Order-parameter holes and theory of microwave conductivity in $YBa_2Cu_3O_{7-\delta}$

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We propose that the low-temperature discrepancy between simple *d*-wave models of the microwave conductivity and existing experiments on single crystals of $YBa_2Cu_3O_{7-\delta}$ can be resolved by including the scattering of quasiparticles from ''holes'' of the order parameter at impurity sites. Within a framework proposed previously, we find in particular excellent agreement with data of Hosseini *et al.* on slightly overdoped $YBa_2Cu_3O_{7-\delta}$ samples over the entire temperature range down to about 2–3 K, and for a wide range of frequencies. Remaining discrepancies in the ''universal'' regime at very low temperatures are discussed.

INTRODUCTION

One of the few areas of the high-temperature superconductivity problem where a well-defined theoretical description is available is the superconducting state of the optimally doped materials. Although the normal state of the cuprates cannot be described in terms of weakly interacting Landau quasiparticles as in a simple metal, it appears that such states are well defined below the critical temperature,[1] due in part to the well-known[2] collapse of the quasiparticle scattering rate.[3,4] This justifies the application of the BCS theory, with a dominant pairing component that is now widely agreed to correspond to $d_{x^2-y^2}$ symmetry. The successes of the *d*-wave theory are many, and have been amply reviewed.[5] The agreement of experiment and theory is particularly impressive in the $YBa_2Cu_3O_{7-\delta}$ (YBCO) system, where steady advances in the quality of single-crystal growth in the past several years have allowed the clean *d*-wave superconducting state to be probed.

One qualitative discrepancy that remains in the comparison of *d*-wave theory with bulk measurements probing the *ab* plane concerns the low-temperature microwave conductivity $\sigma(\Omega,T)$. Measurements on yttria-stabilized zirconia crucible-grown, nominally pure, YBCO crystals at low frequencies Ω of the order of a few GHz showed an apparent linear temperature dependence $\sigma\sim T$ for temperatures T sufficiently far below a large peak at 30–40 K.[4,6] Theories of the dynamical conductivity in the *d*-wave state[7,8] have been successful in explaining roughly the size and position, as well as the frequency and disorder dependence of the peak. However, at low temperatures and small microwave frequencies, where transport is dominated by elastic scattering and the theory should be simplest, the theoretical prediction is $\sigma\sim T^2$, not T.

A pure linear temperature dependence turns out to be very difficult to obtain within the framework of the BCS theory, however. In the original work of Bonn *et al.*,[4] it was suggested that $\sigma\sim T$ is a natural result at low temperatures since the assumed Drude form of the conductivity $\sigma \sim(e^2/m)n_{qp}(T)\tau(T)$ yields $\sigma\sim T$ if the quasiparticle density varies as $n_{qp}\sim T$ as expected for a *d*-wave superconductor at low energies, and if the effective quasiparticle scattering time $\tau(T)$ saturates at low temperatures, as in a normal metal. While the assumption of a Drude form of the conductivity was supported by microscopic analysis,[7] it was shown that pair correlations in the usual impurity scattering models generically lead to strong temperature dependence of the scattering time, e.g., $\tau(T)\sim T$ (unitarity limit) or $\tau(T) \sim 1/T$ (Born limit). Attempts to resolve this problem by choosing intermediate scattering strengths[8] have not provided obviously better results.

Ultimately, the problem can be traced back to the fact that the BCS Green's function has quasiparticle poles at $\omega=\pm E_{\mathbf{k}}$, where $E_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$, $\xi_{\mathbf{k}}$ is the single-particle band energy, and $\Delta_{\mathbf{k}}=\Delta_0\cos 2\phi$ is the *d*-wave order parameter (OP) over an isotropic two-dimensional Fermi surface. This leads naturally to an analytic expansion of the $\Omega\rightarrow 0$ conductivity in powers of T^2, regardless of band structure or phase shift (though the range where this expansion is possible can vary dramatically). The leading term in the *d*-wave case is the ''universal'' (disorder-independent) constant $\sigma(\Omega\rightarrow 0,T\rightarrow 0)\equiv\sigma_{00}=ne^2/(m\pi\Delta_0)$,[9] hence the T^2 result obtained for the subleading term in Ref. 7. While initially microwave cavity experiments did not have the resolution required to determine this constant, its analog in the case of thermal conductivity was confirmed recently by Taillefer et al.[10] Whether the same discrepancy regarding the subleading temperature corrections exists in the case of thermal currents is not known, since the electronic corrections are obscured by the phonon contribution.

The microwave conductivity impasse was broken very recently with data on extremely pure $BaZrO_3$ crucible-grown $YBa_2Cu_3O_{6.99}$ single crystals by Hosseini *et al.*[11] In addition to observing the increase in peak height and decrease in peak temperature predicted by the Drude picture for purer samples, it was noted that the very-high-resolution data did *not* support the $\sigma(\Omega\rightarrow 0,T)\sim T$ result anticipated on the basis of the earlier measurements. Rather, the T dependence of the lowest frequency (~ 1 GHz) data was slightly sublinear, crossing over to superlinear dependence above a crossover frequency of about 13 GHz. This unusual behavior has led us to reconsider a proposal we advanced recently,[12] that the standard *d*-wave theory of impurity scattering should be modified, particularly in the case of transport properties, to include the effects of order parameter ''holes'' near the impurity sites.[12–14] This leads to additional scattering at low energies due to the formation of an additional scattering resonance.[12] A recent calculation on the spatial structure of the local density of states around impurities sites has used similar methods.[15] In this paper we argue that, with the proper inclusion of the corrections due to OP suppressions, nearly all features of the low-T microwave conductivity data can be understood quantitatively. The exception is the value of the residual $\Omega\to 0$ conductivity, which we discuss in some detail.

IMPURITY *t* MATRIX

We assume in our approach[12] that the bare impurity can be described by a δ-function scattering potential, $\hat{U}(\mathbf{R}-\mathbf{R}_{imp})=U_0\delta(\mathbf{R}-\mathbf{R}_{imp})\tau_3$, where the τ_i are the Pauli matrices in particle-hole space. We then argue further[12] that for bulk transport properties the only essential features of the order parameter suppression induced by this potential are that it retains roughly the same symmetry as the background order parameter (induced subdominant pair components can be included but we deem them less important) and deviates substantially from the bulk value over a range of order of the inverse Fermi wave number k_F^{-1} around the impurity site. Since this length scale is small in the cuprates it is justifiable to replace the order parameter suppression by a pointlike potential, $\delta\Delta_{\mathbf{k}}\delta(\mathbf{R}-\mathbf{R}_{imp})$, where $\mathbf{R}_{imp}$ is the impurity site and we take the spatial average of the order parameter fluctuation to have the form $\delta\Delta_{\mathbf{k}}\equiv\delta_d\cos 2\phi$. In Ref. 12 the amplitude δ_d is then determined self-consistently through the BCS gap equation for a single impurity. Both the gap equation and the conductivity, calculated now by standard impurity-averaging methods, then contain the effective impurity potential $\hat{U}(\mathbf{p},\mathbf{p}')=(\hat{U}_0\tau_3+\delta_d\cos 2\phi\tau_1)$. Thus we explicitly account for the fact that electrons moving near the impurity feel an effective one-body potential due not only to the bare impurity but to the order parameter fluctuation around it.

The impurity t matrix is given as usual by (in matrix notation) $\hat{T}=\hat{U}+\hat{U}\hat{G}_0\hat{T}$, with $\hat{U}$ defined above. 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. It becomes momentum dependent in the current theory with d-wave OP suppression.

The solution for the t matrix at $\mathbf{q}=\mathbf{p}'-\mathbf{p}=0$ in the present ansatz for a single impurity may be written

$$\hat{T}_{\mathbf{k}}(\omega)\simeq\frac{U_0^2g_0+U_0\tau_3}{1-U_0^2g_0^2}+\frac{\delta_d^2g_0+(\delta_d-\delta_d^2g_2)\cos 2\phi\tau_1}{(1-\delta_dg_2)^2-(\delta_dg_0)^2}, \tag{1}$$

where g_0 and g_2 are the components of the momentum integrated Green function, $g_0\equiv(1/2)\Sigma_k\mathrm{Tr}\hat{G}(\mathbf{k},\omega)$ and $g_2\equiv(1/2)\Sigma_k\mathrm{Tr}\,\tau_1\cos 2\phi\,\hat{G}(\mathbf{k},\omega)$. Again, subleading OP contributions have been neglected.[12] The disorder-averaged self-energy is now defined in the limit of a density n_i of independent impurities to be $\hat{\Sigma}(\mathbf{k},\omega)\equiv n_i\hat{T}_{\mathbf{k}}(\omega)$, and determined self-consistently with the averaged $\hat{G}$ via the Dyson equation $\hat{G}^{-1}=\omega-\xi_k\tau_3-\Delta_k\tau_1-\hat{\Sigma}(\mathbf{k},\omega)\equiv\tilde{\omega}-\tilde{\xi}_k\tau_3-\tilde{\Delta}_k\tau_1$. The first term in Eq. (1) is the usual dirty d-wave theory result for arbitrary scattering phase shift $\delta_0=-\cot^{-1}[1/(N_0\pi U_0)]$, yielding in particular a resonance at $\omega=0$ in the unitarity limit $U_0\to\infty$.

The denominator in the second term, due to OP scattering, leads to a similar resonance, at a position to be numerically determined. Introducing $c_f=(\pi\delta_dN_0)^{-1}$ we estimated in Ref. 12 the quantity $\omega/\Delta_0=[-2/\pi-c_f]\equiv-\tilde{c}_f$, which determines the position of the off-diagonal resonance to be $\tilde{c}_f\simeq-0.16$ as $U_0\to\infty$. It is important to note that this determination was based on a solution to the one-impurity problem neglecting the average suppression of the gap due to disorder, and without accounting for induced subdominant pair components. We expect $|\delta_d|$ in a complete theory to be somewhat smaller, and for the moment take c_f to be a free parameter. The main point, however, is that some additional spectral weight is shifted from the gap edge down to low and intermediate frequencies[12] when compared to the usual d-wave model. We now investigate how this affects the microwave conductivity and compare to the experimental data of Hosseini *et al.*[11]

MICROWAVE CONDUCTIVITY

In Ref. 12, we discussed the $\Omega\to 0$ conductivity and compared with the expected $\sigma\sim T$ behavior; at that time it was noted that no pure T-linear behavior could be identified in the theory, although the deviations from the theory without off-diagonal scattering were pronounced and of the right qualitative size and sign. The data of Hosseini *et al.*[11] now make it clear that a subtle crossover in the temperature dependence is taking place in the 1–20 GHz regime. We therefore calculate the full frequency-dependent conductivity

$$\begin{aligned}\sigma_{ij}(\Omega)=&-\frac{ne^2}{m\Omega}\int_{-\infty}^{\infty}d\omega[f(\omega)-f(\omega-\Omega)]\mathrm{Im}\\&\times\int\frac{d\phi}{2\pi}\hat{k}_i\hat{k}_j\Bigg[\frac{\tilde{\omega}'_+(\tilde{\omega}_++\tilde{\omega}'_+)+\tilde{\Delta}'_{k+}(\tilde{\Delta}_{k+}-\tilde{\Delta}'_{k+})}{(\xi_{0+}^2-\xi_{0+}'^2)}\\&\times\left(\frac{1}{\xi'_{0+}}-\frac{1}{\xi_{0+}}\right)\\&+\frac{\tilde{\omega}'_-(\tilde{\omega}_++\tilde{\omega}'_-)+\tilde{\Delta}'_{k-}(\tilde{\Delta}_{k+}-\tilde{\Delta}'_{k-})}{(\xi_{0+}^2-\xi_{0-}'^2)}\\&\times\left(\frac{1}{\xi_{0+}}+\frac{1}{\xi'_{0-}}\right)\Bigg],\end{aligned} \tag{2}$$

where $\xi_\pm\equiv\pm\sqrt{\tilde{\omega}_\pm^2-\tilde{\Delta}_{\mathbf{k}\pm}^2}$, the subscripts $\pm$ indicate evaluation at $\omega\pm i0^+$, and primed quantities are evaluated at $\omega-\Omega$. The first term in Eq. (2) gives rise to the ''universal'' $T\to 0$ conductivity σ_{00}, which is unrenormalized with respect to the theory without order parameter scattering, while the second term determines the leading temperature corrections. As in Ref. 7, quasiparticle states are broadened in all calculations by an inelastic scattering term $1/\tau_{inel}(T)$ calcu-

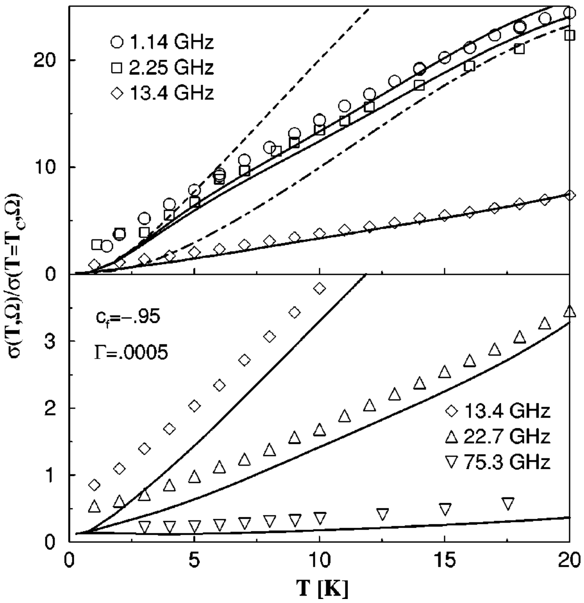

FIG. 1. Normalized microwave conductivity for the frequencies of Ref. 11. Solid lines, theory with $\Gamma/T_c=0.0005$, $c_f=-0.95$, $\Delta_0/T_c=3$. Dashed line, same Γ, $f=2.25$ GHz, without OP scattering. Dot-dashed line, $\Gamma=0.0014$, $f=2.25$ GHz, without OP scattering.

lated from a model of spin-fluctuation scattering as described in Ref. 16.

In Fig. 1 we show the best fit obtained to the low-frequency data of Ref. 11, with normal state scattering rate $\Gamma=0.0005T_c$ in the unitarity scattering limit, and take $c_f\sim-0.95$ and $\Delta_0/T_c=3$. We note that the theory indeed reproduces the slightly sublinear behavior at low frequencies, and crosses over at around 13 GHz to a superlinear behavior and eventually to T^2. At low T the theory curves are consistently below the experimental data, but the relative discrepancy is not large, with the exception of the very low-temperature regime below 2–3 K.

In Fig. 2 we show the frequency dependence of the theory for the same parameters at experimental temperatures; here the agreement is excellent. As noted by Hosseini et al., the most remarkable aspect of the data is the extremely weak temperature dependence of the width in frequency of the residual conductivity peak at low temperatures; this is well reproduced by the theory. In the inset to Fig. 2, we plot the experimental determination of this width, called $1/\tau(T)$, obtained by a fit to a Drude (Lorentzian) spectrum.[11] However, in the microscopic model we propose, the relaxation rate $1/\tau(\omega)$ for nodal quasiparticles is frequency dependent. Furthermore, we find that the momentum dependence of the off-diagonal impurity self-energy *prevents* a derivation similar to Ref. 7 providing a microscopic justification for a Drude or ''two-fluid'' analysis. Thus $1/\tau(T)$ has no well-defined microscopic meaning, but for comparison's sake we have also performed a Drude fit to the theoretical $\sigma(\omega,T)$, the result of which is shown in the inset to Fig. 2. We note that the deep minimum in $1/\tau(T)$ found without OP scattering[7] has been nearly eliminated, but the scattering rate still rises at the lowest temperatures due to the increase of the elastic scattering rate in the unitarity limit (see inset).[7] However, this rise is somewhat misleading as the conductivity spec-

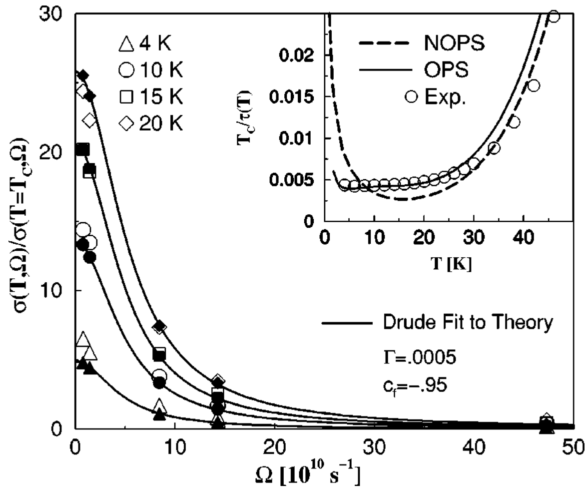

FIG. 2. Normalized $\sigma(\Omega)$ at various T. The open symbols are experimental data from Ref. 11, the solid symbols are results from our theory, with $\Gamma/T_c=0.0005$ and $c_f=-0.95$. Inset: effective scattering rate $\tau(T_c)/\tau(T)$ vs T. The solid line corresponds to theory with parameters as above, the dashed line is the theory without OP scattering. The symbols are data from Ref. 11.

trum becomes distinctly non-Lorentzian below $\gamma\sim\sqrt{\Gamma\Delta_0}\sim2-3$ K, indicating a further breakdown of the Drude interpretation. We note that in the present theory the minimum of $1/\tau(T)$ occurs at an energy of roughly $1/\tau_{min}=(\Gamma^3\Delta_0)^{1/4}$.

Finally, in Fig. 3 we show the behavior of the conductivity over the entire temperature range, where the inelastic scattering plays a much more crucial role. It is remarkable that with the same parameters used to describe the entire frequency range at low temperatures, the peak position is also well described. However, the theoretical curves rise *faster* than the experimental data below T_c and fall faster than experiment below the peak temperature. At first glance this seems to be a shortcoming of our treatment of the inelastic scattering following Ref. 16. On the other hand, the inset of Fig. 3 shows that the scattering rate extracted from

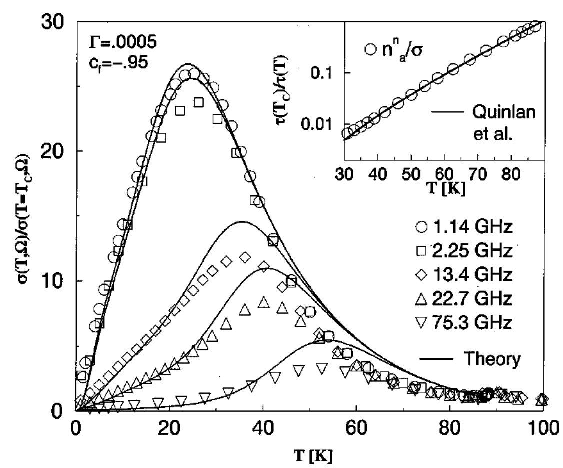

FIG. 3. $\sigma(T)$ at various external frequency Ω. The symbols are experimental data (Ref. 11, with the sharp peak at T_c truncated). The solid lines are results of our theory with $\Gamma/T_c=0.0005$, $c_f=-0.95$. Inset: comparison of inelastic scattering rate after Ref. 16 and the experimental ratio of normal fluid fraction and conductivity at 1.14 GHz. For the considered temperature range the impurity contributions to the scattering rate are unimportant.

the experimental a-axis penetration depth and conductivity data via $1/\tau(T) \sim n_a^n(T)/\sigma(T)$ is in excellent agreement with the result of Ref. 16 in the T range dominated by inelastic scattering [here, $n_a^n(T) = 1 - \lambda_a^2(T=0)/\lambda_a^2(T)$ is the normal fluid fraction]. We therefore believe that the neglect of band-structure effects in the calculation of the density of states is the major source of the discrepancy at higher temperatures.

CONCLUSIONS

We have shown that the inclusion of the order parameter suppression $\delta\Delta_{\mathbf{k}}$ at impurity sites dramatically improves the fit of the weak-coupling BCS d-wave theory of the microwave conductivity to recent experiments on very pure samples of $YBa_2Cu_3O_{7-\delta}$. The excellent fit over a wide range of temperatures and frequencies is found for an impurity scattering rate of approximately $\Gamma/T_c = 0.0005$, confirming that the samples measured by Hosseini *et al.* are significantly purer than the previous generation of yttria-stabilized zirconia $YBa_2Cu_3O_{6.95}$ crystals. Although our treatment of $\delta\Delta_{\mathbf{k}}$ is crude, it captures the basic physics of the curate superconductors, namely, that the bulk order parameter is significantly suppressed over a very short length scale.

There are two sources of concern that suggest that the current approach needs to be refined still further. The first is that we were forced to treat the position $\tilde{c}_f$ of the off-diagonal resonance as a fit parameter rather than determining it self-consistently, as originally proposed in Ref. 12. We have suggested that the facts that (i) the value determined from the fit is quite close to the self-consistently determined value ($c_f \sim -0.8$ with weak T dependence in the strong scattering limit), and (ii) the approximations made, namely, neglecting the effect of disorder on the average gap value in the determination of c_f as well as induced subdominant pair components, tend in the right direction to account for the discrepancy, but we have no estimate of the magnitude of this error. Both a more complete, self-consistent calculation within our framework, as well as a full calculation of the disorder-averaged one-electron spectral function in the framework of the Bogoliubov–de Gennes equation are desirable.

The second problematic aspect is the limiting value and behavior of the conductivity for $T \lesssim 2-3$ K. As seen in Fig. 1, the $T \to 0$ value appears to be 3–5 times the calculated $\sigma_{00}/\sigma(T_c) = \tau^{-1}(T_c)/(\pi\Delta_0)$. We have considered several kinds of corrections to the theory as described herein that tend to increase σ_{00}, or the extrapolated $\sigma(T \to 0)$. The first are nonlocal corrections, which are negligible in the geometry considered by Hosseini *et al.* The second are deviations from the unitarity limit, which have been discussed by in Ref. 8. We find, as these authors did, that such deviations rapidly lead to increasing positive curvature in σ vs T and are never consistent with the measured $\sigma(T)$ when $\sigma(T \to 0)$ is large enough to resemble experiment. More likely sources of error include the neglect of vertex corrections due to anisotropic impurity scattering and Fermi liquid corrections, which may change the residual conductivity by a factor of order unity.[18] The final possibility is that a few twin boundaries are present within the skin depth of the experiment. Twins have been shown to dramatically increase the residual conductivity in poorer samples,[17] and lead to an ''extrinsic'' contribution to the transport that is poorly understood at present.

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