# Effect of the impurity scattering on the zero-temperature penetration depth in $d_{x^2-y^2}$ symmetry

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(Received 12 January 1994)

We have calculated the effect of impurity scattering in the Born (weak) and unitary (strong) limits on the absolute value of the zero-temperature penetration depth  $\lambda(0)$ . The gap is taken to exhibit  $d_{x^2,y^2}$ symmetry in the copper-oxygen planes and a model two-dimensional tight-binding band structure is used with nearest-neighbor hopping only. Impurities depress the value of the critical temperature and, at the same time, increase the value of  $\lambda(0)$ . Weak and strong scattering are compared. The predicted increase in  $\lambda(0)$  is smaller than indicated in recent experiments.

# I. INTRODUCTION

There is considerable experimental evidence for the idea that the gap in the copper-oxide planes of the high-T<sub>c</sub> oxides may exhibit  $d_{x^2,y^2}$  symmetry. Earlier evidence was reviewed by Annett and Goldenfeld.<sup>1</sup> Among the evidence is NMR and Knight-shift data,<sup>2</sup> temperature dependence of the penetration depth,<sup>3</sup> which is found to be linear at low T over a wide temperature range in high-quality  $YBa_2Cu_3O_{7-\delta}$  samples, some tunneling data,<sup>4,5</sup> angle-resolved photoemission,<sup>6,7</sup> inelastic polarized neutron-scattering data on the spin susceptibility,<sup>8</sup> and the superconducting quantum interference device experiments of Wollman et al. and Sigrist and Rice.9,10 Another set of important experiments are those relating to the collapse of the scattering rates in the superconducting state which would be qualitatively consistent with an antiferromagnetic spin-fluctuation mechanism in as much as the spin susceptibility, which plays the role of the pairing interaction in these theories, is expected to be modified by the onset of superconductivity. These experiments include the microwave work of Bonn et al.<sup>11</sup> and Nuss *et al.*, <sup>12</sup> the thermoconductivity data of Yu *et al.*, <sup>13</sup> and the optical data of Romero *et al.* <sup>14</sup> There is also data on the effect of atomic substitutions on various properties which indicate *d*-wave superconductivity. We mention here explicitly the NMR and Knight-shift work of Ishida *et al.* and Hotta.<sup>15,16</sup>

The experiments of Hardy *et al.*<sup>3</sup> were carried out on single-crystal samples of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$ </sub>. Similar experiments on thin films often give a  $T^2$  dependence<sup>17-20</sup> instead of the *T*-dependence characteristic of a pure *d*-wave superconductor. This observation can be interpreted qualitatively as due to disorder scattering which changes the predicted *T* law to  $T^2$  for a dirty *d*-wave superconductor.<sup>21-25</sup> In particular, Hirschfeld and Goldenfeld<sup>25</sup> have discussed the crossover temperature *T* at which the change from *T* to  $T^2$  law comes about in impure samples with resonant impurity scattering. Very recently, this crossover problem has been investigated experimentally by Lee *et al.*<sup>26</sup> and Bonn *et al.*<sup>27</sup> The change in the value of the zero-temperature penetration depth has been measured as a function of Ni and Zn concentrations, in par-

ticular, by Ulm and co-workers.<sup>28,29</sup>

In this paper, we consider a strong-coupling formulation of the problem of a  $d_{x^2-y^2}$  superconductor within a tight-binding band and calculate the effect of impurity scattering in both Born and unitary scattering limits on the value of the penetration depth at zero temperature with a view at a comparison with experiment. The earlier work of Hirschfeld and Goldenfeld<sup>25</sup> involves the weakcoupling limit and an infinite band approximation with a constant electronic density of states at the Fermi surface and spherical symmetry for the electronic bands in the copper-oxide plane. These approximations are not used in this work. Here, we will not be concerned directly with the crossover between the T and  $T^2$  law but concentrate on the impurity dependence of the zero-temperature penetration depth. In Sec. II, we present some of the necessary formalism and give results for the critical temperature as a function of impurity content. The penetration depth is discussed in Sec. IV where numerical results are presented. A brief conclusion is included in Sec. IV.

#### II. FORMALISM AND RESULTS FOR $T_c$

Strong-coupling equations for a superconductor with gap exhibiting  $d_{x^2,y^2}$  symmetry with a planar Brillouin zone and with impurity scattering have been given by Arberg, Mansor, and Carbotte.<sup>24</sup> They are a set of two equations for the momentum **k**, dependent pairing potential  $\tilde{\Delta}_{\mathbf{k}}(n)$ , and renormalized Matsubara frequencies  $\tilde{\omega}_{\mathbf{k}}(n)$  with bare frequencies  $\omega_n = \pi T(2n-1) \ n = 0, \pm 1, \pm 2, \ldots$  and T the temperature. The equations are

 $\widetilde{\Delta}_{\mathbf{k}}(n) = Tg \sum_{m} \eta_{\mathbf{k}} \widetilde{\lambda}(n-m) \sum_{\mathbf{k}'} \eta_{\mathbf{k}'} \widetilde{D}_{\mathbf{k}'}(m)$ 

and

$$\widetilde{\omega}_{\mathbf{k}}(n) = \omega_{n} + T \sum_{m} \widetilde{\lambda}(n-m) \sum_{\mathbf{k}'} \widetilde{\Omega}_{\mathbf{k}'}(m) + n_{I} \frac{\sum_{\mathbf{k}'} \widetilde{\Omega}_{\mathbf{k}'}(n)}{\widetilde{c}^{2} + \left[\sum_{\mathbf{k}'} \widetilde{\Omega}_{\mathbf{k}'}(n)\right]^{2} + \left[\sum_{\mathbf{k}'} \widetilde{D}_{\mathbf{k}'}(n)\right]^{2}} .$$
(2)

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(1)

In these equations, the impurities enter only in the renormalization channel [Eq. (2)] and not in the gap channel [Eq. (1)] because the scattering is assumed to be isotropic and is therefore orthogonal to the  $d_{x^2-y^2}$  gap function with

$$\eta_{\mathbf{k}} = \left[\cos(k_{x}a) - \cos(k_{y}a)\right], \qquad (3)$$

where a is the lattice parameter in the CuO<sub>2</sub> plane and k is momentum restricted to the first two-dimensional Brillouin zone. In Eq. (2),  $n_I$  is the impurity concentration and  $\tilde{c} = 1/V_I$ , that is, the inverse of the impurity potential taken to be constant in momentum space. The limit  $\tilde{c} \rightarrow 0$  corresponds to the unitary limit which is also referred to as resonant scattering and  $\tilde{c} \rightarrow \infty$  is the Born approximation. In these two limits, the impurity team in (2) reduces to

$$\frac{\widetilde{\Gamma}\sum_{\mathbf{k}'}\widetilde{\Omega}_{\mathbf{k}'}(n)}{\left[\sum_{\mathbf{k}'}\widetilde{\Omega}_{\mathbf{k}'}(n)\right]^2 + \left[\sum_{\mathbf{k}'}\widetilde{D}_{\mathbf{k}'}(n)\right]^2}$$
(4a)

and

$$\widetilde{t}_{+} \sum_{\mathbf{k}'} \widetilde{\Omega}_{\mathbf{k}'}(n) , \qquad (4b)$$

respectively, with  $\tilde{\Gamma} = n_I$  and  $\tilde{t}_+ = n_I / \tilde{c}^2 = n_I V_I^2$ . In these expressions, the sum over momentum

$$\sum_{\mathbf{k}'} \rightarrow \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} d\mathbf{k}'_x \int_{-\pi}^{\pi} d\mathbf{k}'_y , \qquad (5)$$

where it is implied that momentum ranges over  $(-\pi,\pi)$  in the first Brillouin zone rather than  $(-\pi/a,\pi/a)$ . By definition

$$\widetilde{\Omega}_{\mathbf{k}}(n) = \frac{\widetilde{\omega}_{\mathbf{k}}(n)}{\epsilon_{\mathbf{k}}^{2} + \widetilde{\omega}_{\mathbf{k}}(n)^{2} + \widetilde{\Delta}_{\mathbf{k}}(n)^{2}}$$
(6)

and

$$\widetilde{D}_{\mathbf{k}}(n) = \frac{\widetilde{\Delta}_{\mathbf{k}}(n)}{\epsilon_{\mathbf{k}}^{2} + \widetilde{\omega}_{\mathbf{k}}(n)^{2} + \widetilde{\Delta}_{\mathbf{k}}(n)^{2}}$$
(7)

with  $\epsilon_k$  the electron energies. For a tight-binding band with hopping matrix element t and up to second-nearest-neighbor interactions

$$\epsilon_{\mathbf{k}} = -2t \left[ \cos(\mathbf{k}_{x}) + \cos(\mathbf{k}_{y}) - 2B \cos(\mathbf{k}_{x}) \cos(\mathbf{k}_{y}) \right] - \mu$$
(8)

with B the second-nearest-neighbor hopping in units of t and  $\mu$  the chemical potential.

Finally, to completely satisfy our basic Eqs. (1) and (2), it is necessary to define  $\tilde{\lambda}(n-m)$  and the parameter g. If one introduces some electron boson spectral density  $\tilde{\alpha}^2 F(\omega)$  to describe the pairing and uses the same spectral density in the gap and renormalization channel except for a constant of proportionality g (often set equal to 1.0 in our work as its value does not change things much), then

$$\widetilde{\lambda}(n-m) = 2 \int \frac{\omega \widetilde{\alpha}^2 F(\omega) d\omega}{\omega^2 + (\omega_n - \omega_m)^2} .$$
(9)

The absolute size of  $\tilde{\alpha}^2 F(\omega)$  is adjusted to get the desired value of critical temperature  $T_c$  for a given choice of spectral weight which, for simplicity, we will take as a  $\delta$  function at the boson energy  $\omega_E$ . This choice is not important in our numerical work and the size of the ratio  $T_c/\omega_E$  is the strong-coupling index.

It is of interest to look at more familiar limits of Eqs. (1) and (2). The BCS limit corresponds to neglecting the  $\tilde{\lambda}(n-m)$  renormalization in Eq. (2). If, in addition, we ignore impurities, the renormalized Matsubara frequencies  $\tilde{\omega}_{\mathbf{k}}(n)$  reduces to their bare values  $\omega_n$ . Further, if  $\tilde{\lambda}(n-m)$  is assumed to be constant and equal to  $\tilde{\lambda}$  and we introduce a cutoff  $\omega_c$  on the energy in the sum over  $\mathbf{k}'$  so as to get a finite result, we obtain a gap  $\tilde{\Delta}_{\mathbf{k}}(n)$  which does not depend on  $\omega_n$  and satisfies the equation

$$\widetilde{\Delta}_{\mathbf{k}} = g \widetilde{\lambda} \eta_{\mathbf{k}} \sum_{\mathbf{k}'}^{\omega_{c}} \eta_{\mathbf{k}'} \frac{\widetilde{\Delta}_{\mathbf{k}'}}{2\sqrt{\epsilon_{\mathbf{k}'}^{2} + \Delta_{\mathbf{k}'}^{2}}} \tanh\left\{\frac{\sqrt{\epsilon_{\mathbf{k}'}^{2} + \widetilde{\Delta}_{\mathbf{k}'}^{2}}}{2T}\right\}, \quad (10)$$

where we have explicitly carried out the sum over Matsubara frequencies to greatly simplify our Eqs. (1) and (2).

Another limit of interest is to go to the infinite band case with constant density of states around the Fermi surface. In this case, the sum over k can be replaced by an integral over the electronic density of state  $N(\epsilon)$  and taken out pinned to its value at the chemical potential  $\mu=0$ leaving only an integration over angles denoted by  $\langle \rangle$ and which is assumed to be normalized. We then obtain from (1) and (2)

$$\widetilde{\Delta}_{\mathbf{k}}(n) = \eta_{\mathbf{k}} \pi T g \sum_{m} \lambda(n-m) \langle \eta_{\mathbf{k}'} D_{\mathbf{k}'}(m) \rangle$$
(11)

and

$$\widetilde{\omega}_{\mathbf{k}}(n) = \omega_{n} + \pi T \sum_{m} \lambda(n-m) \langle \Omega_{\mathbf{k}'}(m) \rangle + \pi \Gamma \frac{\langle \Omega_{\mathbf{k}'}(n) \rangle}{c^{2} + [\langle \Omega_{\mathbf{k}'}(n) \rangle]^{2} + [\langle D_{\mathbf{k}'}(n) \rangle]^{2}}, \qquad (12)$$

which are the equations used by Prohammer and Carbotte<sup>23</sup> and are a strong-coupling version of those used by Hirschfeld and Goldenfeld.<sup>25</sup> In Eqs. (11) and (12),  $\lambda \equiv N(0)\tilde{\lambda}$ ,  $\Gamma = n_I / N(0)\pi^2$ , and  $c = [1/N(0)\pi V_I]^2$  and by definition

$$\Omega_{\mathbf{k}}(n) = \frac{\widetilde{\omega}_{\mathbf{k}}(n)}{\sqrt{\widetilde{\omega}_{\mathbf{k}}(n)^2 + \widetilde{\Delta}_{\mathbf{k}}(n)^2}}$$
(13)

and

$$D_{\mathbf{k}}(n) = \frac{\widetilde{\Delta}_{\mathbf{k}}(n)}{\sqrt{\widetilde{\omega}_{\mathbf{k}}(n)^2 + \widetilde{\Delta}_{\mathbf{k}}(n)^2}} .$$
(14)

At the critical temperature, the gap is infinitesimal and Eqs. (1) and (2) can be linearized and the impurity term in the unitary and Born limit reduce, respectively, to [Eqs. (4a) and (4b)]

$$\widetilde{\Gamma}\left[\sum_{\mathbf{k}'}\widetilde{\Omega}_{\mathbf{k}'}(T_c,n=0)\right]^{-1} \text{ and } \widetilde{t}_+\sum_{\mathbf{k}'}\widetilde{\Omega}_{\mathbf{k}'}(T_c,n=0),$$

where the temperature dependence of  $\tilde{\Omega}_{\mathbf{k}}(n)$  has been made explicit and taken at  $T_c$ . In the infinite band limit, we have, instead,  $\pi\Gamma \operatorname{sgn}(\omega_n)$  and  $\pi t_+ \operatorname{sgn}(\omega_n)$  with  $t^+ = n_I N(0) V_I^2$ , which are constants independent of temperature. When the density of states is not constant and a Van Hove singularity can exist in the electronic density of states, however, the impurity term in (2), as we have seen, is more complicated and will depend on the value of  $T_c$  as well as Matsubara frequency  $\omega_n$  even in the normal state. To get a single measure of the strength of the scattering, we can use

$$\widetilde{\Gamma}\left[\sum_{\mathbf{k}'}\widetilde{\Omega}_{\mathbf{k}'}(T_c, n=0)\right]^{-1} \text{ and } \widetilde{t}_+\sum_{\mathbf{k}'}\widetilde{\Omega}_{\mathbf{k}'}(T_c, n=0)$$

for unitary and Born scattering, respectively, which we denote by  $\pi\overline{\Gamma}$  and  $\pi\overline{t}_+$ . These are the two quantities that naturally replace  $\pi\Gamma$  and  $\pi t_+$  in the more familiar infinite band case. Returning, for a moment, to Eqs. (11) and (12) at  $T_c$  and assuming that  $\lambda(n-m)$  is constant up to a cutoff  $\omega_c$  and zero, otherwise we recover familiar BCS equations, namely

$$\widetilde{\Delta}_{\mathbf{k}} = \eta_{\mathbf{k}} \pi T g \lambda \sum_{m}^{\omega_{c}} \left\langle \eta_{\mathbf{k}'} \frac{\widetilde{\Delta}_{\mathbf{k}'}(n)}{|\widetilde{\omega}_{\mathbf{k}'}(m)|} \right\rangle$$
(15)

and the gap is independent of frequency and

$$\widetilde{\omega}_{\mathbf{k}}(n) = \omega_n (1+\lambda) + \pi \Gamma \frac{\operatorname{sgn}(\omega_n)}{1+c^2}$$
(16)

independent of **k**. Note that for unitary scattering  $\pi\Gamma/(1+c^2) \rightarrow \pi\Gamma$  and for Born scattering  $\rightarrow \pi t^+$ . Substitution of (16) into (15) and cancelling out the gap gives a single equation for the critical temperature  $T_c$  of the form

$$1 = 2g\lambda\pi T \sum_{m=0}^{\omega_c} \frac{1}{\omega_n (1+\lambda) + \pi\Gamma/(1+c^2)} , \qquad (17)$$

where we have made use of the normalization  $\langle \eta_k^2 \rangle = 1$ . Equation (17) can be rewritten as

$$-\ln\left[\frac{T_c}{T_c^0}\right] = \psi\left[\frac{1}{2} + \rho\right] - \psi\left[\frac{1}{2}\right] . \tag{18}$$

In this equation,  $\psi$  is the digamma function and

$$\rho = \frac{\pi\Gamma}{1+c^2} \times \frac{1}{2\pi T_c(1+\lambda)} \tag{19}$$

is called the pair-breaking parameter. Equation (18) is the classic equation of Abrikosov and Gorkov<sup>30</sup> which describes the effect of paramagnetic spin-flip impurity scattering in an s-wave superconductor. It has recently been used by Radtke et al.<sup>31</sup> to discuss the sensitivity of the d-wave state to the presence of normal impurities. Previous treatments have always used Born scattering. Here, we see that the same simple form also applies to arbitrary strength of the impurity potential. In this simplified form, the critical concentration of impurities that reduce  $T_c$  to zero is given by

$$\pi \left[ \frac{\Gamma}{1+c^2} \right]^{\text{crit}} = \left[ \frac{1+\lambda}{1\times 13} \right] T_c^0 .$$
 (20)

From (20), we see that the strong-coupling renormalization parameter  $\lambda$  increases the value of the critical scattering rate above its BCS value, a well-known result for paramagnetic impurities in s-wave superconductivity.<sup>32</sup> For Born scattering,  $\Gamma/(1+c^2)$  reduces to  $t^+ = 1/2\pi\tau^{\text{imp}}$  with  $\tau^{\text{imp}}$  the impurity scattering time. It is important to note that for paramagnetic impurities in the s-wave case, the parameter  $\pi t^+$  occurs in both the equation for the gap and the equation for the renormalization channel.<sup>33</sup> When the second of these is substituted into the first to get a single equation for the critical temperature, the two impurity terms add up and what enters the pair-breaking parameter  $\rho$  is  $2\pi t^+$ . Here, the impurities do not contribute to the gap channel and so it is  $\pi t^+$ that enters so that the impurities are now half as effective as the paramagnetic impurities in the s-wave case. All these results apply only to the infinite band case. When the density of state cannot be assumed to be constant, no simple analytic results are possible but the physics does not change much except for the important difference that impurities affect not only the gap and its anisotropy but also smear out the Van Hove singularity in the electronic density of states. This leads to additional changes in  $T_c$ but not to qualitative differences in its variation with impurities as can be seen in Fig. 1. What is shown is the ratio of  $T_c$  (with impurities) to its value  $T_c^0$  (in the pure case) as a function of the parameters  $\pi \overline{\Gamma} / T_c^0$  for unitary scattering (dotted curve) and  $\pi \overline{t} / T_c^0$  for Born scattering



FIG. 1. The ratio of the impure critical temperature  $T_c$  to its pure value  $T_c^0$  as a function of impurity scattering rate for Born scattering (solid line) and unitary scattering (dotted line). More precisely, the horizontal axis is  $\pi \overline{t}_+ / T_c^0$  and  $\pi \overline{\Gamma} / T_c^0$  for solid and dotted curve, respectively.

(solid curve). These two parameters play the role in the finite band case of  $\pi\Gamma/T_c^0$  and  $\pi t_+/T_c^0$  in the infinite band case. While in our numerical work we have varied  $g, \mu, \omega_E, t$ , and the value of the critical temperature  $T_c^0$ , here we present results only for t = 100.0 meV, g = 1,  $\mu = 25.0 \text{ meV}, \omega_E = 100.0 \text{ meV}$ , and  $T_c^0 \cong 9.88 \text{ meV} \cong 115$  K. The curves in Fig. 1 are quite similar to the familiar Abrikosov Gorkov case and the critical impurity scattering rate roughly obeys Eq. (20). Since our calculations fully account for the Van Hove singularity and the effect of impurities on it, Eq. (20) does not strictly apply. These more complicated effects, however, seem not to be very large. Finally, Born and unitary scattering are not very different when plotted in this way.

## **III. PENETRATION DEPTH**

In the London limit, the penetration depth  $\lambda_{ij}(T)$  can be written as<sup>22</sup>

$$\lambda_{ij}^{-2}(T) = 4\pi \frac{e^2}{c^2} \left[ 2T \sum_{n\mathbf{k}} v_{\mathbf{k}i} v_{\mathbf{k}j} \left\{ \frac{\left[ \widetilde{\Delta}_{\mathbf{k}}(n)^2 + \epsilon_{\mathbf{k}}^2 - \widetilde{\omega}_{\mathbf{k}}(n)^2 \right]}{\left[ \widetilde{\Delta}_{\mathbf{k}}(n)^2 + \epsilon_{\mathbf{k}}^2 + \widetilde{\omega}_{\mathbf{k}}(n)^2 \right]^2} - \frac{\left[ \epsilon_{\mathbf{k}}^2 - \widetilde{\omega}_{\mathbf{k}}^0(n)^2 \right]}{\left[ \epsilon_{\mathbf{k}}^2 + \widetilde{\omega}_{\mathbf{k}}^0(n)^2 \right]^2} \right\} \right].$$
(21)

Here, e is the charge on the electron and c is the velocity of light. In formula (21),  $v_{ki}$  is the *i*th component of the Fermi velocity and  $\tilde{\omega}_{k}^{0}(n)$  is  $\tilde{\omega}_{k}(n)$  evaluated in the normal state, i.e., obtained from Eq. (2) setting  $\tilde{\Delta}_{k}(m)$  zero everywhere on the right-hand side of the equation which makes (2) an explicit expression for  $\tilde{\omega}_{k}^{0}(n)$  and not a coupled equation. To make contact with previous work, several limits of Eq. (21) are of interest. First, we consider the case of an infinite band with constant density of states taken out at the Fermi energy and the velocities pinned to the Fermi surface. We get from a contour integration over energy  $\epsilon$ 

$$\lambda_{ij}^{-2}(T) = \frac{4\pi}{c^2} e^2 \left[ \pi T 2N(0) \sum_{n} \left\langle v_{\mathbf{k}_{F_i}} v_{\mathbf{k}_{F_j}} \frac{\widetilde{\Delta}_{\mathbf{k}}^2(n)}{(\sqrt{\widetilde{\omega}_{\mathbf{k}}(n)^2 + \widetilde{\Delta}_{\mathbf{k}}(n)^2})^3} \right\rangle \right].$$
(22)

The second term, referring to the normal state, has dropped out as it is zero after the energy integration has been performed. If the gap is assumed to be isotropic, we recover the well-known result quoted by Carbotte<sup>34</sup> in his review, namely

$$\lambda_{ij}^{-2}(T) = \frac{4\pi}{c^2} 2e^2 \pi \frac{2}{3} v_F^2 N(0) T \sum_{n=1}^{\infty} \frac{\tilde{\Delta}^2(n)}{[\tilde{\Delta}(n)^2 + \tilde{\omega}(n)^2]^{3/2}} .$$
(23)

Using the fact that the electron density  $n = \frac{2}{3}N(0)mv_F^2$ and that the classical London penetration depth  $\lambda_0^{-2} = (4\pi e^2/c^2)(n/m)$  (unrenormalized quantities), we obtain

$$\lambda^{-2}(T) = \lambda_0^{-2} 2\pi T \sum_{n=1}^{\infty} \frac{\Delta^2(n)}{\left[\tilde{\Delta}(n)^2 + \tilde{\omega}(n)^2\right]^{3/2}}$$
(24)

with *m* the electron mass. If we take the BCS limit,  $\tilde{\Delta}(n)$  becomes independent of *n* and  $\tilde{\omega}(n) = \omega_n$ , in which case at T = 0

$$\lambda^{-2}(T) = \lambda_0^{-1} \int_0^\infty \frac{\tilde{\Delta}^2}{(\tilde{\Delta}^2 + \omega^2)^{3/2}} d\omega . \qquad (25)$$

The integral in (25) is equal to one giving  $\lambda(T=0)=\lambda_0$ , as expected.

Another interesting limit of (22) is the pure BCS limit. Using the formula

$$\frac{\partial f(y)}{\partial y} = T \sum_{n} \frac{y^2 - \omega_n^2}{(y^2 + \omega_n^2)^2} , \qquad (26)$$

we immediately obtain from (21)

$$\lambda_{ij}^{-2}(T) = \frac{4\pi e^2}{c^2} 2 \sum_{\mathbf{k}} v_{\mathbf{k}i} v_{\mathbf{k}j} \left[ -\frac{\partial f}{\partial \epsilon_{\mathbf{k}}} + \frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}} \right] \quad (27)$$

with  $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$ . It is clear that the last term in (27) vanished at  $T \rightarrow 0$  and we recover  $\lambda_0^{-2}$  as before.

In Fig. 2, we present our main results. The parameters are the same as those used in the previous section during our discussion of  $T_c$  and its variation with impurities. What is plotted is

$$[\lambda_{xx}(T=0,n_I=0)/\lambda_{xx}(T,n_I)]^2$$

versus reduced temperature for four samples in the range  $T/T_c = (0 \text{ to } 0.8)$ . The solid line is for the pure case and shows an almost perfectly linear behavior throughout the temperature range displayed. The dotted line is for an impure sample with  $T_c/T_c^0=0.96$ , i.e., a 4% reduction in  $T_c$ , while the short dashed and long dashed lines are for  $T_c/T_c^0=0.92$  and 0.84, respectively. Unitary scattering has been assumed in all cases. Note that in the last case with a 16% reduction in  $T_c$  value, the deviation from linearity starts at rather high values of reduced temperature and it is not clear that a linear region can even be identified.

It is also of interest to note the effect of impurities on the zero-temperature intercept of the curves of Fig. 2. In Fig. 3, we show the ratio of the value of the zerotemperature penetration depth at finite impurity concentration to its pure value. On the horizontal axis, we use



FIG. 2. The square of the pure system penetration depth  $\lambda_{xx}(T=0,n_I=0)$  at zero temperature to its impure value  $\lambda_{xx}(T,n_I)$  at finite T as a function of reduced temperature  $T/T_c$  for four cases labeled by the ratio of impure  $T_c$  to pure  $T_c^0$  critical temperature, namely  $T_c/T_c^0=1.0$  (solid),  $T_c/T_c^0=0.96$  (dotted),  $T_c/T_c^0=0.92$  (short dashed), and  $T_c/T_c^0=0.84$  (long dashed curve).

the parameter  $1 - T_c / T_c^0$  to monitor the amount of impurity used (i.e., instead of  $\eta_I$ ). The dotted curve is for unitary scattering, while the solid curve is for Born scattering. It is clear that unitary scattering changes the value of the zero-temperature penetration depth more strongly than does Born scattering.

We now give a comparison of our work with the exper-



FIG. 3. The ratio of the impure penetration depth at T=0,  $\lambda(T=0, n_I)$  to its value in the pure case  $\lambda(T=0, n_I=0)$  as a function of one minus the ratio of impure to pure critical temperature, i.e.,  $1-T_c/T_c^0$ . The dotted curve is for resonant scattering, while the solid is for Born scattering.

imental results of Ju Young Lee et al.<sup>26</sup> In terms of reduction in  $T_c$  from the ideal clean value, their sample A and B, which do not differ much, correspond roughly to the short dashed curve of Fig. 2 and their sample A' to the long dashed curve. In the latter case, comparing A'to the pure case, we find a change in  $\lambda(0)^2$  of about a factor of 2, while the experiment is about 3. Strictly speaking, our theory needs modification in the case of sample A' which involves oxygen depletion and hence, probably should be modeled with a change in chemical potential. For the former case, comparing A or B to the pure sample, we find a factor of about 1.5 as compared to an experimental value of roughly 1.6 which is quite good agreement. In both these comparisons, we have simply used Fig. 3 of Ju Young Lee et al.<sup>26</sup> Thus, for these samples, there is qualitative and even semiquantitative agreement between theory and experiment.

The more extensive very recent results of Ulm and coworkers<sup>28,29</sup> on Al, Ni, and Zn substitution show variations in value of  $\lambda(0)$  which are always larger than those calculated in this work. In some case, the discrepancy is as much as a factor of 2 in the ratio of impure to pure penetration depth  $\lambda(0)$  when plotted against the measured attendant reduction in value of  $T_c$  as impurities are added. While the data show considerable fluctuations when plotted in this way, it would nevertheless appear that some modifications to the simple theory presented here are needed in order to make the theoretical value of  $T_c$  less sensitive to impurity scattering, as emphasized particularly by Radtke *et al.*,<sup>31</sup> while at the same time increasing the sensitivity of the magnitude of the zerotemperature penetration depth by perhaps as much as a factor of 2 from these two effects combined. More accurate data on the value of  $\lambda(0)$  would be valuable and might reduce the quantitative disagreement found here.

After this work was submitted, we became aware of similar calculations by Kim, Preosti, and Muzikar.<sup>35</sup> These authors use a BCS formalism with a constant density of state and an infinite band approximation. Here, we use a strong-coupling formalism, make no Fermi-surface approximation, but rather integrate over the entire Brillouin zone properly accounting for the underlying band structure and attendant Van Hove singularity. Despite these differences, our results for the impurity dependence of the zero-temperature penetration depth are in qualitative agreement with those of Kim, Preosti, and Muzikar.<sup>35</sup> Their results, however, show less variation than do ours, as a function of reduction in  $T_c$  value.

#### **IV. CONCLUSIONS**

In a model of a tight-binding two-dimensional band with a Van Hove singularity and for which the gap is assumed to have  $d_{x^2,y^2}$  symmetry, we have calculated the effect of impurities on the penetration depth  $\lambda(T)$  with emphasis on the change in its zero-temperature value  $\lambda(0)$ . In our model, impurity scattering, in Born or unitary limit, affects the size of  $\lambda(0)$  not only through changes in superconducting parameters as it would in models with a constant density of states, but also because the Van Hove singularity is being affected. While unitary scattering is more effective at increasing  $\lambda(0)$  than is Born scattering for the same reduction in  $T_c$ , the calculated changes are not as large as are observed in recent experiments on Al, Zn, and Ni substitutions on the Cu site in  $YBa_2(Cu_{1-x}M_{\lambda})_3O_7$ .<sup>27,28</sup> The experiments generally give increases in the  $\lambda(0)$  value that are larger than expected in our work on the basis of the corresponding change in  $T_c$ . It would appear that this data, while easily understood qualitatively, does present some challenge for simple *d*-wave theories of the type described here (and used extensively in the literature) if they are to be quantitative. More accurate data would be very helpful at this stage. A similar, and perhaps related, problem has been noted by Radtke et al.<sup>31</sup> who have pointed out that the experimental value of  $T_c$  in the high- $T_c$  oxide appears not to be sufficiently dependent on variations in residual resistivity if they are *d*-wave superconductors. Here, we find that the observed changes in value of the zero-

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temperature penetration depth on alloying are larger than predicted for resonant scattering from impurities in a *d*-wave superconductor sometimes by as much as a factor of 2. We hope that further, perhaps more exact, determinations of the value of  $\lambda(0)$  in impure systems will be forthcoming so that more definitive conclusions can be made. From a theoretical point of view, it may be that it is necessary to include in the theory the large amount of inelastic scattering at  $T_c$  that is known to be present in such systems as this might lead to less sensitivity of  $T_c$  to elastic scattering.

## ACKNOWLEDGMENTS

Research was supported in part by the Natural Sciences and Engineering Council of Canada (NSERC) and by the Canadian Institute of Advanced Research (CIAR).

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