

Enhancement of thermal transport in the degenerate periodic Anderson model

V. Zlatić,^{1,2} R. Monnier,³ and J. K. Freericks⁴

¹*Institute of Physics, Bijenička c. 46, 10001 Zagreb, Croatia*

²*International School for Advanced Studies (SISSA), Via Beirut 2-4, I-34014 Trieste, Italy*

³*ETH Hönggerberg, Laboratorium für Festkörperphysik, 8093 Zürich, Switzerland*

⁴*Department of Physics, Georgetown University, Washington, D.C. 20057, USA*

(Received 7 April 2008; revised manuscript received 21 June 2008; published 22 July 2008)

The low-temperature transport coefficients of the degenerate periodic $SU(N)$ Anderson model are calculated in the limit of infinite correlation between f electrons, within the framework of dynamical mean-field theory. We establish the Fermi-liquid (FL) laws in the clean limit, taking into account the quasiparticle damping. The latter yields a reduced value of the Lorenz number in the Wiedemann-Franz law. Our results indicate that the renormalization of the thermal conductivity and of the Seebeck coefficient can lead to a substantial enhancement of the electronic thermoelectric figure of merit at low temperature. Using the FL laws, we discuss the low-temperature anomalies that show up in the electrical resistance of the intermetallic compounds with cerium and ytterbium ions when studied as a function of pressure. Our calculations explain the sharp maximum of the coefficient of the T^2 term of the electrical resistance and the rapid variation in residual resistance found in a number of Ce and Yb intermetallics at some critical pressure.

DOI: 10.1103/PhysRevB.78.045113

PACS number(s): 75.30.Mb, 72.15.Jf, 75.30.Kz

I. INTRODUCTION

The low-temperature charge and thermal transport of heavy fermions and valence fluctuators with Ce, Eu, Yb, and U ions display interesting and complex behavior, such as a striking correlation^{1,2} between the low-temperature Seebeck coefficient $\alpha(T)$ and the specific-heat coefficient $\gamma=C_V/T$. In many of these systems, the dimensionless ratio $q=|e|\lim_{T\rightarrow 0}\alpha/\gamma T$ is nearly the same, although the absolute values of γ and α/T vary by orders of magnitude. In metallic systems, the data show³⁻⁷ small deviations from this universal behavior, due to the variation in carrier concentration; in bad metals, q can become quite large.^{1,2} The Kadowaki-Woods (KW) ratio,⁸ which is defined as $\rho(T)/(\gamma T)^2$, where $\rho(T)$ is the electrical resistivity, exhibits similar universal features if one takes into account the effective low-temperature degeneracy of the f multiplet, as defined by the multiplicity of the crystal-field (CF) ground state,^{9,10} the carrier concentration, and the unit-cell volume.¹¹

The near constancy of the KW and q ratios brings to the fore the validity of the Wiedemann-Franz (WF) law, $\kappa\rho/T=\mathcal{L}_0$, and the possibility of enhancing the electronic thermoelectric figure of merit in strongly correlated materials, $ZT=\alpha^2T/\kappa\rho$, where κ is the electronic contribution to the thermal conductivity and $\mathcal{L}_0=\pi^2k_B^2/3e^2$ is the Fermi-liquid (FL) Lorenz number. When the WF law holds, metals must have a thermopower larger than 155 $\mu\text{V}/\text{K}$ to achieve $ZT>1$; to date no metal has been found with so large a thermopower. In the temperature window where the effective Lorenz number ($\mathcal{L}=\kappa\rho/T$) is reduced, one can achieve $ZT>1$ with substantially lower thermopowers, which might make it possible to find strongly correlated metals that can be used for cooling applications at low temperature.

The above-mentioned universality of the KW and q ratios, typical of a FL state, attracted considerable theoretical attention. Kontani⁹ explained the KW ratio by using the orbitally degenerate periodic Anderson model that he solved by the

quasiparticle (QP) approximation of Yamada and Yosida¹² and Yamada.¹³ Neglecting both the vertex corrections and the momentum dependence of the self-energy, he derived a KW ratio that depends on the degeneracy of the f states and brought the experimental data closer to the universal (theoretical) curve.¹⁰ Miyake and Kohno¹⁴ calculated the q ratio for the same QP dispersion as in Ref. 12, using an effective N -fold-degenerate free-electron model in which the on-site correlation U_{ff} is accounted for by the renormalized hybridization between the c and f states. Restricting the average number of f electrons to $n_f\leq 1$, they treated the QPs as free fermions and assumed that the repeated impurity scattering gives rise to an energy-dependent relaxation rate. Neglecting the QP damping due to Coulomb repulsion, Miyake and Kohno¹⁴ calculated the low-temperature thermopower as a logarithmic derivative of the frequency-dependent conductivity¹⁵ and showed that the q ratio is a quasiuniversal number.

The effect of electron-electron scattering on the transport coefficients was recently studied by Grenzebach *et al.*,¹⁶ using the dynamical mean-field theory¹⁷ (DMFT) of the periodic spin-1/2 Anderson model. The auxiliary impurity problem generated by the DMFT was solved by the numerical renormalization-group (NRG) method, which discretizes the energy spectrum and defines the temperature as the difference between the two lowest-energy states. This provides accurate results for the static properties at arbitrary temperature but cannot provide the thermal transport in the FL regime. The DMFT+NRG calculations indicate an enhancement of the figure of merit when the temperature is reduced below its value at the resistivity maximum and show a breakdown of the WF law due to electron correlations. Recently, we calculated the thermopower and the q ratio of the periodic Anderson model, taking into account the CF splitting¹⁸ and enforcing $n_f\leq 1$ at each lattice site (a realistic description of the CF states requires a local constraint). Solving the auxiliary impurity problem in the noncrossing approximation (NCA), we obtained a semiquantitative description of the

experimental data on heavy fermions and valence fluctuators in the incoherent regime. However, a detailed analysis of the DMT+NRG and the NCA results shows that either method can neither describe the thermal transport much below the Kondo temperature T_K nor establish the FL laws.

In this paper, we discuss the coherent thermal transport of the periodic Anderson model with $SU(N)$ symmetry in the limit of an infinitely large Coulomb repulsion between f electrons. Such an effective N -fold-degenerate model applies to intermetallic compounds with Ce, Eu, Yb, and U ions in the FL regime, where the excited CF states can be neglected.¹⁹ For a given compound, the number of effective channels depends on the pressure and doping. We assume that the model has been solved in thermal equilibrium, so that the FL scale $T_0 \sim 1/\gamma$ is known. The total particle number per unit cell $n(\mu)$ is also n known; μ denotes the chemical potential. Alternatively, we can assume that the values of γ and n are taken from experiment. Using these equilibrium quantities and enforcing the constraint $n_f \leq 1$ at each lattice site, we construct an analytic solution for the stationary heat and charge transport in the FL regime.

Unlike in the previous work, we do not calculate the transport properties in the QP representation because the operator algebra in the projected Hilbert space is not fermionic and the representation of the exact charge and heat current-density operators is cumbersome. In the original fermionic representation, Mahan²⁰ demonstrated that the correlation functions between the above current-density operators can be expressed in terms of transport integrals which differ only by powers of the excitation energy in their integrand, so that the same techniques can be used for their evaluation as in weakly correlated systems.

The transport coefficients are obtained by the DMFT and expressed in terms of the average conduction-electron velocity, the renormalized density of conduction states, and the frequency and temperature-dependent relaxation rate which explicitly takes into account the QP damping. Since we are considering the FL regime, we use the QP approximation of Yamada and Yosida¹² to relate all these quantities to the FL scale T_0 and to the unrenormalized density of c states, $\mathcal{N}_c^0(\omega)$, evaluated at the shifted chemical potential $\mu_L = \mu + \Delta\mu$. The shift $\Delta\mu$ is determined by the Luttinger theorem. Using the Sommerfeld expansion, we obtain the universal FL laws which show that the KW ratio depends not only on the multiplicity of the f state and the average FS velocity but also on the carrier concentration and the unit-cell volume, as observed experimentally.¹¹ As regards the q ratio, we find that changes in the carrier concentration, induced by pressure or chemical pressure, lead to deviations from universality. We also find large deviations from the WF law due to the lowering of the effective Lorenz number, which can lead to a substantial enhancement of the thermoelectric figure of merit $ZT > 1$. The change in the effective degeneracy of the model induced by pressure explains the pronounced maximum of the coefficient of the T^2 term of the electrical resistance^{21–24} and the rapid variation in residual resistance,^{21,22} found in a number of Ce and Yb intermetallics at some critical pressure.

The usefulness of the approximate analytic solution of the DMFT equations becomes apparent when we realize that a numerical calculation of the above-mentioned universal ra-

tios encounters serious difficulty. Neither the NRG nor exact diagonalization nor quantum Monte Carlo approaches provide accurate transport coefficients in the FL regime (especially when the coherence temperature is low). Combining analytical and numerical results enables a reliable estimate of transport coefficients at arbitrary temperatures, which is needed if the model is to be compared with experimental data.

The rest of this paper is organized as follows: Section II describes the DMFT calculations of transport coefficients in the low-temperature limit. In Sec. III we use the QP approximation to calculate the renormalized density of states and transport relaxation time in the FL regime. Section IV establishes the FL laws. In Sec. V we use our results to discuss the experimental data, and Sec. VI provides the summary and conclusions.

II. FORMALISM FOR THE TRANSPORT COEFFICIENTS

The $SU(N)$ -symmetric periodic Anderson model is written in the standard form,¹⁹

$$\mathcal{H} = \mathcal{H}_{\text{band}} + \mathcal{H}_{\text{imp}} + \mathcal{H}_{\text{mix}} - \mu\mathcal{N}. \quad (1)$$

Here, $\mathcal{H}_{\text{band}}$ describes the conduction (c) band with unperturbed dispersion $\epsilon_{\mathbf{k}}$, assumed to be an even function of \mathbf{k} . Because we have an $SU(N)$ symmetric model, there are N distinct flavors of conduction electrons, which are labeled by the index σ , so that

$$\mathcal{H}_{\text{band}} = \sum_{\sigma=1}^N \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \quad (2)$$

The operators $c_{\mathbf{k}\sigma}^\dagger$ ($c_{\mathbf{k}\sigma}$) create (annihilate) a band electron with momentum \mathbf{k} and flavor σ . The noninteracting density of conduction states, $\mathcal{N}_c^0(\omega)$, is calculated for each flavor and any $\epsilon_{\mathbf{k}}$ as $\mathcal{N}_c^0(\omega) = 1/(\mathcal{N}_i\mathcal{V}) \sum_{\mathbf{k}} \delta(\omega - \epsilon_{\mathbf{k}})$, where \mathcal{N}_i is the number of lattice sites and \mathcal{V} is the volume of the primitive unit cell. The characteristic bandwidth of the unperturbed c density of states (DOS) is W . The number of conduction electrons is Nn_c (per unit cell); i.e., there are n_c conduction electrons of each flavor. We assume an infinite Coulomb repulsion, $U_{ff} \rightarrow \infty$, and describe the localized $4f$ states by \mathcal{H}_{imp} ,

$$\mathcal{H}_{\text{imp}} = \sum_{\sigma=1}^N \sum_i E_f^\sigma \mathcal{P} f_{i\sigma}^\dagger f_{i\sigma} \mathcal{P}, \quad (3)$$

where E_f^σ labels the site energy of flavor σ and \mathcal{P} projects onto the subspace with zero or one total f electrons per site. The number of f electrons is restricted to $n_f \leq 1$; i.e., there are n_f/N localized electrons per flavor. The hybridization between same flavor c and f electrons is described by \mathcal{H}_{mix} ,

$$\mathcal{H}_{\text{mix}} = \sum_{\sigma=1}^N \sum_{ij} V_{ij}^\sigma \mathcal{P} (f_{i\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger f_{i\sigma}) \mathcal{P}, \quad (4)$$

where the conduction-electron operators are now written in real space. The total electron number operator is $\mathcal{N} = \sum_{\sigma} \sum_i (c_{i\sigma}^\dagger c_{i\sigma} + f_{i\sigma}^\dagger f_{i\sigma})$, and the chemical potential μ is ad-

justed to keep the total particle number $n = Nn_c + n_f$ constant (as a function of temperature or pressure). For a degenerate paramagnetic state, all flavors are equivalent and the label σ can be dropped.

The intermetallic compounds with $4f$ ions are described by the N -fold-degenerate model with on-site hybridization, $V_{ij} = V\delta_{ij}$, which simplifies the calculations. For large N , an exact solution is provided by the mean-field or the slave-boson solution;¹⁹ but for small N the correlations give rise to the Kondo effect, which cannot be described by mean-field theories. The physically relevant value of N depends on the effective degeneracy of the $4f$ state. A single electron (or hole) in the lowest spin-orbit state of the $4f$ shell of Ce (Yb) is $2J+1$ -fold degenerate, where $J=5/2$ for Ce and $J=7/2$ for Yb. This degeneracy is further reduced by CF splitting; for small hybridization and temperatures at which the excited CF states are unoccupied, the value of N is determined by the degeneracy of the lowest CF state. If the hybridization is such that the CF splitting does not occur, or the excited states are thermally occupied, the effective degeneracy is defined by the lowest spin-orbit multiplet, which is a sextet for Ce and an octet for Yb. In all the physically relevant cases, $2 \leq N \leq 8$; the system exhibits the Kondo effect.

At high temperatures, the qualitative solution can be obtained by perturbative scaling,¹⁹ which shows that the properties depend on an exponentially small energy scale $T_K \approx W \exp(-1/Ng)$, where g is the dimensionless coupling constant $g = V^2 \mathcal{N}_c^0(\mu) / E_f$. At temperature T_K the perturbation theory breaks down. The low-temperature thermodynamic quantities of the $SU(N)$ model are given very accurately by the DMFT+NRG and we assume that we know the numerical value of Fermi-liquid scale $T_0 = \pi^2 k_B^2 / 3\gamma\lambda$, where the linear coefficient of the low-temperature specific heat γ is measured per unit volume. Alternatively, T_0 can be estimated from the slave-boson solution or taken from experiment. Unlike the situation for the static thermodynamic quantities, no currently available numerical method provides a reliable solution for the transport coefficients at low temperatures. In this paper, we evaluate the heat and charge transport of the $SU(N)$ symmetric Anderson model by the Fermi-liquid theory,¹² which holds for $T \leq T_0$.

For the static and uniform transport, we need the $\mathbf{q} \rightarrow 0$ component of the charge and heat current-density operators, which are obtained by commuting the Hamiltonian with the appropriate polarization operators.²⁵ The total current density obtained in such a way satisfies

$$\mathbf{j}_c = \lim_{\tau, \tau' \rightarrow 0} \frac{eN}{\mathcal{V}\mathcal{N}_i} \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger(\tau) c_{\mathbf{k}\sigma}(\tau'), \quad (5)$$

where $\mathbf{v}_{\mathbf{k}} = \nabla \epsilon_{\mathbf{k}} / \hbar$ is the band velocity of the noninteracting (and unhybridized) c states. For constant hybridization the energy current density is given by a similar expression which shows that the model satisfies the Jonson-Mahan theorem.²⁰ This allows us to express the charge conductivity by $\sigma(T) = e^2 N L_{11}$, the thermopower by $\alpha(T) |e| T = -L_{12} / L_{11}$, and the electronic contribution to the thermal conductivity by $\kappa(T) T = N(L_{22} - L_{12}^2 / L_{11})$. In each of these expressions, we have introduced the (single-flavor) transport integrals:

$$L_{mn} = \int d\omega \left(-\frac{df}{d\omega} \right) \omega^{m+n-2} \Lambda(\omega, T), \quad (6)$$

where $f(\omega) = 1 / [1 + \exp(\beta\omega)]$ is the Fermi-Dirac distribution function, ω is measured with respect to the chemical potential μ , and $\Lambda(\omega, T)$ is a function calculated in Appendix A by the Kubo linear-response theory.

At low temperature ($-df/d\omega$) approaches a delta function and the main contribution to the integrals in Eq. (6) comes from the low-energy excitations within the Fermi window, $|\omega| \lesssim k_B T$, and with the wave vectors in the vicinity of the Fermi surface. In the Fermi-liquid state, $\Lambda(\omega, T)$ can be calculated in a straightforward way (for details see Appendix A) which yields in the $\omega, T \rightarrow 0$ limit

$$\Lambda(\omega, T) = \frac{1}{3} v_F^2 \mathcal{N}_c(\omega) \tau(\omega, T), \quad (7)$$

for a three-dimensional system. Here, v_F^2 denotes the average of $v_{\mathbf{k}}^2$ over the renormalized Fermi surface of hybridized states; $\tau(\omega, T)$ is the transport relaxation time, given by the momentum-independent self-energy of the c electrons,

$$\tau(\omega, T) = \frac{-\hbar}{\text{Im} \Sigma_c(\omega^+, T)}, \quad (8)$$

and $\mathcal{N}_c(\omega)$ is the renormalized DOS of c electrons (for a single flavor),

$$\mathcal{N}_c(\omega) = \frac{1}{\mathcal{V}\mathcal{N}_i} \sum_{\mathbf{k}} A_c(\mathbf{k}, \omega). \quad (9)$$

The spectral function of the c electrons,

$$A_c(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G_c(\mathbf{k}, \omega^+). \quad (10)$$

is obtained by evaluating the retarded Green's function $G_c(\mathbf{k}, z)$ just above the real axis, where $z = \omega^+ = \omega + i\delta$ and $\delta \rightarrow 0$ from positive values.

The Green's functions of the periodic Anderson model are defined by the time-ordered thermal averages in the usual way and are cast in the Dyson form by using the equation of motion or the diagrammatic expansion. The Dyson equations for c and f Green's function read^{12,13}

$$G_c(\mathbf{k}, z) = \frac{z - E_f - \Sigma_f(z) + \mu}{[z - \epsilon_{\mathbf{k}} + \mu][z - E_f - \Sigma_f(z) + \mu] - V^2} \quad (11)$$

and

$$G_f(\mathbf{k}, z) = \frac{z - \epsilon_{\mathbf{k}} + \mu}{[z - \epsilon_{\mathbf{k}} + \mu][z - E_f - \Sigma_f(z) + \mu] - V^2}, \quad (12)$$

where z denotes a variable in the complex energy plane and $\Sigma_f(z)$ is the local self-energy of f electrons which describes the renormalization of the (hybridized) f states due to local Coulomb interaction. The Dyson equation for the conduction electrons can also be written in the alternative form

$$G_c(\mathbf{k}, z) = \frac{1}{z - \epsilon_{\mathbf{k}} + \mu - \Sigma_c(z)}, \quad (13)$$

where the local self-energy of the conduction electrons satisfies

$$\Sigma_c(z) = \frac{V^2}{z - E_f + \mu - \Sigma_f(z)}. \quad (14)$$

This self-energy describes the renormalization of the unhybridized c states due to the scattering on the f states; i.e., Σ_c includes the hybridization *and* the correlation effects. The DMFT condition ensures $\Sigma_f(\omega^+, T)$ to be local but the locality of $\Sigma_c(\omega^+, T)$ also requires the hybridization to be momentum independent. The dc transport relaxation time is obtained by substituting $\Sigma_c(\omega^+, T)$ into Eq. (8), which yields

$$\frac{\tau(\omega, T)}{\hbar} \simeq \frac{(\omega - E_f - \text{Re } \Sigma_f + \mu)^2 + (\delta - \text{Im } \Sigma_f)^2}{V^2(\delta - \text{Im } \Sigma_f)}, \quad (15)$$

where the T, ω dependence is due to $\Sigma_f(\omega, T)$. To account for the residual impurity scattering, which is present in any sample, we assume that δ in Eq. (15) has a small but finite value. For temperatures such that $|\text{Im } \Sigma_f(\omega, T)| \gg \delta$, this additional scattering is neglected; we discuss the temperature dependence of transport coefficients by setting $\delta=0$. At $T=0$ the self-energy vanishes and $\tau(\omega, T)$ becomes a constant. The pressure dependence of the residual resistance is discussed using Eq. (7) with a constant relaxation time, which neglects the renormalization effects due to the repeated scattering on the impurities. Where appropriate, the clean limit implies we are in the regime where $\delta \ll |\text{Im } \Sigma_f(\omega, T)|$, whereas we must examine the dirty limit, where $\delta > |\text{Im } \Sigma_f(\omega, T)|$, to describe residual resistance data.

III. FERMI-LIQUID APPROACH

In the FL regime, the imaginary part of Σ_f is small and can be neglected when discussing the renormalized excitation spectrum in the limit $T, \omega \rightarrow 0$. Expanding $\Sigma_f(\omega)$ through linear order in frequency, we find in that limit

$$\omega - [E_f + \text{Re } \Sigma_f(\omega) - \mu] \approx (\omega - \tilde{\omega}_f)Z_f^{-1} + \mathcal{O}(\omega^2), \quad (16)$$

with $Z_f^{-1} = [1 - \partial \Sigma_f / \partial \omega]_{\omega=0}$ as the enhancement factor ($0 \leq Z_f \leq 1$) and $\tilde{\omega}_f = [E_f + \text{Re } \Sigma_f(0) - \mu]Z_f$. The parameters $\tilde{\omega}_f$ and Z_f appear in the description of the model at low temperatures.

If we ignore the imaginary part of the self-energy, both Green's functions in Eqs. (11) and (12) develop poles¹² which define the QP excitations with wave vector \mathbf{k} . Using Eq. (16), we can write the secular equation for the QP excitations in terms of the renormalized quantities as

$$(\omega - \epsilon_{\mathbf{k}} + \mu)(\omega - \tilde{\omega}_f) - \tilde{V}^2 = 0, \quad (17)$$

with $\tilde{V} = V\sqrt{Z_f}$ as the renormalized hybridization. The roots $\omega = \Omega_{\mathbf{k}}^{\pm}$ describe two QP branches,

$$\Omega_{\mathbf{k}}^{\pm} = \frac{1}{2}[(\epsilon_{\mathbf{k}} - \mu + \tilde{\omega}_f) \pm \sqrt{(\epsilon_{\mathbf{k}} - \mu - \tilde{\omega}_f)^2 + 4\tilde{V}^2}], \quad (18)$$

separated by the hybridization gap $2\tilde{V}$. These excitations are defined only for energies close to the chemical potential, where $\text{Im } \Sigma_f$ can be neglected. For large ω the QP approximation breaks down and Eq. (17) is unphysical. At the FS we have $\Omega_{\mathbf{k}_F}^- = 0$ or $\Omega_{\mathbf{k}_F}^+ = 0$, depending on the value of $Nn_c + n_f$. For Ce and Eu systems, we place the bare f level below the chemical potential, which puts μ close to the top of the lower QP branch. From $\Omega_{\mathbf{k}_F}^- = 0$ we see that \mathbf{k}_F is then close to the zone boundary, where $\epsilon_{\mathbf{k}_F} - \mu \simeq W$ (W denotes the half-width of the unperturbed c band). For Yb compounds, the bare level is above μ , so that the lower QP branch is full and the chemical potential is close to the bottom of the upper branch. The equation $\Omega_{\mathbf{k}_F}^+ = 0$ gives \mathbf{k}_F close to the zone center, such that $\epsilon_{\mathbf{k}_F} - \mu \simeq -W$. Close to the FS, the QP dispersion is very weak and $\Omega_{\mathbf{k}}^{\pm}$ describes two heavy QP bands with a half-width equal to \tilde{V}_f^2/W .

The above derivation treats the QP as a noninteracting Fermi gas with effective parameters $\tilde{\omega}_f$ and Z_f (or \tilde{V}). These parameters can be related to the linear coefficient of the specific heat, which is assumed to be known. Using the expression for total QP density of states,

$$\mathcal{N}^{\text{QP}}(\omega) = \frac{1}{\mathcal{V}N_i} \sum_{\mathbf{k}} \delta(\omega - \Omega_{\mathbf{k}}^{\pm}), \quad (19)$$

and the fact that the QP excitations defined by Eq. (17) are infinitely long lived [$\text{Im } \Sigma_f(\omega) = 0$ at $T=0$], we write

$$\gamma = \frac{\pi^2 k_B^2}{6} N \mathcal{N}^{\text{QP}}(0) = \frac{\pi^2 k_B^2}{3\mathcal{V}} \frac{1}{k_B T_0}, \quad (20)$$

where the N -fold degeneracy of the system has been taken into account. The relationship between γ and \mathcal{N}^{QP} is derived assuming that thermally excited QPs increase the average energy per unit volume by approximately $\Delta E \simeq (k_B T)^2 N \mathcal{N}^{\text{QP}}(0)$. The FL parameter T_0 introduced in Eq. (20) defines the low-temperature scaling behavior of all physical quantities. In many systems, it also sets the temperature at which the QP description breaks down. This temperature might or might not coincide with the high-temperature Kondo scale of the system. By definition, the inverse of T_0 is given by the specific-heat coefficient or, equivalently, by the density of the QP excitations of the $SU(N)$ model, which can be calculated very accurately in thermal equilibrium. As shown below, the low-temperature thermal transport is also characterized by T_0 .

The FL scale T_0 can be related to the partial densities of f and c states¹² by expanding Eqs. (11) and (12) for small ω . This yields the spectral functions

$$A_c(\mathbf{k}, \omega) \approx a_{\mathbf{k}}^c(\omega) \delta(\omega - \Omega_{\mathbf{k}}^{\pm}) \quad (21)$$

and

$$A_f(\mathbf{k}, \omega) \approx a_{\mathbf{k}}^f(\omega) \delta(\omega - \Omega_{\mathbf{k}}^{\pm}), \quad (22)$$

where we used the fact that $\omega = \Omega_{\mathbf{k}}^{\pm}$ can be satisfied with only one of the roots and introduced the coefficients

$$a_{\mathbf{k}}^c(\omega) = \left[1 + \frac{\tilde{V}^2}{(\omega - \tilde{\omega}_f)^2} \right]^{-1} \quad (23)$$

and

$$a_{\mathbf{k}}^f(\omega) = Z_f \frac{\tilde{V}^2}{(\omega - \tilde{\omega}_f)^2} a_{\mathbf{k}}^c(\omega). \quad (24)$$

These coefficients satisfy the FL sum rule,¹²

$$a_{\mathbf{k}}^c(\omega) + Z_f^{-1} a_{\mathbf{k}}^f(\omega) = 1. \quad (25)$$

When we substitute Eq. (25) into Eq. (19) and use Eq. (20), the summation of $A_c(\mathbf{k}, \omega)$ and $A_f(\mathbf{k}, \omega)$ over the first Brillouin zone yields

$$\frac{2}{\mathcal{V} N k_B T_0} = \mathcal{N}_c(0) + Z_f^{-1} \mathcal{N}_f(0), \quad (26)$$

which shows that the FL scale is set by the product of the large enhancement factor $1/Z_f$ and $\mathcal{N}_f(0)$.

To relate T_0 to the renormalized parameters $\tilde{\omega}_f$ and Z_f , we express, first, the renormalized c and f DOS in terms of the density of unhybridized band states. Using the identities $\delta(\omega - \Omega_{\mathbf{k}}^{\pm}) = \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}}^{\pm}) / |d\Omega_{\mathbf{k}}^{\pm} / d\epsilon_{\mathbf{k}}|$ and $d\Omega_{\mathbf{k}}^{\pm} / d\epsilon_{\mathbf{k}} = a_{\mathbf{k}}^c(\omega)|_{\omega=\Omega_{\mathbf{k}}^{\pm}}$, where $\epsilon_{\mathbf{k}}^{\pm}$ is the solution of Eq. (17) for a given (small) ω , we obtain from Eqs. (21) and (22) the results

$$\mathcal{N}_c(\omega) = \mathcal{N}_c^0 \left(\omega + \mu - \frac{\tilde{V}^2}{\omega - \tilde{\omega}_f} \right) \quad (27)$$

and

$$\mathcal{N}_f(\omega) = \frac{Z_f \tilde{V}^2}{(\omega - \tilde{\omega}_f)^2} \mathcal{N}_c(\omega). \quad (28)$$

The expressions in Eqs. (27) and (28) are similar in spirit and in form to those in Refs. 26 and 27, where the fully interacting DOS of the periodic Anderson model is equated with the DOS of a noninteracting $U=0$ model. The Green's functions of that model are defined by Eqs. (11) and (12) for $\Sigma_f(\omega) = 0$. Here, we find it more convenient to relate $\mathcal{N}_c(\omega)$ to the DOS of an *unhybridized* conduction band which is obtained from Eq. (13) for $\Sigma_c(\omega) = 0$. At low temperatures, where only the hybridized bands have physical relevance, this auxiliary conduction band is just a convenient mathematical construct. However, at high temperatures, where the model has to account for the scattering of conduction states on localized paramagnetic f states, the unhybridized conduction band is physically relevant.

The auxiliary model provides the renormalized Fermi surface (FS) of the periodic Anderson model simply by the Luttinger theorem, i.e., from the fundamental Fermi-liquid relation, which states that the volume of the FS cannot be changed by interactions. Using the standard form of the c -electron Green's function [in Eq. (13)] and the fact that

$\Sigma_c(z)$ is momentum independent (this holds for momentum-independent hybridization in infinite dimensions), we immediately learn that the FS of the auxiliary band model (with $n = Nn_c + n_f$ electrons per unit cell) coincides with the FS of the periodic Anderson model with the same number of electrons per cell. The shape of the renormalized FS is obtained by solving Eq. (17) at $\omega=0$, which yields the implicit equation

$$\epsilon_{\mathbf{k}_F} = \mu + \frac{\tilde{V}^2}{\tilde{\omega}_f} \quad (29)$$

in terms of the noninteracting dispersion. We recall that μ is fixed by the condition

$$n = Nn_c + n_f = N\mathcal{V} \int_{-\infty}^{\mu} d\omega [\mathcal{N}_c(\omega) + \mathcal{N}_f(\omega)]. \quad (30)$$

The auxiliary model has exactly the same FS, determined by the equation

$$\epsilon_{\mathbf{k}_F} = \mu_L, \quad (31)$$

where μ_L is obtained from the integral

$$n = N\mathcal{V} \int_{-\infty}^{\mu_L} d\omega \mathcal{N}_c^0(\omega); \quad (32)$$

i.e., μ_L is the chemical potential of a conduction band with $n = n_c + n_f$ electrons. The same chemical potential μ (μ_L) appears in Eqs. (29) and (30) [Eqs. (31) and (32)] because the Luttinger theorem ensures that the number of \mathbf{k} points enclosed by the FS coincides with the total number of electrons in the system. Equations (29) and (31) give the shift

$$\Delta\mu = \mu_L - \mu = \frac{\tilde{V}^2}{\tilde{\omega}_f}. \quad (33)$$

Substituting Eqs. (27) and (28) into Eq. (26) and using Eq. (33) to eliminate $\tilde{V}^2/\tilde{\omega}_f$, we find the relationship between $\tilde{\omega}_f$ and T_0 ,

$$\tilde{\omega}_f = \Delta\mu \frac{N\mathcal{N}_c^0(\mu_L) \mathcal{V} k_B T_0 / 2}{1 - N\mathcal{N}_c^0(\mu_L) \mathcal{V} k_B T_0 / 2} \approx \frac{N}{2} \Delta\mu \mathcal{N}_c^0(\mu_L) \mathcal{V} k_B T_0, \quad (34)$$

where the last expression neglects the exponentially small term in the denominator. The sign of $\tilde{\omega}_f$ is set by $\Delta\mu$, which is positive for Ce and Eu compounds and negative for Yb compounds. The enhancement factor is obtained from Eq. (33) as $Z_f = \Delta\mu \tilde{\omega}_f / \tilde{V}^2$.

The ratio $2\tilde{\omega}_f/T_0 = \Delta\mu \mathcal{N}_c^0(\mu_L)$ depends for a given $n(\mu)$ on the renormalized chemical potential μ , the auxiliary one μ_L , and the unit-cell volume \mathcal{V} . While μ_L is easily obtained from $n(\mu)$, the value of μ is difficult to find without numerical calculations except for very small \tilde{V} , large N , and for $n_f \approx 1$ and $n_c \approx 1/2$, when each conduction band is close to half filling. In that case, the renormalization does not change much the partial occupancies of the f and c states, and we can approximate $n_c \approx \mathcal{V} \int_{-\infty}^{\mu} d\omega \mathcal{N}_c^0(\omega)$, which yields

$$N\mathcal{V} \int_{\mu}^{\mu_L} d\omega \mathcal{N}_c^0(\omega) \approx n - Nn_c = n_f, \quad (35)$$

where we have implicitly assumed $\mu_L > \mu$, which applies to Ce and Eu compounds. A similar result can be obtained for Yb compounds after an electron-hole transformation. For large N the integral is small and since the integrand has a maximum around μ (the auxiliary band is close to half filling), it follows that $\Delta\mu$ is small. Using $\mathcal{N}_c^0(\mu_L) \approx \mathcal{N}_c^0(\mu)$, we estimate

$$\mathcal{V} \int_{\mu}^{\mu_L} d\omega \mathcal{N}_c^0(\omega) \approx \Delta\mu \mathcal{V} \mathcal{N}_c^0(\mu_L) \approx \frac{n_f}{N}. \quad (36)$$

Thus, for large N and $n_f \approx 1$, we have the simple relation $\tilde{\omega}_f \approx n_f k_B T_0 / 2$. For small N and/or small n_f , Eq. (35) still holds but we cannot claim that $\Delta\mu$ is small. If $\mathcal{N}_c^0(\omega)$ decreases rapidly for $\omega > \mu$, as it usually does, we can conclude that $\Delta\mu \mathcal{V} \mathcal{N}_c^0(\mu_L) \ll n_f / N \ll \Delta\mu \mathcal{V} \mathcal{N}_c^0(\mu)$ but we cannot express $\Delta\mu \mathcal{V} \mathcal{N}_c^0(\mu_L)$ in terms of n_f or relate $\tilde{\omega}_f$ to T_0 in a simple way, as in the large- N limit.

The auxiliary model with unhybridized conduction electrons has a simple physical interpretation for systems with small hybridization and $n_f \approx 1$, i.e., for heavy fermions with very low Kondo temperature. In such systems the $4f$ ions are in a well-defined valence state, the low-energy dynamics is dominated by spin fluctuations and n_f is temperature independent.¹⁹ At low temperatures, the renormalized FS is defined by the set of \mathbf{k} vectors satisfying $\epsilon_{\mathbf{k}} = \mu + \Delta\mu$. This FS is large because it encloses $(n_c + n_f/N)$ states of each flavor. At high temperatures, the Fermi surface is small because it encloses only n_c conduction states (f states are localized and do not contribute to the Fermi volume). Ignoring the fact that thermal fluctuations remove the discontinuity in the Fermi distribution function, we approximate the renormalized FS by the FS of unhybridized conduction states. (This holds for $T \ll W$.) On the other hand, the condition $\epsilon_{\mathbf{k}} = \mu$ defines a set of \mathbf{k} vectors which are close to the FS of the auxiliary band with n_c electrons. This FS is also small because it encloses only n_c states of each flavor. Since n_f and n_c are temperature independent, the shift $\Delta\mu$ provides the difference between the FS of the high-temperature paramagnetic phase with Nn_c conduction electrons (and n_f localized states) and the FS of the low-temperature FL phase with N bands containing each $n_c + n_f/N$ hybridized states. The above considerations show that the formation of the coherent QP bands is accompanied by a ‘‘jump’’ of the Fermi volume from a small to a large value and that the large FS encloses n_f/N additional states. The auxiliary model approximates the conduction band of the periodic Anderson model and allows us to estimate this jump.

So far, we neglected the imaginary part of self-energy, since we considered only the low-energy excitations at $T = 0$. In order to calculate the transport properties at low but nonzero temperature, we have to include the QP damping, which is given by the imaginary part of the self-energy (in the clean limit). To estimate $\text{Im} \Sigma_f(\omega, T)$ at low temperatures, we use the diagrammatic analysis of Yamada and Yosida.¹²

In infinite dimensions, the expansion is in terms of the local Green’s functions and produces the FL expression^{9,12}

$$-\text{Im} \Sigma_f(\omega, T) \approx \frac{\pi}{2} [\omega^2 + (\pi k_B T)^2] (N-1) [\mathcal{V} \mathcal{N}_f(0)]^3 \Gamma_f^2, \quad (37)$$

where Γ_f is the irreducible four-point scattering vertex for electrons with different flavors. Equation (37) is a straightforward generalization of the result produced by second-order perturbation theory, in which the bare interaction U_{ff} is replaced by the scattering vertex Γ_f . In the limit of large correlations, when the charge fluctuations are suppressed, the Ward identity^{12,13} gives $Z_f^{-1} = (N-1) \mathcal{V} \mathcal{N}_f(0) \Gamma_f$, such that $\gamma = (\pi^2 k_B^2 / 6) N(N-1) \mathcal{V} [\mathcal{N}_f(0)]^2 \Gamma_f$, where we neglect the much smaller conduction-electron contribution to γ . Substituting into Eq. (37) yields in the $T, \omega \rightarrow 0$ limit⁹

$$\text{Im} \Sigma_f(\omega, T) \approx -2\pi \frac{\omega^2 + (\pi k_B T)^2}{(N-1) N^2 \mathcal{V} \mathcal{N}_f(0) (k_B T_0)^2}. \quad (38)$$

Expanding $\Sigma_c(\omega, T)$ in Eq. (14) into a power series [with the real and imaginary parts of $\Sigma_f(\omega, T)$ given by Eqs. (16) and (38), respectively], we obtain the self-energy of c electrons in the FL form. That is, in the FL regime, the real part of $\Sigma_c(\omega, T)$ is a constant and the imaginary part is a quadratic function of T and ω .

Inserting $\Sigma_f(\omega, T)$ into Eq. (15) for $\tau(\omega, T)$ and using $Z_f \tilde{V}^2 / \mathcal{N}_f(0) = \tilde{\omega}_f^2 / \mathcal{N}_c(0)$ yields for $T, \omega \rightarrow 0$ the leading term

$$\begin{aligned} \tau(\omega, T) &= \frac{\hbar(N-1) N^2 \mathcal{V} \mathcal{N}_c^0(\mu_L) k_B^2 T_0^2}{2\pi \tilde{\omega}_f^2} \frac{(\omega - \tilde{\omega}_f)^2}{(\pi k_B T)^2 + \omega^2} \\ &\approx \tau_0(T) \left(1 - \frac{\omega}{\tilde{\omega}_f}\right)^2 \left(1 - \frac{\omega^2}{\pi^2 k_B^2 T^2}\right), \end{aligned} \quad (39)$$

where

$$\tau_0(T) = \frac{\hbar(N-1) N^2 \mathcal{V} \mathcal{N}_c^0(\mu_L) T_0^2}{2\pi^3 T^2}. \quad (40)$$

The second line in Eq. (39) emphasizes the fact that the limit $\omega \rightarrow 0$ is taken before $T \rightarrow 0$ and that $\Sigma_f(\omega^+, T)$ is known only up to the ω^2 terms, so that the Sommerfeld expansion cannot be extended beyond the second order (up to that order both forms produce the same result). The first (second) bracket in Eq. (39) is due to the real (imaginary) part of $\Sigma_f(\omega^+, T)$. Unlike $\Sigma_c(\omega, T)$, the FL laws produced by the Sommerfeld expansion of transport coefficients are affected not only by the ω dependence of $\text{Im} \Sigma_f(\omega, T)$ but also that of $\text{Re} \Sigma_f(\omega, T)$ as well.

In order to make an estimate of the slope of the renormalized f DOS, which is needed for thermal transport, we invoke the DMFT condition. This condition also provides a physical interpretation of the low-energy parameter $\tilde{\omega}_f$. In DMFT, we compute the local Green’s function from the local self-energy,

$$\begin{aligned}
 G_f(z) &= \sum_{\mathbf{k}} G_f(\mathbf{k}, z) \\
 &= \mathcal{V} \int d\epsilon \mathcal{N}_c^0(\epsilon) \frac{1}{z - E_f + \mu - \Sigma_f(z) - \frac{V^2}{z - \epsilon + \mu}}; \quad (41)
 \end{aligned}$$

map it onto the Green's function of an effective single impurity Anderson model with a hybridization function $\Delta(z)$,

$$F(z) = \frac{1}{z - E_f + \mu - \Delta(z) - \Sigma_f(z)}; \quad (42)$$

and adjust $\Delta(z)$ to make $G_f(z)$ and $F(z)$ identical. The DMFT procedure works because the large-dimensional limit guarantees that the functional relationship between the local self-energy and the local Green's function for the lattice is identical to the functional relationship between the self-energy for the impurity and the impurity Green's function. In the limit where $T=0$ and $\omega \rightarrow 0$, we approximate $\Delta(\omega) = i\Delta_0$ with the constant $\Delta_0 < 0$ and write the DMFT condition at low frequencies as

$$\mathcal{N}_f(\omega) = -\frac{1}{\pi} \text{Im} F(\omega^+) \approx \frac{1}{\pi |\Delta_0|} \frac{\tilde{\Delta}_f^2}{(\omega - \tilde{\omega}_f)^2 + \tilde{\Delta}_f^2}, \quad (43)$$

where $\tilde{\Delta}_f = \Delta_0 Z_f$. This Kondo-type form of $\mathcal{N}_f(\omega)$ holds only for $\omega \ll \tilde{\omega}_f$, just like the quasiparticle dispersion makes sense only for $\omega \ll T_0$. It cannot be extrapolated to higher frequencies, where the approximation $\Delta(\omega) = i\Delta_0$ does not hold. The approximate form given by Eq. (43) has a maximum at $\tilde{\omega}_f$, where the exact f DOS has a gap; the exact DMFT spectral function has a maximum between μ and $\tilde{\omega}_f$. The width of effective Kondo resonance is $\tilde{\Delta}_f$. In the FL regime, $\omega \leq k_B T \ll \tilde{\omega}_f$; the transport coefficients depend on the characteristic energy scales defined by this effective Kondo resonance.

The width $\tilde{\Delta}_f$, like $\tilde{\omega}_f$, can be related to the FL scale T_0 of the periodic Anderson model. Equating the f DOS and the effective single impurity DOS at $\omega=0$ yields

$$\pi \Delta \mu \mathcal{V} \mathcal{N}_c^0(\mu_L) = \frac{x}{1+x^2}, \quad (44)$$

where $x = \tilde{\omega}_f / \tilde{\Delta}_f$. Solving for x produces the result

$$\tilde{\Delta}_f = \frac{2\pi \Delta \mu \mathcal{V} \mathcal{N}_c^0(\mu_L)}{1 \pm \sqrt{1 - [2\pi \Delta \mu \mathcal{V} \mathcal{N}_c^0(\mu_L)]^2}} \tilde{\omega}_f, \quad (45)$$

and we choose the negative sign. Since $\Delta \mu \mathcal{V} \mathcal{N}_c^0(\mu_L)$ was shown to be very small [see the discussion around Eqs. (35) and (36)], the root in the above expression can be expanded to produce the lowest-order result,

$$\tilde{\Delta}_f = \frac{\tilde{\omega}_f}{\pi \Delta \mu \mathcal{V} \mathcal{N}_c^0(\mu_L)} \approx \frac{1}{2\pi} N k_B T_0. \quad (46)$$

The above expression, which follows from the DMFT condition, ensures that the initial slope of the renormalized f DOS is very small,

$$\left[\frac{\partial \mathcal{N}_f(\omega)}{\partial \omega} \right]_{\omega=0} \approx \frac{\tilde{\omega}_f}{\tilde{\Delta}_f} \approx \pi \Delta \mu \mathcal{V} \mathcal{N}_c^0(\mu_L) \ll 1. \quad (47)$$

Finally, we remark that the FS average of the unrenormalized velocity squared, $v_{\mathbf{k}}^2$, can be found from the integral

$$v_F^2 = \langle v_{\mathbf{k}_F}^2 \rangle = \int d^d \mathbf{k} \delta(\mathbf{k} - \mathbf{k}_F) v_{\mathbf{k}}^2, \quad (48)$$

where the δ function restricts the integral to the renormalized FS. In infinite dimensions v_F^2 is a constant for all fillings, but in lower dimensions the change in the Fermi volume with pressure or temperature can modify v_F^2 and affect thermal transport. Numerical calculations for the three-dimensional periodic Anderson model with nearest-neighbor hopping on a simple cubic lattice give $v_F^2 = (ta_1/\hbar)^2 v^2$, where $v^2 \approx 1.4$ for $n \approx 1/2$ and $v^2 \ll 1$ for $n \approx 1$.

IV. FERMI-LIQUID LAWS

The transport coefficients of the periodic $SU(N)$ Anderson model with infinite correlation between f electrons are obtained in the FL regime by making the lowest-order Sommerfeld expansion of transport integrals, Eq. (6), and expressing the integrand $\Lambda(\omega)$ in terms of the known expressions for $v_{\mathbf{k}_F}^2$, $\mathcal{N}_c^0(\omega)$, and $\tau(\omega, T)$. The algebra is straightforward (for details see Appendix B) and yields the transport coefficients as simple powers of reduced temperature T/T_0 .

The specific resistance of N parallel channels obtained in such a way is

$$\rho(T) = \frac{9\pi^3 \mathcal{V}}{\hbar e^2 v_F^2 N(N-1) [N \mathcal{V} \mathcal{N}_c^0(\mu_L)]^2} \left(\frac{T}{T_0} \right)^2, \quad (49)$$

which holds for $N \geq 2$ and arbitrary $\mathcal{N}_c^0(\omega)$.

The resistivity expression in Eq. (49) neglects terms on the order of $(T/T_0)^4$ and is valid only for $T \ll T_0$. Even in that temperature range, $\rho(T)$ deviates from the universal (KW) form because the prefactor of the $(T/T_0)^2$ term has an explicit parameter dependence. The value of these parameters depends on the Fermi volume of the system, which can be changed in several ways. For example, additional impurity scattering or lattice expansion (negative pressure) can localize the f states and exclude them from the Fermi volume. Another possibility is to increase the effective degeneracy of the f states (by pressure or thermal population of the excited states), which changes the number of resonant channels and shifts the Fermi surface away closer to the zone center. The jumps in the Fermi volume changes μ_L and v_F^2 , which has a strong impact on the resistivity. This feature can be used to explain the resistivity anomalies that accompany the localization or delocalization of f electrons in heavy fermions, i.e., the breakdown or the formation of the QP bands. The rapid change in the coefficient of the T^2 term in the resistivity following the pressure- or doping-induced jump of the Fermi volume in cerium compounds is discussed in detail below. On the other hand, if we tune the model parameters of the $SU(N)$ model in such a way that the Fermi volume is preserved (by keeping N/n constant), the Luttinger theorem

ensures that μ_L and v_F^2 do not change. In that case, the prefactor of $(T/T_0)^2$ is constant but $\rho(T)$ changes due to variations in T_0 , which can be exponentially fast.

For large N , the approximation $N\mathcal{V}\mathcal{N}_c^0(\mu_L) \approx n_f/\Delta\mu$ yields the expression

$$\rho(T) \approx \frac{81(\Delta\mu/n_f)^2\mathcal{V}^3}{\hbar N(N-1)\pi k_B^2 v_F^2} (\gamma T)^2, \quad (50)$$

which simplifies the discussion of heavy fermions in the Kondo limit, $n_f \approx 1$. The Luttinger theorem ensures $n_f/\Delta\mu$ is constant even when the tuning of the external parameters gives rise to a charge transfer between the f and c states and thereby changes the renormalized chemical potential. As long as the tuning does not affect the degeneracy of the ground state, the prefactor of the $(\gamma T)^2$ term of the resistivity is always the same.

The Seebeck coefficient is obtained by using the Sommerfeld expansion for L_{12} and L_{11} , which gives

$$\alpha(T) \approx \frac{4\pi^2 k_B}{|e|N\Delta\mu\mathcal{V}\mathcal{N}_c^0(\mu_L)} \frac{T}{T_0}. \quad (51)$$

The enhancement of L_{12} is solely due to the real part of the self-energy. The imaginary part corrects L_{11} and gives a factor of 3/2 enhancement of $\alpha(T)$ with respect to the $U=0$ case. This factor does not arise in mean-field theory or in slave-boson approximations based on quadratic Hamiltonians with renormalized parameters.¹⁴ The above result corrects the expression used in our previous paper,¹⁸ which was derived neglecting the energy dependence of the density of states. The term $\Delta\mu$, which does not occur in the low-temperature resistivity expression in Eq. (49), has an explicit parameter dependence, so that, strictly speaking, $\alpha(T)$ is not a universal function of T/T_0 . In bad metals and systems with a low-carrier concentration, μ_L is close to the band edge, where $\mathcal{N}_c^0(\mu_L)$ could be very small, so that $\alpha(T)$ could be very large.

The Seebeck coefficient of heavy fermions with $n_f \approx 1$ and large N assumes the simple form

$$\alpha(T) = \mp \frac{4\pi^2 k_B}{n_f |e|} \frac{T}{T_0}. \quad (52)$$

Since the doubly occupied f states are removed from the Hilbert space, the model is highly asymmetric, and the initial slope $\lim_{T \rightarrow 0} \alpha(T)/T$ never vanishes. As a matter of fact, the closer the system is to half filling, the larger is the slope, $\alpha/T \propto 1/T_0$. This, however, does not necessarily imply a large thermopower, since the FL laws are valid only for $T \ll T_0$ and close to half filling T_0 is exponentially small.

The FL result for the thermal conductivity in the clean limit reads

$$\kappa(T) = T\sigma(T)\mathcal{L}_0(T), \quad (53)$$

where the usual Lorentz number, $\mathcal{L}_0 = \pi^2 k_B^2/3e^2$, has been replaced by the effective one,

$$\mathcal{L}_0(T) = \bar{\mathcal{L}}_0 \left[1 - \frac{32\pi^2}{n_f^2} \left(\frac{T}{T_0} \right)^2 \right], \quad (54)$$

and $\bar{\mathcal{L}}_0 = \pi^2 k_B^2/2e^2$. This change is due to the imaginary part of the self-energy and is therefore not obtainable by mean-field or slave-boson calculations which neglect the QP damping. The $T \rightarrow 0$ limit yields the Wiedemann-Franz law, $\kappa(T) \propto T\sigma(T)$, but the correction given in the square brackets leads to deviations even at low temperatures. Since the factor multiplying the T^2 term is very large, we find a reduction in $\kappa(T)$ and substantial deviations from the WF law much below T_0 .

Before closing this section, we summarize the procedure for calculating the transport coefficients of the periodic Anderson model in the FL regime. The model is specified by the hybridization V , the bare f -level position E_f , the degeneracy N , the center of the bare conduction band E_0 , the unperturbed dispersion $\epsilon_{\mathbf{k}}$, and the restriction $n_f \leq 1$. The unperturbed density of conduction states, $N_c^0(\omega)$, is easily obtained from $\epsilon_{\mathbf{k}}$. For a given total electron density n (per cell), we use the DMFT+NRG or some simpler scheme, such as the slave bosons, to find the renormalized chemical potential, the number of f electrons, and the low-temperature coefficient of the specific heat, which sets the FL scale T_0 . These static quantities can be calculated in thermal equilibrium to a very high accuracy. For constant hybridization, we can make separate DMFT+NRG runs for $n_c(\mu)$ and $n_f(\mu)$ and we do not have to calculate the spectral function, which is not given very accurately (for all ω) by the NRG. From $n = Nn_c + n_f$, we obtain μ , μ_L , and $\Delta\mu$, which provide the renormalized FS and the average v_F^2 . From T_0 , μ_L , and $\Delta\mu$, we obtain the Kondo scale $\tilde{\omega}_f$ and specify completely the low-energy behavior of $N_c(\omega)$ and $\tau(\omega)$. The FL laws follow at once. For heavy fermions with large N , $n_f \approx 1$, and small \tilde{V} , the procedure simplifies considerably, since we can approximate $\Delta\mu N\mathcal{V}\mathcal{N}_c^0(\mu_L) \approx n_f$ and obtain all the renormalized quantities by using $\tilde{\omega}_f \approx n_f k_B T_0/2$.

V. DISCUSSION OF EXPERIMENTAL RESULTS

A. Universal ratios

The FL laws in Eqs. (49)–(53) describe coherent charge and heat transport in stoichiometric compounds in a way analogous to the phase-shift expressions for dilute Kondo alloys.¹⁹ They explain the near-universal behavior of the KW ratio^{8,10} reported for many heavy fermions and valence fluctuators. The ratio $\rho(T)/(\gamma T)^2$ obtained from Eq. (49) exhibits an explicit dependence on the ground-state degeneracy and the average velocity (squared) and an implicit dependence on the Fermi volume, i.e., on the carrier concentration. The N dependence as well as the dependence on carrier concentration of the KW ratio were recently emphasized by Kontani⁹ and Tsujii *et al.*,¹⁰ who obtained the power law $n^{-4/3}$ for the latter by using the free-electron approximation for the average velocity and the density of states in the expression for the resistivity. Our formulation leads to a similar N dependence [see also Eq. (50)]. However, it includes also the dependence on the average velocity, the renormalized Fermi volume, and the carrier concentration, which are implicit

functions of the degeneracy and have to be taken into account when discussing the pressure or doping experiments on strongly correlated electron systems.¹¹

As regards the thermal transport, Eq. (51) gives $q = \lim_{T \rightarrow 0} |e\alpha|/\gamma T \approx 12/[N\Delta\mu\mathcal{N}_c^0(\mu_L)]$, which has an explicit parameter dependence, so that the q ratio, like the KW ratio, can deviate from the universal value.^{1,2} In bad metals and systems with a low-carrier concentration, μ_L is close to the band edge, where $\mathcal{N}_c^0(\mu_L)$ could be very small, making $\alpha(T)$ large. For a given system, the q ratio can be pressure dependent due to the transfer of f electrons into conduction band. The data on the pressure dependence are not available, but the deviations from the universal value are indicated by recent chemical pressure data.²

A further remarkable consequence of correlations is the enhancement of the low-temperature figure of merit due to the deviations from the WF law. Using Eq. (53) and neglecting phonons in the FL regime, we express the figure of merit as a ratio, $ZT = \alpha^2(T)/\mathcal{L}(T)$. For constant Lorenz number, the maximum of ZT is defined by the thermopower; but in correlated systems, the temperature dependence of the effective Lorenz number can lead to an additional enhancement. Even though our FL result is valid only for $T \ll T_0$, it captures the essential features: an increase in α^2 and a decrease in $\mathcal{L}(T)$ that ultimately give rise to $ZT > 1$. The enhancement of ZT is due to the renormalization of the thermopower and the Lorenz number; i.e., $ZT > 1$ is not restricted to metallic systems with $\alpha(T) > 155 \mu\text{V/K}$. We expect large ZT for small T_0 ; but to find the optimal situation, one should tune the parameters and study the border of the FL regime by numerical methods.

B. Pressure dependence of the low-temperature resistivity

The FL laws derived for the periodic Anderson model explain the changes observed in the transport coefficients of heavy fermions under applied pressure. As an illustration, we consider the pressure dependence of the coefficient of the T^2 term in the resistivity, defined as $A(p) = (\rho - \rho_0)/T^2$, where ρ_0 is the residual resistivity. In the case of the two heavy fermion antiferromagnets $\text{CePd}_{2-x}\text{Ge}_{2-x}$ (Ref. 23) and CeRu_2Ge_2 ,²⁴ $A(p)$ is small and nearly pressure independent for $p \leq 4$ GPa. Above 4 GPa, $A(p)$ increases rapidly and reaches a maximum value for pressure between 4 and 8 GPa. At the critical pressure p_c , the maximum of $A(p_c)$ is typically 1 order of magnitude higher than at ambient pressure. For $p > p_c$, the value of $A(p)$ drops to the ambient pressure one. A somewhat different behavior is found in the heavy fermion superconductor CeCu_2Si_2 and in the antiferromagnet CeCu_2Ge_2 when analyzed in the normal state.^{21,22} The values of $A(p)$ are large at initial pressure, which is applied in order to restore the FL behavior; above that pressure $A(p)$ decreases to a plateau and then drops by nearly 2 orders of magnitude.^{21,22}

A sharp maximum of $A(p)$ is observed for systems in which the ground state of the $4f$ ion is characterized at ambient pressure by a CF doublet well separated from the excited CF states. The Néel temperature of such systems is much higher than the Kondo temperature and the large para-

magnetic entropy of Ce ions is removed at T_N by an antiferromagnetic (AFM) transition rather than by a Kondo crossover. The low-entropy state involves large unscreened moments which correspond to the $4f$ ions frozen in the high-temperature (magnetic) configuration. Below T_N , the conduction electrons are essentially free except for some magnon and impurity scattering, such that the resistivity at ambient pressure is small and weakly temperature dependent, as shown by $\text{CePd}_{2-x}\text{Ge}_{2-x}$ and CeRu_2Ge_2 data.

To explain the experimental data, we assume that an increase in pressure leads at p_c to the delocalization of the $4f$ states²⁸ and the formation of hybridized bands, which can be described by the SU(2) Anderson model. The two channels (sub-bands) in which the lowest $4f$ doublet hybridizes with the conduction states of the appropriate symmetry, accommodate nearly one electron per site, $n_c + n_f/2 \approx 1$, for each flavor. The renormalized Fermi volume is large and the FS is close to the edge of the Brillouin zone, where v_F^2 is small. The corresponding value of μ_L is on the order of the bandwidth [see Eqs. (31) and (32)], such that $\mathcal{N}_c^0(\mu_L)$ is also small. [The maximum of $\mathcal{N}_c^0(\omega)$ is assumed to be close to the center of the band.] Since T_0 is small ($T_0 < T_N$), the coefficient of the T^2 term in the resistivity, given by Eq. (49) for $N=2$, is large. The enhancement of $A(p)$ with respect to the values at ambient pressure (where the f states are localized) is due to the delocalization of the f states by applied pressure. In a system with delocalized f states, the main effect of pressure is to increase the hybridization and T_0 provided the degeneracy of the lowest occupied CF level is preserved. We can understand the increase in T_0 by recalling that the FL scale of the lattice is proportional to the low-energy scale of the auxiliary impurity model [see Eq. (34)] and that an increase in the Kondo scale with hybridization (pressure) is a typical feature of any Kondo system. An increase in T_0 can also be inferred from the experimental data,^{21,22} which show that in $\text{CePd}_{2-x}\text{Ge}_{2-x}$ and CeRu_2Ge_2 the value of T_0 scales with the high-temperature Kondo scale.

A qualitative change occurs at the point where the hybridization becomes so large that the system cannot sustain the CF excitations and the degeneracy of the f level changes from two to six. To estimate the resistivity of this high-pressure state, we use the SU(6) model, in which a single f electron is distributed over six equivalent hybridized channels. In that case, our FL solution shows that the FS is shifted away from the zone boundary, μ_L is decreased, and $\mathcal{N}_c^0(\mu_L)$ is increased with respect to the values obtained for $N=2$. The average squared velocity, v_F^2 , and the FL scale T_0 are also increased for $N=6$, which reduces $A(p)$ to small values, in agreement with the experimental data.²¹⁻²⁴ The drop in $A(p)$ for $p > p_c$ signifies the doublet-sextet crossover and is mainly due to the prefactor in Eq. (49), which has an explicit and implicit dependence on N . At the crossover, the Fermi volume changes and the KW ratio is strongly pressure dependent. Once the degeneracy of the f state is stabilized at a higher value, a further increase in pressure reduces $A(p)$ by increasing T_0 but does not change v_F^2 or μ_L , which are fixed by the Luttinger theorem for $(n_c + n_f/6)$ states per channel. Eventually, at very high pressure, the system is transformed into a valence fluctuator with an enormously enhanced FL scale, such that $A(p)$ drops to a very small value.

As regards CeCu_2Si_2 (Ref. 22) and CeCu_2Ge_2 ,²¹ we can explain the data by using the same reasoning as above if we assume that the f states are delocalized at the initial pressure which restores the FL state. The value of $A(p)$ at the initial pressure is large because the temperature dependence of the resistivity is due to two degenerate sub-bands with very heavy fermions. The FS of these sub-bands is close to the zone boundary, where v_F^2 , μ_L , and $\mathcal{N}_c^0(\mu_L)$ are very small. The hybridized bands which involve the excited CF states have a small Fermi volume and their low-energy properties are free-electron-like. They carry most of the current but have temperature-independent resistivity and do not affect $A(p)$. The first decrease in $A(p)$ occurs at a pressure at which an increase in the hybridization removes the CF excitations, such that the effective degeneracy of the f state increases from 2 to 4 or 6. For large N , the expression in Eq. (49) gives small A . The final drop in $A(p)$ is due to the crossover into the valence fluctuating regime and an exponential increase in the FL scale T_0 . If we assume a proportionality between T_0 and the Kondo scale T_K , which is indicated by the experimental data, our calculations would explain the $A(p)$ versus T_K scaling reported in Ref. 22.

The above scenario also offers an explanation for the peak observed in the residual resistivity of CeCu_2Ge_2 (Ref. 21) and CeCu_2Si_2 (Ref. 22) for pressures at which the degeneracy of the f level changes and $A(p)$ drops from the maximum value. At such a pressure, the formerly nonresonant channels responsible for the low residual resistivity transform into resonant ones, which reduces v_F^2 and $\mathcal{N}_c^0(\mu_L)$. For a constant impurity scattering rate, this leads to a drastic increase in ρ_0 . A further increase in pressure transforms the system into a valence fluctuator with nearly free conduction states and small ρ_0 . An alternative explanation for this peak was suggested by Miyake and Maebashi,²⁹ who attributed it to critical valence fluctuations. In our approach, these would occur at higher pressure, and we expect the resulting feature to be narrower than the one observed experimentally. A peak in $\rho_0(p)$ is also observed in YbCu_2Si_2 .²¹ In this case, the mechanism that leads to it is the “mirror image” of the preceding one:³⁰ Starting from a valence fluctuating regime at ambient pressure, the system is driven into a state with a well-defined valence in which all eight components of the $J=7/2$ $4f$ multiplet hybridize with conduction states, so that ρ_0 is very large. A further increase in pressure stabilizes the magnetic $4f^{13}$ configuration,³¹ inhibits the charge fluctuations, and gives rise to the CF excitations. This reduces the effective degeneracy of the f hole by splitting off the doubly degenerate “resonant” sub-band with heavy QPs from the “nonresonant” sub-bands with nearly free electrons. For the reasons given above, ρ_0 is reduced yet larger than at ambient pressure.

VI. SUMMARY AND CONCLUSIONS

A detailed understanding of the thermoelectric properties of the periodic Anderson model in the full temperature range and for arbitrary parameters is of a considerable interest, as it might facilitate the search for new thermoelectrics with a useful low-temperature figure of merit. The model with the

$\text{SU}(N)$ symmetry and an infinitely large Coulomb repulsion between f electrons captures the low-temperature features of the intermetallic compounds with Ce, Eu, and Yb ions, which exhibit often a large thermopower, and might have a potential for applications.

The thermoelectric response of the $\text{SU}(N)$ model with $n = Nn_f + n_c$ particles is calculated in the FL regime assuming that the FL scale T_0 is known. The value of T_0 can be obtained from the numerical DMFT results for the linear coefficient of the specific heat or estimated from an analytic expression for the QP DOS given by the slave-boson approximation.³² The transport integrals are related to the current-current correlation function and calculated by using the Luttinger theorem and the DMFT condition. The low-temperature transport coefficients are obtained from the Sommerfeld expansion as power series in terms of the reduced temperature T/T_0 . The coefficients in the expansion depend on the average conduction-electron velocity; the unit-cell volume; the effective degeneracy of the f state; the unrenormalized density of c states, $\mathcal{N}_c^0(\mu_L)$; and the shift in the chemical potential, $\Delta\mu = \mu_L - \mu$, which also has a simple physical interpretation. The chemical potential μ corresponds to n interacting particles. For a flat low-energy dispersion, μ is not much different from the chemical potential of Nn_c conduction states decoupled from the f states. The FS of such a conduction band encloses Nn_c points in the \mathbf{k} space and is considered to be “small.” The FS of the Anderson model, determined by the Luttinger theorem, accommodates f electrons in addition to c electrons and is considered to be “large.” For \mathbf{k} -independent hybridization, this large FS coincides with the FS of a free conduction band with n electrons and chemical potential μ_L . Obviously, the FS of a noninteracting conduction band with n electrons differs from the FS of Nn_c electrons, so that the shift $\Delta\mu$ measures the jump in the Fermi volume due to the hybridization.

The parameter dependence of the coefficients multiplying various powers of reduced temperature corrects the simple scaling behavior and explains the deviations of the KW and the q ratios from the universal constants. The FL law for the conductivity gives the KW ratio (which depends on the multiplicity of the f state), the unit-cell volume, the average FS velocity, and the carrier concentration, in agreement with the experimental data.¹¹ The FL law for the thermopower gives the q ratio, which depends on the concentration of f electrons. From these results we conclude that in some systems, pressure or chemical pressure can cause a substantial shift of the “universal ratios” from the common values. We also find that the quasiparticle damping leads to the breakdown of the WF law due to the temperature dependence of the effective Lorenz number. In the absence of the thermal current due to phonons, this would lead to a substantial enhancement of the thermoelectric figure of merit, $ZT > 1$. Assuming that pressure changes the hybridization and the effective degeneracy of the f state, we explained the pronounced maximum of the coefficient of the T^2 term of the electrical resistance^{21–24} and the rapid variation in residual resistance^{21,22} found in a number of Ce and Yb intermetallics at some critical pressure.

Our results describe the main features of thermal transport that one finds in heavy fermions in the FL regime but do not indicate the temperature at which the FL description breaks

down nor relate the FL scale to the Kondo scale, which characterizes the high-temperature behavior. A complete discussion should explain the low- and high-temperature behaviors on equal footing, provide all the relevant energy scales of the system, and account for the change in the effective degeneracy of the low-energy states due to applied pressure, doping, or temperature. The change in the effective degeneracy can have a dramatic effect on the transport coefficients and seems to be responsible for complicated thermoelectric response of intermetallic compounds with Ce and Yb ions. The realistic modeling should remove the $SU(N)$ symmetry, take into account the excited CF states, consider the details of the band structure, and/or include additional interactions. Unfortunately, none of the presently available methods can solve such more realistic models, explain the crossovers between various physical states, and describe the behavior of the correlation functions in the full temperature and pressure range.

A rough description of the high-temperature regime, which takes into account the CF splitting, can be obtained by assuming that the conduction electrons scatter incoherently on the $4f$ ions. This reduces the lattice model with n electrons per unit cell to an effective Anderson impurity model which can be solved very accurately by the noncrossing approximation (NCA).^{18,30} The NCA solution leads to an exponentially small Kondo scale and explains the main features that one finds in the thermoelectric response of heavy fermions and valence fluctuators for $T \geq T_K$. In particular, the NCA shows that the effective degeneracy of the model changes as the excited CF states become thermally populated. Some justification for applying an effective single impurity model to the stoichiometric compounds is provided by the fact that in the temperature range we are concerned with, the resistivity of most heavy fermions is very large and the mean free path is not much longer than a few lattice spacings. Furthermore, the NCA solution for an effective twofold-degenerate impurity model^{18,30} agrees for $T \geq T_K$ with recent DMFT+NRG results for the twofold-degenerate periodic Anderson model.¹⁶ For an N -fold-degenerate model, the NCA gives $\alpha(T)$ and the power factor $P(T) = \alpha^2(T)/\rho(T)$ with a pronounced maximum and $\mathcal{L}(T)$ with a shallow minimum around T_K , which supports our previous conclusions regarding the enhancement of the thermoelectric figure of merit. The agreement between the perturbative solution of an effective single impurity model and the experimental data indicates that the high-temperature state of heavy fermions and valence fluctuators can be represented by a nearly free conduction band, which is weakly perturbed by localized (paramagnetic) f states. Ignoring the thermal broadening of the Fermi distribution function, we find that this FS is much smaller than the low-temperature one, which must include the f electrons in order to satisfy the Luttinger theorem. The perturbative solution breaks down in the coherent regime, as it cannot describe the change in the Fermi volume. For a periodic model, the reduction in the paramagnetic entropy, the crossover from the high-temperature perturbative regime into the FL regime, and the relationship between T_K and T_0 can only be obtained by nonperturbative methods.

The DMFT+NRG method describes, in principle, the crossover from the high-entropy state formed above T_K to the

low-entropy FL ground state. It provides the Kondo scale T_K which governs the high-temperature behavior and gives an accurate numerical estimate of the FL scale T_0 and other thermodynamic quantities, such as the number of particles or the chemical potential of the ground state. However, neither the DMFT+NRG nor the effective impurity approach provide a quantitative description of the transport properties of the periodic Anderson model for temperatures below T_K or T_0 . The usefulness of the FL approach is that it gives the low-temperature transport coefficients for a given T_0 and allows us to obtain an overall description by extrapolating between the FL solution and the high-temperature one obtained by the NCA or the DMFT+NRG methods.

It would be interesting to perform an experimental study of the pressure-induced deviations of the q ratio and the KW ratio from their universal values, using the universal behavior of the power factor or the effective Lorenz number as consistency checks. Since $P(T)$ and $\mathcal{L}(T)$ require only transport measurements, they are well suited for pressure experiments. The above discussion makes it clear that pressure experiments provide the most stringent test of the FL laws.

ACKNOWLEDGMENTS

We thank David Logan for pointing out some unclear points in the original manuscript. Useful discussions with K. Yamada, D. Jaccard, and T. Pruschke are gratefully acknowledged. This work was supported by the Ministry of Science of Croatia under Grant No. 035-0352843-2849, the COST P-16 ECOM project, and the National Science Foundation under Grants No. DMR-0210717 and No. DMR-0705266. The work at SISSA was supported by the Central European Initiative. V.Z. and J.K.F. acknowledge the hospitality of the ETH Zurich, where this work was completed.

APPENDIX A: CORRELATION FUNCTION IN THE FERMILIQUID REGIME

To find $\Lambda(\omega, T)$, we use the Kubo formula for the static conductivity which provides L_{11} as the zero-frequency limit of the number current–number current correlation function,²⁵

$$L_{11}^{\alpha\beta} = \lim_{\nu \rightarrow 0} \text{Re} \frac{i}{\nu} \bar{L}_{11}^{\alpha\beta}(\nu), \quad (\text{A1})$$

where

$$\bar{L}_{11}^{\alpha\beta}(i\nu) = \frac{\hbar}{\mathcal{V}\mathcal{N}_i} \int_0^\beta d\tau e^{i\nu\tau} \langle T_{\mathbf{j}} \mathbf{j}_\alpha^\dagger(\tau) \mathbf{j}_\beta(0) \rangle, \quad (\text{A2})$$

$\nu_i = 2\pi k_B T i$ is the bosonic Matsubara frequency, the τ dependence of the operator is with respect to the Hamiltonian in Eq. (1), the subscripts α and β denote the respective spatial indices of the number-current vector \mathbf{j}_c/e ; and we must analytically continue $\bar{L}_{11}^{\alpha\beta}(i\nu)$ to the real axis $\bar{L}_{11}^{\alpha\beta}(\nu)$ before taking the limit $\nu \rightarrow 0$.

Substituting the definition of the particle current operator from Eq. (5) into Eq. (A2) for $\bar{L}_{11}^{\alpha\beta}$ and taking the limit of infinite dimensions, in which the dressed correlation function is equal to the bare one,^{33,34} we obtain

$$\bar{L}_{11}^{\alpha\beta}(i\nu_l) = \frac{-\hbar}{\mathcal{V}\mathcal{N}_i} \int_0^\beta d\tau e^{i\nu_l\tau} \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}\alpha} \mathbf{v}_{\mathbf{k}\beta} G_c(\mathbf{k}, \tau) G_c(\mathbf{k}, -\tau), \quad (\text{A3})$$

where $G_c(\mathbf{k}, \tau)$ is the imaginary time Green's function of the c electrons, which can be expressed as a Fourier series, $G_c(\mathbf{k}, \tau) = k_B T \sum_n \exp(-i\omega_n \tau) G_c(\mathbf{k}, i\omega_n)$. Substituting into Eq. (A3) and integrating over imaginary time provides the result

$$\bar{L}_{11}^{\alpha\beta}(i\nu_l) = \frac{-\hbar}{\mathcal{V}\mathcal{N}_i} k_B T \sum_n \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}\alpha} \mathbf{v}_{\mathbf{k}\beta} G_c(\mathbf{k}, i\omega_n) G_c(\mathbf{k}, i\omega_n + i\nu_l), \quad (\text{A4})$$

which has to be analytically continued to the real axis. Since the Green's functions in Eq. (A4) depend on \mathbf{k} only through $\epsilon(\mathbf{k})$ which is an even function of \mathbf{k} , while $\mathbf{v}_{\mathbf{k}\alpha}$ is odd, the summation over \mathbf{k} vanishes for $\alpha \neq \beta$. We consider only isotropic systems, where $L_{11}^{\alpha\alpha} = L_{11}$. To perform the analytic continuation, we follow closely Ref. 35 and obtain the result (evaluated explicitly for a three-dimensional system)

$$L_{11} = \frac{-\hbar}{\mathcal{V}\mathcal{N}_i} \frac{v_F^2}{3\pi} \int_{-\infty}^{\infty} d\omega \lim_{\nu \rightarrow 0} \frac{f(\omega) - f(\omega + \nu)}{\nu} \times \text{Re} \left[\frac{G_c(\omega) - G_c(\omega + \nu)}{\nu + \Sigma_c(\omega) - \Sigma_c(\omega + \nu)} - \frac{G_c^*(\omega) - G_c(\omega + \nu)}{\nu + \Sigma_c^*(\omega) - \Sigma_c(\omega + \nu)} \right], \quad (\text{A5})$$

where we introduced the local Green's function

$$G_c(\omega) = \sum_{\mathbf{k}} G_c(\mathbf{k}, \omega) \quad (\text{A6})$$

and replaced the square of the α component of velocity by its Fermi-surface average v_F^2/d (d is the spatial dimension, which we can take to be equal to 3 for real systems). This step is justified because the energy integrations in Eq. (A5) is restricted to a narrow interval around the Fermi energy, where the integrand is singular, so that the main contribution to the \mathbf{k} summation comes from the \mathbf{k} points close to the Fermi surface. On the infinite-dimensional hypercubic lattice, the integral can be performed exactly and one finds that the average square velocity is equal to $a_l^2 t^{*2} / 16\hbar^2$ when expressed in terms of the reduced nearest-neighbor hopping $t^* = 2\sqrt{d}t$.

We can now take the limit of $\nu \rightarrow 0$. Writing

$$\lim_{\nu \rightarrow 0} \frac{G_c(\omega) - G_c(\omega + \nu)}{\nu + \Sigma_c(\omega) - \Sigma_c(\omega + \nu)} = - \frac{\partial G_c(\omega)}{\partial \omega} \frac{1}{1 - \frac{\partial \Sigma_c(\omega)}{\partial \omega}} \quad (\text{A7})$$

and

$$\lim_{\nu \rightarrow 0} \frac{G_c^*(\omega) - G_c(\omega + \nu)}{\nu + \Sigma_c^*(\omega) - \Sigma_c(\omega + \nu)} = \frac{\text{Im} G_c(\omega)}{\text{Im} \Sigma_c(\omega)} \quad (\text{A8})$$

produces our final result

$$L_{11} = \int_{-\infty}^{\infty} d\omega \left[- \frac{df(\omega)}{d\omega} \right] \Lambda(\omega, T), \quad (\text{A9})$$

where $\Lambda(\omega, T)$ is defined by

$$\Lambda(\omega) = \frac{\hbar}{\mathcal{V}\mathcal{N}_c} \frac{v_F^2}{3\pi} \left\{ \frac{\text{Im} G_c(\omega)}{\text{Im} \Sigma_c(\omega)} + \text{Re} \left[\frac{\frac{\partial G_c(\omega)}{\partial \omega}}{1 - \frac{\partial \Sigma_c(\omega)}{\partial \omega}} \right] \right\}. \quad (\text{A10})$$

To estimate the relative importance of the two terms in Eq. (A10), we introduce the Hilbert transform of $\mathcal{N}_c(\omega)$,

$$\mathcal{H}_c(\omega) = - \frac{1}{\pi \mathcal{V}\mathcal{N}_i} \text{Re} G_c(\omega). \quad (\text{A11})$$

In the FL regime, where $\mathcal{N}_c(\omega)$ is δ -function-like, the slope of $\mathcal{H}_c(\omega)$ is very large; it is proportional to the c -electron enhancement factor

$$\text{Re} \left[1 - \frac{\partial \Sigma_c(\omega)}{\partial \omega} \right] = Z_c^{-1}.$$

On the other hand, $\text{Im} \partial \Sigma_c(\omega) / \partial \omega$ is small around $\omega = 0$ because $\text{Im} \Sigma_c(\omega)$ is close to its maximum value. Using

$$\text{Im} \frac{\partial \Sigma_c(\omega)}{\partial \omega} \ll Z_c^{-1},$$

we neglect $[\text{Im} \partial \Sigma_c(\omega) / \partial \omega]^2$ in the denominator of the second term for $\Lambda(\omega)$ in Eq. (A10) and approximate

$$\text{Re} \left[\frac{\frac{\partial G_c(\omega)}{\partial \omega}}{1 - \frac{\partial \Sigma_c(\omega)}{\partial \omega}} \right] \simeq Z_c \frac{\partial \mathcal{H}_c(\omega)}{\partial \omega} - \frac{\partial \mathcal{N}_c(\omega)}{\partial \omega} \text{Im} \frac{\partial \Sigma_c(\omega)}{\partial \omega}.$$

This term is small with respect to $\mathcal{N}_c(\omega) / \text{Im} \Sigma(\omega)$, which diverges in the limit $T, \omega \rightarrow 0$. Keeping only the singular term in Eq. (A10), we obtain the result of Eq. (7) used in the text.

APPENDIX B: TRANSPORT COEFFICIENTS

The transport coefficients are obtained by expanding the derivative of the Fermi function in a Sommerfeld expansion, $-\partial f(\omega) / \partial \omega = \delta(\omega) + (\pi^2 k_B^2 T^2 / 6) [\partial^2 \delta(\omega) / \partial \omega^2]$, which gives the following result for the transport integrals:

$$L_{mn} = [\omega^{m+n-2} \Lambda(\omega, T)]_{\omega=0} + \frac{\pi^2 k_B^2 T^2}{6} \left\{ \frac{\partial^2}{\partial \omega^2} [\omega^{m+n-2} \Lambda(\omega, T)] \right\}_{\omega=0}. \quad (\text{B1})$$

For thermal transport we have to evaluate

$$L_{11} = [\Lambda(\omega, T)]_{\omega=0} + \frac{\pi^2 k_B^2 T^2}{6} \Lambda''(\omega, T)|_{\omega=0}, \quad (\text{B2})$$

$$L_{12} = \frac{\pi^2 k_B^2 T^2}{3} \Lambda'(\omega, T)|_{\omega=0}, \quad (\text{B3})$$

$$L_{22} = \frac{\pi^2 k_B^2 T^2}{3} \Lambda(\omega, T)|_{\omega=0}, \quad (\text{B4})$$

where

$$\Lambda(\omega, T) = \frac{1}{3} v_F^2 \mathcal{N}_c(\omega) \tau(\omega, T), \quad (\text{B5})$$

$$\Lambda'(\omega, T) = \frac{1}{3} v_F^2 [\mathcal{N}'_c(\omega) \tau(\omega, T) + \mathcal{N}_c(\omega) \tau'(\omega, T)], \quad (\text{B6})$$

$$\Lambda''(\omega, T) = \frac{1}{3} v_F^2 [\mathcal{N}''_c(\omega) \tau(\omega, T) + 2\mathcal{N}'_c(\omega) \tau'(\omega, T) + \mathcal{N}_c(\omega) \tau''(\omega, T)], \quad (\text{B7})$$

and Λ' and Λ'' denote the first and second derivatives with respect to ω . The first derivative of $\mathcal{N}_c(\omega)$ is

$$\mathcal{N}'_c(\omega) = \frac{2(\omega - \tilde{\omega}_f)}{Z_f \tilde{V}^2} \mathcal{N}_f(\omega) + \frac{(\omega - \tilde{\omega}_f)^2}{Z_f \tilde{V}^2} \mathcal{N}'_f(\omega) \quad (\text{B8})$$

and becomes in the $\omega \rightarrow 0$ limit

$$\mathcal{N}'_c(0) \simeq -2 \frac{\mathcal{N}_c(0)}{\tilde{\omega}_f}, \quad (\text{B9})$$

where the DMFT condition showed that the derivative of the f -electron DOS is small at $\omega=0$. For the second derivative, we obtain

$$\mathcal{N}''_c(0) = \frac{2\mathcal{N}_c(0)}{\tilde{\omega}_f^2}, \quad (\text{B10})$$

using $\mathcal{N}'_f(0)/Z_f \tilde{V}^2 = \mathcal{N}_c(0)/\tilde{\omega}_f^2$ and dropping the terms proportional to $\tilde{\omega}_f \mathcal{N}'_f(0)$ and $\tilde{\omega}_f^2 \mathcal{N}''_f(0)$ which are exponentially small [see also Eq. (47)].

The transport relaxation time given by the expression in Eq. (39) yields at $\omega=0$

$$\tau'(0, T) = -2 \frac{\tau_0(T)}{\tilde{\omega}_f}, \quad (\text{B11})$$

$$\tau''(0, T) = 2\tau_0(T) \left[\frac{1}{\tilde{\omega}_f^2} - \frac{1}{(\pi k_B T)^2} \right]. \quad (\text{B12})$$

The transport integrals are now easy to find. The first one is obtained from Eq. (B7), which gives

$$L_{11} \simeq \frac{1}{3} v_F^2 \mathcal{N}_c(0) \tau_0(T) \left\{ 1 + \frac{\pi^2 k_B^2 T^2}{3} \left[\frac{6\mathcal{N}_c(0)}{\tilde{\omega}_f^2} - \frac{1}{(\pi k_B T)^2} \right] \right\} \\ \simeq \Lambda(0, T) \left[\frac{2}{3} + \mathcal{O}(T^2) \right]. \quad (\text{B13})$$

The last term in the square brackets in the second line grows as $1/T^2$, while the first one is a (large) constant which we neglect at low enough temperature. Since $\Lambda(0, T) \propto 1/T^2$, this approximation amounts to keeping the T^2 terms in the electrical resistance and neglecting the T^4 contribution. The correcting factor $2/3$ in Eq. (B13) originates from the imaginary part of the self-energy and it is well known from the dilute alloy problem;³⁶ hence it arises only in the clean limit. Inserting the expressions for the renormalized c DOS [Eq. (27)] and the relaxation time [Eq. (40)], we obtain the dominant low-temperature contribution to L_{11} :

$$L_{11} = v_F^2 \frac{\hbar(N-1)[N\mathcal{V}\mathcal{N}_c^0(\mu_L)]^2}{9\pi^3\mathcal{V}} \left(\frac{T_0}{T} \right)^2, \quad (\text{B14})$$

which yields for the static conductivity $\sigma(T) = Ne^2 L_{11}$

$$\sigma(T) = \frac{\hbar e^2 v_F^2 N(N-1)[N\mathcal{V}\mathcal{N}_c^0(\mu_L)]^2}{9\pi^3\mathcal{V}} \left(\frac{T_0}{T} \right)^2 \quad (\text{B15})$$

and the resistivity $\rho(T) = 1/\sigma(T)$.

The second transport integral is obtained from Eq. (B6), which gives

$$L_{12} = \frac{\pi^2 k_B^2 T^2}{3} \Lambda(0, T) \left[\frac{\mathcal{N}'_c(0)}{\mathcal{N}_c(0)} + \frac{\tau'(0, T)}{\tau(0, T)} \right] \quad (\text{B16})$$

$$\simeq -2L_{11} \frac{\pi^2 k_B^2 T^2}{\tilde{\omega}_f} \simeq \mp 4L_{11} \frac{\pi^2 k_B T^2}{n_f T_0}. \quad (\text{B17})$$

In the second equation, we used $\tilde{\omega}_f \simeq \pm n_f k_B T_0/2$, which holds for heavy fermions with $n_f \simeq 1$ and large N only.

The thermal conductivity is defined by the expression

$$\kappa(T) = N \frac{L_{11}}{T} \left[\frac{L_{22}}{L_{11}} - \left(\frac{L_{12}}{L_{11}} \right)^2 \right] \quad (\text{B18})$$

and follows from the previous results, which give $L_{11} = 2\Lambda(0, T)/3$, $L_{12}/L_{11} \simeq 2\pi^2 k_B^2 T^2/\tilde{\omega}_f$, $L_{22} = \pi^2 k_B^2 T^2 \Lambda(0, T)/3$, and $L_{22}/L_{11} = \pi^2 k_B^2 T^2/2$. In the heavy fermion limit, this yields the expression in Eq. (53) used in the main text.

¹K. Behnia, D. Jaccard, and J. Flouquet, J. Phys.: Condens. Matter **16**, 5187 (2004).

²J. Sakurai and Y. Isikawa, J. Phys. Soc. Jpn. **74**, 1926 (2005).

³Z. Hossain, C. Geibel, N. Senthilkumaran, M. Deppe, M. Baenitz, F. Schiller, and S. L. Molodtsov, Phys. Rev. B **69**, 014422 (2004).

⁴J. Sakurai, A. Iwasaki, Q. Lu, D. Ho, Y. Isikawa, J. R. Fernández, and C. G. Sal, J. Phys. Soc. Jpn. **71**, 2829 (2002).

⁵M. Očko, D. Drobac, J. L. Sarrao, and Z. Fisk, Phys. Rev. B **64**, 085103 (2001).

⁶M. Očko, J. L. Sarrao, and Z. Šimek, J. Magn. Magn. Mater. **43–46**, 284 (2004).

⁷U. Kohler, N. Oeschler, F. Steglich, S. Maquilon, and Z. Fisk, Phys. Rev. B **77**, 104412 (2008).

⁸K. Kadowaki and S. B. Woods, Solid State Commun. **71**, 1149 (1987).

- ⁹H. Kontani, J. Phys. Soc. Jpn. **73**, 515 (2004).
- ¹⁰N. Tsujii, H. Kontani, and K. Yoshimura, Phys. Rev. Lett. **94**, 057201 (2005).
- ¹¹N. E. Hussey, J. Phys. Soc. Jpn. **74**, 1107 (2005).
- ¹²K. Yamada and K. Yosida, Prog. Theor. Phys. **76**, 681 (1986).
- ¹³K. Yamada, *Electron Correlation in Metals* (Cambridge University, Cambridge, 2004).
- ¹⁴K. Miyake and H. Kohno, J. Phys. Soc. Jpn. **74**, 254 (2005).
- ¹⁵N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Dover, London, 1958).
- ¹⁶C. Grenzebach, F. B. Anders, G. Czycholl, and T. Pruschke, Phys. Rev. B **74**, 195119 (2006).
- ¹⁷A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
- ¹⁸V. Zlatić, R. Monnier, J. Freericks, and K. W. Becker, Phys. Rev. B **76**, 085122 (2007).
- ¹⁹A. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
- ²⁰G. D. Mahan, *Solid State Physics*, edited by H. Ehrenreich and F. Spaepen (Academic, San Diego, 1997), Vol. 51, p. 81.
- ²¹D. Jaccard, E. Vargoz, K. Alami-Yadri, and H. Wilhelm, Rev. High Pressure Sci. Technol. **7**, 412 (1998).
- ²²A. T. Holmes, D. Jaccard, and K. Miyake, Phys. Rev. B **69**, 024508 (2004).
- ²³H. Wilhelm and D. Jaccard, Phys. Rev. B **66**, 064428 (2002).
- ²⁴H. Wilhelm, D. Jaccard, V. Zlatić, R. Monnier, B. Delley, and B. Coqblin, J. Phys.: Condens. Matter **17**, S823 (2005).
- ²⁵G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
- ²⁶N. Vidhyadhiraja and D. Logan, Eur. Phys. J. B **39**, 313 (2004).
- ²⁷D. E. Logan and N. S. Vidhyadhiraja, J. Phys.: Condens. Matter **17**, 2935 (2005).
- ²⁸N. Kernavanois, S. Raymond, E. Ressouche, B. Grenier, J. Flouquet, and P. Lejay, Phys. Rev. B **71**, 064404 (2005).
- ²⁹K. Miyake and H. Maebashi, J. Phys. Soc. Jpn. **71**, 1007 (2002).
- ³⁰V. Zlatić and R. Monnier, Phys. Rev. B **71**, 165109 (2005).
- ³¹K. Alami-Yadri, D. Jaccard, and D. Andreica, J. Low Temp. Phys. **114**, 135 (1999).
- ³²S. Burdin and V. Zlatić (unpublished).
- ³³A. Khurana, Phys. Rev. Lett. **64**, 1990 (1990).
- ³⁴V. Zlatić and B. Horvatić, Solid State Commun. **75**, 263 (1990).
- ³⁵J. K. Freericks and V. Zlatić, Phys. Rev. B **64**, 245118 (2001).
- ³⁶B. Horvatić and V. Zlatić, Phys. Rev. B **30**, 6717 (1984).