Scattering by impurity-induced order parameter “holes” in
d-wave superconductors

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Abstract

Nonmagnetic impurities in d-wave superconductors cause strong local suppressions of the order parameter. We investigate the observable effects of the scattering off such suppressions in bulk samples by treating the order parameter “hole” as a pointlike off-diagonal scatterer treated within a self-consistent t-matrix approximation. Strong scattering potentials lead to a finite-energy spectral feature in the d-wave “impurity band”, the observable effects of which include enhanced low-temperature microwave power absorption and a stronger sensitivity of the London penetration depth to disorder than found previously in simpler “dirty” d-wave models.

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Introduction. The current consensus regarding the d-wave symmetry of the order parameter in the hole-doped cuprates rests to a considerable extent on the success of simple models of the effect of disorder on unconventional superconductors. Theories based on the impurity t-matrix approximation suggest that disorder gives rise to an “impurity band” of extended states near the Fermi level which dominates the low-temperature behavior of the system. Although published data on superconducting properties continue to exhibit a certain variability, such apparent discrepancies can frequently be accounted for within this picture by allowing for the variation in sample quality. Systematic substitution of Copper with nonmagnetic planar defects such as Zn or Ni leads to similar effects. The observed strong temperature dependence of transport properties of nominally pure samples with nearly optimal $T_c$ gives rise to the further conclusion of near-unitarity limit scattering by most simple defects in these systems.

Several puzzles and discrepancies must be understood before the problem of disorder in the superconducting state of the high-temperature superconductors (HTSC’s) may be considered solved even at a purely phenomenological level. The simplest theory of low-temperature transport in a d-wave superconductor predicts an $\omega \to 0$ conductivity $\sigma \simeq \sigma_{00} + aT^2$, where $\sigma_{00} \simeq ne^2/(m\pi\Delta_0)$ is a “universal” constant dependent on the scale set by the order parameter maximum $\Delta_0$ but independent of the relaxation rate $1/\tau$ for weak disorder. Experiments on untwinned samples clean enough to exhibit the linear-$T$ magnetic penetration depth characteristic of a pure d-wave state down to a few degrees are consistent with the universal residual conductivity value, but exhibit a conductivity temperature variation $\delta\sigma \simeq T$ or even sublinear temperature dependence.

Further difficulties include the rather slow measured rate at which the critical temperature itself is suppressed by impurities, (for planar defects, roughly a factor of two slower than predicted by the simplest theory) as well as a considerably more rapid decrease of the low-$T$ superfluid density $\rho_s$ with disorder than predicted. The two effects together result in a ratio $T_c/\rho_s$ which is considerably larger than predicted by “dirty d-wave” theory in many HTSC samples, as pointed out recently by Franz et al. These authors argued
that the usual theory, which assumes a spatially homogeneous disorder-averaged order parameter (OP) $\Delta_{\mathbf{k}}$, neglects an important physical effect, namely the supression of the true order parameter $\Delta_{\mathbf{k}}(\mathbf{R})$ around the positions of the defects. These static fluctuations are expected to be large since the order parameter is d-wave in character, and highly local since the order parameter varies (crudely speaking) on a scale of the coherence length $\xi$, which at low $T$ is of order a few Å in HTSC’s. In a full numerical solution to the Bogoliubov-de Gennes (BdG) equations for a d-wave system with dilute strong potential scatterers, Franz et al. indeed observed an enhancement of $T_c/\rho_s$ consistent with experiment. Very recently [11], a more analytic approach to the effect of order parameter suppression by Zhitomirsky and Walker found a reduction of the $T_c$-suppression in rough agreement with experimental observations. Both approaches work best close to $T_c$. On the other hand, the discrepancy with experiment in the $T$-dependence of the transport properties is most evident at low temperatures. Clearly, a complementary approach for low $T$ is needed.

In the interest of constructing a practical theory of transport in the HTSC’s including these order parameter suppressions, we have attempted to exploit the short range nature of the order parameter supression (at low $T$) by replacing the true, self-consistently determined $\Delta_{\mathbf{k}}(\mathbf{R})$ near the impurity site by a pointlike order parameter “hole” which acts as an off-diagonal (in the Nambu–Gorkov matrix sense) potential scatterer for electrons. The weight of the off-diagonal perturbation is then determined by the bare impurity potential and by the solution to the one-impurity problem for the $\mathbf{R}$-integrated OP suppression. This approximation makes sense at low temperatures, mainly because the zero $T$ coherence length which controls the range of the OP suppressions is at most a few atomic lengths for the HTSC’s. With this approximation, one can perform disorder averages in the usual way and obtain a generalization of the very flexible t-matrix approximation involving a translationally invariant, effective medium.

Having outlined the method, we proceed to show that the failures of the “dirty d-wave” model when compared to experiments on low-$T$ microwave conductivity and the dependence of the absolute penetration depth on disorder are at least partially cured. The results for the
temperature dependence of $\lambda$ and other thermodynamic quantities does change very little. A preliminary account of this research has appeared in Ref. [12].

**Local order parameter suppression by single impurity.** Several authors have solved the BdG equations or equivalent for the local structure of the d-wave $\Delta_k(R)$ around a nonmagnetic impurity. [13] In our approach, we make the usual BCS assumption that the pairing potential is separable, $V_{k,k'} \equiv V\Phi(k)\Phi(k')$, and has d-symmetry, with $\Phi_d(k) \equiv \sqrt{2}\cos 2\phi$ normalized over a model circular Fermi surface. We further neglect so-called “leading loser” components of the pair interaction, e.g. subdominant pairing channels which have been shown to lead to additional fine structure in the order parameter around the impurity site despite being energetically forbidden in the bulk.

The bare impurity itself is described for simplicity by a $\delta$-function potential in real space, $\hat{U}(R-R_{imp}) = U_0\delta(R-R_{imp})\tau_3$, where the $\tau_i$ are the Pauli matrices in particle-hole space. Initially, one might try to find the spatial variation of the order parameter, which is given by the BCS gap equation after subtraction of the bulk limit. The Fourier transform of the (static) order parameter fluctuation $\delta\Delta_k(q)$ is then determined [14,12] by the single-impurity t-matrix $\hat{T}(p,p')$,

$$\delta\Delta_k(q) = V\Phi_d(k)T\sum_\omega \sum_{k'} \Phi_d(k') \times$$
$$\text{Tr}\left\{\frac{\tau_1}{2}\hat{G}_0(k' + q/2)\hat{T}(k' + q/2,k' - q/2)\hat{G}_0(k' - q/2)\right\},$$

where $\hat{G}_0$ is the matrix Green function of the pure system. The t-matrix is given as usual by

$$\hat{T}(p,p') = \hat{U}(p,p') + \sum_{p''}\hat{U}(p,p'')\hat{G}_0(p'')\hat{T}(p'',p'),$$

where $\hat{T}(p,p')$ and $\hat{U}(p,p')$ are Fourier transforms with respect to the electronic momenta. In the usual “dirty d-wave” theory, the t-matrix is taken independent of momentum, $\hat{T} = \hat{T}(\omega)$, for the case of isotropic scatterers. Here, we explicitly account for the fact that electrons moving in the neighborhood of the impurity feel an effective one-body potential due
not only to the bare impurity but to the order parameter modification about the impurity. The effective impurity potential is therefore

\[ \hat{U}_k(q) = \hat{U}_0 \tau_3 + \delta \Delta_k(q) \tau_1 \]  

(4)

where \( k = (p + p')/2 \) is the momentum conjugate to the “fast” relative motion of the electron pair, while \( q = p - p' \) is the momentum conjugate to the slowly varying center of mass position. Solving Eqs. 2–4 self-consistently is equivalent to solving the BdG equations for a single impurity, and will yield a momentum-dependent t-matrix in the d-wave case. The associated order parameter fluctuation \( \delta \Delta_k(q) \) has d-wave symmetry in real space about the impurity site. [13]

Our objective instead is to develop a formalism for calculating observables in the presence of a finite concentration of impurities. To this end, we neglect the \( q \)-dependence of \( \delta \Delta_k(q) \) in Eq. 4 equivalent to replacing the full \( \delta \Delta_k(R - R_{imp}) \) with \( \delta \Delta_k(q = 0) \delta(R - R_{imp}) \). This is certainly a reasonable approximation in the cuprates at temperatures sufficiently far below \( T_c \), since the very short \( T = 0 \) coherence length \( \xi_0 \) on which the order parameter varies becomes comparable to the lattice constant. We then solve Eq. 2 for \( \delta \Delta_k(q = 0) \) under the continued assumption of negligible subdominant pair component, such that \( \delta \Delta_k(q = 0) = \delta_d \cos 2\phi \). We point out that no new parameter has been introduced into the theory by this procedure, since \( \delta_d \) is driven by the impurity scattering strength \( U_0 \).
FIG. 1. Order parameter scattering strength vs. temperature. The dot-dashed and dashed lines are the first order (FO) result \[15\] for \(\delta_d\) with \(U_0 = 10\) and \(U = 20\), respectively, the symbols and solid lines are the self-consistent results for \(U_0 = 10, 20, 50, 1000\), as indicated. For this example, \((N_0)^{-1} = 100T_c\) and \(\Delta_o = 3T_c\). The pairing potential and the cutoff are chosen such that the BCS-expression for \(T_c\) is the unit of energy, \(T_c = 1\).\[14\]

We begin by solving Eqs. \[2\]–\[4\] numerically under the approximations outlined above. In Fig. \[\] we show the temperature dependence of the self-consistent evaluation of \(\delta_d\) in comparison with the result obtained when the \(\tau_1\) part of the t-matrix is iterated only once. \[15\] Close to \(T_c\), the first order (FO) result diverges like \((1 - T/T_c)^{-1/2}\) whereas the self-consistent result vanishes with the bulk order parameter \(\Delta_0\) like \((1 - T/T_c)^{1/2}\). For low \(T\) and the smallest \(U_0 = 10\) the first order and the self-consistent result agree well, as \(\delta_d\) is sufficiently small. But already for \(U_0 = 20\) the discrepancies are obvious even for zero temperature. For small \(U_0\) (and low \(T\)) the first order result underestimates \(|\delta_d|\), however, for large \(U_0\) it overestimates \(|\delta_d|\) (not shown in the figure). Note that \(\delta_d\) can be quite large in the unitarity limit \(U_0 \to \infty\). However, it can never be infinite as its \(U_0\)-dependence saturates like \(U_0^2/(1 + constU_0^2)\). In a similar fashion the nonlinear corrections in \(\delta_d\) prevent the divergence of \(\delta_d\) at the critical temperature (see the expression for the t-matrix below).

**Self-energies in t-matrix approximation.** The solution to Eq. \[3\] at \(q = 0\) in the present ansatz may be written...
\[ \hat{T}_k(\omega) = \frac{U_0^2 g_0 + U_0^2 \tau_3}{1 - U_0^2 g_0^2} + \delta_g \frac{\delta d g_0 + (1 - \delta_d g_2) \cos 2\phi \tau_1}{(1 - \delta_d g_2)^2 - (\delta_d g_0)^2}, \] (5)

where \( g_0 \) and \( g_2 \) are the components of the momentum integrated Green function, \( g_0 \equiv (1/2) \sum_k \text{Tr} \hat{G}(k, \omega) \) and \( g_2 \equiv (1/2) \sum_k \text{Tr} \tau_1 \cos 2\phi \hat{G}(k, \omega) \). This solution is not exact but is obtained under the reasonable assumption of the smallness of higher order scattering terms which have no inhomogeneous driving term. [12] The disorder-averaged self-energy is now defined in the limit of independent scattering centers to be \( \hat{\Sigma}(k, \omega) \equiv n_i \hat{T}_k(\omega) \), and determined self-consistently with the averaged \( \hat{G} \) via the Dyson equation, \( \hat{G}^{-1} = \omega - \xi_k \tau_3 - \Delta_k \tau_1 - \hat{\Sigma}(k, \omega) \equiv \tilde{\omega} - \tilde{\xi}_k \tau_3 - \tilde{\Delta}_k \tau_1 \). The first term in Eq. 5 is the result obtained in the usual dirty d-wave theory for arbitrary scattering phase shift \( \delta_0 = -\cot^{-1}(1/N_0 U_0) \). For strong scattering, \( \delta_0 \simeq \pi/2 \), a resonance occurs at or near the Fermi level, as can be seen by examining the corresponding denominator; this leads to the finite density of states at the Fermi level and “gapless” behavior, as has been discussed extensively in the literature. [2,3]

The denominator in the second term, due to off-diagonal scattering, leads to a similar resonance. To estimate the position of this feature, we examine the clean limit, in which \( g_2 \simeq -\pi N_0[2/\pi + i(\omega^2/\Delta_0^2) \log(4\Delta_0/\omega)] \) and \( g_0 \simeq -\pi N_0[\omega \log(4\Delta_0/\omega) + i\omega/\Delta_0] \) for \( \omega/\Delta_0 \ll 1 \).

The resonance in the second term of Eq. 5 then occurs when \( \omega/\Delta_0 = [-2/\pi + (\pi \delta_d N_0)^{-1}] \equiv \tilde{c}_f \). Our self-consistent determination of \( \delta_d \) given above shows that as \( U_0 \to \infty, \tilde{c}_f \simeq 0.2 \), so the resonance from the off-diagonal channel never occurs at the Fermi level. It is easy to check that on resonance the imaginary part of the denominator is of the same order as the real part, up to log corrections. We therefore expect that the resonance will modify the low-energy behavior of the quasiparticle relaxation time at the lowest energies in the clean limit.

These notions are confirmed by the full numerical evaluation of the self-energies. In Fig. 2 we show the imaginary part of the diagonal self-energy for various values of the impurity scattering rate parameter \( \Gamma \equiv n_i/\pi N_0 \). In the clean limit the two resonances are clearly distinguishable, but they merge with increasing disorder. This is because the zero frequency feature grows only \( \propto \gamma \sim \sqrt{\Gamma \Delta_0} \) but the feature at finite frequencies \( \propto \Gamma \) (at least initially).
Thus, above a certain disorder we no longer expect off-diagonal scattering to qualitatively modify low-temperature transport. There should, however, be novel temperature-dependent effects at small disorder. In addition, the disorder dependence of any quantity which is sensitive to all energy scales, as, e.g. the $T = 0$ superfluid density discussed below, may be substantially modified.

FIG. 2. $\text{Im}\Sigma_0(\omega)$ for several values of $\Gamma$, with and without OP scattering. The resonance at finite energy is a direct consequence of the additional OP scattering. The zero frequency resonance is qualitatively unchanged.

**Microwave conductivity and penetration depth.** In the limit of vanishing external frequency $\Omega = 0$, the quasiparticle conductivity is given by [5]

$$\sigma(T, \Omega = 0) = -\frac{ne^2}{m} \int_{-\infty}^{\infty} d\omega \left( -\frac{\partial f}{\partial \omega} \right) S(\omega, T),$$  

where $n$ is the electron density, $e$ and $m$ the electron charge and mass, respectively, and

$$S(\omega, T) = \int \frac{d\phi}{4\pi} \left[ \text{Im} \frac{\tilde{\omega}^2}{\xi_+^3} - \frac{1}{2} \frac{\tilde{\omega}_+^{\prime 2} + \tilde{\Delta}_{k+}^2}{\tilde{\omega}_+^{\prime} + \tilde{\Delta}_{k+}} \frac{\xi_+'}{\xi_+} \right],$$

where $\xi_+ \equiv \pm \sqrt{\tilde{\omega}_+^2 - \tilde{\Delta}_{k+}^2}$, the subscripts $\pm$ indicate evaluation at $\omega \pm i0^+$, and real and imaginary parts are denoted by $'$ and $''$, respectively. The first term in Eq. [5] gives rise to the "universal" $T \to 0$ conductivity $\sigma_{00}$, while the second term determines the low-temperature behavior.
FIG. 3. Low-\(T\) microwave conductivity at various disorder \(\Gamma\), with full \(T\)-range in inset. Note the quasi–linear behavior of the data with OP scattering. The conductivity without OP scattering is always quadratic in \(T\) at low temperatures.

In Figure 3, we show the results of a numerical evaluation of \(\sigma\) with and without OP scattering. In the absence of OP scattering, \(\sigma \simeq T^2\) for almost the entire region (the conductivity is measured in units of the “universal” zero temperature value \(\sigma_{00}\)). The values of \(\Gamma\) and \(\Delta_o = 3T_c\) have been chosen by fitting the low temperature penetration depth of recent experiments on YBCO single crystals. [8,5]. This result for the conductivity is at odds with the observed dominant linear behavior observed in the same samples. In contrast, the result including OP scattering displays quasi-linear behavior above an energy scale that is a fraction of \(\gamma\) due to the new resonance. This becomes more obvious if we lower the parameter \(\Gamma\) in the case of additional OPS, so that the conductivity at higher temperatures is in rough agreement with the standard theory and the experimental data (not shown in the figure). The additional feature in the self energy can increase the conductivity by more than a factor of two at the appropriate temperatures, and therefore resembles much more the dominant linear behavior of the experimental data.

In the inset to Fig. 3, we show the full temperature range of the conductivity using the model of Ref. [5] for the inelastic scattering. The peak in \(\sigma\) and subsequent drop at higher \(T\) is due to the competition between impurity and inelastic scattering.

The superfluid density and penetration depth are given by evaluating the imaginary part...
of the conductivity at \( \omega = 0, q \to 0 \) if we ignore nonlocal corrections which can
be important for \( T \lesssim 1 K \) in very clean samples: \[10\]

\[
\rho_s = -\int_0^\infty d\omega \tanh \frac{\omega}{2T} \int \frac{d\phi}{2\pi} \text{Re} \frac{\Delta_k^2}{(\tilde{\omega}^2 - \Delta_k^2)^{3/2}}
\]

(8)

Because we have accounted for a new source of scattering, we expect a faster depletion of the
superfluid density for a given impurity concentration. In Figure 4, we show the dependence
of \( \rho_s \) at \( T = 0 \) on disorder with and without OP scattering. The comparison is complicated
by the fact that two cases have different critical concentrations (the concentration at which
\( T_c \) is suppressed to zero temperature). The \( T_c \) (and consequently the critical concentration)
including OP scattering is much suppressed. This is an artifact of our treatment of the OP
scattering which is invalid when the range of the OP suppression becomes large (close to
\( T_c \) or the critical concentration). In order to make the comparison meaningful we scale the
result of the OP scattering case so that \( \Gamma_c = n_c/\pi N_o \) is the same as in the standard case
without OP scattering.

The increase in the initial slope of the \( \rho_s \) suppression over the usual dirty d-wave approach
is about 30–40\%. This is less than the difference noted in Ref. \[9\] in damaged YBCO films.
We are not aware of measurements of the absolute scale of \( \rho_s \) in which the samples are
systematically disordered by, e.g. Zn substitution for Cu. Such experiments would be very
useful to confirm the importance of order parameter scattering for bulk properties.

Low temperature properties dependent primarily on the density of states (DOS) should
be largely unaffected by the new source of scattering. For example, the \( T \to T^2 \) crossover
with disorder in the penetration depth of a d-wave superconductor \[17\] is controlled by the
finite residual density of states at zero energy, \( N(\omega \to 0) \), that arises due to impurities. As
this residual DOS is determined primarily by the resonance of the self energy at the Fermi
level in the unitarity limit, little change from the standard theory is observed.
FIG. 4. Superfluid density $\rho_s$ vs. $\Gamma$ with & w/o OP scattering. In order to eliminate trivial effects due to the suppressed critical concentration in the OP scattering case we scale the corresponding data so that the $\Gamma_c$ are the same $\Gamma_c \sim 0.82$. Note the increased initial slope in the OP scattering case. Close to $\Gamma_c$ our approximate treatment of OP scattering becomes invalid.

Conclusions. The strong suppression of the order parameter around nonmagnetic impurity sites is an important qualitative difference between d-wave systems and classic s-wave superconductors, where such suppressions are small. The spatial structure of the quasiparticle states and condensate in the neighborhood of an impurity in the Cu-O plane will soon be probed with STM as has been achieved for the similar vortex problem. We have posed the complementary question of how disorder in the off-diagonal channel induced by impurities modifies bulk average properties of a d-wave superconductor. By making the plausible assumption of local off-diagonal scattering, we have constructed a simple theory able to describe these effects. We have shown that the measured quasi-linear temperature dependence of the microwave conductivity at low temperatures can be obtained within our theory, as a result of a finite-energy scattering resonance which arises in the unitarity limit. We have also shown that the suppression of the $T = 0$ superfluid density with disorder is enhanced over the usual theory, although the temperature dependence is only weakly affected. Systematic measurements of the disorder dependence of $\lambda(T \to 0)$ or $\rho_s(T \to 0)$ will aid in establishing the validity of our picture.

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REFERENCES

[1] For recent reviews see M. Sigrist, K. Ueda, D.J. Scalapino, Physics Reports 250, 329 (1995); J. Annett, N. Goldenfeld, and A. Leggett, LANL cond-mat/9601060.

[2] P.J. Hirschfeld, D. Vollhardt and P. Wölffle, Solid State Communications, 59, 111 (1986)

[3] S. Schmitt-Rink, K. Miyake and C. M. Varma, Phys. Rev. Lett. 57, 2575 (1986).

[4] R. Joynt, J. of Low Temp. Phys. 109, 811 (1997).

[5] P. J. Hirschfeld, W.O. Putikka, and D. Scalapino, Phys. Rev. Lett. 71, 3705 (1993); P.J. Hirschfeld, W.O. Putikka, and D. Scalapino, Phys. Rev. B50, 10250 (1994).

[6] P.A. Lee, Phys. Rev. Lett. 71, 1887 (1993).

[7] K. Zhang, D. A. Bonn, S. Kamal, R. Liang, D. J. Baar, W. N. Hardy, D. Basov and T. Timusk, Phys. Rev. Lett. 73, 2484 (1994); see also L. Taillefer, B. Lussier, R. Gagnon, K. Behnia and H. Aubin, Phys. Rev. Lett. 79, 483 (1997) for similar features in the thermal conductivity.

[8] D. A. Bonn, R. Liang, T. M. Riseman, D. J. Baar, D. C. Morgan, K. Zhang, P. Donsanjh, T. L. Duty, A. MacFarlane, G. D. Morris, J. H. Brewer, W. N. Hardy, C. Kallin, and A. J. Berlinsky, Phys. Rev. B47, 11314 (1993); D. A. Bonn, S. Kamal, K. Zhang, R. Liang, D. J. Baar, E. Klein and W. N. Hardy, Phys. Rev. B50, 4051 (1994).

[9] P. Arberg and J. Carbotte, Phys. Rev. B50, 3250 (1994); H. Kim, G. Preosti and P. Muzikar, Phys. Rev. B49, 3544, (1994).

[10] M. Franz, C. Callin, A. J. Berlinsky and M. I. Salkola, Phys. Rev. B56, 7882 (1997).

[11] M. E. Zhitomirsky and M. B. Walker, Phys. Rev. Lett. 80, 5413 (1998).

[12] M. H. Hettler, Ph. D. Thesis, University of Florida (1996).

[13] P.C.E. Stamp, J. Magn. Magn. Mat. 63-64,429 (1987). T. Xiang and J.M. Wheatley,
Phys. Rev. B51, 11721 (1995); A. V. Balatsky, M. I. Salkola and A. Rosengren, Phys. Rev. B51, 15547 (1995). Y. Onishi, Y. Ohashi, Y. Shingaki and K. Miyake, J. Phys. Soc. Jpn. 65, 675 (1996); M. Franz, C. Callin and A. J. Berlinsky, Phys. Rev. B54, R6897 (1996);

[14] A. I. Rusinov, Soviet Phys. JETP, 29, 1101 (1969).

[15] C. H. Choi and P. Muzikar, Phys. Rev. B41, 1812 (1990); C. H. Choi, Phys. Rev. B50, 3491 (1994).

[16] I. Kosztin and A. J. Leggett, Phys. Rev. Lett. 79, 135 (1997).

[17] P. J. Hirschfeld and N. Goldenfeld, Phys. Rev. B48, 4219 (1993).