Optical and Thermal Transport Properties of an Inhomogeneous d-Wave Superconductor

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We calculate transport properties of disordered 2D d-wave superconductors from solutions of the Bogoliubov-de Gennes equations, and show that weak localization effects give rise to a finite frequency peak in the optical conductivity similar to that observed in experiments on disordered cuprates. At low energies, order parameter inhomogeneities induce linear and quadratic temperature dependencies in microwave and thermal conductivities respectively, and appear to drive the system towards a quasiparticle insulating phase.

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Introduction. The study of disorder in high \(T_c\) superconductors (HTSC) remains an engaging topic for at least two reasons: first, it is apparent that significant disorder—perhaps originating with charge-donor impurities—is present in nearly all HTSC samples and, second, the controlled doping of substitutional impurities is a powerful means of studying the electronic state. Transport experiments on the cuprates at low \(T\) have given us information on the quasiparticle lifetime in the disordered superconductor and indicated the existence of strong, near-unitarity limit scattering potentials associated with impurities in the CuO\(_2\) plane. The simplest BCS-quasiparticle theories have been successful at describing qualitative features of transport experiments, but fail to explain many of the details. This is the principal motivation for the current work addressing transport properties of dirty d-wave superconductors. The approach taken here is to model the paired state as an inhomogeneous superfluid via the Bogoliubov-deGennes (BdG) equations. We focus most of our attention on optimally doped superconductors at low temperatures, where inelastic processes freeze out\(^1\) and mean-field theory is most applicable.

It is well known that HTSC are strongly affected by disorder because of the d-wave symmetry of the pair order parameter \(\Delta_{ij}\) (\(i\) and \(j\) are site indices of the paired electrons). In a pure sample, the density of states (DOS) \(\rho(\omega)\) is gapless and vanishes as \(|\omega|\) at the Fermi energy (taken to be 0 here). A single strong-scattering impurity produces a pair of subgap resonances at \(\pm \omega_0\) \((\omega_0 < \Delta_{\text{max}}, \Delta_{\text{max}}\) the DOS peak associated with the gap edge in tunneling experiments). When a finite concentration \(n_i\) of impurities with impurity potential \(U\) is present, the isolated resonances are split, and broaden into an “impurity band” centered at the Fermi energy. The energy scale \(\gamma\) of the impurity band, below which \(\rho(E)\) crosses over from linear \((|E| > \gamma)\) to constant \((|E| < \gamma)\), is determined by \(n_i\) and \(U\). These essential features are captured in the widely-used self-consistent T-matrix approximation (SCTMA) for impurity scattering\(^2\). The SCTMA is a perturbative scheme which is useful for treating point-like scatterers. It correctly incorporates physics associated with strong scattering potentials, but ignores correlation effects between impurities (i.e. localization effects), as well as the local response of the superfluid to the impurities. In the SCTMA, \(\gamma\) is also the quasiparticle scattering rate in the impurity band.

While the SCTMA-based notion of an impurity band appears to be fairly consistent with the observed thermodynamic properties of the optimally doped cuprates\(^3\), the simplest theory based on this picture disagree with transport experiments. Notably, the low-temperature behavior of both the thermal and microwave conductivities in several systems disagree with the simple prediction, \(\sigma, \kappa/T \sim T^2\). For example, the low-temperature microwave conductivity in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) appears to vary roughly linearly with temperature, \(\sigma \sim T\). In addition, the optical conductivity of disordered cuprates is observed to have a maximum at a disorder-dependent frequency of order 100 cm\(^{-1}\); this feature is also not found in the simple SCTMA analysis\(^4\). Finally, the SCTMA predicts the universality of residual transport coefficients, i.e. limiting values of \(\kappa/T\) and \(\sigma\) as \(T \to 0\) which depend only weakly on disorder\(^5\). While this has been confirmed in thermal conductivity measurements on YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\); there are other systems where universality is not seen\(^6\). We show below that some of these discrepancies can be understood within a BCS framework by going beyond the SCTMA.

Approach. The BdG equations will be solved at two levels of approximation. Like the SCTMA, non-self-consistent (NSC) solutions assume that \(\Delta_{ij}\) is homogeneous, but unlike the SCTMA, NSC solutions incorporate quantum coherence (i.e. localization) effects associated with scattering from multiple impurities exactly. Self-consistent (SC) BdG solutions involve a further step in which the nonlinear response of \(\Delta_{ij}\) to the local disorder potential is determined. In both cases, the BdG equations are solved on a tight-binding lattice with \(N = 1600\) sites and up to 50 disorder configurations. In matrix...
The mean-field Hamiltonian is

$$\mathcal{H} = \sum_{ij} \Phi_i^\dagger \left[ t_{ij} \Delta_{ij} - t_{ij}^* \right] \Phi_j$$

with $$\Phi_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$$. The subscripts $$i$$ and $$j$$ refer to site indices, and $$t_{ij} = -\delta_{ij} + (U - \mu) \delta_{ij}$$ with $$\delta_{ij} = 1$$ for nearest neighbour sites, and 0 otherwise. All energies in this work are measured in units of $$t$$, and the lattice constant is $$a = 1$$. The bond order-parameter is $$\Delta_{ij} = -V(c_{i\uparrow} \sigma_{ij} c_{j\uparrow}^\dagger)$$ with $$\sigma_{ij}$$ connecting sites $$i$$ and $$j$$, and where $$\Delta_0$$ is the homogeneous d-wave amplitude. Spatial fluctuations arise naturally when one solves $$\Delta_{ij}$$ self-consistently in the presence of a disorder potential. For this work $$V = 3.28$$, making $$\Delta_0 = 0.8$$ which is a factor of $$\sim 4$$ larger than the realistic case. The eigenstates are found using standard linear algebra routines to diagonalise Eq. (1). The quasiparticle DOS is $$\rho(\omega) = N^{-1} \sum_n \delta(\omega - E_n)$$ where $$E_n$$ are the eigenenergies for a given impurity configuration and $$\langle \ldots \rangle$$ represents configuration averaging.

The complex conductivity is

$$\sigma(\omega, T) = \left\langle \frac{\text{e}^{2\hbar}}{\text{i} \omega N} \sum_{n, n'} |\hat{\gamma}_{nn'}^\alpha|^2 \frac{f(E_n) - f(E_{n'})}{\hbar \omega^+ - E_n - E_{n'}} \right\rangle,$$

where $$\hat{\gamma}^\alpha_{nm} \equiv \langle n| (p_x/m) \otimes \sigma^\alpha|m \rangle$$ is the matrix element of the velocity between eigenstates $$n$$ and $$m$$, $$\sigma^\alpha (\alpha = 0, \ldots, 3)$$ is the Pauli matrix in particle-hole space, and $$\omega^+ = \omega + \text{i} \omega^+$$.

We use a binning procedure to evaluate the real part of $$\sigma(\omega, T)$$. Note the expression (2) is not manifestly gauge invariant, but we do not expect this to be a problem since the collective response of the one-component charged order parameter occurs at the plasma frequency.

For numerical reasons, we are restricted to evaluating $$\sigma(\omega, T)$$ in the “gapless regime”, $$\gamma \gtrsim T$$, which has been studied in intentionally damaged samples of YBa$_2$Cu$_3$O$_{7-\delta}$. In this regime, the SCTMA predicts that the real part of the conductivity is $$\sigma_{\text{SCTMA}}(\omega \to 0, T) = \sigma_{00} + \alpha(T/\gamma)^2$$ and $$\sigma_{\text{SCTMA}}(\omega, 0) = \sigma_{00} + \alpha' (\omega/\gamma)^2$$, with a universal value for the residual conductivity: $$\sigma_{00} = e^2v_F^2/(\pi^2\hbar v\Delta)$$. In this expression, $$v_F$$ is the Fermi velocity and $$v\Delta = |\nabla k\Delta_k|$$ is the quasiparticle velocity component parallel to the Fermi surface. Both impurity vertex corrections and Fermi-liquid corrections renormalize $$\sigma_{00}$$ in an approximation where s-wave scattering is generalized to include anisotropic components, but where weak localization corrections and order parameter inhomogeneities are neglected. In this scheme the thermal conductivity is not renormalized, $$\kappa(T)/T = \kappa_{00} + a(T/\gamma)^2$$, with universal value $$\kappa_{00} = \frac{1}{\text{i} \Delta_k} (v_F^2 + v^2) / \hbar v_F^2$$ which survives this class of perturbative corrections.

Results. Typical results for $$\rho(\omega)$$ near unitarity—defined by $$\omega_0 \ll \gamma$$ and corresponding to $$U \approx 10$$ and $$U \approx 5$$ in the NSC and SCTC calculations respectively—are shown in Fig. 1. NSC calculations agree semiquantitatively with SCTMA calculations except below an exponentially small energy. The SC result, by contrast, shows a large disorder-induced suppression of the DOS relative to the SCTMA plateau. As discussed elsewhere, the “disorder-induced pseudogap” (DIP) at the Fermi-energy appears to be a generic feature of SC BdG solutions and has an energy scale related to $$\omega_0$$ but which grows with increasing $$n_i$$. We stress that for typical planar Cu substituents in HTSC, this is an energy scale which is comparable to those explored in transport experiments.

Figure 1 shows the basic low-T result for the conductivity with strong scattering impurities. $$\sigma_{\text{SCTMA}}(\omega)$$ is approximately Drude-like for $$\omega > \gamma$$, but saturates at the universal value $$\Delta_0$$. Numerical solutions of the BdG equations deviate significantly from this with $$\sigma(\omega < \gamma)$$ linear in frequency, and rising to a peak at $$\omega \approx \gamma$$. This is true for both $$\sigma_{\text{SC}}$$ and $$\sigma_{\text{NSC}}$$ (the SC and NSC BdG conductivities respectively), and is therefore the result of weak localization corrections to the SCTMA result. Indeed Fig. (c) shows that $$\delta \sigma(\omega) / \sigma_{00}$$ for $$\sigma_{\text{NSC}}(\omega) - \sigma_{\text{SCTMA}}(\omega)$$ satisfies a scaling relation, $$\delta \sigma(\omega)/\sigma_{00} = F(\omega/\gamma)$$, which is similar to the weak-localization scaling relation for dirty 2D metals. In contrast, $$\sigma_{\text{SC}}(\omega)$$ does not display a simple scaling relation, as we discuss below. At this point, we simply remark...
that $\sigma_{SC}(\omega)$ always has less finite-$\omega$ spectral weight than $\sigma_{SCTMA}(\omega)$ for the same value of $U$ [as illustrated in Fig. 2(a)], with the lost weight appearing in the superfluid response\cite{6}.

The finite-frequency conductivity peak exhibited in Fig. 1 is reminiscent of conductivity measurements in disordered HTSC\cite{8}. Experimentally, the peak is also seen in the normal state $T > T_c$, generally at higher energies, whereas in our approximation it occurs at significantly lower energies, and is much less pronounced than in the superconducting state. It is clear that inelastic scattering is important in the normal state and needs to be incorporated in a complete explanation of the finite-frequency peak. Nevertheless, this is the simplest way of understanding this feature of the optical data, which has not been reproduced in any other approach to our knowledge.

The temperature dependence of the low-frequency conductivity is also of experimental interest. In Fig. 2 we have plotted $\sigma(\omega_1, T)$, where $\omega_1 = 0.0297$ is the lowest nonzero frequency, chosen since $\omega = 0$ suffers from finite-size effects. The strong $T$-dependence of $\sigma_{NSC}(\omega_1, T)$ is similar to the SCTMA result. On the other hand, $\sigma_{SC}(\omega_1, T)$ has a linear-$T$ conductivity, reminiscent of most microwave conductivity experiments\cite{8}. These results are generic for a wide range of $U$ near unitarity. Figure 2 also shows the thermal conductivity

$$\kappa(T) = \frac{1}{2\pi h T} \int dx x^2 \left( -\frac{\partial f}{\partial x} \right) \langle S_T(x) \rangle,$$

(3)

where

$$S_T(x) = \frac{2\pi^2 h^2}{N} \sum_{n, n'} |\langle \hat{v}_g \rangle_{nn'}|^2 \delta(x - E_n)\delta(E_n - E_{n'}),$$

(4)

with quasiparticle group velocity $\hat{v}_g = \hat{v}_g^3 + \hat{v}_g^2 \otimes \tau^1$, and $\langle \hat{v}_g^2 \rangle_{ij} = (1/h)(x_i - x_j)\Delta_{ij}$ in the site representation\cite{2}. For a finite system, the $\delta$-functions in Eq. (4) are broadened to smooth the discreteness of the energy spectrum.

It is apparent in Fig. 3 that the Wiedemann-Franz law $\kappa/\sigma T = L_0 \equiv k_B^2 \pi^2/3e^2$, which is already violated because of differences between the group and Fermi velocity, appears to also be violated at low $T$ (at least in the NSC case) by weak localization corrections. For comparison, we show a similar calculation of the charge-conductivity which becomes exact in the limit $\omega \ll T$,

$$\sigma(T) = \frac{e^2}{2\pi h} \int dx \left( -\frac{\partial f}{\partial x} \right) \langle S_\sigma(x) \rangle,$$

(5)

with $S_\sigma$ identical to $S_T$ with the replacement of $\delta_\rho$ by $\delta^0_\rho$. From the figure, it is clear that Eq. (5) is in good agreement with $\sigma(\omega_1, T)$, and that both $\kappa(T)/T$ and $\sigma(T)$ exhibit a linear $T$-dependence over a wide range of temperatures. The extent of the linear regime is discussed below. Linear power laws have been claimed in thermal conductivity measurements\cite{10} (but other power laws have also been reported), and this work provides a potential mechanism. Conductivities with odd power-laws in $T$ are difficult to achieve in the SCTMA because all quantities increases, in qualitative agreement with $\sigma_{NSC}(\omega)$ at low frequencies.

Finally, in Fig. 3 we study the dependence of $\sigma_{SC}(\omega)$ on impurity concentration. As $n_i$ is increased, the peak position in $\sigma_{SC}$ increases, in qualitative agreement with the scaling of $\sigma_{NSC}(\omega)$. The scaling of $\sigma_{SC}(\omega)$ is not straightforward, however, since low-frequency spectral weight is depleted as $n_i$ increases, in contrast to $\sigma_{NSC}(\omega)$ which depends only weakly on $n_i$ at low $\omega$. The depletion is correlated with the growth of the DIP, shown in Fig. 3(b), reminiscent of disordered interacting met-

![FIG. 2: T-dependent conductivity, normalised to $\sigma_{00}$ for (a) NSC BdG and (b) SC BdG with $n_i = 0.06$, $U = 10$, $\mu = 1.2$, and $\Delta = 0.8$. $\omega_1 = 0.0297$ is the lowest nonzero frequency used in calculating $\sigma$ with Eq. (2). $\kappa/(TL_0) \sigma(T)$ are evaluated using Eqs. (1) and (3).](image)

![FIG. 3: Scaling of $\sigma_{SC}(\omega)$ with $n_i$ at $T = 0$. (a) $\sigma_{SC}(\omega)$ for a range of $n_i$ between 0.02 and 0.14, $U = 5$. (b) Density of states at $n_i = 0.04$ (open circles) and $n_i = 0.14$ (filled circles). (c) Thermal conductivity vs. temperature for same $n_i, U$.](image)
als near the metal-insulator transition. For the model interaction chosen, we never observe a transition to a truly gapped state, and it is doubtful that a quasiparticle metal-insulator transition could be observed in real HTSC since superconductivity is destroyed in heavily damaged samples. However, the current work is strongly suggestive that the physics of disordered cuprate superconductors is influenced by proximity to such a transition.

In Fig. 3(c), we plot the SC thermal conductivity for several impurity concentrations to illustrate the robustness of the (quasi)linear-T regime. The regime is bounded by two disorder-dependent temperature scales; the upper crossover temperature is readily apparent up to $n_i = 0.08$, and is correlated with the weak localization scale $\gamma$, while the lower bound signals a downturn in $\kappa/T$ which appears to scale with the DIP. For $n_i = 0.14$, there is no clear distinction between these scales. With current system sizes it is difficult to determine the lowest energy behavior. If one assumes the matrix elements of $\langle \hat{p}_y \rangle$ have only weak energy dependence near the Fermi surface, then we expect $S_T(x) \sim \rho(x)^2$ which is $\sim x^{2\alpha}$ near $x = 0$ ($\rho \sim x^{\alpha}$) in the SC BdG calculations. For sufficiently small $T$, then, one anticipates a downturn with $\kappa/T \sim T^{2\alpha}$ below the DIP energy scale. It is clear that a strong suppression relative to the universal SCTMA result $\kappa(T) \rightarrow \kappa_{00}$ is to be expected.

Conclusions. We have observed effects with two distinct physical origins in this work. First, there is a pronounced peak in $\sigma(\omega)$ at $\omega \approx \gamma$ arising from localization physics. This occurs whether or not the BdG equations are solved self-consistently, and is consistent with the experimental fact that the peak is only observed in very disordered systems. Since $\gamma \sim \sqrt{n_i}$ for strong scatterers, our work suggests that a systematic study of samples with varying impurity concentrations will provide an experimental means to distinguish between the weak localization mechanism presented here, and other proposed origins for the peak. Second, we have found that important physics associated with the correlated order-parameter response to disorder arises at low energies. Perhaps the most striking result is the observation of linear-$T$ power laws in the charge and thermal conductivities, as observed in some high-$T_c$ systems. In addition, order parameter suppression effects appear to eliminate the residual conductivities at asymptotically low temperatures expected on the basis of SCTMA and other treatments. We note that the current work assumes fairly disordered systems, and the extrapolation to the clean limit ($\gamma < T$) is not obvious. On the other hand, this is the first time that this additional source of off-diagonal scattering has been correctly accounted for in a transport theory, and there appears to be no reason in principle why these effects should also not be important in clean 2D systems and possibly even in higher dimensions. To compare directly with experiments, the effect of realistic Dirac cone anisotropies and inelastic scattering needs to be better understood. Work along these lines is in progress.

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