Spin-Fluctuation-Induced Superconductivity in the Copper Oxides: A Strong Coupling Calculation

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We have carried out a strong coupling calculation of spin-fluctuation-induced superconductivity for $YBa_2Cu_3O_7$ using the experimentally determined spin excitation spectrum. We find that it is extremely important to take full account of the momentum and frequency dependence of the interaction and that while lifetime effects substantially reduce T_c from its value calculated in a weak coupling approximation, it is still possible for spin fluctuations to give rise to high-temperature superconductivity.

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Since the discovery of high-temperature superconductivity in the copper oxides by Bednorz and Mueller [1], a key question has been "what is the physical mechanism responsible for superconductivity in these systems?" In two previous communications [2,3] (hereafter referred to as MBP) we have examined the possibility that antiferromagnetic paramagnons, the low-lying spin excitations which are responsible for the unusual magnetic properties of the normal state of the copper oxides [4], might also give rise to high-temperature superconductivity. We have described the results of weak coupling calculations which demonstrate that the retarded interaction between planar quasiparticles induced by the exchange of antiferromagnetic paramagnons leads uniquely to a transition to a superconducting state with $d_{x^2-y^2}$ symmetry [2,3]. With a spin excitation spectrum and a quasiparticle-paramagnon coupling determined by fits to normal-state experiments, we obtained 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 found that the effective quasiparticle interaction possesses considerable structure in that it is both momentum and frequency dependent, and showed, 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 idea of spin-fluctuation-induced superconductivity is not a new one, since it is believed to be the physical origin of the comparatively low-temperature superconductivity observed in the heavy-electron actinide systems. Theorists have, however, been generally skeptical that it would work for high-temperature superconductivity, primarily because they believed that the short lifetime for the scattering of quasiparticles against spin fluctuations would make it impossible for the quasiparticles to take sufficient advantage of the spin-fluctuation-induced interaction to superconduct at high temperature. However, MBP found by careful numerical calculations that the "starting" temperature for high-temperature superconductors, calculated in a weak coupling theory in which the influence of this scattering on the superconducting transition was neglected, was much higher than earlier approximate calculations had suggested. Still it is essential to carry out a strong coupling calculation using the Eliashberg formalism [5] to demonstrate that high superconducting transition temperatures persist when full account is taken of lifetime effects. We report here on the results of such Eliashberg calculations. We show that the so-called pair-breaking effects of quasiparticle scattering substantially reduce the superconducting transition temperature from what it would have been in their absence, but do not prevent the copper oxides from becoming high-temperature superconductors. We find that as was the case for weak coupling theory, it is essential, in carrying out Eliashberg calculations, to allow for the full momentum and frequency dependence of the retarded quasiparticle interaction; if one fails to do this, the resulting transition temperatures can easily be smaller by 1 order of magnitude.

The 2D Eliashberg equations 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

$$\Sigma(\mathbf{p},i\omega_n)=g^2\frac{k_BT}{N_{\mathbf{q}}^2}\sum_{\Omega_n}\sum_{\mathbf{q}}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)G(\mathbf{q},i\Omega_n)\,, \tag{1}$$

$$G(\mathbf{p},i\omega_n)=\frac{1}{i\omega_n-(\epsilon_{\mathbf{p}}-\mu)-\Sigma(\mathbf{p},i\omega_n)}\,, \tag{2}$$

$$\Phi(\mathbf{p},i\omega_n)=-g^2\frac{k_BT}{N_{\mathbf{q}}^2}\sum_{\Omega_n}\sum_{\mathbf{q}}\chi(\mathbf{p}-\mathbf{q},i\omega_n-i\Omega_n)G(\mathbf{q},i\Omega_n)G(-\mathbf{q},-i\Omega_n)\Phi(\mathbf{q},i\Omega_n)\,, \tag{3}$$

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, $\epsilon_{\mathbf{p}}=-2t[\cos(p_x)+\cos(p_y)]$ is the bare electron spectrum, and μ is the chemical potential. $N_{\mathbf{q}}^2$ is the total number of momenta in the Brillouin zone and $\omega_n=(2n+1)\pi k_BT$, n

$=-\infty,\ldots,-1,0,1,\ldots,+\infty$. The coupling constant g^2 is equal to $2g_{\text{eff}}^2$ as defined by MBP. $\chi(\mathbf{q},iv_n)$ is related to the imaginary part of the spin response function $\mathrm{Im}\chi(\mathbf{q},\omega)$ via the spectral representation

$$\chi(\mathbf{q},iv_n)=-\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\frac{\mathrm{Im}\chi(\mathbf{q},\omega)}{iv_n-\omega},\quad \mathrm{Im}\chi(\mathbf{q},\omega)=\frac{\chi_{\mathbf{Q}}\omega/\omega_{\mathrm{SF}}}{[1+\xi^2(\mathbf{q}-\mathbf{Q})^2]^2+(\omega/\omega_{\mathrm{SF}})^2} \tag{4}$$

on taking the form determined by Millis, Monien, and Pines [4] from their fit to NMR experiments. $\chi_{\mathbf{Q}}\equiv\chi_0\xi^2\beta^{1/2}$ is the susceptibility at wave vector $\mathbf{Q}=(\pi,\pi)$, where χ_0 is the experimentally measured long-wavelength spin susceptibility, ξ is a temperature-dependent antiferromagnetic correlation length, $\beta\approx\pi^2$, and $\omega_{\mathrm{SF}}=\Gamma/\beta^{1/2}\pi\xi^2$, where $\Gamma=0.4$ eV. To get $\chi(\mathbf{q},iv_l)$ to decay faster than $1/v_l$ for large v_l, we introduce a cutoff ω_0 and take $\mathrm{Im}\chi(\mathbf{q},\omega)=0$ for $\omega>\omega_0$. In the following we will adopt the value $\omega_0=0.4$ eV.

The critical temperature for the model is determined from Eq. (3) 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

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

is equal to 1. For the present model the argument presented for the weak coupling case still holds: A solution can only be found for a d-wave gap, $\Phi(\mathbf{p},i\omega_n)\propto\cos(p_x)-\cos(p_y)$.

In practice one has to solve those equations on a finite lattice and with a finite number of Matsubara frequencies. In order not to introduce fictitious temperature dependences one has to keep the upper energy cutoff $\omega_{n_{\max}}(T)$ constant. In the present calculation, the energy cutoff was set to ~ 3 times the bandwidth, that is, ~ 6 eV. Thus, one has to fix the temperature and adjust the coupling constant and the chemical potential until a solution is found. It is especially important in the present case to maintain the area of the Fermi surface constant (i.e., to insure $n=n_0$) since the large momentum transfers (i.e., across the Fermi surface) are those that bring about superconductivity. For a copper oxide plane in $YBa_2Cu_3O_7$, an appropriate value is $n_0\approx 0.75$.

The solution of Eqs. (1)–(3) is obtained iteratively: The most critical part of the algorithm is how to perform the iterations in an efficient manner. Because of the size of the arrays required for an accurate solution, efficiency is essential if one wants to solve the problem at all. In order to minimize finite-size effects, the momentum sums are performed on a 64×64 lattice and the number of Matsubara frequencies is up to 640. The iterations are performed until the difference in all the components of the self-energy between two successive iterations is less than 1 part in 10^4. The same accuracy is imposed on the largest eigenvalue of the superconducting kernel.

The equations are easily seen to be convolutions in momentum and frequency space of various quantities. Therefore, a fast-Fourier-transform algorithm is the best (and so far the only) way to perform the iterations (after a suitable discretization of the equations in imaginary time which amounts to using the trapeze rule to do the integrations over τ). Such an algorithm was first used by Serene and Hess [6] in their propagator-renormalized fluctuation exchange calculations on the Hubbard model.

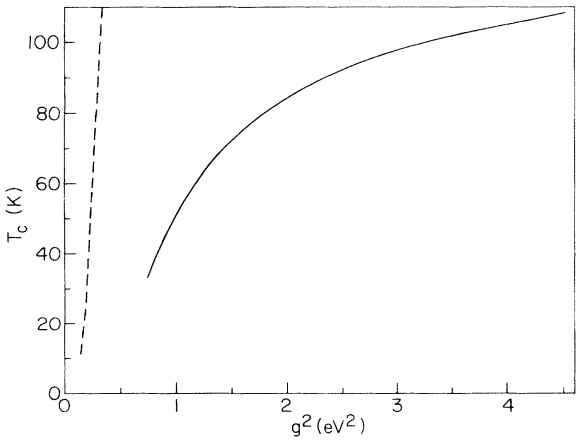

FIG. 1. Critical temperature T_c vs coupling constant squared. The solid line is the result of the strong coupling calculation Eqs. (1)–(3). The dashed line is the weak coupling result (in which the frequency dependence of the gap is ignored and the 2D integral equation is approximated by a 1D integral equation) obtained by MBP.

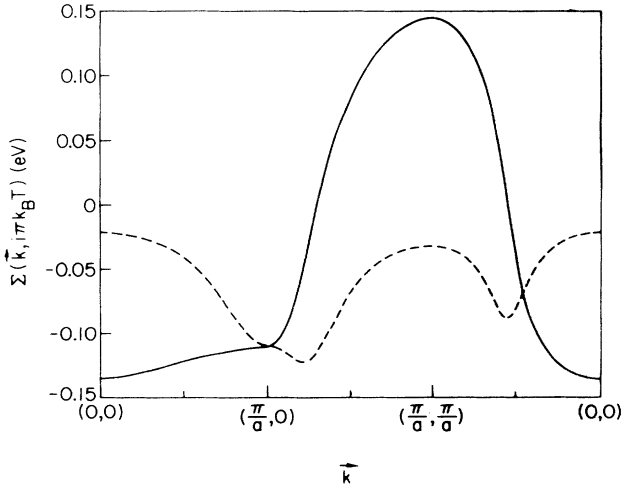

FIG. 2. The real (solid line) and imaginary (dashed line) parts of the self-energy $\Sigma(\mathbf{k},i\omega_n)$ at $T_c=90$ K for the lowest Matsubara frequency $\omega_n=\pi k_BT_c$ as a function of $\mathbf{k}$. The real part would vanish in the case of particle-hole symmetry.

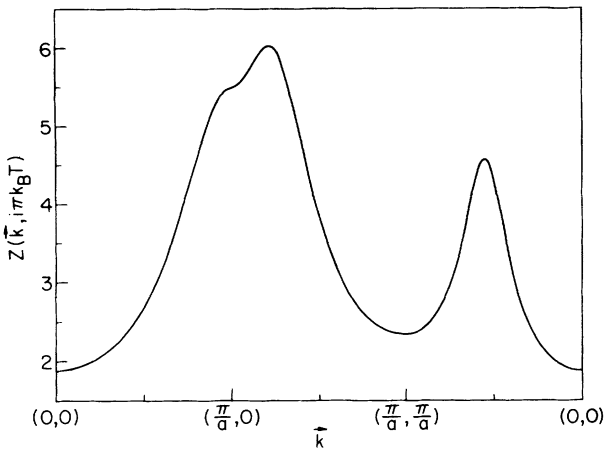

FIG. 3. The renormalization factor $Z(\mathbf{k},i\omega_n)=1-\mathrm{Im}\Sigma(\mathbf{k},i\omega_n)/\omega_n$ at $T_c=90$ K for the lowest Matsubara frequency $\omega_n=\pi k_B T_c$ as a function of $\mathbf{k}$. The two peaks in $Z(\mathbf{k},i\omega_n)$ near $(\pi/a,0)$ and $(\pi/2a,\pi/2a)$ are the result of a perfect match with the maximum of the spin excitation spectrum at $(\pi/a,\pi/a)$. The largest of the two peaks is near the Van Hove singularity $(\pi/a,0)$.

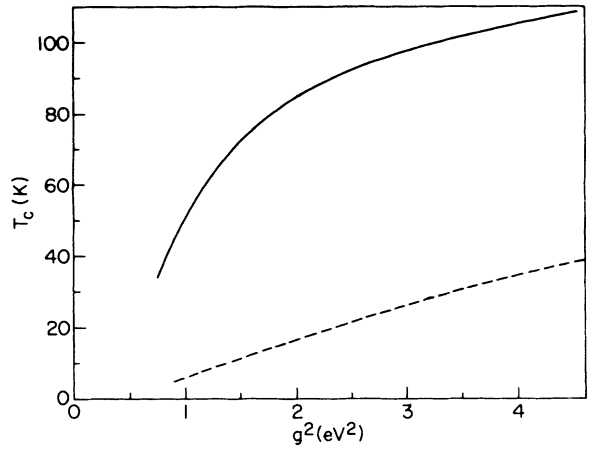

FIG. 4. Comparison of the results from the full Eliashberg calculation, Eqs. (1)–(3) (solid line), and the "phonon-inspired" Eliashberg calculation, Eqs. (5a) and (5b) (dashed line), for the same model parameters.

In the present work we have modified their algorithm in order to obtain smooth Green's functions in imaginary time [7]. The resulting algorithm works extremely well and allows us to solve the Eliashberg equations for large system sizes. When efficiently implemented on a Cray Y-MP computer, the solution of Eqs. (1)–(3) for a choice of coupling constant and chemical potential takes less than a minute for a system size of $64\times64\times256$.

The results of our solution of Eqs. (1)–(3) with the spin-fluctuation spectrum appropriate for $YBa_2Cu_3O_7$ are shown in Figs. 1–3. We see that while lifetime effects substantially reduce T_c from its value calculated in a weak coupling approximation, it is still possible for low-frequency spin fluctuations to give rise to high-temperature superconductivity, albeit with larger coupling constants than those used by MBP. However, we find, in a calculation to be reported elsewhere, that these larger coupling constants are in the range necessary to explain the normal-state properties. One also sees from the plot that for the doping concentration, Fermi surface, and spin excitation spectrum used in the calculation, transition temperatures much higher than 90 K cannot be easily generated.

As we did in the weak coupling case, it is instructive to compare the full solution of the problem to the approximation proposed by Millis [8]. He has argued that because of the smallness of the MBP cutoff Γ/π^2 relative to the bandwidth, one should be able to define a theory in terms of Fermi surface quantities only. In the usual Eliashberg notation, $\Sigma(\mathbf{p},i\omega_n)=i\omega_n[1-Z(\mathbf{p},i\omega_n)]$ when the energy shift is ignored [5]. On parametrizing the Fermi surface with the variables $\epsilon=\mu$ and θ as in MBP one obtains the strong coupling equations [8]

$$\omega_n Z(\theta,i\omega_n)=\omega_n+\frac{g^2k_BT}{\pi B}\int_0^{\pi/2}d\theta'\sum_{\Omega_n}\frac{1}{[(1+|\mu|)^2-(1-|\mu|)^2\cos^2(\theta')]^{1/2}}\times\mathrm{sgn}(\Omega_n)\sum_{\varphi_i}\chi(\mathbf{p}(\mu,\theta)-\varphi_i\mathbf{q}(\mu,\theta'),i\omega_n-i\Omega_n)\,, \tag{5a}$$

$$\bar{\Phi}(\theta,i\omega_n)=-\frac{g^2k_BT}{\pi B}\int_0^{\pi/2}d\theta'\sum_{\Omega_n}\frac{1}{[(1+|\mu|)^2-(1-|\mu|)^2\cos^2(\theta')]^{1/2}}\frac{1}{|\Omega_nZ(\theta',\Omega_n)|}\times\sum_{\varphi_i}(-1)^{\varphi_i}\chi(\mathbf{p}(\mu,\theta)-\varphi_i\mathbf{q}(\mu,\theta'),i\omega_n-i\Omega_n)\bar{\Phi}(\theta',i\Omega_n)\,, \tag{5b}$$

where $\bar{\Phi}(\theta,i\omega_n)=\Phi(\theta,i\omega_n)\cos(\theta)$ is the anomalous self-energy, $\{\varphi_i\}_{i=1,\ldots,8}$ are the transformations that map any wave vector in the Brillouin zone onto the first octant, and $(-1)^{\varphi_i}$ is the parity of the gap under these transformations. μ is the chemical potential in units of half the bandwidth. The solution to these equations for the same model parameters (susceptibility, cutoff ω_0, and doping) used in our strong coupling calculations is shown in Fig. 4 and compared to the results of the more complete calculation. The discrepancy between the two calculations may again be attributed to the neglect of the structure in momentum space. Needless to say, for the problem at hand, the difference in the maximum values of T_c which can be obtained is physically quite important.

We plan to examine various possibilities for $\mathrm{Im}\chi(\mathbf{q},\omega)$

to try to determine what features of this spectral function limit the transition temperature. More precisely, we will explore the functional dependence of T_c on the antiferromagnetic correlation length ξ and the spin fluctuation frequency ω_{SF}, and the wave vector at which the susceptibility is peaked, i.e., commensurate versus incommensurate antiferromagnetic correlations. The influence of the shape of the Fermi surface on T_c is also to be worked out. The role of isotropic elastic impurity scattering on the transition temperature and its interplay with the inelastic scattering due to spin fluctuations is likewise of interest.

We have shown that low-frequency spin fluctuations can be very effective as a mechanism for high-temperature superconductivity. However, we cannot overemphasize the importance, in examining spin fluctuation mechanisms, of paying great attention to the structure of the induced quasiparticle interaction; unless this is done, the transition temperature T_c is seriously underestimated. As a corollary, the McMillan-Rowell inversion scheme is very likely not to work for the present problem; since different experiments probe different momentum structures, information about coupling constants and spectra deduced from one experiment cannot be applied to another. Our demonstration that superconductivity at high temperatures can be achieved with a spin-fluctuation mechanism removes what many had viewed as a major "theoretical" roadblock to using this mechanism to explain superconductivity in the copper oxides. Since we have shown that the resulting pairing state must possess $d_{x^2-y^2}$ symmetry, the proof that these materials are in fact "spin-fluctuation" superconductors will come in experimental verification of our proposed $d_{x^2-y^2}$ pairing state.

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