Universal behavior of the thermopower of heavy-fermion metals

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We reveal and explain a universal scaling behavior of the thermopower $S/T$ in heavy-fermion (HF) compounds. Using the archetypical HF metal YbRh$_2$Si$_2$ as an example, we demonstrate that the scaling behavior of $S/T$ is violated by the antiferromagnetic phase transition, since both the residual resistivity $\rho_0$ and the density of states $N$ experience jumps at the phase transition, making the thermopower experience two jumps and change its sign. Our elucidation is based on flattening of the single-particle spectrum that profoundly affects $\rho_0$ and $N$. To depict the main features of the $S/T$ behavior, we construct the $T$–$B$ schematic phase diagram. Our calculated $S/T$ for YbRh$_2$Si$_2$ and for [BiBa$_{0.66}$K$_{0.36}$O$_2$]CoO$_2$ are in good agreement with experimental observations.

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Heavy-fermion (HF) metals are constantly and intensively studied. It is commonly believed that their behavior is determined by quantum critical point (QCP) that generates non-Fermi liquid (NFL) behavior, revealing vivid deviations from the Landau Fermi liquid (LFL) behavior. QCP is usually associated with a magnetic QCP, see e.g. [1, 2]. The NFL behavior is commonly characterized by a set of exponents of the temperature dependence of the physical properties, such as specific heat, resistivity, susceptibility etc. [3, 4]. These exponents are different from those of ordinary Fermi liquids. The LFL and NFL behaviors, and the crossover region cannot be captured by any single exponent as seen, for example, from Fig. 1 (a), that depicts the behavior of the normalized specific heat $C/T$ extracted from measurements of the specific heat $C$ on YbRh$_2$Si$_2$. In the vicinity of QCP it is helpful to use “internal” scales to measure $C/T$ and the temperature $T$ in order to reveal a universal scaling behavior. A maximum structure $(C/T)_N$ in $C/T$ at temperature $T_M$ appears with the application of magnetic field $B$ and $T_M$ acquires higher values as $B$ is increased. To obtain $(C/T)_N$, we use $(C/T)_M$ and $T_M$ as “internal” scales: $(C/T)_M$ is used to normalize $C/T$, and $T$ is normalized by $T_M$. Fig. 1 (a) shows the resulting $(C/T)_N$ as a function of normalized temperature $\tilde{T}_N = T/T_M$, with different symbols for different magnetic field strengths $B$. It is seen that the LFL and NFL states are separated by a crossover region where $(C/T)_N$ reaches its maximal value. This figure displays the scaling behavior of the normalized experimental curves. The curves for different $B$ values merge into a single curve when viewed in terms of the normalized temperature $\tilde{T}_N = T/T_M$. As evident from Fig. 1 (a), $(C/T)_N$ is not a constant as would be for a LFL; furthermore, it demonstrates the asserted scaling behavior over a wide range of values of the normalized temperature $\tilde{T}_N$. This behavior coincides with that of the magnetic susceptibility $\chi \propto C/T \propto M^*$ revealed in measurements on [BiBa$_{0.66}$K$_{0.36}$O$_2$]CoO$_2$ and incorporated in Fig. 1 (b), where $M^*$ is the effective mass. The solid line tracks the results of the same calculations that describe the universal scaling behavior $(C/T)_N$ shown in Fig. 1 (a). We thus conclude that the solid curve drawn in Figs. 1 (a) and (b) exhibits a universal scaling behavior intrinsic to this system. Calculations carried out within the framework of fermion condensation (FC) theory [5–7] and represented by the solid curve are in good agreement with the data. In this theory, the QCP is interpreted as a fermion-condensation quantum phase transition (FCQPT) at which the quasiparticle effective mass $M^*$ diverges. In such an event, quasiparticles of energy $\epsilon$ remain well-defined excitations near the chemical potential $\mu$, $\epsilon \sim \mu$, while the FC state itself is protected by topological invariants [8, 9]. A study of the thermoelectric power $S$ may deliver new insight into the nature of the quantum phase transition that defines the NFL behavior of the corresponding HF compound. For example, one may reasonably propose that the thermoelectric power $S$ distinguishes between two competing scenarios for quantum phase transitions in heavy fermions, namely the spin-density-wave theory and the breakdown of the Kondo effect [10, 11]. Indeed, $S$ is sensitive to the derivative of the density of electronic states and the change in the relaxation time at $\mu$. Using the Boltzmann equation, the thermopower $S$ can be written as

$$S = -\frac{\pi^2 k_B^2 T}{3 e} \left[ \frac{\partial \ln \sigma(\epsilon)}{\partial \epsilon} \right]_{\epsilon = \mu},$$

where $k_B$ and $e$ are, respectively, the Boltzmann constant and the elementary charge, while $\sigma$ is the dc electric conductivity of the system, given by

$$\sigma(\epsilon) = 2 e^2 \tau(\epsilon) \int \delta(\mu - \epsilon(p)) v(p) v(p) \frac{dp}{(2\pi)^3}.$$
The solid curve represents calculations of \( \frac{C}{T} \) of states \( N \) \( \rightarrow \) nature (b) Scaled susceptibility \( \frac{C}{T} \) and change in the relaxation time at the derivative of the density of electronic states and the \( p \) in the panel (a).

\[ YbRh_{2}Si_{2} \]

FIG. 1: (color online) (a) The normalized specific heat \( \left( C/T \right)_{N} \) versus normalized temperature \( T_{N} \). \( \left( C/T \right)_{N} \) is extracted from the measurements of the specific heat \( C/T \) on \( YbRh_{2}Si_{2} \) in magnetic fields \( B \) listed in the legend. The LFL region, crossover one, and NFL one are depicted by the arrows. The solid curve displays calculations of \( \left( C/T \right)_{N} \). (b) Scaled susceptility \( \chi \) as a function of scaled temperature \( T/(B-B_{c0}) \) for various \( B \) values shown in the legend. The solid curve represents calculations of \( \left( C/T \right)_{N} \) displayed in the panel (a).

\[ \mathbf{p} \] is the electron wave-vector, \( \tau \) is the scattering time, and \( v \) denotes the velocity of electron. Thus, we see from Eq. 2 that the thermoelectric power \( S \) is sensitive to the derivative of the density of electronic states and the change in the relaxation time at \( \varepsilon = \mu \). On the basis of the Fermi liquid theory description, the term in the brackets on the right hand side of Eq. 1 can be simplified, so that one has \( S \propto TN(\varepsilon = \mu) \propto C \) at \( T \to 0 \). In the LFL phase of a HF metal the density of states \( N(\varepsilon) \) is temperature independent, and \( S \propto C \) becomes proportional to \( T \), since both quantities are proportional to the electronic density of states. As a result, that charge and heat currents at low temperatures are transported by quasiparticles in LFL, the ratio \( q \) is approximately constant, \( q = en(S/C) \simeq en(S/S_{enl}) \simeq \pm 1 \), where \( n \) is the number density of the charge carriers and \( S_{enl} \) the entropy density of charge carriers. In this Communication we show that the thermopower \( S/T \) of different HF compounds exhibits universal scaling behavior. This universal behavior coincides with that of the normalized specific heat \( \left( C/T \right)_{N} \) shown in Fig. 1 (a). Using the archetypical HF metal \( YbRh_{2}Si_{2} \) as an example, we also demonstrate that the universal behavior of \( S/T \) is violated by the AF phase transition, since the residual resistivity and the density of states experience jumps at the phase transition. This results in corresponding downward jumps of \( S/T \) and its change of sign. To depict the main features of the \( S/T \) behavior, we construct a schematic \( T-B \) phase diagram. Our calculated \( S/T \) of \( YbRh_{2}Si_{2} \) and of the HF cobalt oxide \([BiBa_{0.66}K_{0.36}O_{2}]CoO_{2}\) are found to be in good agreement with experimental observations.
In calculating the thermopower $S/T$ and its universal behavior, we model the HF as a homogeneous liquid, since this permits us to avoid complications associated with the crystalline anisotropy of solids. To reveal the universal behavior of the thermopower, we normalize $S/T$ in the same way as in the normalization of $C/T$: the normalized function $(S/T)_N$ is obtained by normalizing $(S/T)$ by its maximum value, occurring at $T = T_M$, and the temperature $T$ is scaled by $T_M$. Taking into account that $S/T \propto C/T$ at $T > T_N$, we conclude that $(S/T)_N = (C/T)_N$, provided that the system in question is located away from possible phase transitions. This universal function $(C/T)_N$ is displayed in Fig. 3(a). Figures 3 (a) and (b) report $(S/T)_N$, extracted from measurements on YbRh$_2$Si$_2$\cite{19,20}, as a function of the normalized magnetic field $B_N$ and $T_N$, respectively. In Fig. 3(a),

FIG. 3: (color online) (a) Normalized isotherm $(S(B)/T)_N$ versus normalized magnetic field $B_N$ for different temperatures shown in the legend. The LFL behavior takes place at $B_N > 1$. (b) Temperature dependence of the normalized thermopower $(S/T)_N$ under several magnetic fields shown in the legend. The data confined by the ellipse violate the scaling behavior taken at the AF phase. The data are extracted from measurements on YbRh$_2$Si$_2$\cite{19,20}. The solid curves in (a) and (b) represent calculated $(C/T)_N$ displayed in Fig 4(a).

FIG. 4: (color online) Panel (a): Single-particle energy $\varepsilon(p)$ and distribution function $n(p)$ at $T = 0$. The arrow shows the chemical potential $\mu$. The vertical lines show the area $p_i < p < p_f$ occupied by FC with $0 < n_0(p) < 1$ and $\varepsilon(p) = \mu$. The Fermi momentum $p_F$ satisfies the condition $p_i < p_F < p_f$ and corresponds to the LFL state, indicated by the arrows, that emerges when the FC state is eliminated. The arrow depicts hole states induced by the FC. Panel (b): Schematic $T - B$ phase diagram of YbRh$_2$Si$_2$. The vertical and horizontal arrows, crossing the transition region depicted by the thick lines, show the LFL-NFL and NFL-LFL transitions at fixed $B$ and $T$, respectively. The hatched area around the solid curve $T_{crossover}(B)$ represents the crossover between the NFL and LFL domains. The NFL state is characterized by the entropy excess $S_0$ given by Eq. 3. As shown by the solid curve, at $B < B_{c0}$ the system is in its AF state. The line of AF phase transitions is denoted by $T_{NL}(B)$. The tricritical point, indicated by the arrow, is at $T = T_{c0}$. At $T < T_{c0}$ the AF phase transition becomes of first order. At that transition the thermopower changes its sign, thus $S/T > 0$, for the hole states shown in the panel (a) vanish at $T < T_{c0}$.
the function \((S/T)_N\) is obtained by normalizing \((S/T)\) by its maximum occurring at \(B_M\), and the field \(B\) is scaled by \(B_M\). We note that the LFL behavior takes place at \(B_N > 1\), since \(S/T \propto M^r\), and \(M^r \propto (B - B_0)^{-2/3}\) are \(T\)-independent. At \(B_N < 1\), \(M^r\) becomes \(T\)-dependent and exhibits the NFL behavior. It is seen from Figs. 3 (a) and (b) that the calculated values of the universal function \((C/T)_N\) are in good agreement with the corresponding experimental data over the wide range of the normalized magnetic field. Thus, \((S/T)_N\) exhibits universal scaling behavior over a wide range of its scaled variable \(B_N\) and \(T_N\). Figure 3 (a) also depicts a violation of the scaling behavior for \(B < B_0\) when the system enters the AF phase. Moreover, as seen from Figs. 2 and 3 (a), the scaling behavior is violated at \(T \leq T_{NL}\) by two downward jumps. The first jump, shown in Figs. 2 and 3 (a) and labeled Jump1, takes place at \(T_{NL} > T > 0.3\) K, while the second, occurring at \(T \leq 0.03\) K, is shown in Fig. 2 and labeled Jump2. The latter is accompanied by a change of sign of \((S/T)_N\), which now becomes positive. As we shall see, these two jumps reflect the presence of flat band at \(\mu\) in the single particle spectrum \(\varepsilon(p)\) of heavy electrons in YbRh2Si2.

Before proceeding to the analysis of these jumps, some remarks are in order concerning the flattening of the spectrum \(\varepsilon(p)\) in HF systems, a phenomenon called swelling of the Fermi surface or FC. As indicated in Fig. 3 (a), the ground states of systems with flat bands are degenerate, and therefore the occupation numbers \(n_0(p)\) of single-particle states belonging to a flat band are given by a continuous function on the interval \([0, 1]\), in contrast to the FL restriction to occupation numbers 0 and 1. This property leads to an entropy excess

\[
S_0 = -\sum n_0(p) \ln n_0(p) + (1 - n_0(p)) \ln(1 - n_0(p)), \tag{3}
\]

that does not contribute to the specific heat \(C(T)\). The entropy excess \(S_0\) contradicts the Nernst theorem. To circumvent violation of the Nernst theorem, FC must be completely eliminated at \(T \to 0\). This can happen by virtue of some phase transition, e.g., the AF transition that becomes of first order at some tricritical point occurring at \(T = T_c\). Such a first-order phase transition provides for eradication of the flat portion in the spectrum \(\varepsilon(p)\). As a consequence, both the density of states \(N\) and the hole states, shown by the arrow in Fig. 4 (a), vanish discontinuously, while the occupation numbers \(n(p)\) and the spectrum \(\varepsilon(p)\) revert to those LFL theory, as indicated by the arrows in Fig. 3 (a). Simultaneously, the Fermi surface undergoes an abrupt change on the interval from the Fermi momentum \(p_f\) to \(p_P\), so as to nullify the swelling of the Fermi surface. We note that the abrupt change is observed as the change of the low-\(T\) Hall coefficient. It is seen from Fig. 2 that at \(T = 0.03\) K \(S/T\) abruptly change it sign, for the hole states vanish. The positive sign of \(S/T\) of YbRh2Si2 without the hole states is in agreement with the positive thermopower of the nonmagnetic counterpart LuRh2Si2, lacking the 4f hole states at \(\mu\). Contrary, at \(T_{NL} > T > T_{cr}\) the AF phase transition is of the second order and the entropy is a continuous function at the border of the phase transition. Therefore, both the occupation numbers and the spectrum \(\varepsilon(p)\) become a HF LFL, and keep their FC-like shape, while FC itself is destroyed. This destruction generates the first jump, shown in Fig. 2 - as the FC state is decayed, its contribution \(\rho_0^{FC}\) to the residual resistivity \(\rho_0\) vanishes, resulting in the change of the scattering time \(\tau(\varepsilon = \mu)\). As a result, the thermopower experiences the first jump, as seen from Eqs. 11 and 12. We recall that in the presence of FC, \(\rho_0 = \rho_0^{FC} + \rho_0^{imp}\), where \(\rho_0^{imp}\) is formed by impurities. We also conclude that the second downward jump under decreasing \(B\) is deeper than the first one, since it is caused by elimination of both \(\rho_0^{FC}\) and the hole states. This is consistent with the experimental observations, as seen from Fig. 2.

![FIG. 5](image_url)

**FIG. 5:** (color online) Temperature dependence of \((S(T)/T)_N\) at magnetic field \(B = 0\), extracted from measurements on \([\text{BiBa}_{0.66}\text{K}_{0.36}\text{O}_2]\text{CoO}_2\), is displayed versus \(T_N\). The solid line is the same as one depicted in Fig. 1 (a).

Fig. 1 (b) displays our constructed schematic \(T - B\) phase diagram for YbRh2Si2. Clearly, on the basis of this phase diagram, the behavior of \(S_N(T, B)\), considered as a function of the dimensionless variable \(T_N\) or \(B_N\), is almost universal. Indeed, as seen from Figs. 1 (a), (b), 3 (a), (b), and 5 all the data, extracted from measurements on YbRh2Si2 and \([\text{BiBa}_{0.66}\text{K}_{0.36}\text{O}_2]\text{CoO}_2\), collapse on the single scaling curve. As seen from Figs. 1 (a) and 3 (b), at \(T_N < 1\), \((S/T)_N\) tends to become constant, implying that \(S\) exhibits LFL behavior. However, at \(T_N \approx 1\) the system enters the narrow crossover region, while at growing temperatures, NFL behavior prevails.

We now show that the observed scaling behavior of \((S(T)/T)_N\) is universal by analyzing experimental data on the thermopower for the strongly correlated layered cobalt oxide \([\text{BiBa}_{0.66}\text{K}_{0.36}\text{O}_2]\text{CoO}_2\). By plotting \((S(T)/T)_N\) as a function of \(T_N\) in Fig. 5 the universal scaling behavior and the three regimes are seen to be in a complete agreement with the reported overall behavior.
in both Figs. 1 (a), (b), and Figs. 3 (a), (b) as well.

In summary, we have revealed and explained the universal scaling behavior of the thermopower $S/T$ in different HF compounds. This universal behavior is consistent with such behavior of the specific heat and of the magnetic susceptibility in HF metals. We have also shown that destruction of the flattening of the single-particle spectrum profoundly affects $S/T$, leading to the two jumps and the change of sign of the thermopower occurring at the antiferromagnetic phase transition. Our calculations of $S/T$ for YbRh$_2$Si$_2$ and for [BiBa$_{0.66}$K$_{0.36}$O$_2$]CoO$_2$ are in good agreement with experimental observations.

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