Theory of Thermal Conductivity in High-$T_c$ Superconductors below $T_c$: Comparison between Hole-Doped and Electron-Doped Systems

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In hole-doped high-$T_c$ superconductors, thermal conductivity $\kappa$ increases drastically just below $T_c$, which has been considered as a hallmark of a nodal gap. In contrast, such a coherence peak in $\kappa$ is not visible in electron-doped compounds, which may indicate a full-gap state such as a $d + i s$-wave state. To settle this problem, we study $\kappa$ in the Hubbard model using the fluctuation-exchange (FLEX) approximation, which predicts that the nodal $d$-wave state is realized in both hole-doped and electron-doped compounds. The contrasting behavior of $\kappa$ in both compounds originates from the differences in the hot/cold spot structure. In general, a prominent coherence peak in $\kappa$ appears in line-node superconductors only when the cold spot exists on the nodal line.

Keywords: spin fluctuation theory, thermal conductivity, unconventional superconductivity, FLEX approximation

In strongly correlated electron systems, transport phenomena give us significant information on the many-body electronic states. In high-$T_c$ superconductors (HTSCs), for example, both the Hall coefficient $R_H$ and the thermoelectric power $S$ are positive in hole-doped compounds such as YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) and La$_{2-x}$Sr$_x$CuO$_4$ (LSCO), whereas they are negative in electron-doped compounds like Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO) and Pr$_{2-x}$Ce$_x$CuO$_4$ (PCCO) [1]. These experimental facts originate from the difference in the “cold-spot,” which is the portion of the Fermi surface where the relaxation time of a quasiparticle (QP), $\tau_k$, takes the maximum value [2–4]:

Below $T_c$, electronic thermal conductivity $\kappa$ has been observed intensively since it gives us considerable information on the superconducting state; it is the only transport coefficient which remains finite below $T_c$. For example, the $k$-dependence of the SC gap can be determined by the angle resolved measurement of $\kappa$ under the magnetic field [5, 6]. Also, one can detect the type of nodal gap structure (full-gap, line-node, or point-node) by measuring $\kappa$ at low temperatures ($T \ll T_c$). For $T \gtrsim T_c$, $\kappa$ also shows rich variety of behavior in various superconductors. In conventional full-gap $s$-wave superconductors, the opening of the SC gap rapidly decreases the density of thermally excited QPs, causing $\kappa$ to decrease. On the other hand, $\kappa$ shows “coherence peak” behavior just below $T_c$ in several unconventional superconductors with line-node gaps, e.g., hole-doped HTSC [7–9], CeCoIn$_5$ [10, 11], and URu$_2$Si$_2$ [12]. A previous theoretical study based on a BCS model with $d$-wave pairing interaction [13] discussed that the coherence peak in YBCO originates from the steep reduction in $\tau$ below $T_c$.

In sharp contrast, no coherence peak in $\kappa$ is observed in electron-doped HTSCs [14, 15], irrespective that a recent ARPES measurement [16] suggests that the $d_{x^2-y^2}$-wave state is realized. The observed $k$-dependence of the SC gap function in NCCO, which prominently deviates from $\cos k_x - \cos k_y$, is well reproduced by the fluctuation-exchange (FLEX) approximation [17], which is a self-consistent spin fluctuation theory. On the other hand, recent point-contact spectroscopy for PCCO [18] suggests that a full-gap SC state such as $d_{x^2-y^2} + is$ or $d_{x^2-y^2} + id_{xy}$ state is realized for $\delta = 0.15$ and 0.17. To find out the real SC state in electron-doped HTSC, we have to elucidate whether the “absence of coherence peak in $\kappa$” is a crucial hallmark of the full-gap SC state, or it can occur even in nodal gap superconductors.

In this letter, we present a theoretical study of the electronic thermal conductivity $\kappa$ in HTSCs using the FLEX approximation. This is the first numerical study of transport properties in the SC state based on the repulsive Hubbard model. In deriving the relaxation time $\tau_k$, both the strong inelastic scattering due to Coulomb interaction and weak elastic impurity scattering are taken into consideration, which corresponds to optimally-doped YBCO and NCCO samples, respectively. We find that a sizable coherence peak of $\kappa$ in YBCO originates from the reduction in inelastic scattering. In contrast, the coherence peak is absent in NCCO in spite of that $d_{x^2-y^2}$-wave SC state is realized, since the nodal point does not coincide with the cold spot in the normal state. Thus, contrasting behaviors of $\kappa$ in YBCO and NCCO are explained on the same footing as $d_{x^2-y^2}$-wave superconductors. This result was not derived in the BCS model [13].

Here, we study the following repulsive Hubbard model:

$$\mathcal{H} = \sum_{k,\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \frac{U}{N} \sum_{k, k', q} c_{k+q\uparrow}^\dagger c_{k' - q\downarrow}^\dagger c_{k' \downarrow} c_{k\uparrow}$$ (1)

where $U$ is the Coulomb interaction and $c_{k\sigma} = 2t_0(\cos(k_x) + \cos(k_y)) + 4t_1 \cos(k_x) \cos(k_y) + 2t_2(\cos(2k_x) + \cos(2k_y))$ is the kinetic energy of free electrons. Hereafter, we put $t_0 = -1.0$, $t_1 = 0.167$, and $t_2 = -0.2$ [2] to reproduce the Fermi surface of YBCO and NCCO. We also put $U = 8.0$ for YBCO and $U = 5.4$ for NCCO. Here, no phenomenological fitting parameters are introduced except for $U$. 

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In the FLEX approximation, the normal and anomalous self-energies are given by

\[
\Sigma^n(k, i\epsilon_n) = \frac{U^2 T}{N} \sum_{k,l} G_{q+k}(i\epsilon_n + i\omega_l) \\
\times \left( \frac{3}{2} \chi_s + \frac{1}{2} \chi_c - \chi_0 \right) q,\omega_l
\]

(2)

\[
\Sigma^a(k, i\epsilon_n) = -\frac{U^2 T}{N} \sum_{k,l} F^+_{q+k}(i\epsilon_n + i\omega_l) \\
\times \left( \frac{3}{2} \chi_s - \frac{1}{2} \chi_c - \phi_0 \right) q,\omega_l
\]

(3)

where \( \epsilon_n = \pi T(2n+1) \) and \( \omega_l = 2\pi T l \) are the Matsubara frequencies for fermions and bosons, respectively. \( \chi_s \) and \( \chi_c \) are the dynamical spin and charge susceptibilities, which are given by

\[
\chi_s(q, i\omega_l) = \frac{\chi_0 + \phi_0}{1 - U(\chi_0 + \phi_0)}
\]

(4)

\[
\chi_c(q, i\omega_l) = \frac{\chi_0 - \phi_0}{1 - U(\chi_0 - \phi_0)}
\]

(5)

\[
\chi_0(q, i\omega_l) = -\frac{T}{N} \sum_{k,n} G_{k+q}(i\epsilon_n + i\omega_l) G^*_k(i\epsilon_n)
\]

(6)

\[
\phi_0(q, i\omega_l) = -\frac{T}{N} \sum_{k,n} F^+_{k+q}(i\epsilon_n + i\omega_l) F_k(i\epsilon_n)
\]

(7)

where \( G \) and \( F \) are the normal and anomalous Green function, respectively. They are given by

\[
G(i\epsilon_n) = (i\epsilon_n + \tilde{e}_k + \Sigma^n(-i\epsilon_n))D(\epsilon_n)^{-1}
\]

(8)

\[
F(i\epsilon_n) = \Sigma^a(-i\epsilon_n)D(\epsilon_n)^{-1}
\]

(9)

\[
D(\epsilon_n) = (-\epsilon_n - \tilde{e}_k + \Sigma^n(-i\epsilon_n))(-\epsilon_n + \tilde{e}_k + \Sigma^n(i\epsilon_n))
\]

\[-(\Sigma^n(-i\epsilon_n))^2
\]

(10)

where \( \tilde{e}_k = e_k - \mu \); \( \mu \) is the chemical potential. In the FLEX approximation, we solve eqs. (2)-(10) self-consistently by choosing \( \mu \) to adjust the electron filling \( n \).

In the following numerical study, we use \( 64 \times 64 \) \( k \)-meshes and 2048 Matsubara frequencies. Figure 1 represents the density of states (DOS); \( \rho(\omega) = \frac{1}{N} \sum_k G^R_k(\omega) \). Here, the advanced (retarded) Green function \( G^R_k(\omega) (G^A_k(\omega)) \) is given by the numerical analytic continuation of the Matsubara Green function from the lower (upper) half plane in the complex \( \omega \) space.

Figure 2 shows the location of the hot/cold spots for both YBCO and NCCO in the normal state. The transport phenomena are governed by QPs around the cold spot, where the QP damping rate \( \gamma_k = \text{Im}\Sigma_k(-i\delta) \) takes the minimum value. According to the FLEX approximation, the cold-spot in hole-doped [electron-doped] systems is around \( (\pi/2, \pi/2) \) \( [(\pi, 0)] \) [2]. The position of the cold-spot in electron-doped systems was confirmed by ARPES measurements [19, 20] after the theoretical prediction [2].

Hereafter, we derive the electric thermal conductivity \( \kappa \). According to the linear response theory [21–23],

\[
\kappa = \frac{-1}{T} \int_0^\beta d\tau \sum_{k_1,k_2} \frac{1}{i\omega_l} \langle Q_{k_1}(\tau)Q_{k_2}(0) \rangle e^{i\omega_l \tau} |_{\omega \to 0}
\]

(11)

\[
\hat{Q}_{kxz}(\tau) = \hat{q}_{kxz}^x + \hat{q}_{kxz}^z + \hat{q}_{kxz}^\sigma + \hat{q}_{kxz}^\sigma
\]

(12)

where \( \hat{Q}_{kxz} \) is the heat current operator in the superconducting state: \( \hat{q}_{kxz}^x \) and \( \hat{q}_{kxz}^\sigma \) are given by

\[
\hat{q}_{kxz}^x = \omega \hat{v}_{kxz}^x, \quad \hat{q}_{kxz}^\sigma = \omega \hat{v}_{kxz}^\sigma
\]

(13)

where \( \hat{v}_{kxz}^x \) represents the “Fermi velocity” and \( \hat{v}_{kxz}^\sigma \) is the “gap velocity” [21]:

\[
\hat{v}_{kxz}^x = v_{kxz}^x c_{kxz}^\sigma, \quad \hat{v}_{kxz}^\sigma = v_{kxz}^\sigma c_{kxz}^\sigma
\]

(14)

where \( v_{kxz}^x = \frac{\partial q^{\sigma}}{\partial k_x} \frac{\partial q^{\sigma}}{\partial k_y} \) and \( v_{kxz}^\sigma = \frac{\partial q^{\sigma}}{\partial k_z} \).

As a result, the expression for \( \kappa \) in the SC state with dropping the current vertex correction (CVC) is given by
\[ \kappa = \frac{1}{2T} \sum_{k} \int dz \left( -\frac{\partial f(z)}{\partial z} \right) \{ 2q_{kx}^{2}(G_{k}^{R}(z)G_{k}^{A}(z) - F_{k}^{R}(z)F_{k}^{A}(z)) \\
- 4q_{kx}q_{kz}G_{k}^{A}(z) - 2F_{k}^{R}(z)F_{k}^{A}(z) \} \]  
(15)
where \( f(z) = (e^{z/T} + 1)^{-1} \). In the normal state, heat CVC due to Coulomb interaction is small, as shown in the second-order perturbation theory with respect to \( U \) [23], and in the FLEX approximation [25]. This fact will also be true below \( T_{c} \) since the particle-nonconserving four point vertex is much smaller than the particle-conserving one [26]. Therefore, we neglect the heat CVC in the present numerical study. We find that the first term in eq. (15), which is proportional to \( \{ q_{kx} \}^{2} \), is predominant, and the other terms which contain the gap velocity, \( q_{kz} \), are negligibly small. On the other hand, the charge CVC gives anomalous transport properties for \( R_{H} \) [2], \( S \) [3], magnetoresistance [24] and Nernst coefficient [25] both in hole-doped and electron-doped systems. Anomalous transport phenomena due to charge CVC are also observed in CeMIn \((M=Co,Rh)\) [27] and in \( \kappa \)-(BEDT-TTF)\( _{2}X \) [28].

Here, we include the QP damping due to impurity scattering \( \gamma_{\text{imp}} \) by replacing \( \Sigma^{nR}(\mathbf{k},\omega) \rightarrow \Sigma^{nR}(\mathbf{k},\omega) - \gamma_{\text{imp}}. \) Then, the total QP damping rate is \( \gamma_{\mathbf{k}} =\gamma_{\mathbf{k}}^{\text{FLEX}} + \gamma_{\text{imp}} \) [13, 29], where \( \gamma_{\mathbf{k}}^{\text{FLEX}} = \text{Im}\Sigma^{nR}(\mathbf{k},\omega)\). In the t-matrix approximation, \( \gamma_{\text{imp}} = n_{\text{imp}}\text{Im}\{ -1/(I^{-1} - g_{0}) \}|_{\omega=0} \), where \( n_{\text{imp}} \) is the impurity concentration, \( I \) is the impurity potential, and \( g_{0} \equiv \frac{1}{N} \sum_{\mathbf{k}} G_{k}^{R} \) is the local Green function. Hereafter, we consider the nearly unitary limit case \( I \sim \infty \) where \( \gamma_{\text{imp}}(T = 0) \) takes a constant value in the self-consistent calculation [13, 29], and assume that \( \gamma_{\text{imp}} \ll \gamma_{\mathbf{k}} \) at \( T > T_{c} \). In this case, we are allowed to put \( \gamma_{\text{imp}}(T = 0) = \gamma_{\text{imp}}(T = 0) \) since the \( T \)-dependence of \( \gamma_{\text{imp}} \) affects \( \kappa \) near \( T_{c} \) only slightly. A schematic \( T \)-dependences of \( \gamma_{\mathbf{k}}^{\text{FLEX}} \) and \( \gamma_{\text{imp}} \) are shown in Fig. 3.

Figure 4 represents the temperature-dependence of \( \kappa \) given by eq. (15). In YBCO, \( \kappa \) increases drastically below \( T_{c} \) since the AF fluctuations, which are the origin of inelastic scattering, are reduced due to the SC gap. Since \( \gamma_{\mathbf{k}} \) is much larger than \( \gamma_{\text{imp}} \) at \( T > T_{c} \), \( \kappa \) in the normal state is affected by \( \gamma_{\text{imp}} \) only slightly. For \( T \ll T_{c} \), the other hand, \( \kappa \) is suppressed by \( \gamma_{\text{imp}} \); \( \kappa \) shows the maximum when \( \gamma_{\mathbf{k}}^{\text{FLEX}} \sim \gamma_{\text{imp}} \) is satisfied at the nodal point. The obtained result is consistent with experiments [7–9]. In strong contrast, in NCCO, “coherence peak” in \( \kappa \) is very small even for \( \gamma_{\text{imp}} = 0 \), which is also consistent with experiments [14, 15].

Here, we discuss the reason why the coherence peak in \( \kappa \) is present in YBCO whereas it is absent in NCCO. Below \( T_{c} \), only thermally excited QPs above the SC gap can contribute to \( \kappa \), except at the nodal point. According to eq. (15), thermal conductivities in the normal state (\( \kappa_{n} \)) and in the line-node SC state (\( \kappa_{s} \)), where \( \rho(\epsilon) \propto |\epsilon| \), are approximately given by

\[ \kappa_{n} \propto \frac{T}{\gamma_{\text{cold}}} \]
(16)
\[ \kappa_{s} \propto \frac{T^{2}}{\gamma_{\text{node}}} \]
(17)
FLEX approximation. In YBCO, both $\gamma$ SC when the cold spot and the nodal point are different. In summary, the coherence peak in temperature drops, $\gamma$ T. In under-doped systems, however, the t-matrix approximation is not sufficient since the radius of “effective impurity potential” is enlarged due to electron-electron correlation, which can be described by the GV'-method in Ref. [31]. For a reliable study of $\kappa$ in under-doped systems, it will be necessary to take account of residual disorders using the GV'-method.

In summary, we studied thermal conductivity $\kappa$ in HTSCs. In the hole-doped case, $\kappa$ shows a prominent “coherence peak” below $T_c$, whereas it is absent in the electron-doped case. Based on the FLEX approximation, such a contrasting behavior of $\kappa$ is well explained, although both YBCO and NCCO are pure $d_{x^2-y^2}$-wave superconductors. We do not have to assume a full-gap state in NCCO (such as $d+is$) to explain the absence of a coherence peak, which originates from the fact that the cold spot (line) in the normal state [$\sim (\pi,0)$] is not on the nodal point (line) of the SC gap. The present study will open the way for the theoretical study of $\kappa$ in various interesting unconventional superconductors.

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where $\gamma_{\text{cold}}$ and $\gamma_{\text{node}}$ represent $\gamma_k$ at the cold spot above $T_c$ and that at the nodal point below $T_c$, respectively.

Figure 5 shows the T-dependence of $\gamma_k$ given by the FLEX approximation. In YBCO, both $\gamma_{\text{cold}}$ and $\gamma_{\text{node}}$ are given by $\gamma_k$ at the same point; $k \approx (\pi/2, \pi/2)$. As the temperature drops, $\gamma_{\text{cold}}$ decreases moderately in proportion to $T$ in the normal state. Below $T_c$, $\gamma_{\text{node}}$ quickly approaches zero since inelastic scattering is suppressed by the SC gap. As a result, $\kappa$ shows a prominent coherence peak below $T_c$, as recognized by eqs. (16) and (17). In NCCO, on the other hand, $\gamma_{\text{cold}}$ is given by $\gamma_k$ at $k \approx (\pi,0)$, which is different from the nodal point of the SC gap; $k \approx (\pi/2, \pi/2)$. Since $\gamma_{\text{node}}$ is much larger than $\gamma_{\text{cold}}$ at $T = T_c$ in NCCO as shown in Fig. 5, $\kappa$ is not enhanced in NCCO below $T_c$. Although the numerical accuracy becomes worse for NCCO below $T \sim 0.015$, the obtained result of $\kappa$ will be qualitatively reliable. In summary, the coherence peak in $\kappa$ is absent even in nodal SC when the cold spot and the nodal point are different.

Figure 6 shows the obtained doping dependence of $\kappa$ in YBCO. In over-doped case ($n = 0.8$), the enhancement of $\kappa$ is largest, and it decreases in optimally ($n = 0.85$) and under-doped ($n = 0.9$) cases since the cold spot approaches the AFBZ as $n \to 1$. This tendency is consistent with experiments [7]. Note that in real materials, $T_c$ in under-doped case is smaller than that in optically-doped case. In the FLEX approximation, however, $T_c$ monotonically increases as $n \to 1$ since the pseudo-gap state in under-doped region cannot be described. The characteristic pseudo-gap phenomena are well described by including the self-energy correction due to strong SC fluctuations into the FLEX approximation, which is called the FLEX+$T$-matrix approximation [25, 30].

In the present work, we assumed that the inelastic scattering is dominant, and neglected the temperature dependence of $\gamma_{\text{imp}}$. This assumption will be allowed for clean optimally-doped HTSCs. In dirty samples where elastic scattering is large, we should calculate the T-dependence of $\gamma_{\text{imp}}$ using the self-consistent t-matrix approximation [13, 29]. In under-doped systems, however, the t-matrix approximation is not sufficient since the radius of “effective impurity potential” is enlarged due to electron-electron correlation, which can be described by the GV'-method in Ref. [31]. For a reliable study of $\kappa$ in under-doped systems, it will be necessary to take account of residual disorders using the GV'-method.

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