Anomalous Thermal Conductivity of Semi-Metallic Superconductors with Electron-Hole Compensation

Hiroto ADACHI * and Manfred SIGRIST

Theoretische Physik, ETH-Hönggerberg, Zurich 8093, Switzerland

The effects of low carrier density and carrier compensation on mixed-state thermal transport are investigated beyond the quasiclassical approximation. It is shown that, contrary to the usual observations, the interplay of the two effects leads to an increase in the thermal conductivity immediately below the upper critical field $H_c2$. Our result can account for the anomalous behavior of the mixed-state thermal conductivity near $H_c2$ recently observed in URu$_2$Si$_2$.

KEYWORDS: semi-metallic superconductor, electron-hole compensation, mixed-state thermal conductivity, heavy fermion superconductor

The discovery of the Nernst effect in the normal state region of underdoped cuprates$^{1}$ has initiated renewed interest in magneto-transport phenomena in exotic superconductors. While a fluctuating vortex contribution may be a natural explanation for the unusual Nernst signal in cuprate, two other important aspects for magneto-transport phenomena were recently pointed out by Behnia and coworkers$^{2,3}$: the effects of electron-hole compensation$^{2}$ and low carrier density.$^{3}$ The recent experiments on ultraclean URu$_2$Si$_2$ by Kasahara et al.$^4$ have motivated our study of these two points with regard to mixed-state thermal transport. The most intriguing result of ref. 4 is the increase in the low-temperature thermal conductivity below the upper critical field $H_c2$, showing a hump structure.$^5$ Usually in the low-temperature limit, the thermal conductivity of a clean type-II superconductor decreases below $H_c2$,$^7$ due to the enhancement of the Andreev scattering rate by vortices and the reduction of the density of states at the Fermi energy.$^8,9$

The key feature behind this anomalous behavior lies in the electronic structure of URu$_2$Si$_2$ introduced by the so-called hidden-order phase occurring below $T^*$ = 17.5 K.$^{10–12}$ In this phase, the carrier density is drastically reduced, as seen in several transport measurements.$^{13–15}$ Furthermore, a nearly perfect $H^2$-dependence of the magneto-resistance without any sign of saturation suggests the compensation of electron and hole pockets of the Fermi surface. This interpretation is further supported by the relatively small Hall angle.

In this letter, we address the effects of the low carrier density and carrier compensation on thermal transport in the mixed phase using a simple model of a two-dimensional $s$-wave superconductor. This allows us to explain the unusual magnetic-field dependence of the thermal conductivity below $H_c2$ found in ref. 4 for URu$_2$Si$_2$, at least on a qualitative level. Since in this study it is necessary to go beyond the quasiclassical approximation, we generalize the approximation scheme for obtaining the Brandt-Pesch-Tewordt Green’s function$^{19}$ valid near $H_c2$, by employing the formalism of Vavilov and Mineev$^{17}$ originally developed to describe the mixed-state de Haas-van Alphen effect.

We start by briefly reviewing the method of ref. 17. Gor’kov equations for a two-dimensional $s$-wave superconductor under strong magnetic fields ($k_B = c = \hbar = 1$) are as follows:

$$[\varepsilon_n - H_0(r) - \hat{u}(r) - \hat{\Delta}(r)]\hat{G}(r, r'; \varepsilon_n) = \delta(r - r'),$$

where $H_0 + \hat{u} + \hat{\Delta} = (H_{0,+} + \hat{\Delta}^*_{\theta} - H_{0,-} - \hat{\Delta}_\theta), \hat{G} = (\hat{G}^0, \hat{G}^\tau),$ and $\varepsilon_n = 2\pi T(n + 1/2)$ is the fermionic Matsubara frequency. The short-range impurity potential $u(r)$ obeys the Gaussian ensemble $u(r) = 0; u(r)u(r') = (1/m^*\tau)\delta(r - r')$ with $m^*$ and $\tau$ being the effective mass and the mean free time of quasiparticles, respectively. The single-particle Hamiltonian $H_0$ is expressed as $H_0(r) = \frac{m^*}{2\mu}Q^2 - \mu$, where $Q = -i\nabla + |e|A(r)$ with the vector potential $A(r)$, and $\mu$ is the Fermi energy. For the magnetic field we assume the Landau gauge $A(r) = H x \hat{y}$, i.e., a uniform field as justified near $H_c2$, if the Ginzburg-Landau parameter $\kappa_{GL}$ is large ($\kappa_{GL} \gg 1$ in URu$_2$Si$_2$). For simplicity, we have dropped the Zeeman coupling term, although paramagnetic effects may be non-negligible in URu$_2$Si$_2$.$^{39}$ The paramagnetic limiting effects are, however, beyond the scope of this letter.

The single-particle Hamiltonian $H_0(r)$ can be diagonalized with the eigenvalues $\zeta_N = \omega_c(N + 1/2) - \mu$ and the eigenfunctions$^{20}$

$$\phi_N(r|q) = \pi^{1/4} \sum_{m=-\infty}^{\infty} \exp \left( \frac{\sqrt{\pi m}}{\lambda} (y - \lambda^2 q_x) + i q_y y \right) \times \phi_N \left( \frac{x + (\sqrt{\pi m} + q_y) \lambda^2}{\lambda} \right),$$

where $\omega_c = |e|H/m^*,$ $\phi_N(x) = \frac{1}{\sqrt{2^N N! \sqrt{\pi}}} H_N(x) e^{-x^2},$ $\lambda = (|e|H)^{-1/2},$ $H_N(x)$ is the $N^{th}$ Hermite polynomial, and $q$ represents the quasi-momentum in the magnetic sublattices.$^{31}$ We have chosen a rectangular lattice$^{17}$ with edges $a_x = a$ and $a_y = 2a$ ($a = \sqrt{\pi} \lambda$). We introduce the magnetic sublattice representation

$$G(r_1, r_2; \varepsilon_n)$$
\[ \rho_{\alpha\beta}(q) = \frac{1}{(2\pi)^2} \int \frac{d\xi}{\Delta(\xi)} \frac{1}{\epsilon(\xi) - \xi - q} \]
Fig. 1. Magnetic-field dependences of thermal conductivity. Here, \( \kappa_{0}^{(e+h)} = \left( \frac{4}{7} \right) T \left( k_{F}^{(e)} l_{\text{imp}}^{(e)} + k_{F}^{(h)} l_{\text{imp}}^{(h)} \right) \) is the normal state thermal conductivity at zero magnetic field. \( \tilde{V}_{\text{pair}} = V^{(e)} \left( 1, 0, 1 \right) \) was used.

in which the relations \( k_{F}^{(h)}/k_{F}^{(e)} = 1, l_{\text{imp}}^{(h)}/l_{\text{imp}}^{(e)} = 1, \) and \( \Delta_{0}^{(h)}/\Delta_{0}^{(e)} = 1 \) hold. Figure 1 shows the magnetic-field dependences of \( \kappa_{L}^{\text{EX}} \) for several values of \( k_{F}^{(e)} \zeta_{0}^{(e)} \). For a large value of \( k_{F}^{(e)} \zeta_{0}^{(e)} (= 10) \), the calculated \( \kappa_{L}^{\text{EX}} \) decreases for fields below \( H_{c2} \). This is consistent with the well-known behavior\(^\text{7-9}\) found in quasiclassical calculations (\( k_{F}^{(e)} \zeta_{0}^{(e)} \rightarrow \infty \)). However, as the carrier density (or \( k_{F}^{(e)} \zeta_{0}^{(e)} \)) is reduced, a new property appears. On lowering the magnetic field, \( \kappa_{L}^{\text{EX}} \) initially increases below \( H_{c2} \) and then decreases, forming a hump structure. In case of a single carrier-type without electron-hole compensation, \( \kappa_{L}^{\text{EX}} \) does not show this kind of hump structure even for small values of \( k_{F}^{(e)} \zeta_{0}^{(e)} \) because of the second term in eq. (10).

The hump structure of \( \kappa_{L}^{\text{EX}} \) below \( H_{c2} \) becomes even more pronounced if the sizes of the energy gaps are different, i.e., \( \Delta_{0}^{(h)}/\Delta_{0}^{(e)} \neq 1 \). In this case, the second term in eq. (10) becomes nonzero below \( H_{c2} \) and enhances the size of the hump. This is actually seen in Fig. 2 where \( \kappa_{L}^{\text{EX}} \) is depicted as a function of magnetic field for different ratios of the two gaps. With a decreasing ratio \( \Delta_{0}^{(h)}/\Delta_{0}^{(e)} \), the increase in \( \kappa_{L}^{\text{EX}} \) below \( H_{c2} \) is enhanced. Evidently, the violation of compensation in the superconducting phase enhances the hump structure below \( H_{c2} \).

Finally, we compare our results with the mixed-state thermal conductivity of URu$_{2}$Si$_{2}$. Note that our analysis yields only a qualitative understanding because we employ a simple quasiparticle picture with a two-dimensional isotropic Fermi surface and neglect the paramagnetic effect as well as the correlation effects. We fix the parameters as follows. From the values \( H_{c2} \approx 2.8 \ T \) for \( H \parallel c \) together with \( k_{F} \approx 1.1 \ \text{nm}^{-1} \),\(^\text{3}\) and taking into account the fact that there is a substantial paramagnetic effect\(^\text{10}\) in this material, we have a rough estimate \( k_{F} \zeta_{0} \approx 6.5 \). For the mean free path, we use \( l_{\text{imp}}^{(e)}/l_{\text{imp}}^{(e)} = 60 \) and \( l_{\text{imp}}^{(h)}/l_{\text{imp}}^{(e)} = 5.5 \) in order to reproduce the observed magneto-resistance (\( \Delta_{\rho x}(10T)/\rho_{xx}(0T) \approx 300 \)) with a nearly perfect \( H^{2}\)-dependence (see the inset of Fig. 3). This choice of parameters is consistent with the scenario\(^\text{4}\) in which the Hall effect is dominated by the light hole band. Further, the positive Hall coefficient and the measured value\(^\text{28}\) \( \rho_{xy}(10T)/\rho_{xx}(0T) \approx 50 \) gives an estimate \( k_{F}^{(h)}/k_{F}^{(e)} = 1.01 \). Finally, we have assumed that a larger gap is formed in the electron band following the discussion in ref. 4. For the gap ratio, we use \( \Delta_{0}^{(h)}/\Delta_{0}^{(e)} = 0.31 \).

The main panel of Fig. 3 shows the calculated thermal conductivity of URu$_{2}$Si$_{2}$ as a function of the magnetic field. The peculiar magnetic-field dependence of the thermal conductivity with the hump structure below \( H_{c2} \) is reproduced, with its size being slightly larger than the measured one in our calculation.\(^\text{4}\) The neglected interband impurity scattering would reduce the size of the hump. It should be noted that while the size of the hump is modified by changing the parameters, the appearance of the hump itself is robust for parameters reproducing the magneto-resistance data.\(^\text{4}\) In the experiment, the thermal conductivity increases sharply below \( H_{c2} \), which...
most probably results from a paramagnetic limiting effect in this material, which we neglect here. In our model case, the hump develops more gently. To treat these other effects is beyond the scope of our study and therefore we leave it for future studies.

The special scattering features provide some physical insight into this behavior. For the superclean limit $\omega_c \tau \gg 1$,\(^{29}\) the heat transport along $-\nabla T$ by quasiparticles is only possible through scattering (see Fig. 4(a)), as otherwise the quasiparticles would experience only the drift motion perpendicular to $-\nabla T$. In the normal state at low temperatures, this corresponds mainly to impurity scattering. In the superconducting mixed phase, an additional contribution is derived from Andreev scattering.\(^{8,30}\) Hence, at high magnetic fields, the Andreev scattering tends to increase the thermal conductivity below $H_{c2}$. At lower fields (smaller $\omega_c \tau$), the Andreev scattering plays a different role. The particle and hole trajectories tend to retrace (Fig. 4(b)). Because both quasiparticle types carry heat, a compensation occurs, which decreases the heat current parallel to $-\nabla T$ and $\kappa^E_M$ decreases at lower fields. The overall behavior leads to the characteristic hump feature. Note that this picture of the single-carrier $\kappa_{xx}$ is applicable to $\kappa^E_M$ because electron-hole compensation leads to the suppression of the second term in eq. (10). In the ordinary case without the compensation, this picture cannot be applied to $\kappa^E_M$ because the second term in eq. (10) makes an important contribution to $\kappa^E_M$ at high fields, veiling the hump below $H_{c2}$.

In conclusion, we have examined the effects of the low carrier density and the electron-hole compensation on mixed-state thermal transport. The interplay of these two effects leads to the appearance of a hump structure of $\kappa_{xx}(H)$ below $H_{c2}$, as observed in URu$_2$Si$_2$, whose electronic states incorporate the two features in the hidden-order phase. Our study provides a natural explanation for the unusual magnetic-field dependence of $\kappa_{xx}(H)$ near $H_{c2}$. Moreover, it demonstrates that URu$_2$Si$_2$ provides a rare chance to examine the physics of the mixed phase in the superclean limit, resulting in intriguing magneto-transport phenomena.

We are grateful to Y. Matsuda, T. Shibauchi, Y. Kasahara and N. Hayashi for insightful discussions. This study was financially supported through a fellowship of the Japan Society for the Promotion of Science and the NCCR MaNEP of the Swiss National foundation.

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