Breakdown of universal transport in correlated $d$-wave superconductors

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The prediction and observation of low-temperature universal thermal conductivity in cuprates has served as a cornerstone of theoretical approaches to the superconducting state, but recent measurements on underdoped samples show strong violations of this apparently fundamental property of $d$-wave nodal quasiparticles. Here, we show that the breakdown of universality may be understood as the consequence of disorder-induced magnetic states in the presence of increasing antiferromagnetic correlations in the underdoped state, even as these same correlations protect the nodal low-energy density of states in agreement with recent scanning tunneling experiments.

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Introduction. Thermal conductivity measurements at low temperatures $T$ in the superconducting state have played an important role in strengthening the case for a $d$-wave BCS description of quasiparticles in optimally doped cuprate superconductors. They are bulk probes of the superconducting state, unlike angular resolved photoemission (ARPES) and scanning tunneling microscopy (STM), and can currently be performed at lower $T$ than microwave experiments. One drawback is the need to separate phonon and electron contributions, but in the cuprate superconductors an asymptotic linear term, $\kappa_0/T \sim \text{const}$ which can be attributed solely to quasiparticles, dominates at the lowest $T$. After theoretical predictions of the universality of $\kappa_0/T$, experimental confirmation was obtained in optimally doped materials.$^2$. According to theory, which relies on the disorder-averaged self-consistent $T$-matrix approximation (SCTMA), the low-$T$ thermal conductivity is

$$\kappa_0 = \frac{\kappa_0}{T} \approx \frac{k_B^2}{3\hbar} \left( \frac{v_F}{v_\Delta} + \frac{v_\Delta}{v_F} \right), \quad (1)$$

where $k_B$ is Boltzmann’s constant, and $v_\Delta$, $v_F$ denote the nodal gap slope and Fermi velocity, respectively. This is a remarkable example of a transport coefficient which is unaffected—leading order—by the addition of disorder. Furthermore, this result is insensitive to vertex corrections due to anisotropic impurity scattering and Fermi liquid effects.$^3$. Observation of universal conductivity in optimally doped samples$^4$ was a key step in establishing the existence of nodal quasiparticles and the validity of the SCTMA in this limit. Soon thereafter, however, measurements in underdoped samples exhibited values of the low-$T$ thermal conductivity considerably below predicted universal limits.$^6$. How and why the universal prediction breaks down has never been explained.

Since $v_F$ is generally considered to be well-known from ARPES$^8$, Eq. (1) has also been used to extract the gap slope for a number of cuprates at lower doping as well$^6$, leading to the conclusion that $v_\Delta$ increases with underdoping$^6$. This conclusion is in apparent contradiction to recent Raman$^7$ and ARPES experiments$^8$, so it is even more important to examine physical effects outside the framework of the SCTMA which could lead to a suppression of $\kappa_0/T$ and thereby to a possible erroneous conclusion about the doping dependence of $v_\Delta$.

There are several effects known to lead to a suppression of $\kappa_0/T$. Localization effects were discussed in this context in Ref.$^9$, and effects of bulk subdominant competing orders have been shown to suppress $\kappa_0/T$ but do not immediately eliminate it, despite the removal of the $d$-wave nodes.$^{10}$. Here, we investigate the effects on $\kappa(T)$ by local impurity-induced moments relevant e.g. to the underdoped regime of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO)$^{11,12,13}$. Such moments are formed in the presence of background Hubbard interactions in the host material.$^{14}$

Recently, the effect of strong correlations of this type on the density of states (DOS) of a disordered $d$-wave superconductor was investigated by Garg et al.$^{15}$, in an approach where the Gutzwiller approximation was used to approximately project out the doubly occupied states of a disordered $t-J$ model. They found the rather remarkable result that the low-energy states were “protected” by interactions, i.e. in the presence of the projection the low-energy residual DOS which normally arises from disorder$^{16}$ was strongly suppressed. Experimentally it is indeed observed that the low-energy DOS is surprisingly homogeneous$^{16,17,18}$, reflecting a robustness of the nodal quasi-particles to disorder. Garg et al. speculated that the projection mitigated effects of disorder generally at low energies. Here we show that in the density channel this hypothesis is correct: interactions screen and diminish the disorder potential. In the magnetic channel, however, scattering is enhanced, and properties which are sensitive to spin scattering like the universal thermal conductivity $\kappa(T)$ may be strongly renormalized even in the absence of Anderson localiza-
tion.

Model. The model we use to study disordered $d$-wave superconductors with magnetic correlations is

$$\hat{H} = -\sum_{(ij)\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{i\sigma} \left( U n_{i,-\sigma} + V_{i}^{imp} - \mu \right) \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} + \sum_{(ij)} \left( \Delta_{ij} \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow} + \text{H.c.} \right). \quad (2)$$

Here, $\hat{c}_{i\sigma}^\dagger$ creates an electron on site $i$ with spin $\sigma$, and $t_{ij} = \{t, t'\}$ denote the two nearest neighbor hopping integrals, $V_{i}^{imp} = \sum_{j=1}^P V_{i}^{imp} \delta_{ij}$ is a nonmagnetic impurity potential resulting from a set of point-like scatterers of strength $V_{i}^{imp}$, $\mu$ is the chemical potential adjusted to fix the doping $x$, and $\Delta_{ij}$ is the order parameter on the bond between sites $i$ and $j$. The amplitude of $\Delta_{ij}$ is set by the coupling constant $g/|t| = 1.3$. The Hubbard repulsion is treated by an unrestricted Hartree approximation, and $U$ is taken to be homogeneous. Below we fix $t'/t = -0.3$, $x = 0.1$, and solve Eq. (2) self-consistently by diagonalizing the associated Bogoliubov-de Gennes (BdG) equations on systems of $N = 40 \times 40$ sites.

The model given by Eq. (2) has been used extensively in the literature to study bulk competing phases, field-induced magnetization, as well as novel bound states at interfaces between antiferromagnets and superconductors. It has also been used to study field-induced moment formation around nonmagnetic impurities in correlated $d$-wave superconductors. In the case of many impurities, Eq. (2) was recently used to model static disorder-induced antiferromagnetism as seen, e.g., by neutron scattering measurements.

Results. In the clean case ($V_{i}^{imp} = 0$), magnetic order induced by $U$ will compete with the superconducting order and lead to a bulk magnetic state above a critical value $U_{c2}$. For $U_{c1} < U < U_{c2}$, a single point-like impurity can induce a localized $S = 1/2$ state with staggered magnetization. Here, $U_{c1}$ is the critical $U$ necessary for local moment formation, and depends on band structure and impurity strength. When $U < U_{c1}$ there is no induced magnetization but the magnetic correlations still suppress the charge modulations and shorten the superconducting healing length $\xi$ near the impurity.

The picture becomes considerably more complex for finite impurity concentrations. However, there is still a lower value $U_{c1}^\ast$ below which no magnetism is induced, and an upper $U_{c2}^\ast \simeq U_{c2}$ above which the ground state becomes that of a disordered magnet. As explained in Ref. 21, it is easier for a dirty system to generate antiferromagnetic islands ($U_{c1}^\ast < U_{c1}$), because of clustering of impurities and resulting charge redistributions.

Density of states. We first focus on the DOS of the disordered $d$-wave superconductor in the presence of correlations and compare with the results of Ref. 13. In particular, we would like to ascertain whether the onset of the local magnetic state has a qualitative effect on the total DOS. In Fig. 1, we show the spatially averaged total DOS, $N(\omega) = \sum_{\mathbf{r},\sigma} N_{\mathbf{r},\sigma}(\mathbf{r},\omega)/N$, where

$$N_{\mathbf{r},\sigma}(\mathbf{r},\omega) = \sum_{n\sigma} \left| u_{n\sigma}(i) \right|^2 \delta(\omega - E_{n\sigma}) + \left| v_{n\sigma}(i) \right|^2 \delta(\omega + E_{n\sigma}), \quad (3)$$

for a series of disorder concentrations consisting of weak scatterers $V_{i}^{imp}/t = 1.0$ for the noninteracting case $U = 0$. We see the usual low-energy pile-up of impurity states inside the $d$-wave gap. In order to obtain smooth DOS curves we have used a small artificial smearing factor $\eta/t = 0.025$. Figure 1b displays the results of the same study, but for the correlated $d$-wave superconductor with $U/t = 2.5$. The remarkable result is that even for 25% disorder, the Hubbard correlations "protect" the $d$-wave V-shaped DOS. The origin of this universal low-energy behavior is the suppressed charge modulations near the impurities as shown in Fig. 1c. Therefore, an impurity potential apparently disturbs a correlated superconductor much less than a conventional BCS state. Interestingly, impurities which only modulate the pair interaction will also perturb the electronic structure primarily near the antinodes, while protecting

![FIG. 1: (Color online) (a) Spatially averaged DOS in the uncorrelated $d$-wave superconductor ($U = 0$) for different concentrations of disorder $n_{i}$. One clearly sees the pile-up of low-energy impurity states. (b) Same as (a) but for the correlated $d$-wave superconductor with $U = 2.5t$. For a large range of impurity concentrations (0-25%) any sizable and qualitative change in the $V$-shaped low-energy DOS is completely absent. (c) A line cut through the center of the system showing the total charge density (top black lines) and the $d$-wave order parameter (lower red lines). The dashed (solid) lines display the results without (with) correlations. (d) DOS for 2.5% strong scatterers ($V_{i}^{imp}/t = 10$) as a function of $U$. The inset shows a zoom of the low-energy region $\omega \in [-0.35t, 0.35t]$.](image)
the low-energy DOS universality. This kind of disorder may exist in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$, where dopants seem to enhance the pairing interaction locally\[27\].

The results shown in Fig. 1b-c are for weak scatterers without induced magnetization, i.e. in the regime $U < U_{c1}$. It is also interesting to study the DOS in the cluster spin-glass phase, $U_{c2} < U < U_{c3}$, highly relevant for example for underdoped LSCO\[11, 12, 21\]. The tendency to create impurity-induced magnetic states increases with the impurity potential\[14\], so in Fig. 1d we have compared the DOS with nearest-neighbor limit scatterers with $V_{imp}/t = 10$ and a fixed impurity concentration of $n_i = 2.5\%$. From Fig. 1i it is evident that in the absence of correlations, the conventional plateau in the DOS predicted by the SCTMA is seen. As $U$ is increased, this plateau disappears gradually, and there is no qualitative change in the DOS as $U_{c2}/t \simeq 1.5$ is crossed. Note at this relatively weak value of $U$, the projection of doubly occupied sites has not been fully implemented, but the tendency is clearly the same. As $U$ increases beyond $U_{c3}/t \simeq U_{c2}/t \simeq 2.8$ we enter a regime where bulk magnetic order coexists with superconductivity, and the clean DOS acquires an additional gap of the Mott-Hubbard type. However, as shown recently, even in this regime, disorder can result in low-energy DOS indistinguishable from a $d$-wave superconductor\[29\].

**Thermal conductivity.** For $d$-wave superconductors, a real-space BdG calculation of $\kappa(T)$ was used to study both localization phenomena\[9, 13\] and the vortex state\[30\]. Here we follow the same approach but focus on the correlation effects and the role of disorder-induced magnetization using a realistic band structure for cuprate superconductors. For an inhomogeneous system we define the total thermal conductivity $\kappa(T)$ as

$$\kappa(T) = \frac{1}{N} \sum_{\mathbf{r}, \mathbf{r}'} \kappa_{xx}(\mathbf{r}, \mathbf{r}', T),$$

where $\kappa_{xx}(\mathbf{r}, \mathbf{r}, T) = \frac{h}{\nabla_z T}$ is the ratio of the thermal current along the $x$ axis at position $\mathbf{r}$ and the uniform temperature gradient applied along the $x$ direction. Within linear response we have

$$\kappa(T) = \frac{1}{T} \text{Im} \left[ \frac{d}{d\Omega} \frac{1}{N} \sum_{\mathbf{r}, \mathbf{r}'} Q_{xx}(\mathbf{r}, \mathbf{r}', i\Omega_n \rightarrow \Omega + i0^+) \right]_{\Omega \rightarrow 0},$$

where $Q_{xx}$ is the heat current-heat current correlation function. The quantity inside the parenthesis in Eq. 4 reads in compact form

$$\frac{d}{d\Omega} \frac{1}{N} \sum_{\mathbf{r}, \mathbf{r}'} Q_{xx}(\mathbf{r}, \mathbf{r}', i\Omega_n \rightarrow \Omega + i0^+) \equiv \frac{1}{4N} \sum_{n,m} \left[ F(E_n, E_m) \sum_{\mathbf{r}, \mathbf{r}'} \psi_*(n) \hat{v}_g \psi_m(l) \right]^2,$$

where the vector $\psi_*(n) = [u_n(t), v_n(i)]$, and $\hat{v}_g$ denotes the discretized group velocity operator given by $\hat{v}_g = \hat{v}_{kin} \tau_3 + \hat{v}_\Delta \tau_1[9]$. Here the kinetic velocity $\langle \hat{v}_{kin}^\tau \rangle = -it_{il}(x_i - x_l)$ with $t_{il} = t(t' / \sqrt{2})$ for $i,l$ being nearest(next-nearest) neighbors (in the flow direction), and similarly the gap velocity is given by $\langle \hat{v}_\Delta^\tau \rangle = i\Delta_0(x_i - x_l)$. In Eq. 6 we have introduced the spatially independent thermal function $F(E_n, E_m)$ given by

$$F(E_n, E_m) = \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \delta_\tau(\omega - E_n) \delta_\tau(\omega' - E_m) \left[ \frac{\omega^2 f(\omega) - \omega'^2 f(\omega')}{(\omega - \omega')^2} + i\pi \omega^2 f'(\omega) \delta(\omega - \omega') \right],$$

where $\delta_\tau(\omega) = 2\eta/(\omega^2 + \eta^2)[30]$. The spin index (and the sum over spin) is implicit in Eqs. (6)-7.

Numerical solution of Eqs. (6)-7 is computationally demanding, and we are restricted to systems of order $40 \times 40$ sites. To study the low $T$ regime, one needs to have a sufficient number of states within the $d$-wave gap. Therefore, for the discussion below we have increased the coupling constant to $g/t = 2.8$, giving $\Delta_0/t = 0.4$ per link in the homogeneous case. This value of $\Delta_0/t$ gives a universal value $\kappa_00 = 1/3 (v_F / v_\Delta + v_\Delta / v_F) = 0.88$ ($k_B = h = 1$) for the band used here. We stress that the increase of the superconducting gap, which is a factor 6-8 larger than cuprate materials, is merely a means to calculate $\kappa(T)/T$ at low $T$ and is not important for the discussion below. However, the corresponding critical $U$’s will be larger as well (as discussed below).

In Fig. 2a (Fig. 2b), we show the low-$T$ thermal conductivity for the case of $n_i = 2.5\%$ ($15\%$) scatterers with $V_{imp}/t = 10$ ($V_{imp}/t = 3$) averaged over 20 different random impurity configurations (which is enough for configurational convergence). For $U = 0$ the result in Fig. 2a agrees well with those obtained previously for the dilute impurity limit: in the non-self-consistent (NSC) calculation (with homogeneous $\Delta=0.4$), $\kappa(T)/T = \kappa_00 + \alpha T^2[31]$, whereas in the self-consistent (SC) case the spatial inhomogeneity of $\Delta_{ij}$ causes a reduction of $\alpha$ and leads to a more linear $T$ dependence of $\kappa/T$. The case with $V_{imp}/t = 3.0$ in Fig. 2a, is an example of one of the weak-
...disorder potentials we are able to study since further reduced $V^{imp}$ leads to mean-free-path larger than our system. As seen from Figs. 2a-b, an increase of the correlations $U$, initially increases $\kappa(T)/T$ towards the NSC result. The origin of this enhancement is the $U$-suppression of the charge- and gap-modulations: the self-consistent mean fields approach the NSC result. As $U$ increases further and magnetic scattering centers are induced near the defects (Fig. 2c-d), $\kappa(T)/T$ is continuously suppressed, and $\kappa_0/T$ eventually vanishes in the bulk magnetic state. In BCS $d$-wave superconductors the universal ratio of $\kappa_0/T$ arises from a cancellation of the increased disorder-induced scattering rate and a concomitant increase in the density of low-energy quasi-particles. In the present case, the universality is broken because the disorder-induced moments increase the scattering rate whereas the resulting low-energy DOS remains unchanged.

In the two cases shown in Fig. 2a-b, $U_{c1}^*/t \approx 1.9$ for $V^{imp}/t = 10.0$, and $U_{c2}^*/t \approx 3.1$ for $V^{imp}/t = 3.0$, whereas $U_{c2}/t = 3.9$ in both cases. Density of states corresponding to the magnetization plots in Fig. 2a-d are shown in the inset of Fig. 2b. Thus, there exists a large spin-glass regime where the DOS remains universal in the sense that it maintains the characteristic V-shape gap for a $d$-wave superconductor, but the thermal conductivity is simultaneously suppressed due to the creation of additional effective magnetic scatterers. Therefore, impurity-driven local moment formation present in the underdoped regime may explain the doping dependence of $\kappa_0/T$ measured in LSCO. Since the low-T thermal conductivity is strongly suppressed, a naive use of the "universal" clean $d$-wave result for $\kappa_0$ in Eq. (1) would lead to an erroneous estimate of the superconducting gap slope at the node. Thus the conclusion that $v_\Delta$ is reduced with decreasing doping as found by recent Raman and ARPES measurements is not necessarily inconsistent with thermal conductivity measurements within the picture presented here. Note that since the mean field theory employed here overestimates the tendency towards static magnetic order, our results suggest that the thermal conductivity in the presence of low-energy dynamical spin fluctuations not quite pinned by impurities, as apparently true in YBCO, will also be suppressed relative to the universal limit.

In summary, we studied the effects of disorder in correlated $d$-wave superconductors, and calculated the DOS and thermal conductivity in different regimes of the Hubbard repulsion $U$. Although the low-energy DOS is protected due to screening of the disorder by interactions, disorder induced magnetism in the presence of correlations can lead to enhanced scattering which may strongly modify transport properties, in agreement with experiments on thermal conductivity in underdoped cuprates.

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[1] P. A. Lee, Phys. Rev. Lett. 71, 1887 (1993); M. J. Graf et al., Phys. Rev. B 53, 1514 (1996).
[2] L. Taillefer et al., Phys. Rev. Lett. 79, 483 (1997).
[3] A. C. Durst and P. A. Lee, Phys. Rev. B 62, 1270 (2000).
[4] M. Chiao et al., Phys. Rev. Lett. 82, 2943 (1999).
[5] S. Nakamae et al., Rev. B 63, 184509 (2001).
[6] M. Sutherland et al., Phys. Rev. Lett. 94, 147004 (2005); X. F. Sun et al., Phys. Rev. Lett. 96, 017008 (2006).
[7] M. Le Tacon et al., Nature Phys. 2, 537 (2006).
[8] J. Mesot et al., Phys. Rev. Lett. 83, 840 (1999); K. Tanaka et al., Science 314, 1910 (2006); T. Kondo et al., Phys. Rev. Lett 98, 267004 (2007).
[9] W. A. Atkinson and P. J. Hirschfeld, Phys. Rev. Lett. 88, 187003 (2002).
[10] V. P. Gusynin and V. A. Miransky, Eur. Phys. J. B 37, 363 (2004).
[11] B. Lake et al., Nature (London) 415, 299 (2002).
[12] M.-H. Julien, Physica B 329-333, 693 (2003).
[13] B. M. Andersen and P. J. Hirschfeld, Physica (Amsterdam) 460C, 744 (2007).
[14] H. Alloul, J. Bobroff, M. Gabay and P. J. Hirschfeld, arXiv:0711.0877v1.
[15] A. Garg, M. Randeria, and N. Trivedi, arXiv:cond-mat/0609666.
[16] S. H. Pan, et al., Nature (London) 413, 282 (2001).
[17] K. McElroy, et al., Nature (London) 422, 592 (2003); Phys. Rev. Lett. 94, 197005 (2005); Science 309, 1048...
(2005).

[18] M. Vershinin et al., Science 303, 1048 (2004).

[19] A.V. Balatsky, I. Vekhter and J.-X. Zhu, Rev. Mod. Phys. 78, 373 (2006).

[20] J. W. Harter et al., Phys. Rev. B 75, 054520 (2007).

[21] B. M. Andersen et al., Phys. Rev. Lett. 99, 147002 (2007).

[22] I. Martin et al., Int. J. Mod. Phys. 14, 3567-3577 (2000); M. Ichioka, M. Takigawa, and K. Machida, J. Phys. Soc. Jpn. 70, 33 (2001); J.-X. Zhu, I. Martin, and A. R. Bishop, Phys. Rev. Lett. 89, 067003 (2002); B. M. Andersen and P. Hedegård, ibid. 95, 037002 (2005); H.-Y. Chen and C. S. Ting, Phys. Rev B 71, 220510(R) (2005); B. M. Andersen et al., ibid. 72, 184510 (2005).

[23] Y. Ohashi, Phys. Rev. B 66, 054522 (2002).

[24] Y. Chen and C. S. Ting, Phys. Rev. Lett. 92, 077203 (2004).

[25] H. Tsuchiura et al., Phys. Rev B 64, 140501(R) (2001); Z. Wang and P. A. Lee, Phys. Rev. Lett. 89, 217002 (2002).

[26] W. A. Atkinson, P. J. Hirschfeld, and A. H. MacDonald, Phys. Rev. Lett. 85, 3922 (2000).

[27] T. S. Nunner et al., Phys. Rev. Lett. 95, 177003 (2005); Phys. Rev. B 73, 104511 (2006).

[28] B. M. Andersen et al., Phys. Rev. B 74, 060501(R) (2006).

[29] W. A. Atkinson, Phys. Rev. B 75, 024510 (2007).

[30] M. Takigawa, M. Ichioka, and K. Machida, Eur. Phys. J. B 27, 303 (2002); J. Phys. Soc. Jpn. 73, 2049 (2004).

[31] P. J. Hirschfeld and W. O. Putikka, Phys. Rev. Lett. 77, 3909 (1996).

[32] J. Takeya et al., Phys. Rev. Lett. 88, 077001 (2002).