

## Predictions for impurity-induced $T_c$ suppression in the high-temperature superconductors

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We address the question of whether anisotropic superconductivity is compatible with the evidently weak sensitivity of the critical temperature  $T_c$  to sample quality in the high- $T_c$  copper oxides. We examine this issue quantitatively by solving the strong-coupling Eliashberg equations numerically as well as analytically for  $s$ -wave impurity scattering within the second Born approximation. For pairing interactions with a characteristically low energy scale, we find an approximately universal dependence of the  $d$ -wave superconducting transition temperature on the planar residual resistivity which is independent of the details of the microscopic pairing. These results, in conjunction with future systematic experiments, should help elucidate the symmetry of the order parameter in the cuprates.

A growing body of experimental evidence has been interpreted as supporting an anisotropic pairing state in the high-temperature superconductors.<sup>1</sup> There are indications, however, that the measured values of the superconducting critical temperature  $T_c$  do not depend strongly on sample quality. Because both magnetic and nonmagnetic impurities are pair breaking in anisotropic superconductors,<sup>2</sup> this latter statement appears to be incompatible with anisotropic pairing.

Two arguments can be offered to explain this apparent contradiction, but neither is quantitative enough to settle the issue. First, the coherence lengths  $\xi \approx 10 \text{ \AA}$  in the cuprates, while the mean free paths  $l \approx 100\text{--}200 \text{ \AA}$ .<sup>3</sup> Since one expects  $T_c$  to be affected by impurities only when  $\xi \sim l$ , the small ratio  $\xi/l \approx 0.1$  suggests that  $T_c$  should not be sensitive to defects. However, for magnetic impurities in  $s$ -wave superconductors, superconductivity is completely destroyed for  $\xi/l \cong 0.12\text{--}0.17$ ,<sup>4</sup> implying that  $\xi/l$  in the cuprates may not be small enough to avoid an impurity-induced reduction of  $T_c$ . Second, one observes significant inelastic scattering in these materials which could act to mask impurity effects. Inelastic scattering would only be able to screen the defects effectively if the inelastic mean free path were much shorter than the impurity mean free path. Estimates of these quantities<sup>3,5</sup> indicate that they are comparable in high-quality samples.

In this paper, we examine quantitatively the effect of impurities in the cuprates by generalizing the Abrikosov-Gor'kov scaling law<sup>4</sup> to anisotropic strong-coupling superconductors. We present model-independent predictions of  $T_c$  as a function of planar residual resistivity due to nonmagnetic impurities for a 90 K  $d$ -wave superconductor and compare these results to the response of an  $s$ -wave superconductor. We also check the validity of

this analytical result by calculating numerically the suppression of  $T_c$  induced by structureless impurities treated within the second Born approximation and in strong-coupling Eliashberg theory. Finally, we discuss how these predictions may be tested experimentally. Other authors have examined this question using analytical<sup>2</sup> as well as numerical techniques.<sup>6-8</sup> The goal of the present work, however, is to quantify the expected  $T_c$  suppression for  $d$ -wave models of the high-temperature superconductors, so that the  $d$ -wave hypothesis can be more directly tested.

We compute  $T_c$  in the presence of impurities from the standard mean field formalism<sup>9</sup> in which the electron self-energy is solved self-consistently from the single-exchange graph. This approach is justified if Migdal's theorem<sup>10</sup> applies, which is the case in conventional, phonon-mediated superconductors,<sup>11</sup> but it is not clear whether a similar result holds in the high-temperature superconductors.<sup>12</sup> Nonetheless, we follow other authors<sup>6-8,13-15</sup> and assume that this result holds in what follows.

In most of our calculations, we employ the standard set of approximations to this mean-field theory in order to simplify the resulting Eliashberg equations.<sup>9,11</sup> These simplified equations are discussed in more detail in Ref. 15. The central approximation to this approach is to limit the wave vectors of the electron self-energy and pairing potential to the Fermi surface, so we refer to the solution of these approximate equations as the Fermi-surface-restricted solution. For comparison, we have also solved the Eliashberg equations without these approximations on two-dimensional lattices of small size ( $64 \times 64$ ,  $32 \times 32$ ) using recently developed fast Fourier transform techniques.<sup>6,13,16</sup> We refer to the solution of these equations as the exact solution.

Of the models of  $d$ -wave superconductors avail-

able,<sup>6,7,13–15,17</sup> we employ a spin-fluctuation-mediated pairing interaction with a spectrum constrained by neutron scattering in  $\text{YBa}_2\text{Cu}_3\text{O}_{6.7}$ .<sup>15</sup> Solving the Fermi-surface-restricted equations with the pairing potential and band structure discussed in Ref. 15 gives us the critical temperature as a function of the bare impurity scattering rate  $\tau_{\text{imp}}^{-1}$ . (Throughout this paper, we set  $\hbar = k_B = 1$ .) We compute  $T_c$  vs  $\tau_{\text{imp}}^{-1}$  for a variety of critical temperatures in the absence of impurities  $T_{c0}$  and in both the weak- (inelastic scattering ignored) and strong- (inelastic scattering included) coupling cases. Although we vary the  $T_{c0}$ 's in this paper, constraints on the electron-spin fluctuation coupling constant imposed by ac conductivity require that  $T_{c0} = 7.2$  K in this model.<sup>15</sup> For comparison, we also compute the impurity-induced  $T_c$  suppression from the exact Eliashberg equations for the Monthoux-Pines spin-fluctuation model<sup>6,13</sup> with a coupling constant chosen so that  $T_{c0} = 100$  K.

We will show that these numerical results can be approximately collapsed to a universal curve. One can deduce that the form of this curve for  $d$ -wave superconductors is

$$-\ln\left(\frac{T_c}{T_{c0}}\right) = \psi\left(\frac{1}{2} + \frac{\alpha T_{c0}}{2\pi T_c}\right) - \psi\left(\frac{1}{2}\right), \quad (1)$$

where  $\psi(z)$  is the digamma function,  $\alpha = 1/[2(1 + \lambda_Z)\tau_{\text{imp}}T_{c0}]$  is the strong-coupling pair-breaking parameter, and  $\lambda_Z = 1 - \langle \text{Im}[\Sigma^{\text{boson}}(\mathbf{k}, i\omega_0)] \rangle / \omega_0$ . In this last equation,  $\Sigma^{\text{boson}}(\mathbf{k}, i\omega_0)$  refers to the self-energy of the pairing boson at the lowest fermionic Matsubara frequency  $\omega_0 = \pi T_{c0}$ , and the angle brackets denote an average over the Fermi surface. We note that, for an  $s$ -wave superconductor with magnetic impurities, Eq. (1) would still apply, but without the factor of 2 in  $\alpha$ . We note that individual aspects of this formulation have appeared in the works of other authors;<sup>2,4,9</sup> in particular, this form of the pair-breaking parameter can be found in Ref. 2.

In order to make contact with experiment, we represent the pair-breaking parameter  $\alpha$  in terms of the planar residual resistivity  $\rho_0$ . From the Kubo formula under the standard assumptions that the pairing boson energy is small compared to the electronic energies and that vertex corrections are not important,<sup>18</sup> the real part of the low frequency residual electrical conductivity is given by

$$\text{Re } \sigma(\omega) = \frac{\omega_{\text{pl}}^{*2}}{4\pi} \frac{\tau_{\text{imp}}^*}{1 + \omega^2 \tau_{\text{imp}}^{*2}}. \quad (2)$$

In this equation,  $\omega_{\text{pl}}^{*2} = \omega_{\text{pl}}^2 / (1 + \lambda)$  is the renormalized plasma frequency which is measured experimentally,

$$\frac{1}{\tau_{\text{imp}}^*} = \frac{1}{1 + \lambda} \frac{1}{\tau_{\text{imp}}} \quad (3)$$

is the renormalized scattering rate due to impurities, and  $\lambda = -\langle \partial \text{Re} \Sigma^{\text{boson}}(\mathbf{k}, \omega) / \partial \omega \rangle |_{\omega=0}$  is the mass renormalization parameter due to the pairing bosons. At zero temperature,  $\lambda$  is equal to the inelastic scattering parameter from the Eliashberg equations  $\lambda_Z$ . Since the characteristic energy of the pairing boson is low compared to other electronic energy scales (i.e., of the order of  $T_c$ ), we find

that  $\lambda \cong \lambda_Z$  to within 5–10 % at  $T_c$ . Combining this result with Eq. (2) and the definition of the pair-breaking parameter  $\alpha$ , we see that

$$\rho_0 \cong \frac{4\pi}{\omega_{\text{pl}}^{*2}} 2T_{c0} \alpha. \quad (4)$$

We emphasize that Eq. (4) allows us to predict the  $T_c$  suppression as a function of planar residual resistivity from the experimentally observed plasma frequency  $\omega_{\text{pl}}^{*2}$  and the critical temperature  $T_{c0}$  *independently* of any microscopic model.

Having set up the formalism for our calculations, we will now discuss the results. Figure 1 shows  $T_c/T_{c0}$  vs scattering rate from nonmagnetic impurities for a selection of  $T_{c0}$ 's in the model  $d$ -wave superconductor of Ref. 15. Since  $T_{c0}$  is inversely proportional to the coherence length  $\xi$ , the different curves in each figure correspond to different  $\xi$ 's. Both weak- [Fig. 1(b)] and strong- [Fig. 1(a)] coupling calculations show that, as  $T_{c0}$  increases ( $\xi$  decreases), the superconductor becomes

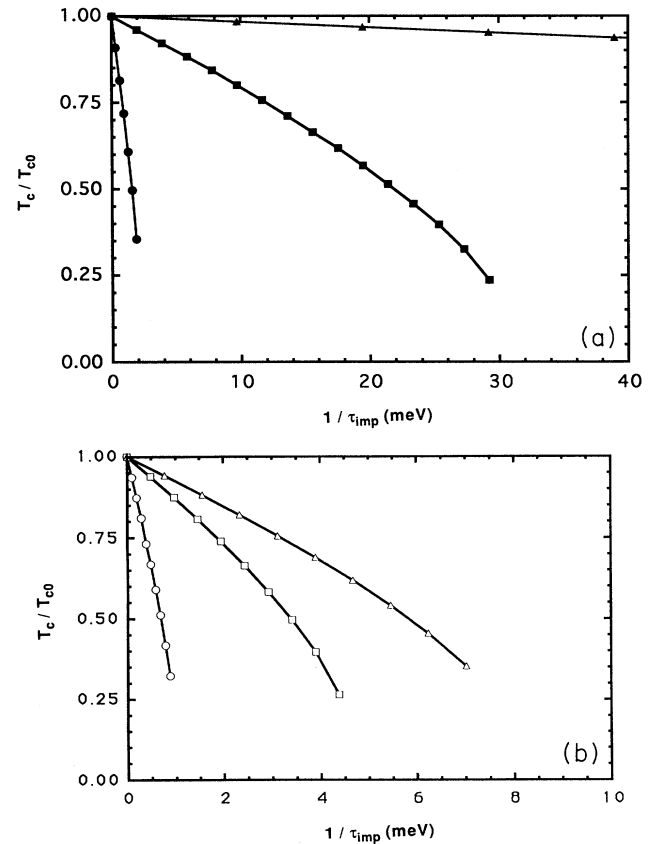


FIG. 1. Critical temperature  $T_c$  normalized by the critical temperature in the absence of impurities  $T_{c0}$  vs the bare impurity scattering rate  $\tau_{\text{imp}}^{-1}$  in meV for the model of Ref. 15 in the (a) strong-coupling and (b) weak-coupling cases calculated in the Fermi-surface-restricted Eliashberg formalism. The  $T_{c0}$ 's are 7.2 K (circle), 31.6 K (box), and 50.2 K (triangle); solid symbols denote strong-coupling results and empty symbols denote weak-coupling results. The solid lines are to guide the eye.

less sensitive to the presence of nonmagnetic impurities. In addition, by comparing curves in Figs. 1(a) and 1(b) with the same  $T_{c0}$ , we see that the strong-coupling curves (which include the effects of inelastic scattering) are less sensitive to impurities than the weak-coupling results.<sup>19</sup> These trends conform to the qualitative expectations discussed in the introduction.

To confirm the validity of our analytical results for the scaling function Eq. (1), we plot in Fig. 2 the numerical data in Fig. 1 in terms of the scaled variables  $T_c/T_{c0}$  and  $\alpha$ . As can be seen from the figure, all of the scaled curves cluster near the scaling function. Note that the data in Fig. 2 include both weak- and strong-coupling results; moreover, even the curve from Fig. 1(a) with nearly the maximum achievable  $T_{c0} = 50$  K falls near the scaling curve. In the inset to Fig. 2, we display the impurity-induced suppression of a 100 K  $d$ -wave superconductor in the Monthoux-Pines model computed from the exact Eliashberg equations. When plotted in terms of  $T_c/T_{c0}$  and  $\alpha$ , this model also produces a  $T_c$  suppression which is close to the scaling function Eq. (1).

Having established the validity of the scaling law, we use this relation to predict the response of a 90 K superconductor to nonmagnetic impurities. In Fig. 3, the shaded region corresponds to the  $d$ -wave  $T_c$  computed from Eqs. (1) and (4) for plasma frequencies  $\omega_{pi}^*$  ranging from 1.1 to 1.4 eV as a function of the planar residual resistivity  $\rho_0$ . These plasma frequencies are chosen to reflect the range of experimental uncertainty in  $\omega_{pi}^*$  in  $\text{YBa}_2\text{Cu}_3\text{O}_7$ .<sup>20</sup> For comparison, Fig. 3 also shows the expected response of an  $s$ -wave superconductor to nonmagnetic impurities (dashed line); in accordance with Anderson's theorem,<sup>21</sup> these impurities have no effect on  $T_c$ .

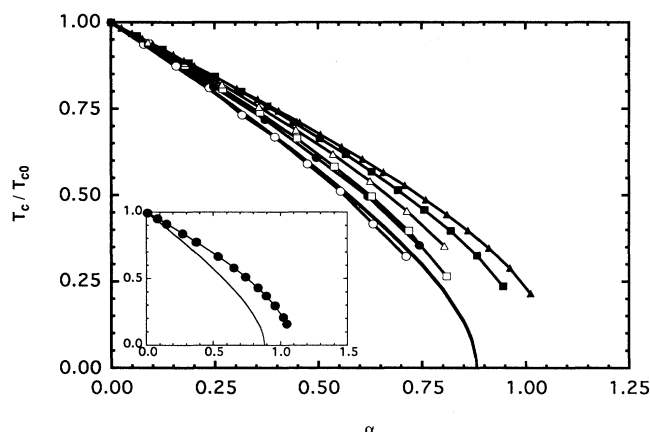


FIG. 2. Normalized critical temperature  $T_c/T_{c0}$  vs pair-breaking parameter  $\alpha = 1/2(1 + \lambda_Z)\tau_{\text{imp}}T_{c0}$  for the data in Fig. 1. Plot symbols are the same as in Fig. 1 with the solid symbols denoting strong-coupling calculations and the open symbols denoting weak-coupling calculations. For comparison, the analytic form of the scaling function [Eq. (1)] is plotted as a plain solid line. Inset: Normalized critical temperature vs pair-breaking parameter for the model of Refs. 6 and 13 calculated from the exact Eliashberg equations with the coupling chosen so that  $T_{c0} = 99.4$  K.

In addition to the uncertainty in the plasma frequency, the accuracy of the prediction in Fig. 3 is affected by the applicability of the scaling law and the assumption of structureless impurities. From Fig. 2, one can see a systematic trend away from the scaling curve as  $T_{c0}$  increases. For a 90 K superconductor, this error amounts to roughly a 20 % correction to the horizontal scale in Fig. 3, which is about the same magnitude as the uncertainty in the plasma frequency. The effect of ignoring the wave-vector dependence of the impurity scattering matrix element is more difficult to estimate. In extreme cases, impurities with wave-vector structure could alter the scale on the horizontal axis by a factor of 2.<sup>2</sup> Even considering these caveats, if the superconducting order parameter has  $d$ -wave symmetry, then the prediction in Fig. 3 should give the correct scale for the residual resistivity at which significant depression of the critical temperature will occur in  $\text{YBa}_2\text{Cu}_3\text{O}_7$ .

Experimentally, one can estimate the residual resistivity  $\rho_0$  by extrapolating the measured linear resistivity vs temperature for temperatures  $T$  greater than  $T_c$  to  $T = 0$ . It is found that this extrapolated planar  $\rho_0$  is about  $20 \mu\Omega \text{ cm}$  in high-quality twinned crystals of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and is roughly  $-20 \mu\Omega \text{ cm}$  in the best untwinned crystals. A negative extrapolated value of  $\rho_0$  means that the resistivity in the absence of superconductivity could not remain linear all the way down to zero temperature, but must turn over to some higher power law. The  $T_c$ 's of twinned and untwinned crystals are about the same, despite the fact that the change in residual resistivity is of order  $20 \mu\Omega \text{ cm}$  between the two types of samples. By contrast, if  $\text{YBa}_2\text{Cu}_3\text{O}_7$  were a  $d$ -wave superconductor, then, according to Fig. 3,  $T_c$  would be strongly suppressed.

This naive argument against the  $d$ -wave scenario is not strictly correct, since our calculations have focused entirely on a single  $\text{CuO}_2$  plane, which implies that the residual resistivity in Fig. 3 represents only the planar

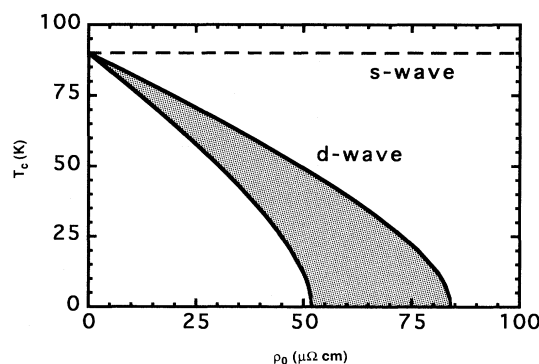


FIG. 3. Prediction of  $T_c$  as a function of the in-plane residual resistivity  $\rho_0$  due to nonmagnetic impurities in a 90 K superconductor with a  $d$ -wave (shaded area) or an  $s$ -wave (dashed line) order parameter. The  $d$ -wave curve is computed from the generalized Abrikosov-Gor'kov form [Eqs. (1) and (4)] for experimental plasma frequencies  $\omega_{pi}^*$  between 1.1 and 1.4 eV, and the  $s$ -wave curve is simply a straight line due to Anderson's theorem.

contribution to  $\rho_0$  and does not include the contribution from the CuO chains. For this reason, one cannot simply take existing measurements of  $T_c$  and  $\rho_0$  in polycrystalline or untwinned samples and infer unambiguous evidence for or against  $d$ -wave superconductivity; more systematic experiments are required.

Currently, two methods could be used to perform such systematic experiments: substitution and irradiation. Substitutional studies<sup>22-24</sup> are able to introduce defects mainly in the CuO<sub>2</sub> planes, as required, but find that the induced defects are generally magnetic. Abrikosov-Gor'kov-like behavior given by Eq. (1) is then to be expected and provides no qualitative distinction between  $s$ - and  $d$ -wave pairing. Alternatively, defects can be induced by irradiation,<sup>25-27</sup> but the location of these defects is often uncontrolled. Recent experiments,<sup>28</sup> though, suggest that low-energy electrons may preferentially disorder the Cu or O in the planes, which would enable a comparison of irradiation data with our predictions. Current irradiation

studies show that  $T_c$  decreases linearly with fluence, as one would expect for weak disorder in the scaling curve of Eq. (1), but it is not known how the fluence is correlated to the residual resistivity or whether the induced defects carry magnetic moments or not. Thus, although it is not yet possible to make a quantitative comparison of our results with current experiments, such a comparison should be possible with future systematic measurements. We hope that the present paper will serve as a stimulus for such experiments.

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