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Thermal conductivity, Fermi pockets and superconductivity in underdoped cuprates

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Abstract

The electronic contribution to thermal conductivity is studied in models of underdoped cuprates where the normal state has a pocketed Fermi surface with circumference $\sim x$ (hole concentration) and the superconducting state is formed by opening a gap in the Fermi pocket. The physical consequences of the Fermi pocket are studied by comparing the thermal conductivity computed in four different models: (1) an ordinary d-wave superconductor with four Dirac Fermi points; (2) a normal metal with a pocketed Fermi surface; (3) a superconductor formed by spinon–holon binding in the t–J model; (4) a phenomenological d-wave Bardeen–Cooper–Schrieffer (BCS) superconductor with superconductivity formed by opening a gap on the pocketed Fermi surface. Our results suggest that thermal conductivity provides useful information to distinguish between different scenarios of the normal-to-superconducting transition in underdoped cuprates.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

It is now generally believed that the physics of the underdoped cuprates holds the key to the understanding of high-T_c cuprates [1–3]. The normal (pseudo-gap) state of underdoped high-T_c is rather unconventional [2]. Instead of a normal Fermi surface that obeys the Luttinger theorem [4], the pseudo-gap state has a segmented or pocketed [5] Fermi surface with length of the segment (Fermi arc) $\sim x$, the hole concentration [5–8]. An interesting question that arises naturally is how can a superconductor be formed from a segmented or pocketed Fermi surface? Is the mechanism responsible for the formation of the pseudo-gap the same as the mechanism that eventually leads to superconductivity?

In this paper, we compute the electronic contribution to the thermal conductivity for a series of related models: (1) an ordinary d-wave superconductor with four Dirac Fermi points; (2) a normal metal with a pocketed Fermi surface; (3) a superconductor arising from spinon–holon binding in the t–J model [9]; (4) a phenomenological d-wave BCS superconductor with superconductivity formed by opening a gap on the pocketed Fermi surface. By comparing the results between these different models, we show that the behavior of thermal conductivity at a range of temperatures from zero to above T_c provides useful information about the questions raised above.

2. Model Hamiltonian and formalism

We first introduce a phenomenological model for the normal state of underdoped cuprates with a pocketed Fermi surface,

$$H_{\text{eff}} = \sum_{\vec{k},\sigma} \varepsilon_1(\vec{k}) c^{(1)\dagger}_{\vec{k}\sigma} c^{(1)}_{\vec{k}\sigma} + \varepsilon_2(\vec{k}) c^{(2)\dagger}_{\vec{k}\sigma} c^{(2)}_{\vec{k}\sigma}, \tag{1}$$

where $\varepsilon_{1(2)}(\vec{k}) = +(-)E^{\text{p}}_{\vec{k}} + \varepsilon_c$, as shown in figure 1, and $E^{\text{p}}_{\vec{k}} = \sqrt{\xi^2_{\vec{k}} + (\Delta^{\text{p}}_{\vec{k}})^2}$. The above Hamiltonian describes two branches of fermions with dispersions $\pm E^{\text{p}}_{\vec{k}} + \varepsilon_c$ where $\varepsilon_c \sim x$ is a phenomenological parameter. We shall consider $\xi_{\vec{k}} = -t_{\text{eff}}[\cos(k_x) + \cos(k_y)] - \mu_{\text{f}} + \varepsilon_c$ and $\Delta^{\text{p}}_{\vec{k}} = \Delta_{\text{p}}(T)[\cos(k_x) - \cos(k_y)]$ hereafter, corresponding to a fermion system with kinetic energy $\xi_{\vec{k}}$ and chemical potential μ_{f} gapped by a pseudo-gap $\Delta^{\text{p}}_{\vec{k}}$ with $d_{x^2-y^2}$ symmetry [2, 3, 10]. The electron

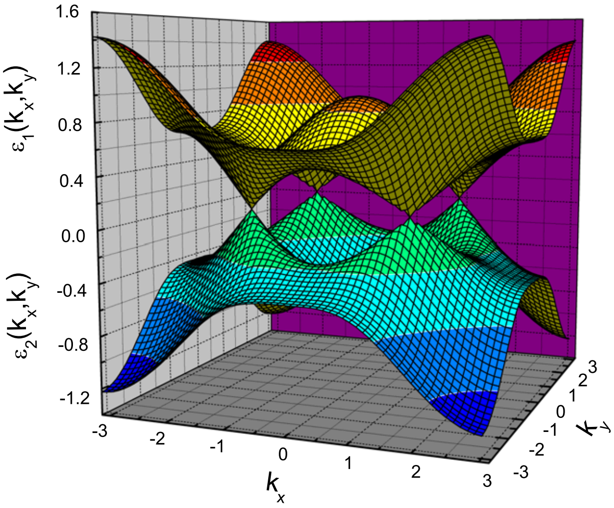


Figure 1. Dispersion relation of $\epsilon_1(\vec{k})$ and $\epsilon_2(\vec{k})$, where we set $x = 0.05$ and the corresponding chemical potential $\mu_f = -0.125$. There are two branch of fermions. The dispersion relation of the up band is $\epsilon_1(\vec{k})$ and the low band dispersion relation is $\epsilon_2(\vec{k})$.

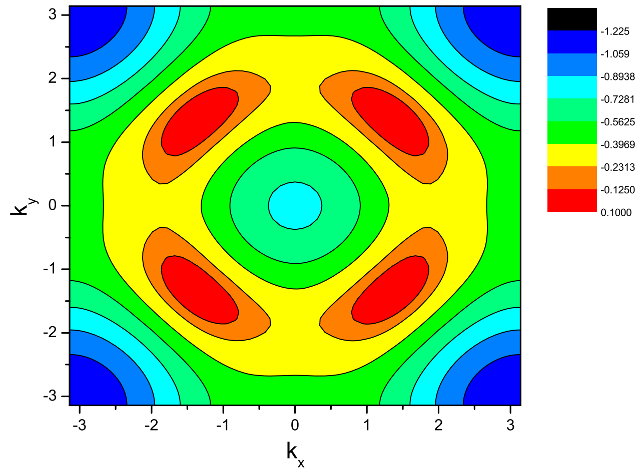


Figure 2. Contour line of $\epsilon_2(\vec{k})$, where we set $x = 0.05$ and the corresponding $\mu_f = -0.125$. The smallest red energy contour loop around $(k_x, k_y) = (\pm\pi/2, \pm\pi/2)$ represents the Fermi surface.

operator in this model is related to the fermion operators $c^{1(2)}_{\vec{k}\sigma}$s by $c_{\vec{k}\sigma} = u^{(1)}_{\vec{k}} c^{(1)}_{\vec{k}\sigma} + u^{(2)}_{\vec{k}} c^{(2)}_{\vec{k}\sigma}$, where $u^{1(2)}_{\vec{k}}$s are coherent factors given by

$$u^{1(2)}_{\vec{k}} = \sqrt{\frac{1}{2}\left(1 + (-)\frac{\xi_{\vec{k}}}{E^{\mathrm{p}}_{\vec{k}}}\right)}.$$

The dispersion $\epsilon_2(\vec{k})$ describes hole pockets around the nodal points $\vec{k}_n$, with $k_{nx} = \pm k_{ny}$ and $\xi_{\vec{k}_n} = 0$. The size of the hole pocket is proportional to the hole concentration $x \sim \varepsilon_c \sim \mu_f$, as shown in figure 2. The coherent factors $u^{1(2)}_{\vec{k}}$s lead to spectral weight differences between the 'inner' and 'outer' region of the hole pocket [3], with larger spectral weight in the 'inner' region, leading to the observation of a Fermi arc in the electron occupation number and photo-emission experiments [2, 9] (see figure 1). The above form of H_{eff} can be derived, for example, from the spinon–holon binding theory of the t–J model [3, 9], a model with a phenomenological ansatz [11] and can also be obtained in a d-density wave state (for $\mu = \epsilon_c$) [12].

Superconductivity can be introduced in the model by adding an effective d-wave BCS pairing term to H_{eff},

$$H_{\text{eff}} \to \sum_{i=1,2}\left[\sum_{\vec{k},\sigma} \varepsilon_i(\vec{k}) c^{(i)\dagger}_{\vec{k}\sigma} c^{(i)}_{\vec{k}\sigma} - \bar{\Delta}_{\vec{k}} c^{(i)}_{-\vec{k}\downarrow} c^{(i)}_{\vec{k}\uparrow} - \bar{\Delta}_{\vec{k}} c^{(i)\dagger}_{\vec{k}\uparrow} c^{(i)\dagger}_{-\vec{k}\downarrow}\right] \tag{2}$$

where $\bar{\Delta}_{\vec{k}} = \Delta_s(T)[\cos(k_x) - \cos(k_y)]$. We assume here that $\bar{\Delta}_{\vec{k}}$ has the same d-wave symmetry as the pseudo-gap but has a different temperature-dependent magnitude governed by $\Delta_s(T)$. The precise nature of $\Delta_s(T)$ and other parameters will be discussed when we consider different models. We assume for simplicity that the pairing gap $\bar{\Delta}_{\vec{k}}$ is the same for both branches of fermions. The resulting energy dispersion relations are $E^2_{1(2)} = |\bar{\Delta}_{\vec{k}}|^2 + [\epsilon_c + (-)E^{\mathrm{p}}_{\vec{k}}]^2$ as shown in figure 3. We note that the first branch of the fermion is fully gapped but nodes exist on the second branch.

Starting from the above effective Hamiltonian, we can compute the thermal conductivity with the Kubo formula [13]. For a system of fermions with a diagonalized BCS Hamiltonian,

$$H = \sum_{\vec{k}} \Psi^{\dagger}_{\vec{k}} h_{\vec{k}} \Psi_{\vec{k}} \tag{3}$$

where

$$\Psi_{\vec{k}} = \begin{pmatrix} \gamma_{\vec{k}\uparrow} \\ \gamma^{\dagger}_{-\vec{k}\downarrow} \end{pmatrix}, \qquad h_k = \begin{pmatrix} E_1(\vec{k}) & 0 \\ 0 & -E_2(\vec{k}) \end{pmatrix}. \tag{4}$$

The thermal conductivity is given by

$$\frac{\kappa_0(T)}{T} = \frac{1}{V}\frac{1}{4\pi}\frac{1}{T^2}\sum_{\vec{k}}\int_{-\infty}^{+\infty} \mathrm{d}\omega \left[-\frac{\partial}{\partial\omega} n_{\mathrm{F}}(\omega)\right]\omega^2 \times \mathrm{Tr}\left[\frac{\partial h_{\vec{k}}}{\partial\vec{k}} A(\vec{k},\omega)\frac{\partial h_{\vec{k}}}{\partial\vec{k}} A(\vec{k},\omega)\right] \equiv \sum_{\vec{k}} \frac{\kappa_0(T,\vec{k})}{T} \tag{5}$$

where $n_{\mathrm{F}}(\omega) = 1/(\mathrm{e}^{\beta\omega} + 1)$ is the fermion occupation number and $A(\vec{k},\omega) = -2\,\mathrm{Im}\,G_{\text{ret}}(\vec{k}, \mathrm{i}\omega)$ is the spectral function of the matrix Green's function [14]. The formula can be generalized to the present case with two independent branches of fermions straightforwardly, where

$$h_k \to \begin{pmatrix} h^{(1)}(\vec{k}) & 0 \\ 0 & h^{(2)}(\vec{k}) \end{pmatrix}$$

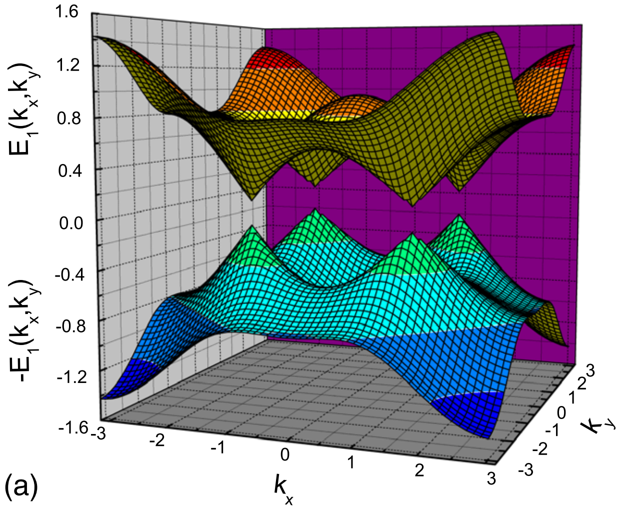
and

$$G_{\text{ret}}(\vec{k}, \mathrm{i}\omega) \to \begin{pmatrix} u^{(1)2}_{\vec{k}} G^{(1)}_{\text{ret}}(\vec{k}, \mathrm{i}\omega) & 0 \\ 0 & u^{(2)2}_{\vec{k}} G^{(2)}_{\text{ret}}(\vec{k}, \mathrm{i}\omega) \end{pmatrix},$$

where $h^{(i)}(\vec{k})$ and $G^{(i)}_{\text{ret}}(\vec{k}, \mathrm{i}\omega)$ are the BCS Hamiltonian matrix and Green's function matrix for the branch (i) fermion, respectively. Putting these together we obtain

$$\frac{\kappa(T)}{T} = \sum_{i=1,2}\sum_{\vec{k}} (u^{(i)}_{\vec{k}})^2 \left(\frac{\kappa^{(i)}_0(T,\vec{k})}{T}\right) \tag{6}$$

where $\kappa^i_0(T,\vec{k})$ $(i = 1, 2)$ is the $\vec{k}$ component of thermal conductivity for the branch (i) BCS superconductor.



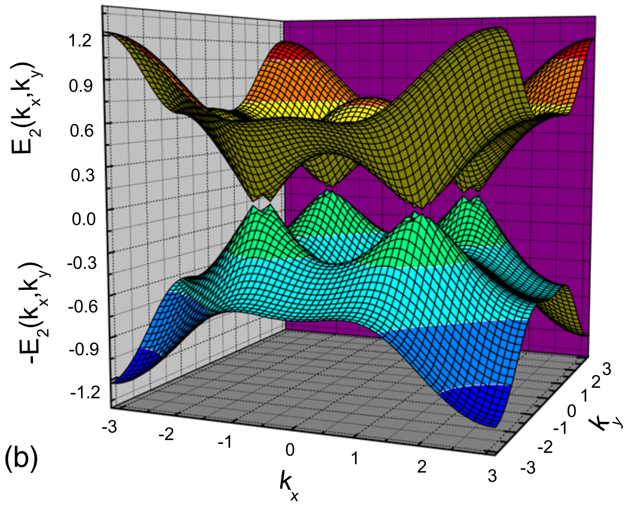


Figure 3. Dispersion relation of $\pm E_i(\vec{k})(i = 1, 2)$, with $x = 0.05$ and the corresponding chemical potential $\mu_f = -0.125$. $\pm E_i(\vec{k})$ are two quasi-particle bands from branch (i) fermions. (a) Dispersion relation of $E_1(\vec{k})$ and $-E_1(\vec{k})$; (b) dispersion relation of $E_2(\vec{k})$ and $-E_2(\vec{k})$.

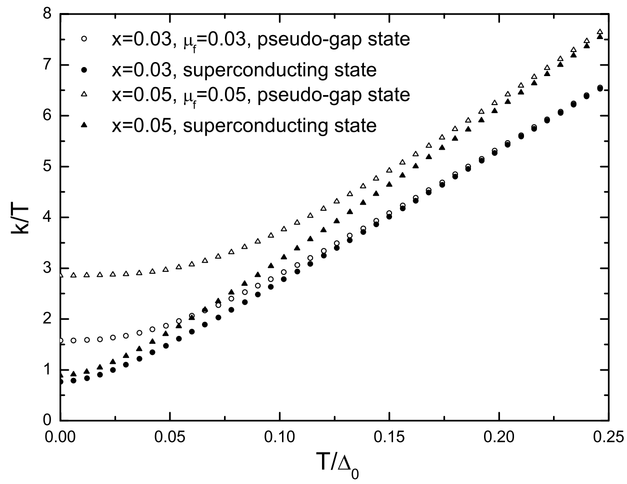


Figure 4. Thermal conductivity for (1) a pure d-wave superconducting state with four Dirac Fermi points and (2) a normal metal with segmented Fermi surface (pseudo-gap state). We set $t_{\mathrm{eff}} \sim (0.75 + 18.0x)\Delta_0$, $\Gamma = 0.15\Delta_0$ and $\varepsilon_c = 6x\Delta_0$ in the numerical calculation.

We shall assume that we are deep in the pseudo-gap regime where $k_B T \ll \Delta_p$ or Δ_s in our following calculations. In this limit we can linearize the fermion dispersion around the nodal points and concentrate on the qualitative effect of superconductivity and the Fermi pocket on thermal conductivity. Notice our purpose is very different from the work in [15] which performed detailed analysis of the thermal conductivity in conventional d-wave superconductors.

3. Thermal conductivity

To begin with, we first revisit ordinary d-wave superconductors where the Fermi surface consists of four Dirac Fermi points. In this case we set $\Delta_p(T) = 0$ and $\Delta_s(T) = \Delta_0 > 0$. We note that thermal conductivity is a measure of quasi-particle excitations only and the same expression for thermal conductivity is obtained if we replace the d-wave superconductor by a pseudo-gap metal with $\Delta_p(T) = \Delta_0$, $\varepsilon_c = 0$ and $\Delta_s(T) = 0$. To illustrate this, we show in figure 4 our numerical results for two different values of hole concentration $x = 0.03, 0.05$ (solid circles and triangles). We consider $k_B T \ll \Delta_0$, and have chosen $t_{\mathrm{eff}} \sim (0.75+18.0x)\Delta_0$, which are parameters obtained from the slave-boson mean-field theory of the t–J model. We also introduce an inverse lifetime $\tau^{-1} = \Gamma = 0.15\Delta_0$ in the electron spectral functions in our calculation. We note that in a realistic calculation of thermal conductivity the temperature dependence of τ^{-1} has to be included for quantitative comparison with experimental data [15]. We have not included this here because we are interested only in the qualitative effects of the Fermi pocket on thermal conductivity that are insensitive to the precise behavior of the parameters we have chosen. In the limit $T \to 0$ we recover the Γ-independent universal thermal conductivity for d-wave superconductors,

$$\frac{\kappa_0(T)}{T} = \left(\frac{\pi^2}{3}k_B^2\right)\frac{1}{\pi^2}\frac{v_f^2 + v_2^2}{v_f v_2}, \tag{7}$$

where v_f and v_2 are the Fermi velocities perpendicular and parallel to the 'Fermi surface' at the nodal points, respectively [14, 15].

Next we consider a normal metal with a pocketed Fermi surface by setting $\Delta_p(T) = \Delta_0$ and $\Delta_s(T) = 0$. The pocket circumference is determined by setting $\varepsilon_c = 6\Delta_0 x$. It is expected that the thermal conductivity will be enhanced compared with the d-wave superconductor at low temperature because the presence of the Fermi surface leads to a larger number of quasi-particles available at low temperature ($k_B T \leqslant \epsilon_c$). The enhancement of thermal conductivity is obvious in figure 4 (open circles and triangles) where we see a clear 'up-turn' in the thermal conductivity at low temperature. The 'up-turn' magnitude is larger for higher doping in our calculation because of the larger Fermi pocket. In the limit $T \to 0$, the thermal conductivity can be calculated analytically with the

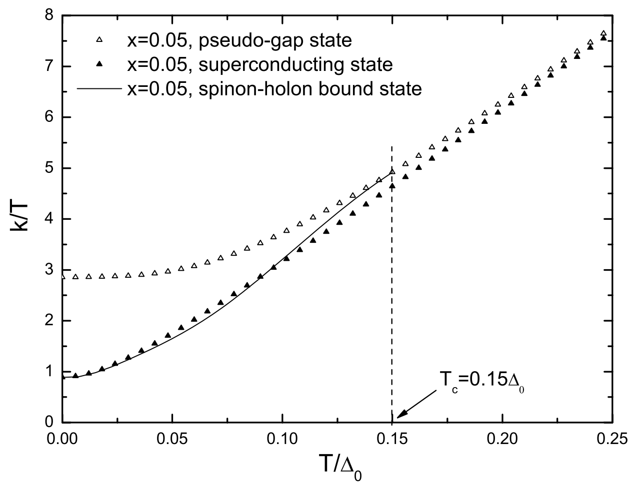


Figure 5. Thermal conductivity of the spinon–holon superconductor (solid line). We choose $\Gamma = 0.15\Delta_0$ and $T_c = 0.09\Delta_0$ in the numerical calculation. The corresponding thermal conductivity for the pure superconductor (solid triangle) and normal metal with segmented Fermi surface (open triangle) are drawn for comparison.

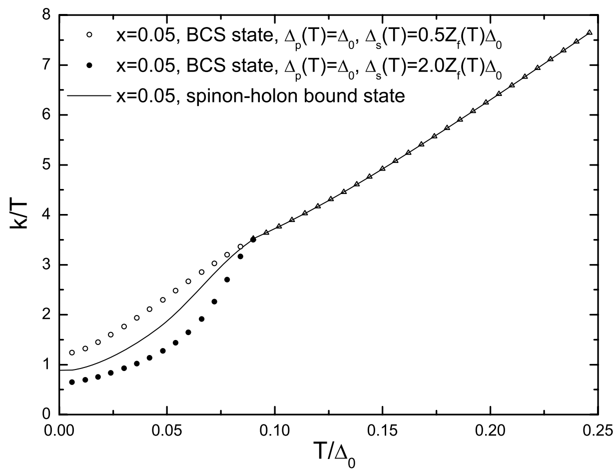


Figure 6. The thermal conductivity of phenomenological d-wave BCS superconductors with different values of superconducting gap $\Delta_s(T) = \alpha Z_f(T)\Delta_0$, $\alpha = 0.5, 1, 2$. Other parameters remain the same as in figure 5. The thermal conductivity of the corresponding s–h superconductor is also shown for comparison.

following result,

$$\frac{\kappa_0(T)}{T} = \left(\frac{\pi^2}{3}k_B^2\right)\frac{1}{\pi^2}\frac{v_f^2+v_2^2}{v_f v_2}\left[1+\frac{\epsilon_c}{\Gamma}\arctan\left(\frac{\epsilon_c}{\Gamma}\right)\right]. \quad (8)$$

The first term in equation (8) is the usual contribution from a d-wave superconductor, whereas the second term can be understood as the contribution from a Drude metal with a Fermi surface of length $\sim x$, assuming $\epsilon_c \gg \Gamma$. This contribution is proportional to Γ^{-1}. The thermal conductivity becomes indistinguishable between the superconductor and the pseudo-gap states at higher temperature because we have set the gap magnitudes (Δ_0) to be the same.

We proceed to compute the thermal conductivity of a specific model where the normal state with the Fermi pocket is formed by bound states of spinons and holons, and the superconducting state is formed by Bose condensation of holons at $T = T_c$ which leads to formation of electron Cooper-pairs (s–h superconductor) [9]. In this case, the system has the special feature that the pseudo-gap merges smoothly into the superconducting gap and the two gaps become indistinguishable in the limit $T \to 0$. Mathematically, the pseudo-gap and superconducting gaps are related to each other by

$$\Delta_s(T) = Z_f(T)\Delta_0, \qquad \Delta_p(T) = [1 - Z_f(T)]\Delta_0 \quad (9)$$

where $Z_f(T) \sim$ the Bose-condensation magnitude in slave-boson mean-field theory. We shall assume $Z_f(T) = 1 - (\frac{T}{T_c})^{3/2}$ in the following calculations, corresponding to a three-dimensional free boson gas where $Z_f(T) = 0$ at $T > T_c$, and goes to 1 smoothly as $T \to 0$ [9]. The results of the calculation are shown in figure 5 for $x = 0.05$, where we also show the corresponding results for a pure d-wave superconductor ($\Delta_s(T) = \Delta_0$, $\Delta_p = 0$) and a normal metal with a pocketed Fermi surface ($\Delta_s = 0$, $\Delta_p = \Delta_0$) for comparison. We find that the s–h superconductor thermal conductivity merges with the thermal conductivity of the corresponding pure d-wave superconductor at $T \to 0$ as a result of merging of the two gaps ($Z_f \to 1$), increases faster than the thermal conductivity of the corresponding d-wave superconductor at low temperature and merges eventually with that of the pseudo-gap metal ($Z_f \to 0$) at $T > T_c$. In particular, a 'bump'-like feature appears in the thermal conductivity at around T_c in the s–h superconductor, which is absent in the thermal conductivity of pure d-wave superconductors. As we shall see below, the 'bump' feature indicates a crossover of thermal conductivity from the (normal state) Fermi pocket behavior at $T \geqslant T_c$ to the behavior of a normal d-wave superconductor at $T \ll T_c$ and is quite independent of the microscopic details of the models.

Lastly, we consider a phenomenological d-wave superconductor where $\Delta_p(T)$ and $\Delta_s(T)$ come from different microscopic origins and have no particular relation to one another. In this case the thermal conductivity at $T \to 0$ will be given by formula equation (7) with different values of $\tilde{v}_f$ and $\tilde{v}_2$ which have no definite relation to the effective values v_f and v_2 extracted from the pseudo-gap phase.

To illustrate this we compute in figure 6 the thermal conductivity for superconductors with $\Delta_s(T) = \alpha Z_f(T)\Delta_0$, $\Delta_p(T) = \Delta_0$ for different values of $\alpha = 0.5, 1, 2$. The existence of a 'bump' feature and a change in qualitative behavior of thermal conductivity below T_c is quite apparent. In particular, we note that the $T \to 0$ values of thermal conductivity differ quite a lot from the corresponding values of the s–h superconductor for $\alpha \neq 1$.

The thermal conductivity at very low temperature can be computed analytically for our models (3) ($\alpha = 1$) and (4) ($\alpha \neq 1$) in a Sommerfeld expansion. We obtain to order T^2,

$$\frac{\kappa_0(T)}{T} = \left(\frac{\pi^2}{3}k_B^2\right)\frac{1}{\pi^2}\frac{v_f^2+(\bar{v}_2(T))^2}{v_f\bar{v}_2(T)}\left[1+\frac{7\pi^2}{5}\left(\frac{k_BT}{\Gamma}\right)^2\right], \quad (10)$$

where $\bar{v}_2(T) = \alpha Z_f(T)v_2$. In general, $Z_f(T) \sim 1 - aT^\beta$ at low temperature where a, β are positive numbers and the expression differs qualitatively from that of ordinary d-wave superconductors where $\kappa_0(T)/T \sim a' + b'T^2$ [16] as long as $\beta < 2$.

4. Discussion

We note that we consider only the electronic contribution to the thermal conductivity in our above analysis. However, phonons also contribute significantly to the thermal conductivity except at very low temperatures and a challenging question is how we can separate the two contributions at the intermediate range of temperature in which we are interested. It was suggested in [17] that the phonon contributions can be separated by studying the magnetic field dependence of thermal conductivity. The technique suggested in the paper may be too crude to pin down the fine structures in thermal conductivity but is probably sufficient for identifying the broad features suggested in our paper.

A frequently asked question in the study of high-T_c cuprates is whether a small Fermi surface really exists in the normal state of underdoped cuprates as is observed in photo-emission [8] and magnetic oscillation [5] experiments. By comparing the results from the different models we studied above, we find that thermal conductivity at a range of temperatures from zero to above T_c provides useful insight into this question. We observe that thermal conductivity of a normal metal with a small Fermi surface has an 'up-turn' at low temperature, with the magnitude of the 'up-turn' being similar in size to that of the Fermi pocket. The corresponding superconductor formed from this normal state will exhibit a 'bump' structure in thermal conductivity at temperatures around T_c. This structure will disappear if the Fermi pocket disappears and thermal conductivity provides a test of its existence. A more direct test for the Fermi pocket can be performed for cuprate superconductors with very low T_c where superconductivity can be destroyed by a strong magnetic field. In this case we expect that an up-turn in the thermal conductivity with magnitude $\sim x$ will be observed at low temperature if the Fermi pocket exists. We note, however, that new electronic states may form in the presence of strong magnetic field and would invalidate our prediction.

Another frequently asked question is whether the microscopic mechanism responsible for the pseudo-gap is the same mechanism that eventually leads to superconductivity. Our study suggests that if the superconductivity and pseudo-gap are arising from the same microscopic origin, the two gaps will become indistinguishable at low temperature and the $T \to 0$ value of thermal conductivity will be close to the thermal conductivity value extrapolated from the $T \gg T_c$ data to $T \to 0$. This 'coincidence' will not occur in general if the two gaps arise from different microscopic origins. We note, however, that we have assumed a constant Γ in our calculation, and the extrapolation will not be accurate if $\Gamma(T)$ has a strong temperature dependence.

5. Conclusion

Summarizing, using a phenomenological model, we examine in this paper the electronic contribution to thermal conductivity in several different situations: (1) an ordinary d-wave superconductor with four Dirac Fermi points; (2) a normal metal with a pocketed Fermi surface; (3) a superconductor formed from spinon–holon binding in the t–J model; (4) a phenomenological d-wave BCS superconductor formed by opening a gap in a normal metal with a pocketed Fermi surface. By comparing the results from these different models, we find that the behavior of thermal conductivity at a range of temperatures from zero to above T_c may provide useful information to some of the frequently asked questions in the study of underdoped high-T_c cuprates. We note that reliable experimental data for thermal conductivity is so far available only at $T \ll T_c$ and accurate data at the whole range of temperatures between $T = 0$ to T_c do not yet exist because of large contributions to thermal conductivity from non-electronic origins [17, 18]. However, a recent experimental study of the impurity effect on low temperature thermal conductivity indicates a breakdown of universal thermal conductivity predicted for pure d-wave superconductors [15, 19] and a separate experiment indicates that a Fermi pocket does not exist in a underdoped LSCO sample which is metallic but shows no superconductivity [20]. The latter experimental result is in agreement with our model (3), which assumes that the normal state is a state with no Bose condensation ($Z_f = 0$, $\Delta_s(T) = 0$, $\Delta_p(T) = \Delta_0$). These results suggest that thermal conductivity is indeed a useful tool to probe the physics behind high-T_c cuprates and our phenomenological analysis provides useful guidance to interpret the experimental results.

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