Higher-Order Fermi-Liquid Corrections for an Anderson Impurity Away from Half Filling

Akira Oguri
Department of Physics, Osaka City University, Sumiyoshi-ku, Osaka 558-8585, Japan

A. C. Hewson
Department of Mathematics, Imperial College London, London SW7 2AZ, United Kingdom

(Received 19 September 2017; revised manuscript received 20 December 2017; published 23 March 2018)

We study the higher-order Fermi-liquid relations of Kondo systems for arbitrary impurity-electron fillings, extending the many-body quantum theoretical approach of Yamada and Yosida. It includes, partly, a microscopic clarification of the related achievements based on Nozières' phenomenological description: Filippone, Moca, von Delft, and Mora [Phys. Rev. B **95**, 165404 (2017)]. In our formulation, the Fermi-liquid parameters such as the quasiparticle energy, damping, and transport coefficients are related to each other through the total vertex $\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)$, which may be regarded as a generalized Landau quasiparticle interaction. We obtain exactly this function up to linear order with respect to the frequencies ω and ω' using the antisymmetry and analytic properties. The coefficients acquire additional contributions of three-body fluctuations away from half filling through the nonlinear susceptibilities. We also apply the formulation to nonequilibrium transport through a quantum dot, and clarify how the zero-bias peak evolves in a magnetic field.

DOI: 10.1103/PhysRevLett.120.126802

Introduction.—Universal low-energy behavior of interacting Fermi systems has been one of the most fascinating properties in condensed matter physics. Landau's Fermi liquid theory [1–3] phenomenologically explains transport properties of electrons in a wide class of metals and normal liquid ^{3}He successfully [4], and may also be applied to exotic systems such as neutron stars and ultracold Fermi gases [5]. It starts with an expansion of the energy E with respect to the deviation of the momentum distribution function $\delta n_{p\sigma}$ from the ground state,

$$E = E_0 + \sum_{p\sigma} \varepsilon_{p} \delta n_{p\sigma} + \frac{1}{2} \sum_{\substack{p\sigma \\ p'\sigma'}} f_{p\sigma,p'\sigma'} \delta n_{p\sigma} \delta n_{p'\sigma'}. \quad (1)$$

The single quasiparticle energy ε_{p} and the interaction between quasiparticles $f_{p\sigma,p'\sigma'}$ can microscopically be related to the four-point vertex function, defined explicitly in the many-body quantum theory [2,3]. The field theoretic description has advantages over the phenomenological approach: the transport equations can be derived directly using the Green's function without relying on empirical assumptions nor the collision integral with the Boltzmann equation [6,7]. For instance, through a microscopic consideration about the antisymmetry properties of the vertex function [3], sufficient conditions for the collective zero sound mode to exist have been derived [8].

Nozières extended the phenomenological Fermi-liquid description to Kondo systems [9], expanding the scattering phase shift δ with respect to a deviation of the occupation number of the impurity level in a way analogous to Eq. (1). Fully microscopic description was constructed by Yamada and Yosida, Shiba, and Yoshimori [10–13], and has also been extended to out-of-equilibrium quantum dots driven by a bias voltage V [14,15]. The two different types of descriptions complement each other and explain the universal behavior at temperatures T much lower than the Kondo energy scale T_K. It is successful especially in the particle-hole symmetric case, i.e., at half filling, where the phase shift is locked at $\delta = \pi/2$ and the quadratic ω^2, T^2, and $(eV)^2$ corrections emerge only through the quasiparticle *damping*.

Away from half filling, however, the Kondo resonance peak deviates from the Fermi energy $\omega = 0$, and as a consequence, the quadratic corrections emerge also through the real part of the self-energy due to the Coulomb interaction U [13,16]. It makes the problem difficult, and such corrections have not been fully understood for a long time. Recently, there has been a significant breakthrough which shed light on this problem by extending Nozières' phenomenological description [17,18]. Specifically, Filippone, Moca, von Delft, and Mora (FMvDM) determined especially the quadratic coefficients of the self-energy away from half filling [19].

In this Letter, we provide a microscopic Fermi-liquid description for the nonequilibrium Anderson impurity [20] away from half filling. One of the most pronounced merits of this formulation is that the real and imaginary parts of the transport coefficients are derived together from an explicit expression for the total vertex $\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)$ at low frequencies. It gives a clear answer to the long-standing problem. Specifically, an asymptotically exact expression is obtained, up to linear order in ω and ω', using the antisymmetry and analytic properties with the Ward identities. The low-energy Fermi-liquid behavior is characterized by the expansion coefficients which are shown to be expressed in terms of the linear $\chi_{\sigma\sigma'}$ and nonlinear $\chi^{[3]}_{\sigma_1\sigma_2\sigma_3}$ susceptibilities.

These susceptibilities can be calculated using methods such as the numerical normalization group (NRG) [21] and the Bethe ansatz solution [22,23]. We apply the microscopic formulation to nonequilibrium current I through a quantum dot in the Kondo regime, and calculate the coefficients using the NRG. The result shows that the zero-bias peak of dI/dV splits at a magnetic field of the order of T_K, and resolves a controversial issue about the splitting [18]. There are other numerical methods which work efficiently at different energy scales, such as the quantum Monte Carlo method [24], time-dependent NRG [25], and density-matrix renormalization group [26]. Our approach has a numerical advantage at low energies as both the linear and nonlinear susceptibilities can be deduced from the flow of energy eigenvalues near the fixed point of the NRG [27].

The microscopic theory gives exact relations between different response functions and has given theoretical support for the universal scaling observed in the nonequilibrium currents through quantum dots in the Kondo regime [28,29]. Furthermore, recent ultrasensitive current noise measurements have successfully determined the Fermi-liquid parameters [30], i.e., the Wilson ratio R_W and the renormalization factor of quasiparticles. However, such comparisons so far have relied on the theoretical predictions at half filling. The exact formula of transport coefficients, presented in Eqs. (22) and (23), overcomes this restriction and can be applied to quantum dots for arbitrary electron fillings. Our formulation also has potential application for a wide class of Kondo systems such as dilute magnetic alloys and quantum impurities with various kinds of internal degrees of freedom.

Nonlinear three-body susceptibilities for impurity levels.—We consider the single Anderson impurity coupled to two noninteracting leads ($\lambda = L, R$);

$$\mathcal{H} = \sum_\sigma \epsilon_{d\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\lambda=L,R}\sum_\sigma \int_{-D}^{D} d\epsilon\, \epsilon c^\dagger_{\epsilon\lambda\sigma} c_{\epsilon\lambda\sigma} + \sum_{\lambda=L,R}\sum_\sigma v_\lambda (\psi^\dagger_{\lambda,\sigma} d_\sigma + d^\dagger_\sigma \psi_{\lambda,\sigma}). \tag{2}$$

Here, $d^\dagger_\sigma$ creates an impurity electron with spin σ and $n_{d\sigma} = d^\dagger_\sigma d_\sigma$. Conduction electrons in each lead are normalized such that $\{c_{\epsilon\lambda\sigma}, c^\dagger_{\epsilon'\lambda'\sigma'}\} = \delta_{\lambda\lambda'}\delta_{\sigma\sigma'}\delta(\epsilon-\epsilon')$. In a magnetic field h, the impurity level is given by $\epsilon_{d\sigma} = \epsilon_d - \sigma h$, where $\sigma = +1$ (-1) for $\uparrow$ $(\downarrow)$ spin. The hybridization v_λ between $\psi_{\lambda\sigma} \equiv \int_{-D}^{D} d\epsilon \sqrt{\rho_c}\, c_{\epsilon\lambda\sigma}$ and impurity electrons broadens the impurity level: $\Delta \equiv \Gamma_L + \Gamma_R$ with $\Gamma_\lambda = \pi\rho_c v_\lambda^2$ and $\rho_c = 1/(2D)$. We consider the parameter region, where the half bandwidth D is much greater than the other energy scales, $D \gg \max(U, \Delta, |\epsilon_{d\sigma}|, |\omega|, T, eV)$.

We use the $T=0$ causal impurity Green's function $G_\sigma(\omega)$ and self-energy $\Sigma_\sigma(\omega)$ defined at $eV = 0$:

$$G_\sigma(\omega) = \frac{1}{\omega - \epsilon_{d\sigma} + i\Delta \mathrm{sgn}(\omega) - \Sigma_\sigma(\omega)}. \tag{3}$$

The phase shift $\cot\delta_\sigma \equiv [\epsilon_{d\sigma} + \Sigma_\sigma(0)]/\Delta$, or the density of states $\rho_{d\sigma} \equiv -\mathrm{Im}G_\sigma(0^+)/\pi$ at $\omega = 0$, is a primary parameter which characterizes the Fermi-liquid ground state. The Friedel sum rule relates δ_σ to the occupation number which can also be given by the first derivative of the free energy $\Omega \equiv -T \log[\mathrm{Tr} e^{-\mathcal{H}/T}]$,

$$\langle n_{d\sigma}\rangle = \frac{\partial\Omega}{\partial\epsilon_{d\sigma}} \xrightarrow{T\to 0} \frac{\delta_\sigma}{\pi}. \tag{4}$$

The leading Fermi-liquid corrections are determined by the static susceptibilities [10],

$$\chi_{\sigma\sigma'} \equiv -\frac{\partial^2\Omega}{\partial\epsilon_{d\sigma'}\partial\epsilon_{d\sigma}} = -\frac{\partial\langle n_{d\sigma}\rangle}{\partial\epsilon_{d\sigma'}} \xrightarrow{T\to 0} \rho_{d\sigma}\tilde{\chi}_{\sigma\sigma'}. \tag{5}$$

It can also be expressed as $\chi_{\sigma\sigma'} = \int_0^{(1/T)} d\tau \langle\delta n_{d\sigma'}(\tau)\delta n_{d\sigma}\rangle$, and $\tilde{\chi}_{\sigma\sigma'} \equiv \delta_{\sigma\sigma'} + \partial\Sigma_\sigma(0)/\partial\epsilon_{d\sigma'}$ is an enhancement factor similar to the Stoner factor. The usual spin and charge susceptibilities, $\chi_s \equiv -\frac{1}{4}[(\partial^2\Omega)/(\partial h^2)]$ and $\chi_c \equiv -[(\partial^2\Omega)/(\partial\epsilon_d^2)]$, are given by linear combinations of $\chi_{\sigma\sigma'}$ [31]. These susceptibilities also determine the characteristic energy scale $4T^* \equiv 1/\sqrt{\chi_{\uparrow\uparrow}\chi_{\downarrow\downarrow}}$ and the Wilson ratio $R_W \equiv 1\text{–}4T^*\chi_{\uparrow\downarrow}$ which corresponds to a dimensionless quasiparticles interaction [21,32].

Away from half filling, the third derivatives of the free energy also contribute to the next leading Fermi-liquid corrections, as we will show later

$$\chi^{[3]}_{\sigma_1\sigma_2\sigma_3} \equiv -\frac{\partial^3\Omega}{\partial\epsilon_{d\sigma_1}\partial\epsilon_{d\sigma_2}\partial\epsilon_{d\sigma_3}} = \frac{\partial\chi_{\sigma_2\sigma_3}}{\partial\epsilon_{d\sigma_1}}. \tag{6}$$

It can also be expressed as a static three-point function of the impurity occupation $\delta n_{d\sigma} \equiv n_{d\sigma} - \langle n_{d\sigma}\rangle$,

$$\chi^{[3]}_{\sigma_1\sigma_2\sigma_3} = -\int_0^{\frac{1}{T}} d\tau_3 \int_0^{\frac{1}{T}} d\tau_2 \langle T_\tau \delta n_{d\sigma_3}(\tau_3)\delta n_{d\sigma_2}(\tau_2)\delta n_{d\sigma_1}\rangle. \tag{7}$$

Higher-order Fermi-liquid corrections at $T = 0$.—The Ward identity, which reflects the current conservation for each spin component σ, plays a central role [13],

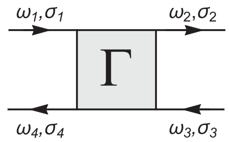

FIG. 1. Total vertex $\Gamma_{\sigma_1\sigma_2;\sigma_3\sigma_4}(\omega_1,\omega_2;\omega_3,\omega_4)$ satisfies the antisymmetry property: Eq. (9) with $\omega_1+\omega_3=\omega_2+\omega_4$.

$$\frac{\partial\Sigma_\sigma(\omega)}{\partial\omega}\delta_{\sigma\sigma'}+\frac{\partial\Sigma_\sigma(\omega)}{\partial\epsilon_{d\sigma'}}=-\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,0;0,\omega)\rho_{d\sigma'}. \quad (8)$$

Here, the total vertex $\Gamma_{\sigma_1\sigma_2;\sigma_3\sigma_4}(\omega_1,\omega_2;\omega_3,\omega_4)$ includes all contributions of multiple scattering, and Fig. 1 shows the assignment of arguments. The antisymmetry properties of the total vertex also impose strong restrictions on the low-energy behavior as a consequence of the exclusion principle [2,3,8,33],

$$\begin{aligned}&\Gamma_{\sigma_1\sigma_2;\sigma_3\sigma_4}(\omega_1,\omega_2;\omega_3,\omega_4)\\&\quad=-\Gamma_{\sigma_3\sigma_2;\sigma_1\sigma_4}(\omega_3,\omega_2;\omega_1,\omega_4)\\&\quad=\Gamma_{\sigma_3\sigma_4;\sigma_1\sigma_2}(\omega_3,\omega_4;\omega_1,\omega_2)\\&\quad=-\Gamma_{\sigma_1\sigma_4;\sigma_3\sigma_2}(\omega_1,\omega_4;\omega_3,\omega_2).\end{aligned} \quad (9)$$

For instance, at zero frequencies the parallel-spin component vanishes $\Gamma_{\sigma\sigma;\sigma\sigma}(0,0;0,0)=0$, and the leading Fermi-liquid relations [34] follow from Eq. (8).

Another important clue is the analytic property. The nonanalytic part of the vertex function is accompanied by the "sgn" functions and is purely imaginary, while the analytic part is real. Thus, the low-frequency expansion of the real part of $\Gamma_{\sigma\sigma;\sigma\sigma}(\omega_1,\omega_2;\omega_3,\omega_4)$ starts with a homogeneous polynomial of degree one. However, such a homogeneous polynomial of linear form cannot satisfy the antisymmetry property Eq. (9) provided $\omega_1+\omega_3=\omega_2+\omega_4$. Therefore, the parallel-spin component does not have an analytic part of linear order. Thus, for $\omega_2=\omega_3=0$,

$$\frac{\partial}{\partial\omega}\mathrm{Re}\Gamma_{\sigma\sigma;\sigma\sigma}(\omega,0;0,\omega)\rho_{d\sigma}\Big|_{\omega\to0}=0. \quad (10)$$

To our knowledge, this property has not explicitly been recognized so far. We have also calculated the skeleton diagrams for $\Gamma_{\sigma\sigma;\sigma\sigma}(\omega,0;0,\omega)$ up to order U^4 and have confirmed Eq. (10) perturbatively [35]. In the linear order, the nonanalytic part shows the $|\omega|$ dependence [12] with a coefficient determined by Yamada and Yosida [11]:

$$\Gamma_{\sigma\sigma;\sigma\sigma}(\omega,0;0,\omega)\rho_{d\sigma}^2=i\pi\chi_{\uparrow\downarrow}^2\omega\ \mathrm{sgn}(\omega)+O(\omega^2). \quad (11)$$

A series of higher-order Fermi-liquid relations follow from this property of the total vertex for parallel spins.

We obtain an identity between the double derivatives of the real part of the self-energy using Eqs. (8) and (10),

$$\mathrm{Re}\frac{\partial^2\Sigma_\sigma(\omega)}{\partial\omega^2}\Big|_{\omega\to0}=\frac{\partial^2\Sigma_\sigma(0)}{\partial\epsilon_{d\sigma}^2}. \quad (12)$$

Note that $\partial^2\Sigma_\sigma(0)/\partial\epsilon_{d\sigma}^2\equiv\partial\tilde{\chi}_{\sigma\sigma}/\partial\epsilon_{d\sigma}$ by definition, and Eq. (12) agrees with FMvDM's result given in Eq. (B8b) of Ref. [18]. Furthermore, using Eqs. (8) and (12), the total vertex for antiparallel spins can be calculated exactly up to terms of order ω^2,

$$\begin{aligned}&\Gamma_{\sigma,-\sigma;-\sigma,\sigma}(\omega,0;0,\omega)\rho_{d\sigma}\rho_{d,-\sigma}\\&\quad=-\chi_{\uparrow\downarrow}+\rho_{d\sigma}\frac{\partial\tilde{\chi}_{\sigma,-\sigma}}{\partial\epsilon_{d\sigma}}\omega\\&\qquad+\frac{\rho_{d\sigma}}{2}\frac{\partial}{\partial\epsilon_{d,-\sigma}}\left(-\frac{\partial\tilde{\chi}_{\sigma\sigma}}{\partial\epsilon_{d\sigma}}+i\pi\frac{\chi_{\uparrow\downarrow}^2}{\rho_{d\sigma}}\mathrm{sgn}(\omega)\right)\omega^2+\cdots.\end{aligned} \quad (13)$$

Note that the ω-linear contribution is real and analytic.

We see in Eqs. (12) and (13) that expansion coefficients depend on $\partial\tilde{\chi}_{\sigma\sigma'}/\partial\epsilon_{d\sigma''}$ which includes contributions from three-body fluctuations $\chi_{\sigma\sigma'\sigma''}^{[3]}$. The three-body correlations vanish in the particle-hole symmetric case since the spin (charge) susceptibility takes a maximum (minimum): $\partial\chi_s/\partial\epsilon_d=0$ and $\partial\chi_c/\partial\epsilon_d=0$ at $\epsilon_d=-U/2$ and $h=0$. We also find that the ω^2 term of Eq. (13) involves four-body fluctuations in the real part through $\partial^2\tilde{\chi}_{\sigma\sigma}/\partial\epsilon_{d\sigma}\partial\epsilon_{d,-\sigma}$ which remains finite even in the particle-hole symmetric case. The four-body fluctuations will also contribute to higher-order terms of the parallel-spin vertex.

We have also calculated the total vertex for two independent frequencies up to linear order in ω and ω':

$$\Gamma_{\sigma\sigma;\sigma\sigma}(\omega,\omega';\omega',\omega)\rho_{d\sigma}^2=i\pi\chi_{\uparrow\downarrow}^2|\omega-\omega'|+\cdots, \quad (14)$$

$$\begin{aligned}&\Gamma_{\sigma,-\sigma;-\sigma,\sigma}(\omega,\omega';\omega',\omega)\rho_{d\sigma}\rho_{d,-\sigma}\\&\quad=-\chi_{\uparrow\downarrow}+\rho_{d\sigma}\frac{\partial\tilde{\chi}_{\sigma,-\sigma}}{\partial\epsilon_{d\sigma}}\omega+\rho_{d,-\sigma}\frac{\partial\tilde{\chi}_{-\sigma,\sigma}}{\partial\epsilon_{d,-\sigma}}\omega'\\&\qquad+i\pi\chi_{\uparrow\downarrow}^2(|\omega-\omega'|-|\omega+\omega'|)+\cdots.\end{aligned} \quad (15)$$

The analytic real part can be deduced from Eqs. (11) and (13) using the antisymmetry properties, Eq. (9). The nonanalytic part has been obtained through an additional consideration about the singular Green's-function products [7,13,15]. Specifically, the $|\omega-\omega'|$ and $|\omega+\omega'|$ contributions emerge from the intermediate particle-hole and particle-particle pair excitations, respectively. We note that the total vertex, Eqs. (14) and (15), can be regarded as a quantum-impurity analogue of Landau's phemomenological interaction $f_{p\sigma,p'\sigma'}$, and can also be compared with Nozières' function $\phi_{\sigma\sigma'}(\varepsilon,\varepsilon')$ [1,9]. One of the advantages of the microscopic formulation to the phenomenological descriptions is that the real and imaginary parts, which contribute to the energy-shift and damping of quasiparticles, are described in a unified way with clearly defined correlation functions.

The T^2 and $(eV)^2$ self-energy corrections.—The T^2 correction of the retarded self-energy $\Sigma_\sigma^r(\omega,T)$ can be deduced from the derivative of $\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)$ with respect to ω' using the formula [2,11,35]

$$\Sigma_\sigma^r(0,T)-\Sigma_\sigma^r(0,0)=\frac{(\pi T)^2}{6}\lim_{\omega\to 0^+}\Psi_\sigma(\omega)+\cdots \qquad (16)$$

$$\Psi_\sigma(\omega)\equiv\lim_{\omega'\to 0}\frac{\partial}{\partial\omega'}\sum_{\sigma'}\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)\rho_{d\sigma'}(\omega'). \qquad (17)$$

Substituting Eqs. (14) and (15) into Eq. (17) [36], we obtain

$$\lim_{\omega\to 0}\Psi_\sigma(\omega)=\frac{1}{\rho_{d\sigma}}\frac{\partial\chi_{\uparrow\downarrow}}{\partial\epsilon_{d,-\sigma}}-i3\pi\frac{\chi_{\uparrow\downarrow}^2}{\rho_{d\sigma}}\mathrm{sgn}(\omega). \qquad (18)$$

Here, the real part, $\partial\chi_{\uparrow\downarrow}/\partial\epsilon_{d,-\sigma}$, emerges from the analytic part of the total vertex for antiparallel spins.

In a previous work, we have diagrammatically shown that the low-bias $(eV)^2$ self-energy can be calculated taking a variational derivative of the equilibrium self-energy with respect to the internal Green's functions [15,37]. Revisiting the details of the calculation, we find exactly the same quantum-mechanical intermediate states, which consequently lead to Eq. (18), determine both the $(eV)^2$ and T^2 corrections [38]. The relation between these two corrections had been first pointed out by FMvDM using Nozières' description [18]. Our result provides a complete proof for this observation.

Using the above results, low-energy behavior of the retarded self-energy $\Sigma_\sigma^r(\omega,T,eV)$ is exactly determined up to terms of order ω^2, T^2, and $(eV)^2$. To be specific, the bias voltage $eV\equiv\mu_L-\mu_R$ is applied through the chemical potentials of the left and right leads, $\mu_L=\alpha_L eV$ and $\mu_R=-\alpha_R eV$, with additional parameters satisfying $\alpha_L+\alpha_R=1$. Thus, the self-energy generally depends not only on eV but also $\alpha\equiv(\alpha_L\Gamma_L-\alpha_R\Gamma_R)/(\Gamma_L+\Gamma_R)$ [15]. The asymptotically exact imaginary and real parts of the retarded self-energy are given by

$$\mathrm{Im}\Sigma_\sigma^r(\omega,T,eV)=-\frac{\pi\chi_{\uparrow\downarrow}^2}{2\rho_{d\sigma}}\left[(\omega-\alpha eV)^2+\frac{3\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2}(eV)^2+(\pi T)^2\right]+\cdots. \qquad (19)$$

$$\epsilon_{d\sigma}+\mathrm{Re}\Sigma_\sigma^r(\omega,T,eV)=\Delta\cot\delta_\sigma+(1-\tilde{\chi}_{\sigma\sigma})\omega+\frac{1}{2}\frac{\partial\tilde{\chi}_{\sigma\sigma}}{\partial\epsilon_{d\sigma}}\omega^2+\frac{1}{6\rho_{d\sigma}}\frac{\partial\chi_{\uparrow\downarrow}}{\partial\epsilon_{d,-\sigma}}\left[\frac{3\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2}(eV)^2+(\pi T)^2\right]$$
$$-\tilde{\chi}_{\sigma,-\sigma}\alpha eV+\frac{\partial\tilde{\chi}_{\sigma,-\sigma}}{\partial\epsilon_{d\sigma}}\alpha eV\omega+\frac{1}{2}\frac{\partial\tilde{\chi}_{\sigma,-\sigma}}{\partial\epsilon_{d,-\sigma}}\alpha^2(eV)^2+\cdots. \qquad (20)$$

We note that Eq. (20) is consistent with the previous result of ours [15], derived for general electron fillings without the knowledge of Eq. (12) [39]. Equation (20) is a generalized formula of the real part, which also extends FMvDM's result [18] to asymmetric junctions $\alpha\neq 0$ [35].

Nonequilibrium magnetotransport.—We next consider the current flowing through the Anderson impurity I [40], using the Meir-Wingreen formula [41] with Eqs. (19) and (20). Specifically, we examine a symmetric junction with $\Gamma_L=\Gamma_R$ and $\mu_L=-\mu_R=eV/2$, for which the conductance can be expressed in the form

$$\frac{dI}{dV}=\frac{e^2}{2\pi\hbar}\sum_\sigma[\sin^2\delta_\sigma-c_{T,\sigma}(\pi T)^2-c_{V,\sigma}(eV)^2], \qquad (21)$$

$$c_{T,\sigma}=\frac{\pi^2}{3}\left[-\cos 2\delta_\sigma(\chi_{\sigma\sigma}^2+2\chi_{\uparrow\downarrow}^2)+\frac{\sin 2\delta_\sigma}{2\pi}\left(\frac{\partial\chi_{\sigma\sigma}}{\partial\epsilon_d}+\sigma\frac{\partial\chi_{\uparrow\downarrow}}{\partial h}\right)\right], \qquad (22)$$

$$c_{V,\sigma}=\frac{\pi^2}{4}\left[-\cos 2\delta_\sigma(\chi_{\sigma\sigma}^2+5\chi_{\uparrow\downarrow}^2)+\frac{\sin 2\delta_\sigma}{2\pi}\left(\frac{\partial\chi_{\sigma\sigma}}{\partial\epsilon_d}+\frac{\partial\chi_{\uparrow\downarrow}}{\partial\epsilon_d}+\sigma 2\frac{\partial\chi_{\uparrow\downarrow}}{\partial h}\right)\right]. \qquad (23)$$

Here, contributions of the three-body fluctuations enter through the derivatives of susceptibilities with respect to ϵ_d or h, which are accompanied by the factor $\sin 2\delta_\sigma$. For the magnetoconductance in the Kondo regime, there is a controversial issue [18]: whether or not the zero-bias peak of dI/dV splits at a magnetic field of the order of the Kondo energy scale T_K. We demonstrate in the following that calculations with the exact conductance formula, Eqs. (22) and (23), resolve the problem [35].

We have calculated the phase shift δ_σ and the enhancement factor $\tilde{\chi}_{\sigma\sigma'}$ as functions of h at $\epsilon_d=-U/2$ using the NRG [42,43]. The dimensionless coefficients $\bar{C}_T=T_K^2\sum_\sigma c_{T,\sigma}/2$ and $\bar{C}_V=T_K^2\sum_\sigma c_{V,\sigma}/2$ have been determined substituting the NRG results into Eqs. (22) and (23). The result is shown in Fig. 2 as a function of h/T_K, using $T_K=1/4\chi_{\uparrow\uparrow}$ defined at $h=0$ for each case of $U/\pi\Delta$ ($=3.0, 3.5, 4.0$) [44]. We see that both $\bar{C}_T$ and $\bar{C}_V$ show the universal Kondo behavior. This is consistent with the behavior of the Wilson ratio which is almost saturated to the strong-coupling value $R_W\simeq 2$ for $U/\pi\Delta\gtrsim 3$ [42]. Furthermore, $\bar{C}_T$ and $\bar{C}_V$ change sign at h of order T_K: at very close magnetic-field values $h\simeq 0.38T_K$. This means that the zero-bias peak does split for $h\gtrsim 0.38T_K$ because dI/dV increases from the zero-bias value as eV increases.

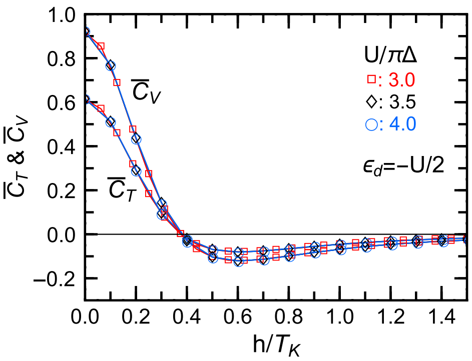

FIG. 2. Magnetic field dependence of the coefficients $\bar{C}_T = T_K^2 \sum_\sigma c_{T,\sigma}/2$ and $\bar{C}_V = T_K^2 \sum_\sigma c_{V,\sigma}/2$ at $\epsilon_d = -U/2$. $T_K = z_0 \pi\Delta/4$ is defined at $h = 0$ with the renormalization factor $z_0 \simeq 0.08$, 0.05, and 0.03 for $U/\pi\Delta = 3.0$, 3.5, and 4.0, respectively. At $h = 0$, the coefficients approach $\bar{C}_T \to \pi^2/16$ and $\bar{C}_V \to 3\pi^2/32$ in the $U \to \infty$ limit.

These observations are consistent with the previous second-order renormalized perturbation result [45].

Conclusion.—We have provided a many-body quantum theoretical description of the Fermi-liquid state in the particle-hole asymmetric case. The Fermi-liquid corrections away from half filling are characterized by additional contributions of the three-body fluctuations which enter through the nonlinear response function $\chi^{[3]}_{\sigma_1\sigma_2\sigma_3}$. The asymptotically exact expression of the total vertex $\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)$ describes low-energy properties in a unified way: this function and its derivatives with respect to ω or ω' determine the quasiparticle interaction, energy shift, damping, and transport coefficients can be generated systematically up to order ω^2, T^2, and $(eV)^2$, with the Ward identities given in Eqs. (8) and (17). Furthermore, the nonequilibrium self-energy Eq. (20) is applicable to the asymmetric tunneling couplings, and has potential application for real quantum dots [28–30]. We have also demonstrated an application to the nonlinear magnetoconductance through a quantum dot in the Kondo regime, and have shown that the zero-bias peak of dI/dV splits naturally at a magnetic finite field of order T_K. Our description can be extended, and may be used, to explore a wide class of Kondo systems and more general quantum impurities.

We wish to thank J. Bauer and R. Sakano for valuable discussions, and C. Mora and J. von Delft for sending us Ref. [18] prior to publication. This work was supported by JSPS KAKENHI Grant Nos. JP26400319, JP26220711.

[1] L. D. Landau, Sov. Phys. JETP **3**, 920 (1957).
[2] A. A. Abrikosov, I. Dzyaloshinskii, and L. P. Gorkov, *Methods of Quantum Field Theory in Statistical Physics* (Pergamon, London, 1965).
[3] L. D. Landau, E. M. Lifshitz, and L. P. Pitaevskii, *Statistical Physics, Part 2* (Butterworth-Heinemann, Oxford, 1991).
[4] A. J. Leggett, Rev. Mod. Phys. **47**, 331 (1975).
[5] I. Bloch, J. Dalibard, and S. Nascimbène, Nat. Phys. **8**, 267 (2012).
[6] G. M. Eliashberg, Sov. Phys. JETP **14**, 886 (1962).
[7] G. M. Eliashberg, Sov. Phys. JETP **15**, 1151 (1962).
[8] N. D. Mermin, Phys. Rev. **159**, 161 (1967).
[9] P. Nozières, J. Low Temp. Phys. **17**, 31 (1974).
[10] K. Yamada, Prog. Theor. Phys. **53**, 970 (1975).
[11] K. Yamada, Prog. Theor. Phys. **54**, 316 (1975).
[12] H. Shiba, Prog. Theor. Phys. **54**, 967 (1975).
[13] A. Yoshimori, Prog. Theor. Phys. **55**, 67 (1976).
[14] S. Hershfield, J. H. Davies, and J. W. Wilkins, Phys. Rev. B **46**, 7046 (1992).
[15] A. Oguri, Phys. Rev. B **64**, 153305 (2001).
[16] B. Horvatić and V. Zlatić, Phys. Status Solidi B **111**, 65 (1982).
[17] C. Mora, C. P. Moca, J. von Delft, and G. Zaránd, Phys. Rev. B **92**, 075120 (2015).
[18] M. Filippone, C. P. Moca, J. von Delft, and C. Mora, Phys. Rev. B **95**, 165404 (2017).
[19] Parameter correspondence: $\alpha_{1\sigma}/\pi = \chi_{\sigma\sigma}$, $\phi_1/\pi = -\chi_{\uparrow\downarrow}$, $2\alpha_{2\sigma}/\pi = -\partial\chi_{\sigma\sigma}/\partial\epsilon_{d\sigma}$, and $\phi_{2\sigma}/\pi = 2\partial\chi_{\uparrow\downarrow}/\partial\epsilon_{d\sigma}$.
[20] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[21] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980).
[22] N. Kawakami and A. Okiji, Solid State Commun. **43**, 467 (1982).
[23] P. B. Wiegmann and A. M. Tsvelick, J. Phys. C **16**, 2281 (1983).
[24] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Rev. Mod. Phys. **83**, 349 (2011).
[25] F. B. Anders and A. Schiller, Phys. Rev. B **74**, 245113 (2006).
[26] S. Kirino, T. Fujii, J. Zhao, and K. Ueda, J. Phys. Soc. Jpn. **77**, 084704 (2008).
[27] A. C. Hewson, A. Oguri, and D. Meyer, Eur. Phys. J. B **40**, 177 (2004).
[28] M. Grobis, I. G. Rau, R. M. Potok, H. Shtrikman, and D. Goldhaber-Gordon, Phys. Rev. Lett. **100**, 246601 (2008).
[29] G. D. Scott, Z. K. Keane, J. W. Ciszek, J. M. Tour, and D. Natelson, Phys. Rev. B **79**, 165413 (2009).
[30] M. Ferrier, T. Arakawa, T. Hata, R. Fujiwara, R. Delagrange, R. Weil, R. Deblock, R. Sakano, A. Oguri, and K. Kobayashi, Nat. Phys. **12**, 230 (2016).
[31] $\chi_s = \frac{1}{4}(\chi_{\uparrow\uparrow} + \chi_{\downarrow\downarrow} - \chi_{\uparrow\downarrow} - \chi_{\downarrow\uparrow})$ and $\chi_c = \chi_{\uparrow\uparrow} + \chi_{\downarrow\downarrow} + \chi_{\uparrow\downarrow} + \chi_{\downarrow\uparrow}$. $\chi_{\sigma\sigma'} = \chi_{\sigma'\sigma}$ and Ω is an even function of h.
[32] A. C. Hewson, J. Phys. Condens. Matter **13**, 10011 (2001).
[33] G. Rohringer, A. Valli, and A. Toschi, Phys. Rev. B **86**, 125114 (2012).
[34] $\tilde{\chi}_{\sigma\sigma'} + \Gamma_{\sigma\sigma';\sigma'\sigma}(0,0;0,0)\rho_{d\sigma'} = (1 - \partial\Sigma_\sigma(\omega)/\partial\omega|_{\omega=0})\delta_{\sigma\sigma'}$.
[35] Details will be given elsewhere: A. Oguri and A. C. Hewson, Phys. Rev. B **97**, 035435 (2018); **97**, 045406 (2018).
[36] Here, $\rho_{d\sigma}(\omega) \equiv (-1/\pi)\mathrm{Im}G^r_\sigma(\omega)$, in the retarded form.
[37] A. Oguri, J. Phys. Soc. Jpn. **74**, 110 (2005).
[38] Equation (17) of this Letter is identical to Eq. (14) of Ref. [15], i.e., $\Psi_\sigma(\omega) = \hat{D}^2\Sigma_\sigma(\omega)$ with $\hat{D}^2$ defined in Ref. [15].

[39] Substituting the ω^2 real part given in Eq. (12) into Eq. (19) of Ref. [15], we obtain the expression which agrees with Eq. (20) at $h \to 0$.
[40] $I = [e/(2\pi\hbar)]\sum_\sigma \int d\omega [(4\Gamma_R \Gamma_L)/(\Gamma_R + \Gamma_L)][f_L(\omega) - f_R(\omega)] \times \pi\rho_{d\sigma}(\omega)$, where $f_\lambda(\omega) \equiv f(\omega - \mu_\lambda)$ and $f(\omega) = [e^{\omega/T} + 1]^{-1}$. See also Ref. [36].
[41] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
[42] A. C. Hewson, J. Bauer, and W. Koller, Phys. Rev. B **73**, 045117 (2006).
[43] A. C. Hewson, A. Oguri, and J. Bauer, in *Physical Properties of Nanosystems*, edited by J. Bonca and S. Kruchinin (Springer Netherlands, Dordrecht, 2011), pp. 11–23.
[44] We used $\Lambda = 2.0$ for the discretization parameter and keep 3600 states per iteration [21].
[45] A. C. Hewson, J. Bauer, and A. Oguri, J. Phys. Condens. Matter **17**, 5413 (2005).