for the frequency dependence of the optical conductivity (calculated with vertex corrections and for the same coupling constant) is shown in Fig. 13 where it is compared with that calculated with a slightly different choice of spin-fluctuation parameters, coupling constant, and hole doping, and is also compared with the experimental results of Orenstein *et al.*[32] It turns out to be difficult to fit both the optical-conductivity results of Orenstein *et al.* and the resistivity results of Ginsberg, Lee, and Stupp. The reason is that the electrical resistivity for the sample in the experiment of Ref. 31 is larger than that measured by Ginsberg, Lee, and Stupp. As can be seen from Fig. 13, the frequency dependence of the optical conductivity is very sensitive, as is the electrical resistivity, to the spin-fluctuation spectrum parameters, especially to the spin-fluctuation frequency ω_{SF}. Thus, until one has measurements of both the electrical resistivity and optical conductivity on the same high-quality sample, it is very difficult to pin down the correct spin-fluctuation parameters for $YBa_2Cu_3O_7$. It is gratifying that the agreement between theory and experiment for the resistivity has been considerably improved by incorporating vertex corrections and the "new" spin-fluctuation spectrum required by T_2 experiments. We also note that despite the fact that the temperature-dependent spin-fluctuation energy[33,34]

$$\omega_{SF}(T)\cong\{9.5+4.75[T\ (\mathrm{K})/100]\}\ \mathrm{meV} \tag{37}$$

is somewhat greater than T for $T\leq 200$ K, the resistivity remains linear in T.

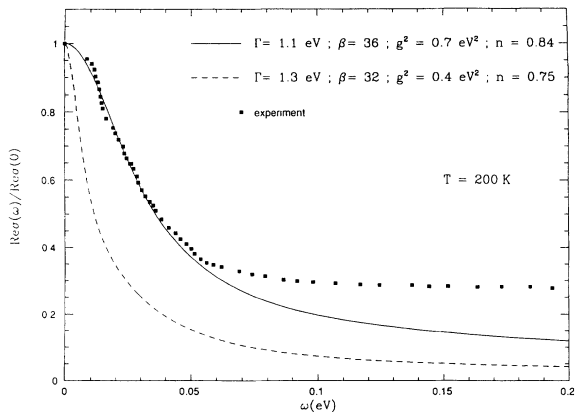

FIG. 13. Comparison of our calculated results for the normalized frequency-dependent optical conductivity $[\sigma(\omega,T)/\sigma(0,T)]$ at 200 K for two choices of parameters with the experimental results of Orenstein *et al.* (Ref. 32). A small change in the spin-fluctuation parameters produces a significant change in the width of the peak of $\sigma(\omega)$. For the parameters that produce a good fit to the experiment, the resistivity turns out to be about 130 $\mu\Omega$ cm at $T=200$ K, which is larger than the experimental results of Ginsberg, Lee, and Stupp (Ref. 31), but rather close to the resistivity measured by Orenstein *et al.* (Ref. 32).

Since the spin fluctuations are two dimensional and confined to the CuO layers and since we are assuming they are the dominant source of scattering for the quasiparticles, one may calculate the c-axis resistivity from the planar Green's function. When a hopping $t_\perp$ between the layers is included, the quasiparticle dispersion [Eq. (3)] is modified and becomes

$$\epsilon_{\mathbf{p}}=-2t[\cos(p_x a)+\cos(p_y a)] -4t'\cos(p_x a)\cos(p_y a)-2t_\perp\cos(p_z c)\ , \tag{38}$$

where c is the lattice constant in the z direction. We still take the two plane bands to be degenerate and assume that the hopping in the z direction is independent of p_x and p_y. When calculating the zz component of the current-current correlation function, the virtual particle-hole pair is such that the particle and hole are in different layers. Since the spin fluctuations are confined to the CuO layers, it follows that the virtual particle and hole cannot exchange a spin fluctuation. Therefore there are no vertex corrections to the c-axis resistivity, since as in the case of the in-plane resistivity, the RPA-like diagrams do not contribute to the current-current correlation function when the interaction is spin dependent. Thus the optical conductivity along the c axis is given by

$$\sigma_c(\omega)=\frac{2e^2c}{i\hbar^2a^2\omega}[R_c(\omega)-R_c(0)]\ , \tag{39}$$

where a and c are the lattice constants along the x and z directions, respectively, and the factor of 2 comes from the two CuO planes per unit cell. $R_c(\omega)$ is the analytic continuation of

$$R_c(i\nu_n)=-\frac{2k_BT}{N_{\mathbf{p}}^3}\sum_{\mathbf{p}}\sum_{\omega_n}\left[\frac{\partial\epsilon_{\mathbf{p}}}{\partial p_z c}\right]^2 G(\mathbf{p},i\omega_n) \times G(\mathbf{p},i\omega_n+i\nu_n)\ , \tag{40}$$

where $G(\mathbf{p},i\omega_n)$ is the quasiparticle propagator, $N_{\mathbf{p}}^3$ is the number of points in the Brillouin zone, and the momentum sum is over p_x, p_y, and p_z. It turns out that $t_\perp$ is much smaller than the nearest-neighbor hopping t, and thus the p_z dependence of the Green's function $G(\mathbf{p},i\omega_n)$ can be ignored. The p_z integral can then be done analytically, and one has

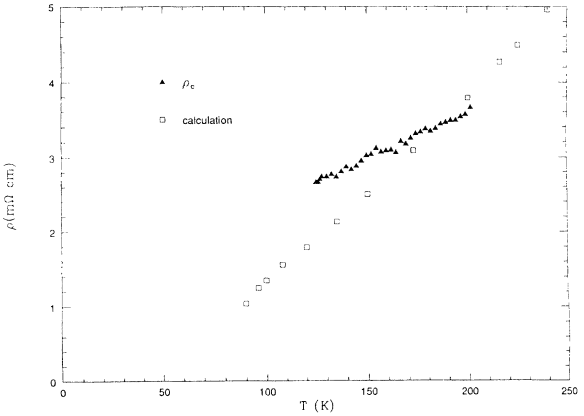

FIG. 14. Comparison of our calculated results for the c-axis resistivity $\rho_c(T)$ with the experimental results of Ginsberg, Lee, and Stupp (Ref. 31).

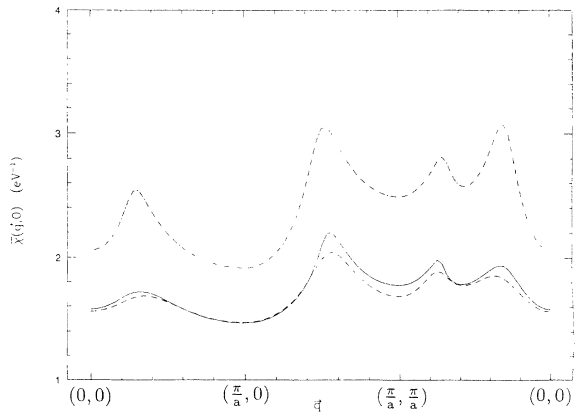

FIG. 15. Irreducible particle-hole susceptibility $\tilde{\chi}(\mathbf{q},0)$, calculated using bare propagators (dot-dashed line) and in the Eliashberg approximation at $T=90$ K (solid line) and at $T=200$ K (dashed line).

$$R_c(i\nu_n)=-\frac{4k_BT}{N_{\mathbf{p}}^2}t_\perp^2\sum_{\mathbf{p}}\sum_{\omega_n}G(\mathbf{p},i\omega_n)G(\mathbf{p},i\omega_n+i\nu_n)\ . \tag{41}$$

The momentum sums are now two dimensional, and the quasiparticle propagators can be calculated from Eqs. (6) and (7). Our results for the c-axis resistivity are shown in Fig. 14, with a hopping between layers, $t_\perp=8$ meV. The coupling constant $g=0.64$ eV is chosen such that the Eliashberg transition temperature is 90 K. As may be seen, the agreement between our theoretical calculation and the experimental results of Ginsberg, Lee, and Stupp[31] is again quite reasonable, given our simplifying assumptions. One notes that the calculation overestimates the slope of $\rho(T)$.

VIII. LOW-FREQUENCY MAGNETIC EXCITATION SPECTRUM

We turn now to a consideration of the low-frequency magnetic properties of the system of coupled quasiparticles and spin fluctuations. In the Matsubara frequency representation, the irreducible particle-hole spin susceptibility $\tilde{\chi}(\mathbf{q},\omega)$ is given by

$$\tilde{\chi}(q,i\nu_n)=-\frac{2k_BT}{N_{\mathbf{p}}^2}\sum_{\mathbf{p},\omega_n}G(\mathbf{p},i\omega_n)G(\mathbf{p}+\mathbf{q},i\omega_n+i\nu_n)\ , \tag{42}$$

where $N_{\mathbf{p}}^2$ is the number of points in the Brillouin zone. We obtain $\tilde{\chi}(\mathbf{q},0)$ by the same procedure used in MP I. Our results at $T=90$ K are given in Fig. 15, where they are compared with the irreducible free-quasiparticle static spin susceptibility $\tilde{\chi}_0(\mathbf{q},0)$ obtained by neglecting the coupling of the quasiparticles to spin fluctuations [i.e., setting $g=0$ in Eq. (2)]. The considerable structure present in $\chi_0(\mathbf{q},0)$ reflects the Kohn anomalies produced by transitions that span the Fermi surface. We find, as was the case for a comparable calculation (using the earlier MMP spin-fluctuation parameters) carried out in MP I, that quasiparticle lifetime effects resulting from the coupling of the quasiparticles to the spin fluctuations act both to reduce the magnitude of $\tilde{\chi}_0(\mathbf{q},0)$ and to smear out the Kohn anomaly peaks.

The experimentally measurable static spin susceptibility $\chi(\mathbf{q},0)$ differs considerably from $\tilde{\chi}(\mathbf{q},0)$ since, as we have seen, it is sharply peaked at the commensurate wave vector $\mathbf{Q}$ [recall that $\chi_{\mathbf{Q}}\cong 75$ states/eV, while $\tilde{\chi}(\mathbf{Q},0)\cong 1.8$ states/eV]. To understand the difference, which is produced by the magnetic coupling between the particles, let us parametrize the effects of the coupling using a RPA-like expression. We thus assume

$$\chi(\mathbf{q},\omega)=\frac{\tilde{\chi}(\mathbf{q},\omega)}{1-J(\mathbf{q})\tilde{\chi}(\mathbf{q},\omega)}\ , \tag{43}$$

where $J(\mathbf{q})$, the *effective* magnetic coupling between the quasiparticles, includes the effect of exchange and vertex corrections and may be temperature dependent. In the limit of low frequencies of interest to us here, we then obtain

$$\chi(\mathbf{q},0)=\frac{\tilde{\chi}(\mathbf{q},0)}{1+F_{\mathbf{q}}^a}\ , \tag{44}$$

$$\lim_{\omega\to 0}\frac{\chi''(\mathbf{q},\omega)}{\omega}=\lim_{\omega\to 0}\frac{\tilde{\chi}''(\mathbf{q},\omega)/\omega}{(1+F_{\mathbf{q}}^a)^2}\ , \tag{45}$$

where

$$F_{\mathbf{q}}^a=J(\mathbf{q})\tilde{\chi}(\mathbf{q},0) \tag{46}$$

measures the enhancement of $\tilde{\chi}(\mathbf{q},0)$ by spin-spin interactions. If we further write

$$\lim_{\omega\to 0}\tilde{\chi}''(\mathbf{q},\omega)=\frac{\pi\omega\tilde{\chi}_q}{\tilde{\Gamma}_q}\ , \tag{47}$$

we can then make a direct connection, for $\mathbf{q}=\mathbf{Q}$, between the spin-fluctuation parameters $\chi_{\mathbf{Q}}\equiv\chi(\mathbf{Q},0)$ and ω_{SF}, the irreducible quasiparticle-quasihole spin spectrum characterized by $\tilde{\chi}(\mathbf{Q},0)$ and $\tilde{\Gamma}_{\mathbf{Q}}$:

$$\chi_{\mathbf{Q}}=\frac{\tilde{\chi}(\mathbf{Q},0)}{1+F_{\mathbf{Q}}^{a}}\ , \tag{48}$$

$$\omega_{\mathrm{SF}}=\frac{\tilde{\Gamma}_{\mathbf{Q}}}{\pi}\frac{\tilde{\chi}(\mathbf{Q},0)}{\chi_{\mathbf{Q}}}\equiv\frac{\tilde{\Gamma}_{\mathbf{Q}}}{\pi}[1+F_{\mathbf{Q}}^{a}]\ . \tag{49}$$

From Eq. (47) we obtain a significant constraint on the quasiparticle Fermi surface:

$$\lim_{\omega\to 0}\frac{\tilde{\chi}''(\mathbf{q},\omega)}{\omega}\neq 0\ ; \tag{50}$$

the Fermi surface must be such that, for values of $\mathbf{p}$ within $k_B T$ of the Fermi surface,

$$\epsilon(\mathbf{p}+\mathbf{Q})-\epsilon(\mathbf{p})=0\ ; \tag{51}$$

otherwise, enhancement would be ineffective. This constraint is satisfied by the open Fermi surface one obtains with $t'=-0.45t$; it is *not* satisfied for the Fermi surface which obtains, for all values of hole doping (apart from half-filling), with $t'=0$, unless one has both very low doping and very high temperatures, $2k_B T\sim\mu$, the chemical potential with respect to that of the half-filled system.

It is instructive to consider the behavior of $J(\mathbf{q})$ in the vicinity of Q. At Q, on making use of our calculated value $\tilde{\chi}(\mathbf{Q},0)|_{T=90\ \mathrm{K}}\cong 1.8$ states/eV and the fit to the NMR experiments, $\chi_{\mathbf{Q}}(T=90\ \mathrm{K})=75$ states/eV, we find

$$J(\mathbf{Q},T=90\ \mathrm{K})=0.54\ \mathrm{eV}\ , \tag{52}$$

$$F_{\mathbf{Q}}^{a}(T=90\ \mathrm{K})=-0.976\ . \tag{53}$$

Rather similar values, based on the earlier MMP fit to the spin excitation spectrum, were obtained in MP I. Thus, even though $[\xi\ (90\ \mathrm{K})/a]$ is not large, one is, in fact, very close to an antiferromagnetic instability ($F_{\mathbf{Q}}^{a}=-1$) even for $YBa_1Cu_3O_7$. The fact that in Sec. IV we found that the assumed spin-fluctuation spectrum is rather far from causing an instability in the quasiparticle response, while the $F_{\mathbf{Q}}^{a}$ [Eq. (53)] found here is close to -1, indicates that we do not yet have a fully self-consistent account of spin and quasiparticle properties.

We next note that since $\tilde{\chi}(\mathbf{q},0)$ exhibits comparatively little structure in the vicinity of $\mathbf{Q}$ (and in fact possesses a local minimum there) and if, as shown in MP I, $\tilde{\Gamma}_{\mathbf{q}}$ also possesses comparatively little structure in the vicinity of $\mathbf{Q}$, then $J(\mathbf{q})$ must fall off quite rapidly as one goes away from $\mathbf{Q}$. This follows from the NMR constraint that the ratio of the ^{63}Cu relaxation rate [which is determined by $F_{\mathbf{q}}^{a}$ in the vicinity of $\mathbf{Q}$, according to Eq. (45)] to the ^{17}O relaxation rate [the latter is determined primarily by the values of $\chi''(\mathbf{q},\omega)$ at wave vectors for which the antiferromagnetic enhancement is not substantial] is quite large at low temperatures (~ 20 near T_c). Hence $F_{\mathbf{q}}^{a}$ must be sharply peaked, and $J(\mathbf{q})$ even more so, to bring this about.

As noted in MP I, for a given calculation of $\tilde{\chi}''(\mathbf{q},\omega)$, at a given temperature, one can easily find a $J(\mathbf{q})$ which is sufficiently peaked at $\mathbf{Q}$ to yield a spectral density of the MMP form [Eq. (4)]. To the extent that one succeeds in doing this, one arrives at a self-consistent picture, since the output calculated quasiparticle spin-fluctuation spectrum would then agree with the assumed input spectrum [Eq. (4)] for values of $\mathbf{q}$ in the vicinity of $\mathbf{Q}$. This output quasiparticle spectrum possesses the further advantage that it provides a microscopic basis for the quasiparticle-like portion of the low-frequency magnetic excitation spectrum, i.e., that obtaining for wave vectors well away from $\mathbf{Q}$. It is this part of $\chi''(\mathbf{q},\omega)$ which is responsible for the spin-lattice relaxation rate of the ^{17}O and ^{89}Y nuclei. Our preliminary calculations, reported in MP I, suggest that this part of $\chi''(\mathbf{q},\omega)$ is also enhanced. Thus a comparison of our calculated values of $\tilde{\chi}_0=1.6$ states/eV with that measured experimentally leads us to conclude that

$$F_0^{a}\cong -0.4\ ; \tag{54}$$

in other words, the effective spin-spin interaction must be such that at long wavelength the measured static spin susceptibility is ferromagnetically enhanced compared to the calculated value $\tilde{\chi}_0$. The exact amount of this enhancement will depend on the details of the hole concentration and coupling constant required to yield $T_c=90$ K. Inspection of Eq. (45) shows that the quasiparticlelike portion of $\chi''(\mathbf{q},\omega)$ takes the approximate form

$$\lim_{\omega\to 0}\frac{\chi''(\mathbf{q},\omega)}{\omega}\cong\lim_{\omega\to 0}\frac{[\tilde{\chi}''(\mathbf{q},\omega/\omega]}{(1+F_0^{a})^2},\quad |\mathbf{q}-\mathbf{Q}|\geq\frac{q}{\xi}\ . \tag{55}$$

A preliminary study of the fit to experiment for the ^{17}O relaxation rates[34] shows that an enhancement of the order of that found from Eq. (55) is required to explain the measured experimental results.

We further note that Eq. (49) may be used to test the extent to which the present calculation of the normal-state magnetic properties is self-consistent for spin fluctuations in the vicinity of $\mathbf{Q}$. On making use of the result $\tilde{\chi}(\mathbf{Q},0)\cong 1.8$ states/eV and the NMR-constrained fit ω_{SF} (90 K)$=14$ meV, we see that to be fully consistent one must have

$$\tilde{\Gamma}_{\mathbf{Q}}=\pi[\chi_{\mathbf{Q}}/\tilde{\chi}(\mathbf{Q},0)]\omega_{\mathrm{SF}}\cong 1.7\ \mathrm{eV}\ , \tag{56}$$

which is close to the value $\tilde{\Gamma}_{\mathbf{Q}}=1.3$ eV, calculated in MP I. This suggests that a self-consistent calculation of $J(\mathbf{q})$ which includes exchange and vertex corrections may lead to quite reasonable results.

We expect the general character of the results based on the model Hamiltonian [Eq. (4)] to be comparatively insensitive to the choice of the nearest-neighbor and next-nearest-neighbor hopping parameters t and t', the choice of n_e, the coupling constant g which yields $T_c=90$ K, or the exact form of the assumed spin-fluctuation spectral density, provided the shape of the Fermi surface is such that Eq. (51) is satisfied. It is natural to inquire how the physical properties calculated using the model Hamiltonian [Eq. (4)] compare with those obtained using the Hubbard model.

Nearly all of the pioneering calculations of the properties of strongly correlated planar quasiparticles have been carried out using the Hubbard and the closely related t-J model. Detailed calculations have been carried out by

Scalapino for the case of nearest-neighbor hopping only, i.e., $t'=0$.[35] These show that qualitative and, sometimes, quantitative agreement with NMR experiments can be obtained if one fine-tunes the choice of n_e and uses the equivalence of the exact Monte Carlo calculations (valid for $T \geq 300$ K) with a RPA expression at high temperatures to extrapolate the RPA-equivalent result to the lower temperatures of primary experimental interest for the $YBa_2Cu_3O_7$ system. For example, Bulut, Scalapino, and White[36] find that an expression of the form

$$\chi(\mathbf{q},\omega)=\frac{\chi_0(\mathbf{q},\omega)}{1-\bar{U}\chi_0(\mathbf{q},\omega)}\ , \tag{57}$$

where $\bar{U}=2t$ and $\chi_0(\mathbf{q},\omega)$ is the noninteracting particle-hole susceptibility calculated for $n_e=0.85$ and $t'=0$, provides an excellent fit to the $\mathbf{q}$, $i\omega_n$, and T dependence of the Monte Carlo results for $\chi(\mathbf{q},i\omega_n)$ obtained on a 8×8 lattice with $U=4t$ and $\langle n \rangle = 0.85$. Bulut and Scalapino[37] have then used Eq. (57) and a suitable choice of gap parameters $[\Delta(0)/kT_c \cong 3-4]$ to compute spin-lattice relaxation and T_2 for ^{63}Cu nuclei in the superconducting state.

One might therefore have reason to hope that the corresponding calculation of the superconducting transition would yield good agreement with experiment. This, however, appears not to be the case. For values of doping for which the proposed susceptibility yields a fit to experiment, the corresponding values of the largest eigenvalue of the superconducting kernel λ_{SC} (see Sec. II) obtained with that susceptibility are much less than 1 for temperatures in the vicinity of 90 K.[38]

We believe there are two reasons why one does not seem to obtain high T_c with a Hubbard-like expression of the form of Eq. (57). First, and probably most important, until one carries out the calculations with a t' which is sufficiently large to yield a Fermi surface which meets the criterion of Eq. (49) at low temperatures and low frequencies, one will not find a peak at $(\pi/a,\pi/a)$ no matter what the value of $\bar{U}$. Second, even if one then adopts a tight-binding spectrum which yields a Fermi surface which meets the criterion of Eq. (49), one will not obtain a commensurate peak in $\chi''(\mathbf{q},\omega)/\omega$ at low frequencies and low temperatures with a featureless restoring force $\bar{U}$; rather, one would find two incommensurate peaks at wave vectors determined by the Kohn anomaly. Thus, with a featureless $\bar{U}$, the maximum values of $F_{\mathbf{q}}^a$ occur at the Kohn anomaly, rather than at $\mathbf{Q}$, and the resulting low-temperature low-frequency $\chi''(\mathbf{q},\omega)$ cannot provide a quantitative explanation of the ^{63}Cu and ^{17}O NMR relaxation rates. We speculate that these difficulties are interrelated, that unless one uses a sharply peaked commensurate spin-fluctuation spectrum with sufficient antiferromagnetic enhancement to explain the NMR experiments, one will not be able to obtain a high T_c.

IX. DISCUSSION AND CONCLUSIONS

The Hamiltonian [Eq. (2)] we have considered in this paper has been chosen to take into account at the outset two key experimental aspects of the metallic superconducting cuprates: the existence of a planar quasiparticle Fermi surface and the presence of strong short-range antiferromagnetic correlations between these planar quasiparticles. It makes possible a detailed examination of the physical consequences of the magnetic interaction between the quasiparticles, since one is at liberty to explore what happens when one changes the shape of the quasiparticle Fermi surface, the hole concentration, the effective coupling g between the quasiparticles and the low-frequency spin excitations, and the spectral density of those spin excitations. Thus one can calculate the way in which changes in these quantities influence the resistivity, optical and other transport properties, and superconducting transition temperature, as well as determining the changes in the normal state of the quasiparticle spectral density and magnetic response functions which are produced by their magnetic interaction.

The results we have obtained for the resistivity- and frequency-dependent optical conductivity provide a quantitative bridge between measurements of the normal-state properties and the high superconducting transition temperature. They illustrate clearly the importance of using an accurate quantitative description of the spin-fluctuation excitation spectrum in calculating both T_c and normal-state properties. We find that when we do so, the effective coupling between quasiparticles and spin fluctuations required to get $T_c \sim 90$ K is substantially reduced, so much so that the corresponding dimensionless coupling constant $\lambda \leq \frac{1}{2}$. We find that the simple form for T_c obtained in MP I persists when one goes to different hole concentration and different spin-fluctuation parameters and that a particularly useful expression for T_c is

$$T_c \cong \{[\xi^2(T_c)/a^2]\omega_{SF}(T_c)(n_e/0.79)\} \times \exp\left[-\frac{1}{0.37N(0)g}\right]\ . \tag{31'}$$

We also find that changes in the spin-fluctuation parameters lead primarily to changes in the prefactor, the cutoff energy for the effectiveness of the spin-fluctuation-induced interaction, $(\omega_{SF}\xi^2)_{T=T_c}$. To a first approximation this quantity is independent of ξ^2, while $\lambda \equiv 0.37N(0)g$ appears to be nearly independent of the details of the spin excitation spectrum.

We have also demonstrated, by explicit calculations, that when a substitutional impurity is located at a planar copper site [Cu(2)], its influence on T_c depends sensitively on whether or not it influences the ^{63}Cu spin-lattice relaxation time. Thus we found that Ni impurities, which Ishida *et al.*[16] have shown do not influence $^{63}T_1$, can be treated, in their influence on T_c, as though they are potential scatterers of strength $U=0.25$ eV. Substitutional Zn impurities, on the other hand, although nonmagnetic, act to disrupt local magnetic order and also change the effective spin-fluctuation-induced interaction responsible for superconductivity; these thereby exert a much larger influence on T_c than their Ni counterparts. The good agreement between our theoretical calculation and experiment provides rather direct experimental evidence for the spin-fluctuation origin of the high-temperature super-

conductivity in $YBa_2Cu_3O_7$.

The model Hamiltonian used in this, and our preceding papers, has not been derived from first principles; indeed, it may be argued that it is only because we have chosen to adopt a more phenomenological experiment-based approach (introducing "experimental" quasiparticles and "experimental" spin fluctuations) that we have been able to make so much progress. Still it would be highly desirable to derive, from first principles, an effective low-energy Hamiltonian of the form of Eq. (2) and to calculate the effective spin coupling $J(\mathbf{q})$ required to bring about a self-consistent description. Also of great interest is the extension of our approach to the "underdoped" 1-2-3 and 2-1-4 systems, to see whether it can provide insight into the magnetic origin of the measured temperature-dependent $\chi_Q(T)$ and modified $\omega_{SF}(T)$ required to explain the NMR experiments,[34] as well as relating the reduced values of T_c to changes in the low-energy spin spectrum.

Other quite desirable extensions of the work described here include a detailed examination of the accuracy of the Eliashberg-Migdal approximation used here (preliminary estimates suggest that, depending on the property, it is valid to between 5% and 25%) and carrying out a conserving approximation of the kind used by Bickers, Scalapino, and White[39] in their pioneering calculations of T_c and other properties (in which they used a $t'=0$ Hubbard model and a value of n_h not far from half-filling).

Calculations which at first sight appear similar to our own have been carried out by Radtke *et al.*[40,41] However, both the resistivity and superconducting transition temperature calculations reported in Ref. 40 are seriously flawed. As we have shown in MP I and the present paper, it is essential, in calculating the resistivity, to solve for the self-energy self-consistently; thus, the Boltzmann equation, relaxation time approximation, adopted by Radtke *et al.*, can lead to serious errors. Second, in computing T_c, these authors limit the wave vectors of the electron self-energy and pairing potential to the Fermi surface. As we have shown by explicit example in MP I, doing so leads, for a given choice of coupling constant, to a serious underestimate of T_c. Thus it is perhaps not surprising that Radtke *et al.* obtain a too large planar resistivity for the normal state of $YBa_2Cu_3O_7$ and find that constraints on the quasiparticle spin-fluctuation coupling constant imposed by the conductivity require that $T_c=7.2$ K instead of the 90 K found here. In their more recent work, Radtke *et al.*[41] report on their predictions for the suppression of T_c by nonmagnetic impurities, based on the model employed in Ref. 40. They find, contrary to the results presented here, what appears to be a significant suppression of T_c; it is likely that this considerable overestimate is a consequence of an inadequate description of the way in which the self-energy of a quasiparticle is modified by its coupling to spin fluctuations, as well as their use of the Born approximation to treat impurity scattering.

The approach to strong-coupling spin-fluctuation-induced superconductivity which may be closest in spirit to that presented here is that developed independently by Moriya, Takahashi, and Ueda,[28] which has recently been reviewed by Ueda, Moriya, and Takahashi.[42] They have reported, at both the Kanazawa conference[43] and a subsequent conference in Tsukuba,[44] on the results of strong-coupling calculations for a Hamiltonian based on the self-consistent renormalization approach of Moriya, Takahashi, and Ueda.[28] However, one cannot at present carry out a comparison between the strong-coupling calculations reported here and those of Ueda, Moriya, and Takahashi,[42] because the details of their computational approach and the sensitivity of their results to the choice of quasiparticle spectrum, spin-fluctuation spectrum, and coupling constant have yet to be published.

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