Quasi-particle Lifetimes in a $d_{x^2-y^2}$ Superconductor

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Abstract

We consider the lifetime of quasi-particles in a d-wave superconductor due to scattering from antiferromagnetic spin-fluctuations, and explicitly separate the contribution from Umklapp processes which determines the electrical conductivity. Results for the temperature dependence of the total scattering rate and the Umklapp scattering rate are compared with relaxation rates obtained from thermal and microwave conductivity measurements, respectively.

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It is now widely accepted that the superconducting state of the high $T_c$ cuprates is characterized by a $d_{x^2-y^2}$-order parameter $[1,2]$. Furthermore, various transport properties such as NMR relaxation times $[3,4]$ and the microwave conductivity $[5]$ have been calculated within a quasi-particle BCS-RPA framework which phenomenologically takes into account the interplay of both the $d_{x^2-y^2}$ pairing and the antiferromagnetic spin correlations. In particular, this approach has previously provided reasonable fits of the temperature dependence of the NMR $T_1$ and $T_2$ relaxation times in optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$ $[6,7]$.

With recent advances in the preparation of YBCO crystals $[8,9]$, microwave measurements $[10]$ at a variety of higher frequencies, and $\kappa_{xy}$ thermal conductivity measurements $[11]$, one has new information on the quasi-particle lifetime involved in the electrical conductivity and the mean-free path associated with the thermal conductivity. Several puzzles have presented themselves. First, microwave measurements appear to indicate that the relaxation rate, long known to collapse rapidly below the critical temperature $[12-14]$, varies as $T^4$, or possibly exponentially, at temperatures $T \ll T_c$. On the other hand, the theory of the quasi-particle relaxation rate in a $d$-wave superconductor due to electron-electron interactions predicts a $T^3$ variation above a scale set by impurity scattering $[3,15,16]$. A solution to this discrepancy has recently been suggested by Walker and Smith $[17]$, who noted that in the absence of disorder, the transport lifetime entering the microwave conductivity arises solely from Umklapp processes, which are always gapped below $T_c$ even in a $d$-wave superconductor, leading to an exponential decay $1/\tau_U \sim \exp(-\Delta_U/T)$. Secondly, while early thermal conductivity experiments extracted quasi-particle mean-free paths in apparent agreement with microwave measurements, recent measurements indicate that on cleaner crystals, where the mean-free path due to inelastic scattering can be probed to lower temperatures, the extracted mean-free path is shorter than in the microwave case $[11]$. Furthermore, the inelastic contribution to the inverse thermal mean free path appears to follow a $T^3$ temperature dependence at low temperatures (see below).

Motivated by the proposal of Walker and Smith $[17]$ regarding the role of Umklapp pro-
cesses, we investigate whether the same type of spin-fluctuation interaction used to fit the NMR data can also provide a quantitative fit to the lifetimes extracted from the microwave and thermal conductivities. In particular, we wish to understand if the discrepancies discussed above can be resolved by recognizing that normal electron-electron interactions conserve the total momentum and therefore cannot degrade the electric current, whereas they can degrade the heat current. We therefore calculate, within a BCS model in which the spin-fluctuation interaction is accounted for in the random phase approximation (RPA), the total quasi-particle lifetime and the Umklapp-only quasi-particle lifetime and compare these with the $\kappa_{xy}$ thermal conductivity and microwave conductivity measurements, respectively. We find that the inelastic lifetimes extracted from thermal transport and charge transport can be accounted for within a BCS-RPA quasi-particle framework. Furthermore, the parameter values which are required are consistent with what is known about the Fermi surface and spin-fluctuations from other measurements. The analysis is based, however, on the subtraction of a constant relaxation rate from both quantities, an approach which must be justified within microscopic theory; we present a brief discussion of these issues and the light shed by our analysis on the behavior of the low-energy impurity scattering amplitude.

In the following, we will assume that we have BCS quasi-particles with a $d_{x^2-y^2}$ gap

$$\Delta_k(T) = \frac{1}{2} \Delta_0(T)(\cos k_x - \cos k_y)$$

(1)

moving on a 2D square lattice with near- and next-near-neighbor one-electron hopping matrix elements $t$ and $t'$, respectively. The effective electron-electron interaction will be modeled by the spin-fluctuation form

$$\text{Im} V(q, \omega) = \frac{3}{2} \bar{U}^2 \frac{\chi_0''(q, \omega)}{(1 - \bar{U} \chi_0'(q, \omega))^2 + (\bar{U} \chi_0''(q, \omega))^2}.$$  

(2)

Here, $\bar{U}$ and the chemical potential, $\mu$, which sets the average site occupation, $\langle n \rangle$, control the strength of the antiferromagnetic spin-fluctuations, and $\chi_0(q, \omega)$ is the BCS susceptibility given by
\[ \chi_0(q, \omega) = \frac{1}{N} \sum_p \left\{ \frac{1}{2} \left[ 1 + \frac{\epsilon_p q + \Delta_p q \Delta_p}{E_{p+q} E_p} \right] \frac{f(E_{p+q}) - f(E_p)}{\omega - (E_{p+q} - E_p) + i0^+} ight. \\
+ \frac{i}{4} \left[ 1 - \frac{\epsilon_p q + \Delta_p q \Delta_p}{E_{p+q} E_p} \right] \frac{1 - f(E_{p+q}) - f(E_p)}{\omega + (E_{p+q} + E_p) + i0^+} \\
+ \frac{i}{4} \left[ 1 - \frac{\epsilon_p q + \Delta_p q \Delta_p}{E_{p+q} E_p} \right] \frac{f(E_{p+q}) + f(E_p) - 1}{\omega - (E_{p+q} + E_p) + i0^+} \right\}, \tag{3} \]

where \( E_p = \sqrt{\epsilon_p^2 + \Delta_p^2} \) and \( \epsilon_p = -2t(cosp_x + cosp_y) - 4t'cosp_xcosp_y - \mu \). The band parameters are taken to be \( t'/t = -0.35 \) with a site filling of \( \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle = 0.85 \), and the temperature dependence of the gap has been parametrized as

\[ \Delta_0(T) = \frac{\Delta_0}{2} \tanh(\alpha \sqrt{T_c/T - 1}). \tag{4} \]

We have used \( \alpha = 3.0 \) to reproduce the rapid onset of the gap below \( T_c \) which is observed experimentally, and set \( 2\Delta_0/k_b T_c = 5 \). Throughout this paper, we use \( t = 1 \) as our energy scale and take \( \bar{U}/t = 2.2 \); this is similar to the \( \bar{U} = 2.0 \) used in previous calculations \cite{3} of the NMR \( T_1 \) and \( T_2 \) relaxation rates, where an RPA form for \( \chi(q, \omega) \) similar to Eq. (3) was employed, but a simple \( (t' = 0) \) tight-binding band assumed.

Using the effective interaction, Eq. (2), the Fermi Golden Rule expression for the quasi-particle lifetime is \[ 15 \]

\[ \tau^{-1}(p, \omega) = \int \frac{d^2p'}{(2\pi)^2} \text{Im} V(p - p', \omega - E_{p'}) (1 + \frac{\Delta_p \Delta_{p'}}{\omega E_{p'}})[n(\omega - E_{p'}) + 1][1 - f(E_{p'})] \\
+ \int \frac{d^2p'}{(2\pi)^2} \text{Im} V(p - p', \omega + E_{p'}) (1 - \frac{\Delta_p \Delta_{p'}}{\omega E_{p'}})[n(\omega + E_{p'}) + 1]f(E_{p'}), \tag{5} \]

where \( n(\omega) \) and \( f(\omega) \) are the usual Bose and Fermi factors. Here the first term arises from quasi-particle scattering resulting from the absorption and emission of a spin-fluctuation. The second term corresponds to a process in which a quasi-particle recombines with another quasi-particle to form a pair and the excess energy is emitted as a spin-fluctuation.

An example of the type of process which this includes is schematically illustrated in Fig. 1(a). Here, a quasi-particle with momentum \( p \) scatters off of another quasi-particle with momentum \( k \) leading to an intermediate state containing quasi-particles of momentum \( p' \) and \( k' \). Momentum conservation on the lattice implies that
\mathbf{p} + \mathbf{k} = \mathbf{p}' + \mathbf{k}' + \mathbf{G} \tag{6}

where \( \mathbf{G} \) is a reciprocal lattice vector and all other momenta are confined to the first Brillouin zone. Since \( E_{\mathbf{k'}} = E_{\mathbf{p}' + \mathbf{k} - \mathbf{G}} = E_{\mathbf{p} - \mathbf{p}' + \mathbf{k}} \), we have the expression for \( \chi_0(\mathbf{q}, \omega) \) given by Eq. (3) with \( \mathbf{q} = \mathbf{p} - \mathbf{p}' \) and with the \( \mathbf{k} \) sum extending over the entire first Brillouin zone. If, however, we had not allowed any reciprocal lattice vectors except \( \mathbf{G} = (0, 0) \), the \( \mathbf{k} \) sum would, for given values of \( \mathbf{p} \) and \( \mathbf{p}' \), extend only over that part of the first Brillouin zone for which \( \mathbf{k}' = \mathbf{p} - \mathbf{p}' + \mathbf{k} \) remains inside the first Brillouin zone. This restriction of \( \mathbf{G} = (0, 0) \) eliminates all of the Umklapp scattering processes, allowing only “normal” processes. In this way, one can introduce a “normal” scattering lifetime \( \tau^{-1}_N(\mathbf{p}, \omega) \). This is obtained by using an interaction with the same denominator as in Eq. (2), but with \( \chi''_0(\mathbf{q}, \omega) \) in the numerator replaced by the imaginary part of Eq. (3) with \( \mathbf{q} = \mathbf{p} - \mathbf{p}' \) for which the sum over \( \mathbf{k} \) is restricted such that \( \mathbf{p} - \mathbf{p}' + \mathbf{k} \) remains in the first Brillouin zone. With this restriction, the resulting “normal”, non-Umklapp, part of \( \chi''_0(\mathbf{q}, \omega) \) depends separately on \( \mathbf{p} \) and \( \mathbf{p}' \) rather than only on the difference of \( \mathbf{p} - \mathbf{p}' \). Having calculated both \( \tau^{-1}(\mathbf{p}, \omega) \) and \( \tau^{-1}_N(\mathbf{p}, \omega) \), one can obtain a lifetime which contains only the Umklapp processes by subtraction

\[
\tau^{-1}_U(\mathbf{p}, \omega) = \tau^{-1}(\mathbf{p}, \omega) - \tau^{-1}_N(\mathbf{p}, \omega). \tag{7}
\]

At temperatures which are small compared with the maximum gap, the thermally excited quasi-particles occupy states close to the \( d_{x^2-y^2} \) gap nodes on the Fermi surface. When two of these thermal quasi-particles scatter, the outgoing states must also occupy states near the nodal region in order to conserve energy. For the Fermi surface shown in Fig. 1(b), these scattering processes must have \( \mathbf{G} = (0, 0) \) and only contribute to the “normal” processes. Umklapp scattering processes are also possible, but these processes are exponentially suppressed at low temperatures. Following Walker and Smith [17], the reason for this is illustrated in Fig. 1(b). Here, we have set the initial quasi-particle momentum \( \mathbf{p} \) to a node and numerically searched for the lowest energy quasi-particle state \( \mathbf{k} \) such that momentum is conserved as in Eq. (3) with the constraint that \( \mathbf{G} = (0, 0) \). For \( t'/t = -0.35 \) and \( \langle n \rangle = 0.85 \) corresponding to the Fermi surface shown, the momentum \( \mathbf{k} \) is the lowest energy state for
which a quasi-particle can have an Umklapp scattering with the nodal quasi-particle \( p \). Since \( \mathbf{k} \) has moved away from the nodal region, \( \Delta_k \) is now finite. When \( k_B T \) is less than \( \Delta_k \), the probability of finding such a quasi-particle varies as \( e^{-\Delta_k/k_B T} \) and the Umklapp scattering is suppressed for temperatures below \( \Delta_k \). We will call this special value the Umklapp gap, \( \Delta_U \). It depends upon the shape of the Fermi surface which is set by \( t'/t \) and \( \langle n \rangle \). Figure 2 shows the Umklapp gap as a function of the strength of the \( t'/t \) for a fixed filling of \( \langle n \rangle = 0.85 \). It is easily seen that an Umklapp gap exists even when \( t'/t = 0 \) and has a magnitude of about 0.07\( t \) for the band with \( t'/t = -0.35 \). We note further that this corresponds to a “Dirac cone anisotropy ratio” \( v_F/v_2 \simeq 12 \), which is consistent with the value determined by low temperature thermal conductivity measurements \cite{19}.

We now compare the absolute values of the relaxation times in question. In Fig. 3(a), we have plotted \( \hbar/k_B T_c \tau_U \) and \( \hbar/k_B T_c \tau \) versus \( T/T_c \) for the parameters discussed above. In order to compare recent thermal conductivity measurements with the total scattering rate, we need to specify a Fermi velocity. For the \( t-t' \) dispersion relation one has \( v_F \simeq 2.16ta \) and taking \( T_c = 0.1t = 90K \), this gives \( v_F \sim 10^7 \text{cm/sec} \). Zhang et. al. \cite{11} have used an effective Fermi velocity \( \eta v_F \sim 10^7 \text{ cm/sec} \) with \( \eta = 0.6 \) and \( v_F = 1.7 \times 10^7 \text{ cm/sec} \). Alternatively, Chiao et. al. \cite{19} have suggested that \( v_F = 2.5 \times 10^7 \text{ cm/sec} \). In the fit of \( \hbar/k_B T_c \tau(T) \) shown as the solid line in Fig. 4(a), we have used \( v_F = 3 \times 10^7 \text{ cm/sec} \) to convert the thermal mean-free path data of Ref. \cite{11} to a quasi-particle relaxation rate shown as the open symbols. Beyond the choice of \( v_F \), the determination of the quasi-particle lifetime from the thermal conductivity measurements is complicated by the phonon contribution to the heat current, and necessitates certain assumptions regarding the nature of quasi-particle scattering in the vortex state \cite{11} which are still controversial. However, we note that the magnitude of the theoretically determined total scattering rate of \( \hbar/\tau(T_c) \sim 3k_B T_c \) at the node is in rough agreement with that determined by ARPES \cite{22}, while \( \hbar/\tau_U(T_c) \sim k_B T_c \) is consistent with optical data. In Fig 3(b), we show the low temperature range of the theoretical predictions, along with the Hosseini et. al. \cite{10} \( 1/\tau \) extracted from microwave data using a two-fluid analysis, shown as open diamonds. Here one sees that taking \( \bar{U}/t = 2 \)
provides a reasonable fit to the magnitude of the low temperature microwave scattering lifetime and the exponential decay of the Umklapp processes also appears to provide a sensible explanation for the observed temperature dependence at low temperatures.

Clearly, there are a number of parameters in this calculation, and the results do vary with their values. Here, we have selected values for $t'/t$ and the filling $\langle n \rangle$ to give a Fermi surface which resembles that seen in ARPES data and various band structure calculations \[20\] for the $d_{x^2-y^2} - p\sigma$ band of YBCO. Specifically, the Fermi surface, as seen in Fig. 1(b), has a diagonal nodal $k$-spacing of $(0.8, 0.8)\pi/2a$, and fixes the size of the Umklapp gap, $\Delta_U$, which determines how $\tau_U^{-1}(p, \omega)$ decreases below the total scattering lifetime. Note that for the Fermi surface pictured in Fig. 1(b), $2\Delta_0/k_BT_c = 5$ corresponds to a maximum of the gap on the Fermi surface near $(\pi, 0)$ of $\max[2\Delta_0(p)/k_BT_c] = 4.7$. The choice of $\bar{U}/t = 2.2$ was made consistent with Refs. [3,4] and because it provided a reasonable fit to the absolute magnitude of the microwave scattering lifetime, as discussed below.

It is important to ask the extent to which the data support the fundamental prediction of this work, that the relaxation rate entering the thermal conductivity data should be the total quasi-particle relaxation rate, which varies as $(T/T_c)^3$ due to spin-fluctuation scattering and recombination processes, in contrast to the activated Umklapp scattering rate which should enter the microwave conductivity. Is Fig. 3 sufficient to conclude that these assertions are correct? In order to examine the true low-$T$ asymptotic forms, we have displayed in Fig. 4 the same curves and data as in Fig. 3 on a log-log plot. From the insert to the figure, it is clear that the low-$T$ behavior of the two experimental relaxation rates is quite different, but although the thermal conductivity data is roughly consistent with the $T^3$ result expected from the spin-fluctuation theory, the microwave data appear to lie considerably above the activated prediction at the lowest temperatures, a behavior hidden by the linear plot in Fig. 3. In the main part of the figure, we show the raw experimental data with no constant subtracted, together with the inelastic rates added to a constant $1/\tau_0$ determined by the experimental data at low $T$.

The most natural interpretation of the residual scattering rates $1/\tau_0$ is in terms of dis-
order. It is striking that the $1/\tau_0$ extracted from the thermal conductivity measurement appears to be significantly larger than that extracted from the microwave measurements, since both measurements were performed on nominally equivalent $BaZrO_3$ crucible-grown samples. The most popular treatment of disorder in the cuprates is the self-consistent $t$-matrix approximation (SCTMA) describing strong scattering by in-plane near-unitarity limit defects. This theory predicts a strong energy dependence of the low-temperature elastic scattering rate, however, inconsistent with the roughly constant behavior observed here [15]. This difficulty was remedied to some extent in Ref. [23] by considering additional scattering from spatial fluctuations of the order parameter. Even in this approach, however, bare scatterers are considered to be isotropic, leading to a vanishing of impurity vertex corrections in local quantities; this implies the same relaxation time for both thermal and microwave conductivities. If the isotropic scattering assumption is relaxed, however, as considered by Durst and Lee [18], the $\omega \to 0$ microwave conductivity is found to be strongly enhanced relative to the thermal conductivity, which is unrenormalized. This may be interpreted as a reduction of the scattering rate in the microwave case, but a full frequency-dependent calculation and proof that a Lorentzian conductivity obtains in analogy to Ref. [5] is required before one may conclude that the observed discrepancy is caused by anisotropic impurity scattering.

To summarize, using a d-wave BCS framework, we have taken a simple spin-fluctuation interaction, which has been used to describe the temperature dependence of the NMR $T_1$ and $T_2$ spin relaxation times in YBCO below $T_c$, and have shown that it can also describe the temperature dependence of both the inelastic charge and heat transport times below $T_c$. The contribution to the quasi-particle lifetime of normal spin-fluctuation scattering processes, which can relax heat currents but not charge currents, as well as Umklapp processes, have been calculated separately. The difference in the two contributions was then shown to account for the difference in experimentally extracted lifetimes in recent microwave and heat conductivity measurements on ultraclean samples of YBCO. Both the predicted temperature dependences in a spin-fluctuation mediated interaction model, the Umklapp scattering rates
$1/\tau_U \sim \exp -\Delta_U/T$ and the total scattering rate $1/\tau \sim T^3$, appear to agree with the data, as do the predicted absolute magnitudes of the two rates. The exponential form of $1/\tau_U$ implies a sensitivity to the Fermi surface shape, which is expected to lead to a significant increase in $1/\tau_U$ at low temperatures upon underdoping. While our results depend upon the band structure and interaction parameters, we have selected these to be consistent with Fermi surface data and NMR measurements, and conclude that the results for the microwave and thermal conductivity inelastic quasi-particle lifetimes are consistent with an effective electron-electron interaction which is mediated by spin-fluctuations.

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FIG. 1. (a) A schematic representation of the scattering process. (b) The non-interacting Fermi surface with $t'/t = -0.35$ at a filling of $\langle n \rangle = 0.85$. The vectors shown correspond to an Umklapp process in which $\bar{p} + \bar{k} = \bar{p}' + \bar{k}' + (0, 2\pi/a)$.

FIG. 2. The size of the Umklapp gap $\Delta_U/t$ (solid curve) and the $v_F/v_2$ ratio (dashed curve) versus the ratio of the next-near-neighbor hopping $t'$ to the near-neighbor hopping $t$. 
FIG. 3. (a) The normalized YBCO quasi-particle scattering rates $\hbar/\tau k_B T_c$ and $\hbar/\tau_U k_B T_c$ versus reduced temperature $T/T_c$. The experimental points for $\hbar/\tau k_B T_c$ were obtained from the thermal conductivity mean-free path measurements by Zhang, et. al. [11] using $v_F = 3 \times 10^7$ cm/sec and are shown as the open circles and squares. The solid line is the total quasi-particle lifetime obtained from Eq. (5) on a $512 \times 512$ lattice with $\bar{U}/t = 2.2, T_c = 0.1 t, t'/t = -0.35, 2\Delta_0/k_B T_c = 5$, and $\langle n \rangle = 0.85$. (b) Same as in (a) for reduced temperatures less than 0.5 with the data of Hosseini, et. al. [10] included as open diamonds. The solid line corresponds to the total lifetime calculated as in (a), while the dashed line represents the lifetime due to Umklapp processes only, Eq. (7). Note a constant term has been subtracted from the experimental data.
FIG. 4. Log-log plot of theoretical predictions for normalized total and Umklapp scattering rates $\hbar/(\tau k_B T_c)$ and $\hbar/(\tau_U k_B T_c)$ obtained from Eq. (5) (solid lines), same parameters as Fig. 3. Data from Refs. [11] and [10] as in Fig. 3. Dashed curves: same theoretical predictions for $\hbar/(\tau k_B T_c)$ and $\hbar/(\tau_U k_B T_c)$ with constants $1/\tau_0 = 5.0 \times 10^{10}$ s$^{-1}$ and $3.3 \times 10^{11}$ s$^{-1}$ added to $1/\tau_U$ and $1/\tau$, respectively. Insert: same as main panel but with $1/\tau_0$ subtracted from data.