Theory of Quasi-Universal Ratio of Seebeck Coefficient to Specific Heat in Zero-Temperature Limit in Correlated Metals

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It is shown that the quasi-universal ratio \( q = \lim_{T \to 0} eS/C \sim \pm 1 \) of the Seebeck coefficient to the specific heat in the limit of \( T = 0 \) observed in a series of strongly correlated metals can be understood on the basis of the Fermi liquid theory description. In deriving this result, it is crucial that a relevant scattering arises from impurities, but not from the mutual scattering of quasiparticles. The systematics of the sign of \( q \) is shown to reflect the sign of the logarithmic derivative of the density of states and the inverse mass tensor of the quasiparticles, explaining the systematics of experiments. In particular, the positive sign of \( q \) for Ce-based and \( f^3 \)-based heavy fermions, and the negative sign for Yb-based and \( f^2 \)-based heavy fermions, are explained. The case of non-Fermi liquid near the quantum critical point (QCP) is briefly mentioned, showing that the ratio \( q \) decreases considerably toward antiferromagnetic QCP while it remains essentially unchanged for the ferromagnetic QCP or QCP due to a local criticality.

KEYWORDS: Seebeck coefficient, specific heat, Fermi liquid, strongly correlated metals, periodic Anderson model

Strongly correlated electron systems exhibit some quasi-universal ratios among various physical quantities. The Wilson ratio, \( \chi/\gamma \), of the magnetic susceptibility \( \chi \) to the Sommerfeld coefficient \( \gamma \), and the so-called Kadowaki-Woods ratio \( A/\gamma^2 \), \( A \) being the coefficient of the \( T^2 \)-term of the resistivity, take a quasi-universal value in a series of strongly correlated electron systems up to logarithmic accuracy. The validity of the Fermi liquid theory and the dynamical nature of the mass enhancement lie behind the universality. Quite recently, Behnia, Jaccard, and Flouquet have revealed that the ratio of the Seebeck coefficient \( S \) to the specific heat \( \gamma T \) takes a quasi-universal value, in the low-temperature limit, for a series of correlated compounds. The purpose of this Letter is to clarify the reason for the universal value for \( eS/\gamma T \) on the basis of the Fermi liquid theory for thermoelectricity.

A firm starting point is that the canonical formula for the Seebeck coefficient \( S \) in the zero-temperature limit is valid even though strong correlations are apparent among the electrons:

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

(1)
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where \( e ( > 0) \) is the elementary charge, \( \sigma(\varepsilon) \) is the conductivity of electrons with energy \( \varepsilon \), and \( \mu \) is the chemical potential at \( T = 0 \). Although the above expression was derived for a single-band Fermi liquid, there is no reason for doubting its validity also in the multiband Fermi liquid. Therefore, we discuss the Seebeck coefficient on the basis of formula (1). Then, we use the conductivity for a multicarrier system:

\[
\sigma(\varepsilon) = \sum_i \sigma_i(\varepsilon),
\]

in the expression of the Seebeck coefficient, (1). Here, \( \sigma_i \) denotes the conductivity due to the \( i \)-th Fermi surface of multicomponent carriers. By some algebra, we obtain the rule of summing the Seebeck coefficient of each component as follows:

\[
S = \sum_i \frac{\sigma_i}{\sigma} S_i.
\]

**Single-Band Fermi liquid**

First, we discuss the case of heavy fermions with a single Fermi surface. The conductivity of a single-band Fermi liquid is approximated as

\[
\sigma(\varepsilon) = e^2 \tau(\varepsilon) \sum_k \delta(\varepsilon - \varepsilon(\vec{k})) \langle v_{\alpha}(\vec{k})v^{*}_{\alpha}(\vec{k}) \rangle,
\]

where \( v^{*} \) denotes the renormalized velocity by vertex corrections due to the many-body effect, and \( \langle \cdots \rangle \) denotes the average over the direction \( \alpha (= x, y, z) \). Here, \( \vec{v}(\vec{k}) \equiv \partial E_{\vec{k}}/\partial \vec{k} \), \( E_{\vec{k}} \) being the dispersion of the quasiparticle, and \( \tau(\varepsilon) \) denotes the transport collision time of the quasiparticles with energy \( \varepsilon \). Hereafter, the renormalized velocity \( v^{*}_{\alpha} \) is approximated by \( v_{\alpha} \), because the impurity scattering plays a dominant role for which such renormalization is not crucial.

The transport collision time for the Fermi liquid is given, around the Fermi level in the zero-temperature limit, as

\[
\tau(\varepsilon)^{-1} = \tau_{\text{imp}}(\varepsilon)^{-1} + B(\varepsilon - \mu)^2,
\]

where \( \tau_{\text{imp}}(\varepsilon) \) is the collision time due to impurity scattering, and \( B \) is a constant of the order of the inverse effective Fermi energy. The second term in the collision rate (5) makes no contribution to \( S \) since the following relation holds:

\[
\lim_{\varepsilon \to \mu} \frac{\partial}{\partial \varepsilon} \ln \tau(\varepsilon) = \lim_{\varepsilon \to \mu} \frac{\partial}{\partial \varepsilon} \ln \tau_{\text{imp}}(\varepsilon).
\]

Therefore, the Seebeck coefficient for a single-band Fermi liquid is expressed as

\[
S = -\frac{\pi^2 k_B^2 T}{3 e} \lim_{\varepsilon = \mu} \left\{ \frac{\partial}{\partial \varepsilon} \ln \tau_{\text{imp}}(\varepsilon) \right. \\
\left. + \frac{\sum_k \delta(\varepsilon - E_{\vec{k}})(\partial v_{\alpha}(\vec{k})/\partial k_{\alpha})}{\sum_k \delta(\varepsilon - E_{\vec{k}})\langle v_{\alpha}(\vec{k})v_{\alpha}(\vec{k}) \rangle} \right\}.
\]
\( \equiv -\frac{\pi^2 k_B^2 T}{3 e} \mathcal{F}. \quad (7) \)

The collision rate due to impurity scattering in the \( t \)-matrix approximation is given by
\[
\tau_{\text{imp}}(\epsilon)^{1-1} = \frac{2\pi z(\epsilon) N^*(\epsilon) u^2}{1 + [\pi z(\epsilon) N^*(\epsilon) u^2]^2} \times c_{\text{imp}}, \quad (8)
\]
where \( c_{\text{imp}} \) is the impurity concentration, \( N^*(\epsilon) \) is the density of states (DOS) of the renormalized quasiparticles, and \( z(\epsilon) \) is the renormalization amplitude. In deriving eq.(8), we have assumed the \( s \)-wave impurity potential and also neglected the real part of the electron self-energy due to impurity scattering. Then, the logarithmic derivative of \( \tau_{\text{imp}} \) is given as
\[
\lim_{\epsilon \to \mu} \frac{\partial}{\partial \epsilon} \ln \tau_{\text{imp}}(\epsilon) = \frac{\pi z(\mu) N^*(\mu) u^2 - 1}{\pi z(\mu) N^*(\mu) u^2 + 1} \times \frac{\partial}{\partial \epsilon} \ln N^*(\epsilon) \bigg|_{\epsilon = \mu}. \quad (9)
\]

Here, we have used the estimation \( \lim_{\epsilon \to \mu} |\partial \ln z(\epsilon)/\partial \epsilon| \ll \lim_{\epsilon \to \mu} |\partial \ln N^*(\epsilon)/\partial \epsilon| \), which has been verified by explicit calculations, e.g., FLEX approximation for \( t-t' \) Hubbard model near the half-filling.\(^{11,12} \) It is noted that \( z(\mu) N^*(\mu) \) is of the same order as the unrenormalized one since the mass enhancement in \( N^* \) is cancelled by the smallness of \( z \), while the logarithmic derivative of \( N^* \) is highly enhanced in a heavy fermion situation.

In order to make the discussion explicit, we proceed with the periodic Anderson model (PAM):
\[
H_{\text{PAM}} = \sum_{\vec{k}} \left\{ \epsilon_{\vec{k}} c_{\vec{k} \sigma}^+ c_{\vec{k} \sigma} + \epsilon_{\vec{f}} f_{\vec{k} \sigma}^+ f_{\vec{k} \sigma} + \left[ V_{\vec{k}} c_{\vec{k} \sigma}^+ f_{\vec{k} \sigma} + \text{h.c.} \right] \right\} + U \sum_i n_{\uparrow i} n_{\downarrow i}, \quad (10)
\]
where the notations are conventional. According to the Fermi liquid theory based on PAM,\(^4 \) the effective Hamiltonian of quasiparticles near the Fermi level is given as
\[
H_{\text{qp}} = \sum_{\vec{k}} \left\{ \epsilon_{\vec{k}} c_{\vec{k} \sigma}^+ c_{\vec{k} \sigma} + \tilde{\epsilon}_{\vec{f}} f_{\vec{k} \sigma}^+ f_{\vec{k} \sigma} + \left[ \tilde{V}_{\vec{k}} c_{\vec{k} \sigma}^+ f_{\vec{k} \sigma} + \text{h.c.} \right] \right\}, \quad (11)
\]
where the renormalized \( f \)-level is determined by the \( f \)-electron self-energy \( \Sigma_{\vec{f}} \) and the renormalization amplitude \( a_{\vec{f}} \) as,
\[
\tilde{\epsilon}_{\vec{f}} \equiv a_{\vec{f}} [\epsilon_{\vec{f}} + \Sigma_{\vec{f}}(\mu)], \quad (12)
\]
and \( \tilde{V}_{\vec{k}} = \sqrt{a_{\vec{f}}} V_{\vec{k}} \). The \( k \)-dependence of \( \Sigma_{\vec{f}} \) should be rather weaker than \( N_F^\text{cond}|V|^2 \), because it is the only way to realize the heavy fermion state by satisfying the two conditions, the Landau-Luttinger sum rule\(^{13,14} \) and the requirement that the \( f \)-electron number \( n_{\vec{f}} \) at each site be nearly unity, \( n_{\vec{f}} \simeq 1 \). Then, the dispersion of the quasiparticles is given as
\[
E_{\vec{k}} = \frac{1}{2} \left[ \epsilon_{\vec{k}} + \tilde{\epsilon}_{\vec{f}} - \sqrt{(\epsilon_{\vec{k}} - \tilde{\epsilon}_{\vec{f}})^2 + 4|\tilde{V}_{\vec{k}}|^2} \right], \quad (13)
\]
where we have assumed the Fermi level is located at the bonding band which is considered to correspond to the Ce-based heavy fermions.
Then, the DOS of the quasiparticles, \( N^*(\epsilon) \equiv 2 \sum_{\vec{k}} \delta(\epsilon - E_{\vec{k}}) \), is given by the standard calculation as follows:

\[
N^*(\epsilon) = 2N^{\text{cond}} \frac{\epsilon^*(\epsilon) - 2\epsilon + \bar{\epsilon}_f}{\bar{\epsilon}_f - \epsilon},
\]

(14)

where \( N^{\text{cond}} \) is the DOS of the conduction electrons, and \( \epsilon^*(\epsilon) \) is determined by the following equation:

\[
\epsilon = \frac{1}{2} \left[ \epsilon^*(\epsilon) + \bar{\epsilon}_f - \sqrt{(\epsilon^*(\epsilon) - \bar{\epsilon}_f)^2 + 4|\vec{V}_{\vec{k}}|^2} \right],
\]

(15)

and is of the order of \( D \), half the bandwidth of conduction electrons. Since \( |\epsilon^*(\epsilon) - \mu| \gg |\bar{\epsilon}_f - \epsilon| \), the DOS is given near the Fermi level, \( \epsilon = \mu \), as

\[
N^*(\epsilon) \sim 2N^{\text{cond}} \frac{D}{|\bar{\epsilon}_f - \epsilon|} = \frac{b}{|\bar{\epsilon}_f - \epsilon|},
\]

(16)

where \( b \) is a constant of \( O(1) \) because \( N^{\text{cond}} D \sim 1 \). Thus, the logarithmic derivative of DOS is given by the following simple expression:

\[
\left. \frac{\partial}{\partial \epsilon} \ln N^*(\epsilon) \right|_{\epsilon=\mu} = -\frac{1}{\mu - \bar{\epsilon}_f}.
\]

(17)

It is noted that the denominator is of the order of the effective Fermi energy.

Now we discuss the second term in the brace of (7). With the use of the dispersion relation (13), the velocity of quasiparticles \( \vec{v}_{\alpha}(\vec{k}) \equiv \partial E_{\vec{k}}/\partial k_{\alpha} \) is estimated near the Fermi level as

\[
\vec{v}_{\alpha}(\vec{k}) = \frac{\bar{\epsilon}_f - E_{\vec{k}}}{\bar{\epsilon}_f + \epsilon_{\vec{k}} - 2E_{\vec{k}}/\partial k_{\alpha}} \approx \frac{\bar{\epsilon}_f - \mu}{\epsilon^*(\mu)} \frac{\partial \epsilon_{\vec{k}}}{\partial k_{\alpha}},
\]

(18)

where we have considered the fact \( |\bar{\epsilon}_f - E_{\vec{k}}| \ll \epsilon^*(\mu) \). The inverse mass tensor is given as

\[
\frac{\partial \epsilon_{\vec{k}}}{\partial k_{\alpha}} \approx -2 \frac{\bar{\epsilon}_f - E_{\vec{k}}}{\epsilon^*(\mu)^2} \left( \frac{\partial \epsilon_{\vec{k}}}{\partial k_{\alpha}} \right)^2 + \frac{\bar{\epsilon}_f - E_{\vec{k}}}{\epsilon^*(\mu)} \frac{\partial^2 \epsilon_{\vec{k}}}{\partial k_{\alpha}^2}.
\]

(19)

Therefore, the second term in the brace of (7) is calculated as

\[
\frac{\sum_{\vec{k}} \delta(\epsilon - E_{\vec{k}}) \partial v_{\alpha}(\vec{k})/\partial k_{\alpha}}{\sum_{\vec{k}} \delta(\epsilon - E_{\vec{k}}) v_{\alpha}(\vec{k}) v_{\beta}(\vec{k})} = 2 - \eta \frac{1}{\epsilon - \bar{\epsilon}_f},
\]

(20)

where \( \eta \equiv \epsilon^*(\mu)(\partial^2 \epsilon_{\vec{k}}/\partial k_{\alpha}^2)/(\partial \epsilon_{\vec{k}}/\partial k_{\alpha})^2 \), which is equal to 1/2 for the free electron dispersion and 0 for the linear dispersion of conduction electrons.

Collecting the relations (9), (17), and (20), the factor \( \mathcal{F} \) in eq.(7) is expressed as

\[
\mathcal{F} = \frac{3 - \eta + (1 - \eta)[\pi z(\mu) N^*(\mu) u^2]}{1 + [\pi z(\mu) N^*(\mu) u^2]} \times \frac{1}{\mu - \bar{\epsilon}_f}.
\]

(21)

Therefore, the ratio \( q \) of the Seebeck coefficient given by eq.(7) to the specific heat \( \gamma T \) is reduced to the concise form of

\[
q \equiv \frac{S e}{T \gamma} = \frac{3 - \eta + (1 - \eta)[\pi z(\mu) N^*(\mu) u^2]}{1 + [\pi z(\mu) N^*(\mu) u^2]} \times \frac{1}{b},
\]

(22)

where \( \gamma \equiv \pi^2 k_B^2 N^*(\mu)/3 \) is the Sommerfeld coefficient, and \( b \equiv N^*(\mu)(\bar{\epsilon}_f - \mu) \). In deriving eq.(22), we have used eq.(16). The ratio \( q \) depends on the character of the impurity scattering:
For a weak impurity potential producing the Born scattering \((zN^*u \ll 1)\), \(q \simeq (3 - \eta)/b\), while \(q \simeq (1 - \eta)/b\) for the impurity with the unitarity scattering \((zN^*u \gg 1)\). The strength of scattering by actual impurities extends from weak to strong coupling. Therefore, we should have taken an average over the impurities when we derived relation (8), rather than simply multiplying the impurity concentration \(c_{\text{imp}}\). If we do so, however, a simple expression as (22) will not be obtained. Therefore, for simplicity, we simply take the average of expression (22) over the strength of the impurity potential. As expected physically, most impurities will have an intermediate character. Therefore, it is reasonable to expect that the ratio is of the order of \(O(1)\), leading to the quasi-universal value for \(q \sim +1\) for Ce-based heavy fermions. A crucial point here is that strong renormalization effects in \(S\) and \(\gamma\) cancel each other out, as in the case of the Kadowaki-Woods ratio.\(^3,4\)

In the case of Yb-based heavy fermions, we should apply the hole version of the above discussions, in which the Fermi level is located on the antibonding band in an electron picture. Even in this case, expressions (14), and (16)-(21), are valid. Since \(\mu > \bar{\varepsilon}_f\), the sign of (22) changes, leading to \(q \sim -1\). These results explain the observed universal behavior of the Yb-based heavy fermion compounds.\(^5\)

**Non-Fermi Liquid near Quantum Critical Point**

In the case near the antiferromagnetic (AF) quantum critical point (QCP), where the quasiparticles are still well defined, the DOS \(N^*(\epsilon)\) is nearly symmetric around the chemical potential. Indeed, near the AF-QCP in 3d, \(N^*(\epsilon) \propto \text{const.} - [(\epsilon - \mu)^2 + \omega_0^2]^{1/4} \times N_{\text{loc}}^*(\epsilon)\), with \(\omega_0\) being the energy scale inversely proportional to the staggered susceptibility and \(N_{\text{loc}}^*(\epsilon)\) being the DOS renormalized by a local correlation effect as discussed above. It is noted that \(\omega_0\) has \(T\)-dependence, \(\propto T^{3/2}\), in general. Therefore, \(\lim_{\epsilon \to \mu} \partial \ln N^*(\epsilon)/\partial \epsilon = \lim_{\epsilon \to \mu} \partial \ln N_{\text{loc}}^*(\epsilon)/\partial \epsilon\). Furthermore, the second term in eq.(7) is shown to remain unenhanced by the AF critical fluctuations. Indeed, the velocity \(v_\alpha\) appearing in eq.(20) depends crucially on the position on the Fermi surface, and vanishes in proportion to the inverse of the logarithm of its energy on the hot lines but remains finite otherwise. Then, the summation with respect to \(\vec{k}\) on the Fermi surface remains of the same order of magnitude as away from the QCP.\(^15\)

Therefore, the ratio \(q\) near the AF-QCP is given as \(|q| \sim N_{\text{loc}}^*(\epsilon)/N^*(\epsilon)|_{\epsilon = \mu}\), which is far less than unity at AF-QCP because \(N^*(\mu)\) is enhanced compared to \(N_{\text{loc}}(\mu)\) by AF critical fluctuations, although it does not diverge. On the other hand, near the ferromagnetic (F) QCP, \(q\) remains of the same order as that away from QCP, because the second term of eq.(7) is proportional to the mass enhancement factor both due to local correlation, given by eq.(20), and the F critical fluctuations which enhance the effective mass equally at all points on the Fermi surface, in contrast to the AF critical fluctuations discussed above. The estimation of the first term in eq.(7) is also valid for F-QCP. Then, the ratio \(q\) exhibits only a small decrease
leaving \( q \sim \pm 1 \) with a logarithmic accuracy.

Thus, the ratio \( q \) considerably decreases toward the AF-QCP but does not change appreciably for the F-QCP. The estimation for F-QCP is also valid for the local quantum criticality, where all the points on the Fermi surface are subject to the effect of critical fluctuations.\(^{16,17}\) These predictions may be explored by experiments around QCP tuned by altering the pressure or the magnetic field.

**Multiband Fermi liquid**

Actual heavy fermion compounds have a multiband structure and plural Fermi surfaces. Therefore, one should calculate \( S_i \), the contribution from the \( i \)-th band, and sum up by using formula (3) with weight \( \sigma_i/\sigma \). In the zero-temperature limit, where only the impurity scattering is relevant to the thermoelectricity, \( \sigma_i/\sigma \) is of the same order for all of the bands because the renormalization effect cancels out for the impurity scattering\(^{18}\) unless a renormalization of the impurity potential due to the quantum critical fluctuations develops.\(^{19,20}\) Indeed, the conductivity of light (\( \ell \)) and heavy (\( h \)) bands is given by

\[
\sigma_{\ell,h} \sim e^2 \tau_{\text{imp}} (v_{F,\ell,h})^2 N_{F,\ell,h},
\]

where the collision time \( \tau_{\text{imp}} \) is given by

\[
(\tau_{\text{imp},\ell,h})^{-1} = 2\pi^2 c_{\text{imp}} u^2 (z_{\ell,h})^2 N_{F,\ell,h}.
\]

It is easy to see that the renormalization factors \( z \) are cancelled among those included in \( v \propto z \) and \( N_F \propto z^{-1} \). Then, \( \sigma_{\ell} \sim \sigma_{h} \) if the impurity potentials for light and heavy carriers are comparable as expected.\(^{21}\) Therefore, the contribution of \( S_i \) from the heavier band dominates because \( |S_{h}| \gg |S_{\ell}| \).

Some heavy fermion compounds such as CeCu\(_2\)Si\(_2\) are compensated metals for which we have to take into account the multiband conduction electrons. Nevertheless, enhancement occurs in the first and second terms in eq. (7) in proportion to \( -\partial \ln N^*(\epsilon)/\partial \epsilon|_{\epsilon=\mu} \) in each heavy fermion band, maintaining the validity of the result for a single-band Fermi liquid. This is because the Fermi level is located just below the level corresponding to the divergence of DOS due to the hybridization effect, which causes the hybridization gap in the case of a single conduction band. A crucial point is that the sign of \( \partial \ln N^*(\epsilon)/\partial \epsilon \) and the inverse mass tensor do not depend on the sign of the velocity but on the curvature of the dispersion of quasiparticles. This explains why the \( q \) value is positive for Sr\(_2\)RuO\(_4\) even though the \( \gamma \)-band (heaviest band) is electron-like with the negative Hall coefficient, \( R_H < 0 \). Indeed, the energy derivative of the DOS of the \( \gamma \)-band is positive due to the van Hove singularity located just above the Fermi level.\(^{22}\) It is also the case in (BEDT-TTF) salt reported in ref. 5. Indeed, the DOS in the Hückel type tight-binding theory seems to explain the difference in the sign of the Seebeck coefficient between the \( b \)- and \( c \)-directions.\(^{23}\)
A prediction based on the above result is that CeRu$_2$Si$_2$ with $q \sim +1$ without the magnetic field $H = 0$ changes the sign of $q$ just above the metamagnetic field $H_M$ for the temperature gradient along the $c$-axis. This is because the singular peak of the DOS arising from the flat band structure around $(0, 0, \pi/c)$, which is located above the Fermi level, is expected to shift down to the Fermi level at $H > H_M$, leading to the reversal of the signs of $\partial \ln N^*(\epsilon)/\partial \epsilon$ and the inverse mass tensor.

$f^2$-Based Heavy Fermions

The above theory for heavy fermions is valid for $f^1$-based compounds. On the other hand, $f^2$-based heavy fermions, such as U- and Pr-based compounds, have a different structure of the quasiparticle band. In such systems, one has to take into account the plural $f$-orbitals split by the crystalline electric field (CEF) effect. It gradually became apparent in the mid 90s that the effective CEF splitting is considerably suppressed to be less than the renormalized energy scale, the effective Fermi energy, while that of the $f^1$-based systems is slightly enhanced due to the correlation effect.$^{26, 27}$ Indeed, this is the only way for the mass of quasiparticles to be highly enhanced by satisfying the two conditions, the Landau-Luttinger sum rule$^{13, 14}$ and the requirement that the $f$-electron number $n_{if}$ of the $i$-th orbital ($i = 1, 2$) at each site be nearly unity, $n_{if} \approx 1$, as seen below. It was shown on the basis of the investigation of the $f^0$-$f^1$-$f^2$ model$^{27}$ that the mass enhancement arises only if the $f$-electron number is nearly 1 or 2, as long as the two $f$-orbitals with a low-lying CEF level are relevant.

The effective Hamiltonian for the quasiparticles of $f^2$-based heavy fermions is given in the form:

$$H_{qp} = \sum_{\vec{k}} \left\{ \epsilon_{\vec{k}} c_{\vec{k}\sigma}^+ c_{\vec{k}\sigma}^+ + \sum_{i=1,2} \tilde{\epsilon}_{if} f_{i\vec{k}\sigma}^+ f_{i\vec{k}\sigma}^+ 
+ \sum_{i=1,2} \tilde{V}_{i\vec{k}}^2 c_{i\vec{k}\sigma}^+ f_{i\vec{k}}^+ + \text{h.c.} \right\},$$

where the renormalized $f$-levels $\tilde{\epsilon}_{if}$’s and the renormalized hybridizations $\tilde{V}_{i\vec{k}}$’s are given by the orbital-dependent $f$-electron self-energy and the renormalization amplitude as

$$\tilde{\epsilon}_{if} \equiv a_{if}[\epsilon_{if} + \Sigma_{if}(\mu)],$$

and $\tilde{V}_{i\vec{k}} \equiv \sqrt{a_{if}} V_{i\vec{k}}$. The dispersion of the quasiparticles $E_{\vec{k}}$ is given as three solutions of

$$\prod_{i=1,2} (\tilde{\epsilon}_{if} - E_{\vec{k}})(\epsilon_{\vec{k}} - E_{\vec{k}}) = \sum_{i=1,2} \tilde{V}_{i\vec{k}}^2 (\tilde{\epsilon}_{if} - E_{\vec{k}}).$$

The schematic behavior of the dispersion is shown in Fig. 1. The renormalized $f$-levels are lifted from their original positions in such a way that the total electrons per site are distributed to two $f$-electrons and the rest to the conduction electrons. The number of correlated electrons is counted using the Landau-Luttinger sum rule, while that of the conduction electrons is...
counted by summing up the $k$-points below the Fermi energy. Then, it is easily seen that the two $f$-electrons occupy the orbital of the lower level $\tilde{\epsilon}_{1f}$ unless the renormalized level splitting $\tilde{\Delta} \equiv \tilde{\epsilon}_{2f} - \tilde{\epsilon}_{1f}$ is far less than the width of each band $\sim a_t|\tilde{V}|^2/D$. On the other hand, if $\tilde{\Delta}$ is significantly smaller than $a_t|\tilde{V}|^2/D$, it is possible to satisfy the above two conditions because the lower level then consists of both $f$-orbitals with nearly equal weight. This is the reason why the renormalized level splitting is considerably reduced to make the $f^2$-based heavy fermion band.\textsuperscript{26,27} It is not difficult to see that eq.(27) has a trivial solution at some $k$ as

$$E_k = \epsilon_k = \tilde{\epsilon} \equiv \frac{\tilde{V}_1^2 \tilde{\epsilon}_{1f} + \tilde{V}_2^2 \tilde{\epsilon}_{2f}}{\tilde{V}_2^2},$$

(28)

where $\tilde{V}_2^2 \equiv (\tilde{V}_1^2 \pm \tilde{V}_2^2)$.

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Fig. 1. Schematic view of the dispersion of $f^2$-based heavy fermions in some direction in the Brillouin zone. The dispersion $\epsilon_k$ of conduction electrons is assumed to be linear, and $k_F$ and $k_B$ denote the Fermi wavevector and the zone boundary, respectively. The dashed curves are for a noninteracting system, and the solid curves are for a renormalized dispersion. The energy scale of the right-hand panel is enlarged compared to the left-hand one. It is noted that effective CEF splitting is reduced to be smaller than the characteristic energy scale $T_0$. 

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Formal solutions of eq.(27) near the renormalized \( f \)-levels are given similarly to eq.(13) as
\[
E_k^\pm = \tilde{\epsilon} + \frac{\hat{V}_k^2}{2\hat{V}_k^2} - \frac{\hat{V}_k^2}{2\hat{\epsilon}_k} \pm \sqrt{\frac{\Delta^2}{4} + \left( \frac{\hat{V}_k^2}{2\hat{\epsilon}_k} \right)^2 - \frac{\hat{V}_k^2}{2\hat{\epsilon}_k} \Delta},
\]
where \( \hat{\epsilon}_k \equiv \epsilon_k - E_k^+ \) and \( |\hat{\epsilon}_k| \sim D \) except for the narrow region \( |\epsilon_k - \tilde{\epsilon}| < \max(\Delta, \hat{V}_k^2/D) \). In the situation shown in Fig. 1, the Fermi level is located in the band \( E^- \) with \( \epsilon_{kF} < \tilde{\epsilon} \), which simplifies the following analysis. In order to avoid the double occupancy of the orbital-1 with a lower CEF energy, \( \epsilon_{kF} \), the energy of the conduction band corresponding to the Fermi wave number should be slightly lower than \( \tilde{\epsilon} \) so that \( |\epsilon_{kF}| > |\epsilon_l - E_k^-|, |\hat{V}_+| \), because the weight in the lower level \( \tilde{\epsilon}_l \) of the orbital-1 is slightly larger than that of orbital-2.

The DOS near the Fermi level is given as
\[
N^\ast(\epsilon) \simeq 4N^\text{cond}(\epsilon_k - \epsilon)^2 \left| \frac{\epsilon - \tilde{\epsilon} + \frac{\Delta_0}{2} + \frac{\hat{V}_k^2}{2(\epsilon_k - E_k^-)}}{\epsilon - \tilde{\epsilon}} \right|, \tag{30}
\]
where \( \Delta_0 \equiv \Delta \hat{V}_k^2/\hat{V}_k^2 \), and the term of \( \mathcal{O}(\hat{V}_k^2/(\epsilon_k - E_k^-)^2) \) has been neglected. Then, the logarithmic derivative of DOS at the Fermi level is expressed as
\[
\left. \frac{\partial \ln N^\ast(\epsilon)}{\partial \epsilon} \right|_{\epsilon=\mu} \simeq -\frac{4}{T_0} \times \frac{(\tilde{\epsilon} - \mu)^2 + (\tilde{\epsilon} - \mu)(T_0 - \Delta_0) + \frac{1}{4}(T_0 - \Delta_0) \left( \frac{T_0}{2} - \Delta_0 \right)}{(\tilde{\epsilon} - \mu) \left( \tilde{\epsilon} - \mu + \frac{T_0 - \Delta_0}{2} \right)} \equiv -\frac{4J}{T_0} < 0, \tag{31}
\]
where the characteristic energy scale \( T_0 \) is defined as \( T_0 \equiv \hat{V}_k^2/|\epsilon_{kF}| \). The inverse mass tensor at the Fermi level is given as
\[
\left. \frac{\partial^2 E_k^-}{\partial k_\alpha^2} \right|_{\epsilon=\mu} \simeq \frac{T_0}{\epsilon_{kF}^2} \times \frac{\tilde{\epsilon} - \mu}{\tilde{\epsilon} - \mu + \frac{T_0 - \Delta_0}{2}} \times \left[ 1 + \frac{T_0(T_0 - \Delta_0)}{8(\tilde{\epsilon} - \mu + \frac{T_0 - \Delta_0}{2})^2} \right] \left( \frac{\partial \epsilon_k}{\partial k_\alpha} \right)^2. \tag{32}
\]
With the use of expression (32) and a similar expression for the velocity \( \partial E_k^-/\partial k_\alpha \), the second term in the brace of eq.(7) is expressed as
\[
\sum_k \delta(\epsilon - E_k^-) \frac{\partial v_\alpha(k)}{\partial k_\alpha} = \frac{4}{T_0} \times \left( \frac{\tilde{\epsilon} - \mu + \frac{T_0 - \Delta_0}{2}}{\tilde{\epsilon} - \mu + \frac{T_0 - \Delta_0}{2}} \right)^2 + \frac{1}{8} \frac{T_0(T_0 - \Delta_0)}{(\tilde{\epsilon} - \mu) \left( \tilde{\epsilon} - \mu + \frac{T_0 - \Delta_0}{2} \right)} \equiv \frac{4H}{T_0} > 0. \tag{33}
\]
Thus, with the use of expressions (31) and (33), the factor \( F \) in eq.(7) is expressed as
\[
F = \frac{4}{T_0} \times \frac{H + J + (H - J)\pi z(\mu)N^\ast(\mu)u^2}{1 + [\pi z(\mu)N^\ast(\mu)u]^2} > 0. \tag{34}
\]
Since \( H \) and \( J \) are positive constants of \( \mathcal{O}(1) \) and \( N^\ast(\mu)T_0 \sim 1 \), the quasi-universal value of
$q \sim -1$ follows as in the argument for the single-band Fermi liquid. This result explains the fact that $q \sim -1$ for UBe$_{13}$ and URu$_2$Si$_2$. A straightforward prediction is that the Pr-based heavy fermions with the filled Skutterudite structure, such as PrFe$_4$P$_{12}$ and PrOs$_4$Sb$_{12}$, will exhibit the universal ratio $q \sim -1$.

In contrast, UPd$_2$Al$_3$ with $q \sim +1$ is considered to be in the $f^3$-configuration and the situation would be the same as in the Ce-based compounds, which is consistent with $q \sim +1$. This is because three $f$-electrons exhibit itinerant-localized dual behavior: two of them are localized to form an $f^2$ CEF level structure and one of them forms the quasiparticles.

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