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1. Introduction

The heavy-electron systems have attracted much attention in condensed matter physics since the localized and itinerant natures of strongly correlated electrons open up unexpected phenomena, which leads to a break through the paradigm to provide a new concept with universality. The emergence of the heavy mass of quasiparticles, their condensation to the superconductivity with essentially "high" transition temperature compared to the renormalized Fermi temperature, and unconventional quantum critical phenomena are such examples.

To make experimental explorations, the measurements of the conductivity and Hall effect have been performed extensively in the heavy-electron systems. Accumulated data for the Ce-based heavy electron systems show that there exists a general tendency that the isothermal resistivity at the measured lowest temperature, i.e., residual resistivity, in the Fermi-liquid regime decreases as pressure increases. On the other hand, in the Yb-based heavy-electron systems, there exits a general tendency that the residual resistivity in the Fermi-liquid regime increases as pressure increases. The mechanism of the pressure dependence of the conductivity and also the Hall conductivity in relation to the valence of Ce and Yb as well as the shape of the Fermi surface has been desired to be clarified theoretically.

Theoretically, the diagonal conductivity and the Hall conductivity were formulated on the basis of the Boltzmann transport theory. The formula of the diagonal conductivity in the system with Coulomb repulsion among electrons was derived microscopically by Eliashberg in the Fermi-liquid theory starting from the Kubo formula. The diagonal conductivity in the periodic Anderson model which is the prototypical model for the Ce- and Yb-based heavy electron systems was formulated on the basis of the Fermi liquid theory by Yamada and Yosida.

The Hall conductivity was formulated by Fukuyama, in the gauge invariant manner starting from the Kubo formula. Later, Eliashberg’s work was extended to the Hall conductivity by Kohno and Yamada, who formulated the general expression in the Fermi liquid theory. Explicit calculation of the diagonal and Hall conductivities was performed by using the conserving approximation in the Hubbard model which contains a single orbital with electron transfer and Coulomb repulsion by Kontani et al.

So far, after the formulation of the diagonal conductivity by Yamada and Yosida, systematic calculations for the diagonal and normal Hall conductivities have not been reported in detail in the periodic Anderson model which contains the two orbitals for f and conduction electrons.

In this paper, we clarify the basic properties of the diagonal and Hall conductivities, and normal Hall effect in the periodic Anderson model. On the basis of the theoretical framework which describes the Fermi liquid correctly, the ground-state properties of the diagonal and Hall conductivities and the Hall coefficient are studied by taking into account the effects of the electron correlation and the weak impurity scattering. By performing the numerical calculation on the square lattice, the dependence on parameters such as the f level, c-f hybridization, the damping rate for f electrons, and the filling is clarified. The relation to the shape of the Fermi surface and the f-electron number per site, corresponding to the valence of Ce and Yb, is also clarified.

The organization of this paper is as follows: In Sect. 2, we review the formalism of conductivity in the periodic Anderson model based on the Fermi-liquid theory. In Sect. 3, exact formulas of the diagonal conductivity and Hall conductivity are derived in the periodic Anderson model for $U = 0$. In Sect. 4, the ground-state properties of the conductivities and the Hall coefficient in the periodic Anderson model with electron correlations and weak-impurity scattering are studied on the basis of the exactly derived formulas. The paper is summarized in Sect. 5.

We take the energy units as $\hbar = 1$, $k_B = 1$, and the light velocity $c = 1$. Note that we denote $e$ as the elementary charge, i.e., $e > 0$. 

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**Basic Properties of Conductivity and Normal Hall Effect in the Periodic Anderson Model**

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2. Formalism of conductivity based on the Fermi liquid theory in the periodic Anderson model

As the simplest minimal model for the electronic state in the Ce- and Yb-based heavy-electron systems, we consider the periodic Anderson model

\[ \mathcal{H} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} \varepsilon_{f,k\sigma} f_{k\sigma} + \sum_{k\sigma} V_k \left( n_{f,k\sigma} + c_{k\sigma}^\dagger f_{k\sigma} + c_{k\sigma} f_{k\sigma}^\dagger \right) + U \sum_{i} n_{i\sigma}^f n_{i\sigma}^c, \]

with \( n_{i\sigma} \equiv f_{i\sigma}^\dagger f_{i\sigma} \) where \( f_{i\sigma} \) is an annihilation (creation) operator of an \( f \) electron at the \( i \)-th site with spin \( \sigma \) and \( c_{k\sigma} \) is an annihilation (creation) operator of a conduction electron at the wave vector \( k \) with spin \( \sigma \). The first term represents the energy band of conduction electrons with a dispersion, \( \varepsilon_k \). The second term represents the energy band of conduction electrons with a dispersion, \( \varepsilon_k \). The third term represents the hybridization between \( f \) and conduction electrons with real \( V_k \). The onsite Coulomb repulsion for \( f \) electrons is expressed in the last term.

Since \( 4f^{15}d^{6}6s^{2} \) configuration is realized in the outermost electrons’ shell of Ce, Ce\(^{13} \) contains the \( 4f^{13} \) electron and Ce\(^{14} \) contains the \( 4f^{14} \) electron. On the other hand, since \( 4f^{16}6s^{2} \) configuration is realized in the outermost electrons’ shell of Yb, Yb\(^{13} \) contains the \( 4f^{13} \) electrons and Yb\(^{14} \) contains \( 4f^{14} \) electrons. Since \( 4f^{14} \) is the closed shell for \( f \) orbital, by taking the hole picture instead of the electron picture, Eq. (1) can be applied to the Yb-based systems and the parallel discussion to the Ce-based systems in the electron picture can be made.

The total filling \( \bar{n} \) is defined as

\[ \bar{n} \equiv n_f + n_c, \]

where \( n_f \) and \( n_c \) are \( f \)-electron number per site and the conduction electron number per site, respectively, defined as

\[ n_f = \frac{1}{N} \sum_{i\sigma} (n_{i\sigma}^f), \]

\[ n_c = \frac{1}{N} \sum_{i\sigma} (n_{i\sigma}^c). \]

Here, \( N \) is the number of the lattice sites and \( n_{i\sigma}^c \equiv c_{i\sigma}^\dagger c_{i\sigma} \). Note that \( \bar{n} = 2 \) is the half filling.

The diagonal conductivity in the periodic Anderson model was formulated on the basis of the Fermi liquid theory by Yamada and Yosida.\(^{17} \) In the following, we review the formalism for the diagonal conductivity.

The retarded Green functions of \( f \) electrons and conduction electrons are given by

\[ G_k^{ff}(\varepsilon) = \left[ \varepsilon + i\delta - \varepsilon_k - \Sigma_k^R(\varepsilon) - \frac{V_k^2}{\varepsilon + i\delta - \varepsilon_k} \right]^{-1}, \]

\[ G_k^{cc}(\varepsilon) = \left[ \varepsilon + i\delta - \varepsilon_k - \left( \Sigma_k^R(\varepsilon) + \frac{V_k^2}{\varepsilon + i\delta - \varepsilon_k} \right) \right]^{-1}, \]

respectively, where \( \Sigma_k^R(\varepsilon) \) is the retarded self energy of \( f \) electrons, which arises from the Coulomb repulsion \( U \), and \( \delta \) is the infinitesimal positive constant.

We consider the case where the Fermi level is located at the lower hybridized band. In the vicinity of the Fermi energy, the Green functions of \( f \) and conduction electrons are described by quasiparticles as

\[ G_k^{ff}(\varepsilon) = a_k^{ff} G_k^{ff}(\varepsilon), \quad G_k^{cc}(\varepsilon) = a_k^{cc} G_k^{cc}(\varepsilon), \]

respectively, where the retarded Green function for the lower hybridized band is given by

\[ G_k^{ff}(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_k + \frac{\partial}{\partial \varepsilon}\Sigma_k(\varepsilon)} \]

and the renormalization factors are given by

\[ a_k^{ff} = \left( 1 - \frac{\partial Re \Sigma_k^R(\varepsilon)}{\partial \varepsilon} \right)^{-1} \varepsilon_{k}, \quad a_k^{cc} = \frac{V_k^2}{\varepsilon_k - \varepsilon_k} a_k^{ff}. \]

The diagonal conductivity is expressed as

\[ \sigma_{xx} = \frac{\varepsilon_f^2}{V_0} \sum_k \int_{-\infty}^{\infty} \frac{de}{\pi} \left( -\frac{\partial f(e)}{\partial \varepsilon} \right) \left| G_k^{ff}(e) \right|^2 v_k(\varepsilon) J_k(\varepsilon) - \text{Re} \left\{ G_k^{ff}(e) \Sigma_k^R(\varepsilon) v_k(\varepsilon) J_k(\varepsilon) \right\}, \]

where \( f(\varepsilon) \) is the Fermi distribution function \( f(\varepsilon) = \frac{e^{\varepsilon - \mu}/T + 1}{e^{\varepsilon - \mu}/T + 1} \) and \( G_k^{ff}(e) \) is the \( f \)-electron Green function for quasiparticles given by Eq. (7). The second term in Eq. (16) was not described in Ref. 17, but this term is necessary quantitatively.\(^{24} \) For example, the exact formula of \( \sigma_{xx} \) derived for \( U = 0 \) in Sect. 3 is correctly reproduced by Eq. (16) with the second term in the brace when we set \( \Sigma_k^R(\varepsilon) = 0 \) [see Eq. (55)]. Here, \( v_k(\varepsilon) \) is the total velocity defined as

\[ v_k(\varepsilon) = v_k^{ff}(\varepsilon) + v_k^{cc}(\varepsilon) = v_k^{ff}(\varepsilon) + \frac{\partial Re \Sigma_k^R(\varepsilon)}{\partial \varepsilon} \varepsilon_k^0 \]

where the velocity of \( f \) electrons and conduction electrons are given by

\[ v_k^{ff}(\varepsilon) = v_k^{ff}(\varepsilon) + \frac{\partial Re \Sigma_k^R(\varepsilon)}{\partial \varepsilon} \varepsilon_k^0, \quad v_k^{cc}(\varepsilon) = v_k^{cc}(\varepsilon) + \frac{\partial Re \Sigma_k^R(\varepsilon)}{\partial \varepsilon} \varepsilon_k^0. \]
Namely, the mass-renormalization factors includes renormalized by the factor with small the resistivity is proportional to Eq. (16), which is denoted by due to electron interaction should diverge in the absence of the last equation is derived for sufficiently low temperatures. Similarly to Eq. (23), enhancement of the density of states of quasiparticles arises from $\delta (\mu - E_k^{\pm})$ by factor $z_k^{-1}$, which cancels out by $a_k^{\pm}$ in Eq. (26). Hence, the mass-renormalization factor does not appear in the expression of the Hall conductivity.

As shown above, the formulas of $\sigma_{xx}$ and $\sigma_{xy}/H$ are obtained in the vicinity of the Fermi level located at the lower hybridized band on the basis of the Fermi liquid theory. In both expressions of $\sigma_{xx}$ and $\sigma_{xy}/H$, the renormalization factors of quasiparticles cancel out.

In the next Sect., we will derive the exact formula of $\sigma_{xx}$ and $\sigma_{xy}/H$ for $U = 0$ in Eq. (1), which give the general formulas in the two-orbital systems, not restricted to the single band as treated in Eqs. (16) and (24). On the basis of the exactly-derived formulas, we will perform the explicit calculation of $\sigma_{xx}$ and $\sigma_{xy}/H$ in the periodic Anderson model with electron correlations to clarify the ground-state properties in Sect.4.

3. Exact formulas of $\sigma_{xx}$ and $\sigma_{xy}$ for $U = 0$

In the case of $U = 0$, Eq. (1) is diagonalized as

$$\mathcal{H} = \sum_{\kappa \sigma} \left[ E_k^{\pm} \delta_{\kappa \sigma} + E_k^{\pm} \gamma_{\kappa \sigma} \right],$$

where $E_k^{\pm}$ is the lower hybridized band and $E_k^{\pm}$ is the upper hybridized band, whose explicit form is given by

$$E_k^{\pm} = \frac{e_k + \epsilon_k^d}{2} \pm \frac{\Delta_k}{2},$$

where $\Delta_k$ is defined as

$$\Delta_k = \sqrt{\left(\epsilon_k - \epsilon_k^d\right)^2 + 4V_k^2}.$$  

Equation (27) is obtained by substituting $\delta_{\kappa \sigma} = u_k \delta_{k \sigma} - w_k \gamma_{k \sigma}$ and $\delta_{\kappa \sigma} = w_k \delta_{k \sigma} + u_k \gamma_{k \sigma}$ to Eq. (1), where $u_k$ and $w_k$ satisfy

$$u_k^2 = a_k^{xx}, \quad \frac{1}{2} \left(1 \pm \frac{\epsilon_k - \epsilon_k^d}{\Delta_k}\right),$$

$$w_k^2 = a_k^{xx}, \quad \frac{1}{2} \left(1 \pm \frac{\epsilon_k - \epsilon_k^d}{\Delta_k}\right),$$

respectively. Here, $a_k^{xx}$ ($a_k^{xx}$) represents the weight factor of the conduction electrons in the lower (upper) hybridized band and $a_k^{xx}$ ($a_k^{xx}$) represents the weight factor of the $f$ electrons in the lower (upper) hybridized band. Note that in the case of $U = 0$ in Eq. (1), i.e., $\sum_{\kappa \sigma} \langle \varepsilon \rangle = 0$, Eqs. (10) and (11) reproduce Eqs. (31) and (30), respectively.

3.1 Derivation of $\sigma_{xx}$ and $\sigma_{xy}$

On the basis of the Kubo formula, the diagonal conductivity is given by

$$\sigma_{xx} = \lim_{\omega \to 0} \frac{\Phi_{xx}(\omega + i\delta) - \Phi_{xx}(0 + i\delta)}{i\omega}.$$  

Here, the kernel $\Phi_{\alpha\alpha}(i\omega_n)$ is expressed as

$$\Phi_{\alpha\alpha}(i\omega_n) = -\frac{e^2}{V_0} \sum_{k} \sum_{\nu} \text{Tr} \left[ G_{k\alpha}(i\omega_n) V_{k\alpha} G_{k\alpha}(i\omega_n + i\omega_n) V_{k\alpha} \right]$$

with $\omega_n = 2\pi n T$ and $\varepsilon_n = (2\pi + 1)n T$ ($m, n$ are integers).

Here, the velocity matrix and the Green-function matrix are given by

$$V_{k\gamma} = \left( \begin{array}{cc} \frac{\partial V_k}{\partial k_x} & \frac{\partial V_k}{\partial k_y} \\ \frac{\partial V_k}{\partial k_y} & \frac{\partial V_k}{\partial k_x} \end{array} \right),$$

$$G_{k\alpha}(i\omega_n) = \left( \begin{array}{cc} G_{k\alpha}^{\sigma\sigma}(i\omega_n) & G_{k\alpha}^{\sigma\bar{\sigma}}(i\omega_n) \\ G_{k\alpha}^{\bar{\sigma}\sigma}(i\omega_n) & G_{k\alpha}^{\bar{\sigma}\bar{\sigma}}(i\omega_n) \end{array} \right),$$

respectively, where

$$G_{k\alpha}^{\sigma\sigma}(i\omega_n) = \left[ i\varepsilon_n - \varepsilon_k - \frac{V_k^2}{i\varepsilon_n - \varepsilon_k} \right]^{-1},$$

$$G_{k\alpha}^{\sigma\bar{\sigma}}(i\omega_n) = \left[ i\varepsilon_n - \varepsilon_k - \frac{V_k^2}{i\varepsilon_n - \varepsilon_k} \right]^{-1},$$

$$G_{k\alpha}^{\bar{\sigma}\bar{\sigma}}(i\omega_n) = \frac{1}{(i\varepsilon_n - \varepsilon_k^2)(i\varepsilon_n - \varepsilon_k)} - \frac{1}{V_k^2},$$

and $G_{k\alpha}^{\sigma\bar{\sigma}}(i\omega_n) = G_{k\alpha}^{\bar{\sigma}\sigma}(i\omega_n)$.

By performing the analytic continuation, the conductivity in the periodic Anderson model for $U = 0$ is derived as

$$\sigma_{xx} = \sigma_{xx}^- + \sigma_{xx}^+ + \sigma_{xx}^+ + \sigma_{xx}^+,$$

where

$$\sigma_{xx}^- = \frac{e^2}{V_0} \int_0^\infty \frac{d\varepsilon}{\pi} \sum_{k} \left( \text{Im} G_{k\alpha}^{\bar{\sigma}\sigma}(\varepsilon) \right)^2,$$

$$\sigma_{xx}^+ = \frac{e^2}{V_0} \int_0^\infty \frac{d\varepsilon}{\pi} \sum_{k} \left( \text{Im} G_{k\alpha}^{\sigma\bar{\sigma}}(\varepsilon) \right)^2,$$

$$\sigma_{xx}^- + \sigma_{xx}^+ = \frac{e^2}{V_0} \int_0^\infty \frac{d\varepsilon}{\pi} \sum_{k} V_k \varepsilon_k^-,\varepsilon_k^+,\varepsilon_k^+,\varepsilon_k^+,$$

where $V_k$ is a volume of the system. The velocity of the hybridized band $v_{k\alpha}^{\sigma\bar{\sigma}} = \partial E_k^{\sigma\bar{\sigma}} / \partial k_\eta$ ($\eta = x, y, z$) is given by

$$v_{k\gamma}^{\sigma\bar{\sigma}} = -\frac{V_k}{\Delta_k} a_{k\alpha}^{\sigma\bar{\sigma}} + d_{k\alpha}^{\sigma\bar{\sigma}} \frac{\partial V_k}{\partial k_\eta} + a_{k\alpha}^{\sigma\bar{\sigma}} \frac{\partial V_k}{\partial k_\eta},$$

where $a_{k\alpha}^{\sigma\bar{\sigma}}$ and $d_{k\alpha}^{\sigma\bar{\sigma}}$ are defined as

$$a_{k\alpha}^{\sigma\bar{\sigma}} = \frac{V_k}{\Delta_k}, \quad d_{k\alpha}^{\sigma\bar{\sigma}} = \frac{V_k}{\Delta_k},$$

$$a_{k\alpha}^{\sigma\bar{\sigma}} = -\frac{V_k}{\Delta_k}, \quad d_{k\alpha}^{\sigma\bar{\sigma}} = \frac{V_k}{\Delta_k},$$

respectively, which satisfies $a_{k\alpha}^{\sigma\bar{\sigma}} + a_{k\alpha}^{\sigma\bar{\sigma}} = 1$ and $a_{k\alpha}^{\sigma\bar{\sigma}} a_{k\alpha}^{\sigma\bar{\sigma}} = a_{k\alpha}^{\sigma\bar{\sigma}} a_{k\alpha}^{\sigma\bar{\sigma}}$. In Eq. (42), the off-diagonal velocity is defined as

$$v_{k\gamma}^{\sigma\bar{\sigma}} = \sqrt{a_{k\alpha}^{\sigma\bar{\sigma}} a_{k\alpha}^{\sigma\bar{\sigma}} v_{k\gamma}^{\sigma\bar{\sigma}}} + \sqrt{a_{k\alpha}^{\sigma\bar{\sigma}} a_{k\alpha}^{\sigma\bar{\sigma}}} v_{k\gamma}^{\sigma\bar{\sigma}},$$

+ \sqrt{a_{k\alpha}^{\sigma\bar{\sigma}} a_{k\alpha}^{\sigma\bar{\sigma}}} v_{k\gamma}^{\sigma\bar{\sigma}} + \sqrt{a_{k\alpha}^{\sigma\bar{\sigma}} a_{k\alpha}^{\sigma\bar{\sigma}}} v_{k\gamma}^{\sigma\bar{\sigma}},$$

for $\alpha = -\alpha$. The retarded Green function $G^{\text{ret}}_{k\alpha}(\varepsilon)$ is given by

$$G^{\text{ret}}_{k\alpha}(\varepsilon) = \frac{1}{\varepsilon - E_k^{\alpha\alpha} + i\Gamma_k^{\alpha\alpha}},$$

where $\Gamma_k^{\alpha\alpha}$ is obtained by the relation of $G^{\alpha\alpha}_{k\alpha}(\varepsilon) = [G^{\text{ret}}_{k\alpha}(\varepsilon)]$. Here, we introduce the imaginary part of the self energy $\Gamma_k^{\alpha\alpha}$ in Eq. (47). This term can arise from the impurity scattering even in the $U = 0$ periodic Anderson model. We discuss the general expression of $\sigma_{xx}$ and $\sigma_{xy}/H$ with the finite damping rate.

On the basis of the formalism in Refs. 18, 19, the Hall conductivity in the periodic Anderson model for $U = 0$ is derived. Hereafter, we show the result for $V_k = V$ in Eq. (1).

The Hall conductivity is given by

$$\sigma_{xy} = \lim_{\varepsilon \to 0} \lim_{\omega \to 0} \frac{\Phi_{xy}(q, \omega + i0^+) - \Phi_{xy}(q, i0^+)}{i\omega},$$

where the kernel $\Phi_{xy}(q, i\omega_n)$ is given by

$$\Phi_{xy}(q, i\omega_n) = (q_x A_{xy} - q_y A_{xy}) \frac{T}{V_0} \sum_{k} \text{Tr} \left[ \frac{\partial V_k}{\partial k_x} G_{k\alpha}(i\omega_n) \right] \frac{\partial V_k}{\partial k_y} G_{k\alpha}(i\omega_n + i\omega_n) + \frac{1}{V_k} \left( v_{k_x} \leftrightarrow v_{k_y} \right).$$

Here $A_{xy}$ is the $\eta$ component of the vector potential by which the magnetic field along the $z$ axis is expressed as $H = i\lim_{\eta \to 0} (q_x A_{xy} - q_y A_{xy})$. By performing the analytic continuation, the Hall conductivity is obtained as follows:

$$\sigma_{xy} = \sum_{\alpha=\bar{\alpha}} \sigma_{xy}^{\alpha\alpha} + \sum_{\alpha=\bar{\alpha}} \sigma_{xy}^{\alpha\bar{\alpha}} + \sigma_{xy}^{\alpha\bar{\alpha}},$$

where

$$\sigma_{xy}^{\alpha\alpha} = H \frac{e^3}{2V_0} \sum_{\alpha=\bar{\alpha}} \int_0^\infty \frac{d\varepsilon}{\pi} \left( -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \left| G^{\text{ret}}_{k\alpha}(\varepsilon) \right|^2 \text{Im} \left[ G^{\text{ret}}_{k\alpha}(\varepsilon) \right] \left| G^{\text{ret}}_{k\alpha}(\varepsilon) \right|^2,$$

$$\sigma_{xy}^{\alpha\bar{\alpha}} = H \frac{e^3}{2V_0} \sum_{\alpha=\bar{\alpha}} \int_0^\infty \frac{d\varepsilon}{\pi} \left( -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \left| G^{\text{ret}}_{k\alpha}(\varepsilon) \right|^2 \text{Im} \left[ G^{\text{ret}}_{k\alpha}(\varepsilon) \right] \left| G^{\text{ret}}_{k\alpha}(\varepsilon) \right|^2,$$

with

$$\sigma_{xy}^{\alpha\bar{\alpha}} = \frac{e^3}{2V_0} \sum_{\alpha=\bar{\alpha}} \int_0^\infty \frac{d\varepsilon}{\pi} \left( -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \left| G^{\text{ret}}_{k\alpha}(\varepsilon) \right|^2 \text{Im} \left[ G^{\text{ret}}_{k\alpha}(\varepsilon) \right] \left| G^{\text{ret}}_{k\alpha}(\varepsilon) \right|^2.$$
Fig. 1. Contours of integration in the complex-$\zeta$ plane. The dots on the imaginary axis represent the Fermionic thermal frequencies $i \omega_n = i(2n+1)\pi T$ with $n$ being integers.

\begin{align*}
+G_{k}^{R}(\epsilon) \left[ G_{k}^{R}(\epsilon) \right]^\dagger \right] Q_{k\sigma y}.
\end{align*}

Here, $\bar{\alpha} = -\alpha$ and $Q_{k\sigma y}$ is defined by

\begin{align*}
Q_{k\sigma y} &= -2\left( \frac{v_{kx}^0 - v_{k}^0}{\Delta_k} \right) \times \left( v_{ky}^0 \frac{\partial v_{ky}^0}{\partial \epsilon} - v_{ky}^0 \frac{\partial v_{ky}^0}{\partial \epsilon} + v_{ky}^0 \frac{\partial v_{ky}^0}{\partial \epsilon} - v_{ky}^0 \frac{\partial v_{ky}^0}{\partial \epsilon} \right) \ .
\end{align*}

In deriving Eq. (39) and Eq. (50), the analytic continuation is performed as shown in Fig. 1. Here, $C_1$ ($C_2$) is the contour from $-\infty$ to $\infty$ (from $\infty$ to $-\infty$) at just above (below) $\text{Im} \zeta = 0$ and $C_3$ ($C_4$) is the contour from $-\infty$ to $\infty$ (from $\infty$ to $-\infty$) at just above (below) $\text{Im} \zeta = -\omega_m$. In Eq. (39) and Eq. (50), the term including $f'(\epsilon)$ term arises from the $C_2 + C_3$ contours, which makes the main contribution from the vicinity of the Fermi level. On the other hand, in Eq. (50), the term including $f_\alpha(\epsilon)$ term arises from the contribution from the $C_1 + C_4$ contours.

It is noted that even when the hybridization has the momentum dependence, $V_k$, Eqs. (51) and (52) hold with the velocities defined in Eqs. (43) and (46). Equations (39) and Eq. (50) are the general expressions for $\sigma_{xx}$ and $\sigma_{xy}/H$, respectively, in the systems with the single-band as well as the two-bands at the Fermi level, which are constituted of two orbitals.

To clarify the fundamental properties of the conductivity and Hall coefficient in the periodic Anderson model, hereafter we discuss the case of the flat dispersion of the $f$ band, $v_{k}^f = v_f$ in Eq. (1) as the simplest typical case of the heavy-electron systems.

An important remark is that in Eqs. (39) and (50) the velocities of the hybridized bands $v_{k}^{\alpha}$ appear, which give rise to the velocity of the “large” Fermi surface which contains contributions from both $f$ and conduction electrons, but not of the “small” Fermi surface for the conduction band.

### 3.2 The limit of small damping rate at low temperatures

When the total filling is less than the half-filling, i.e., $\bar{n} < 2$ and the Fermi level is located at the lower hybridized band, $\sigma_{xx} = \sigma_{xy}^2$ holds in Eq. (39) at low temperatures for the small $V_k$ to satisfy $\mu \tau_k \gg 1$, where the relaxation time $\tau_k$ is defined as $\tau_k = \frac{1}{\mu}$.

In this case, from Eq. (40), we have

\begin{align*}
\sigma_{xx} &\approx \sigma_{xx}^2 = \frac{e^2}{V_0} \sum_{k_0} \left( \frac{\partial f(E_k)}{\partial E_k} \right) \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \frac{1}{2k} \\
&\times \int_0^\infty \frac{d\epsilon}{\pi} \left[ \left( \epsilon - E_k - \Gamma_k \right)^2 + \Gamma_k^2 \right]^{-1}.
\end{align*}

Note that Eq. (16) in the limit of $U = 0$ reproduces the expression of Eq. (55). Since $\frac{\partial f(E_k)}{\partial E_k} = 0$ holds at $T = 0$, we have

\begin{align*}
\sigma_{xx} &= \frac{e^2}{V_0} \sum_{k_0} \delta(\mu - E_k) \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \tau_k, \quad (56)
\end{align*}

in the ground state.

As for the Hall conductivity, in the small $\Gamma_k$ limit at low temperatures, the contribution from the lower hybridized band $\sigma_{xy}$ in Eq. (51) is only the relevant term for $\sigma_{xy}$. Then we have

\begin{align*}
\sigma_{xy} &\approx H \frac{e^2}{2V_0} \sum_{k_0} \left( \frac{\partial f(E_k)}{\partial E_k} \right) \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \times \int_0^\infty \frac{d\epsilon}{\pi} \left[ G_{k}^{R}(\epsilon) \right]^2 \Im G_{k}^{R}(\epsilon),
\end{align*}

\begin{align*}
&= -H \frac{e^2}{2V_0} \sum_{k_0} \left( \frac{\partial f(E_k)}{\partial E_k} \right) \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 2\tau_k.
\end{align*}

Note that Eq. (24) in the limit of $U = 0$ reproduces the expression of Eq. (57). Since $\frac{\partial f(E_k)}{\partial E_k} = 0$ holds at $T = 0$, we have

\begin{align*}
\sigma_{xy} &= -H \frac{e^2}{2V_0} \sum_{k_0} \delta(\mu - E_k) \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 \left( \frac{\partial \epsilon_k^0}{\partial k} \right)^2 2\tau_k, \quad (58)
\end{align*}

in the ground state.

### 3.3 Isotropic free-electron system

To analyze $\sigma_{xx}$ and $\sigma_{xy}$ explicitly, we consider the isotropic free electron system. Namely, the conduction electrons have the free dispersion as $\epsilon_k = \frac{\pi k^2}{2m}$ in the periodic Anderson model in three spatial dimension. Here we assume $\tau = \tau_k$ ($\Gamma = \Gamma_k$) for simplicity of analysis. Equation (56) can be calculated as

\begin{align*}
\sigma_{xx} &= \frac{2e^2}{(2\pi)^3} \int_{S(\mu)} dS \frac{\epsilon_k^0}{|\nabla E_k^0|},
\end{align*}

where the integral is taken as the surface integral over the constant-energy-surface $S(\mu)$ where $\mu = E_k$ is satisfied in the $k$ space. Since we have $|\nabla E_k^0| = \frac{a_{xx}^\infty}{k_F}$ with $v_k^0 \equiv \sqrt{(v_{k}^0)^2 + (v_{k}^0)^2 + (v_{k}^0)^2}$ and $\int_{S(\mu)} dS = 4\pi k_F^2$ with $k_F$ being the Fermi wave number in the isotropic free-electron system,
Eq. (59) leads to

\[
\sigma_{xx} = \frac{2e^2T}{(2\pi)^2} 4\pi k_F^3 \frac{\left(\epsilon_{F,k}\right)^2}{\epsilon_{F,k}} \alpha_{cc,k}, \tag{60}
\]

\[
= \frac{\bar{n}e^2T}{m_e} \alpha_{cc,k}, \tag{61}
\]

where \(\epsilon_{F,k} = k_F/m_e\), \(\epsilon_{F,k} = k_F/m_e\), and \(\tilde{k}_F^2/3\) are used. Here, \(\bar{n}\) is the total filling, which is defined by the total electron number \(N_e\) per the volume of the system:

\[
\bar{n} = \frac{N_e}{V} = 2 \cdot \frac{4\pi}{(2\pi)^3} \int_{0}^{\frac{\pi}{2}} d\kappa^2 = \frac{k_F^3}{3\pi^2}. \tag{62}
\]

Note that the factor \(\tau(a_{cc,k})\) appears in Eq. (61), which implies that the ratio of the amplitude of conduction electrons to the damping rate determines the nature of \(\sigma_{xx}\).

As for the Hall conductivity, Eq. (58) can be calculated as

\[
\sigma_{xy} = -H \frac{2e^2T r_F}{(2\pi)^3 m_e} \int_{\epsilon_{F}} dS \left(\epsilon_{F,k}\right)^2 \frac{\alpha_{cc,k}}{\sqrt{E_F}}, \tag{63}
\]

\[
= -H \frac{2e^2 T r_F}{(2\pi)^3 m_e} \frac{k_F^2}{v_F} \frac{\left(\epsilon_{F,k}\right)^2}{v_F}, \tag{64}
\]

\[
= -\omega_c \tau_{cc,k} \frac{e_{cc,k}}{h}, \tag{65}
\]

where \(\omega_c\) is the cyclotron frequency defined as \(\omega_c = \frac{eH}{m_e}\). Note that in Eq. (64) the factor \(\left(\tau(a_{cc,k})\right)^2\) appears, which implies that the square of the ratio of the amplitude of conduction electrons to the damping rate determines the nature of \(\sigma_{xy}\).

By using Eqs. (61) and (65), the Hall coefficient \(R_H\) under a weak magnetic field \(H\) applied along the \(z\) axis is obtained as

\[
R_H = \frac{\sigma_{xy}/H}{\sigma_{xx}}, \tag{66}
\]

\[
= \frac{\omega_c \tau_{cc,k}}{H \sigma_{xx}}, \tag{67}
\]

\[
= \frac{1}{\bar{n}e}. \tag{68}
\]

Note here that although both \(\sigma_{xx}\) and \(\sigma_{xy}\) include the ratio of the weight factor \(\alpha_{cc,k}\) to the damping rate as Eqs. (61) and (65), the factors \(\tau(a_{cc,k})\) in the Hall coefficient are cancelled so that the resultant \(R_H\) is expressed by the total electron filling \(\bar{n}\). This implies that \(R_H\) is only determined by the total filling irrespective of the weight of conduction electrons component at the Fermi level. Namely, Eq. (68) reproduces the well-known result in the single-orbital system.

Here, two remarks should be made. First, Eq. (68) shows the negative sign and that the magnitude is expressed as inverse of the total filling. We note that Eq. (68) is obtained in the free-electron system with the spherical Fermi surface. In general, \(R_H\) depends on the shape of the Fermi surface, more precisely, the curvature of the Fermi surface. Hence, sign of \(R_H\) and the magnitude itself depend on the shape of the Fermi surface even in the small-\(T_0\) limit at \(T = 0\). This point will be discussed in detail in Sect. 4.2.5.

Second, we note that Eq. (68) is obtained in the small-\(T_0\) limit. If the damping rate \(\Gamma_k\) is not small, it is not guaranteed that \(R_H\) shows a constant behavior as Eq. (68) when \(\epsilon_l\) is varied even at \(T = 0\), as will be discussed in Sect. 4.2.6.

4. Ground-state properties of \(\sigma_{xx}, \sigma_{xy}/H, \) and \(R_H\) on the square lattice

In Sect. 3, we derived exactly the general expressions of diagonal and Hall conductivities in hybridized two-orbital systems with arbitrary band dispersions for non-interacting case. In this Sect. we study the ground-state properties of the diagonal conductivity and normal Hall effect in the periodic Anderson model with onsite Coulomb repulsion between \(f\) electrons. By employing the Fermi liquid theory discussed in Sect. 2, we will discuss that the diagonal and Hall conductivities can be calculated by using the formulas derived in Sect. 3. However, we make an approximation in which the Fermi liquid correction for the current given by Eq. (21) is neglected. Nevertheless, this approximation is considered to be valid for the present purpose that we discuss a qualitative aspect of the diagonal and Hall conductivities. To clarify the general properties realized in Ce- and Yb-based heavy-electron systems, we concentrate on the Fermi-liquid ground state taking into account the effect of weak impurity scatterings.

The imaginary part of the f-electron self energy around the Fermi level is expressed as

\[
\Omega(\epsilon) = \Omega^U(\epsilon) + \Omega^{imp}, \tag{69}
\]

where \(\Omega^U(\epsilon)\) is arising from the onsite Coulomb repulsion in Eq. (1) and \(\Omega^{imp}\) is from the impurity scattering. In the Fermi-liquid regime, \(\Omega^U(\epsilon)\) has the following form at zero temperature:

\[
\Omega^U(\epsilon) = -C_U(\epsilon - \mu)^2, \tag{70}
\]

where \(C_U > 0\) is a constant of the order of the inverse of the effective Fermi energy.\(^{17,30}\) When \(f\) electrons are scattered weakly by a small amount of local impurities, \(\Omega^{imp}\) is calculated within the Born approximation\(^{30,31}\) as

\[
\Omega^{imp} \approx -\pi n_{imp} u^2 \langle \delta_{\epsilon_k} \rangle \times N^*(\mu), \tag{71}
\]

where \(n_{imp}\) is the impurity concentration and \(u\) is the impurity potential. Here, \(N^*(\mu)\) is the density of states of the quasiparticles at the Fermi level defined by \(N^*(\epsilon) = \sum_k \delta(\epsilon - E_{k,\epsilon}/N)\) with \(N\) being the number of lattice sites and \(\langle \delta_{\epsilon_k} \rangle\) is averaged value of the \(f\)-electron weight factor defined in Eq. (10) over the Fermi level. Although \(N^*(\mu)\) is enhanced by the renormalization factor \(\tau_{cc,k}^{-1}\), the enhancement is canceled by the factor \(\langle \delta_{\epsilon_k} \rangle\) within [see Eq. (10)]. Hence, \(\langle \delta_{\epsilon_k} \rangle\) is the quantity in the order of \(\pi V^2 N^*(\mu)^{-1}\), where \(N_e\) is the density of states of conduction electrons at the Fermi level.

As described in the formalism in Sect. 2, the diagonal conductivity in Eq. (16) and Hall conductivity in Eq. (24) are calculated by using the Green function for quasiparticles. Here we consider the \(\Omega^U(\mu)\) in the form of Eq. (69) as the self energy. Since the impurity concentration \(n_{imp}\) and the strength of the impurity potential \(u\) are parameters to be given and the extra factor \(\langle \delta_{\epsilon_k} \rangle\) in \(N^*(\mu)\) in Eq. (71) can be expressed essentially by bare quantities not including renormalization factor and has only weak dependence in \(\epsilon_l\), we treat them as variable input parameters. Namely, we calculate \(\sigma_{xx}\) and \(\sigma_{xy}/H\) by inputting

\[
\Gamma \equiv -\Omega^U(\mu) = -\Omega^{imp} \tag{72}
\]
into the quasiparticle Green function. As the simplest framework to perform such a calculation, we employ the slave-boson mean field theory \(^{(32)}\) since it has been established to describe the fixed point of the Fermi-liquid ground state in the periodic Anderson model correctly.

### 4.1 Slave-boson mean field theory

By applying the slave-boson mean field theory \(^{(32)}\) to Eq. (1), the effective Hamiltonian is obtained as

\[
\hat{\mathcal{H}} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i\sigma} \varepsilon_i f_{i\sigma}^\dagger f_{i\sigma} + V \sum_{i\sigma} \left( \tilde{z}_{i\sigma} f_{i\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger \tilde{z}_{i\sigma} \right) + U \sum_i d_i^\dagger d_i
\]

\[+ \sum_i \lambda^{(1)} \left( e_i^\dagger e_i + p_{i\sigma}^\dagger p_{i\sigma} + p_{i\sigma} p_{i\sigma}^\dagger - d_i^\dagger d_i - 1 \right)\]

\[+ \sum_{i\sigma} \lambda^{(2)} \left( f_{i\sigma}^\dagger f_{i\sigma} - p_{i\sigma}^\dagger p_{i\sigma} - d_i^\dagger d_i \right). \tag{73}\]

Here, \(e_i^\dagger, e_i\) and \(d_i^\dagger, d_i\) are boson creation (annihilation) operators for the empty and doubly-occupied state, respectively and \(p_{i\sigma}^\dagger, p_{i\sigma}\) for the singly-occupied state on the \(i\)-th site. The renormalization factor is defined as

\[
z_{i\sigma} = \left( 1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma} \right)^{-1/2} \left( e_i^\dagger p_{i\sigma} + p_{i\sigma}^\dagger e_i \right) \times \left( 1 - e_i e_i - p_{i\sigma}^\dagger p_{i\sigma} \right)^{-1/2}. \tag{74}\]

The last two terms with the Lagrange multipliers \(\lambda^{(1)}\) and \(\lambda^{(2)}\) in Eq. (73) are introduced to require the constraint for the completeness condition.

Here, we consider the case where \(f\) electrons are subject to the impurity scattering in the form of Eq. (72) as an input parameter.

By approximating the mean fields as uniform ones, \(e = (e_i), p_{\sigma} = (p_{i\sigma}), d = (d_i), \) and the Lagrange multipliers, \(\lambda^{(1)} = \lambda_1, \) and \(\lambda^{(2)} = \lambda_2, \) with \(z_{i\sigma} = (z_{i\sigma}), \) the set of mean-field equations is obtained by \(\partial (\hat{\mathcal{H}})/\partial \lambda^{(1)} = 0, \partial (\hat{\mathcal{H}})/\partial \lambda^{(2)} = 0, \partial (\hat{\mathcal{H}})/\partial p_{\sigma} = 0, \partial (\hat{\mathcal{H}})/\partial d = 0, \) and \(\partial (\hat{\mathcal{H}})/\partial e = 0: \)

\[
e^2 + p_{\sigma}^2 + p_{\sigma}^2 + d^2 = 1, \tag{75}\]

\[
\frac{1}{N} \sum_{k\sigma} \left( f_{k\sigma}^\dagger f_{k\sigma} \right) = p_{\sigma}^2 + p_{\sigma}^2. \tag{76}\]

Then, we end up by solving the mean-field equations of Eqs. (76), (77), and (79) for \(\lambda^{(1)}, \lambda^{(2)}, \) and \(\rho\) simultaneously with Eq. (2) for the chemical potential \(\mu\) in the self-consistent manner. In these equations, the following expectation values are calculated as

\[
\frac{1}{N} \sum_{k\sigma} \langle f_{k\sigma}^\dagger f_{k\sigma} \rangle = \frac{1}{\pi N} \sum_{k\sigma} \oint d\varepsilon f_{R}(\varepsilon) \text{Im} G_{R}(\varepsilon) \tag{85}\]

\[
\frac{1}{N} \sum_{k\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = \frac{1}{\pi N} \sum_{k\sigma} \oint d\varepsilon f_{R}(\varepsilon) \text{Im} G_{R}(\varepsilon) \tag{86}\]

\[
\frac{1}{N} \sum_{k\sigma} \langle f_{k\sigma}^\dagger c_{k\sigma} \rangle = \frac{1}{\pi N} \sum_{k\sigma} \oint d\varepsilon f_{R}(\varepsilon) \text{Im} G_{R}(\varepsilon) \tag{87}\]

Here, \(G_{R}(\varepsilon), G_{cc}(\varepsilon), \) and \(G_{fc}(\varepsilon)\) are the retarded f-electron, conduction-electron, and off-diagonal Green functions, respectively, which are given by

\[
G_{R}(\varepsilon) = \tilde{a}_{R}^\dagger (\tilde{a}_{R}) + \tilde{a}_{R}^\dagger (\tilde{a}_{R}) \tag{88}\]

\[
G_{cc}(\varepsilon) = \tilde{a}_{cc}^\dagger (\tilde{a}_{cc}) + \tilde{a}_{cc}^\dagger (\tilde{a}_{cc}) \tag{89}\]

\[
G_{fc}(\varepsilon) = \tilde{a}_{fc}^\dagger (\tilde{a}_{fc}) + \tilde{a}_{fc}^\dagger (\tilde{a}_{fc}) \tag{90}\]

respectively. In Eq. (88), \(\tilde{a}_{R}^\dagger (\tilde{a}_{R})\) is the amplitude of the f-electron component in the lower (upper)-hybridized band at \(k.\) In Eq. (89), \(\tilde{a}_{cc}^\dagger (\tilde{a}_{cc})\) is the amplitude of the conduction-electron component in the lower (upper)-hybridized band at \(k.\) These are given by

\[
\tilde{a}_{s,k}^\dagger = \tilde{a}_{s,k} = \frac{1}{2} \left( 1 + \frac{\varepsilon_k - \varepsilon_1}{\Delta_k} \right). \tag{91}\]

The weight factor \(\tilde{a}_{s,k}^\dagger (\tilde{a}_{s,k})\) in the lower (upper) hybridized
Here, \( \tilde{\Delta}_k \) is given by
\[
\tilde{\Delta}_k = \sqrt{(\xi_k - \xi_f)^2 + 4\tilde{V}^2},
\]
where \( \tilde{\xi}_f \equiv \xi_f + \lambda (d^{(2)}_f) \) and \( \tilde{V} \equiv V_Z \). We note that the relation \( \delta_{\alpha,k}^{(f)} + \delta_{\alpha,k}^{(c)} = 1 \) holds. In Eqs. (91) and (94), the \( f \) level \( \xi_f \) and the hybridization strength \( \Gamma \) are replaced by \( \tilde{\xi}_f \) and \( \tilde{V} \) in Eqs. (30) and (29), respectively. The retarded Green function \( \tilde{G}_{k\alpha}^{(f)}(\epsilon) \) is given by
\[
\tilde{G}_{k\alpha}^{(f)}(\epsilon) = \frac{1}{\epsilon - \tilde{E}_k^{(f)}(\epsilon) + \tilde{\Gamma}_k^{(f)}},
\]
where \( \tilde{E}_k^{(f)} \) is given by
\[
\tilde{E}_k^{(f)} = \tilde{\xi}_f + \tilde{\xi}_k + \frac{\tilde{\Delta}_k}{2}.
\]

Here we consider the finite imaginary part of the self energy, \( \tilde{\Gamma}_k^{(f)} \), in Eq. (95), as described in Eq. (72). In Sect. 2, Eq. (10) is expressed as
\[
\tilde{\alpha}_{\alpha,k}^{(f)} = \alpha_k \left[ 1 + \frac{\alpha_k V^2}{(\xi_k - \tilde{\xi}_k)^2} \right]^{-1}.
\]

In the present mean-field framework, the renormalization factor is expressed as \( z \) and the quasiparticle band is expressed as \( \tilde{E}_k^{(f)} \). Hence, by setting \( z_k \) as \( z \) and \( \tilde{E}_k^{(f)} \) as \( \tilde{E}^{(f)} \) in Eq. (97), \( \tilde{\alpha}_{\alpha,k}^{(f)} \) is expressed as \( z \tilde{\alpha}_{\alpha,k}^{(f)} \). Then, from Eq. (15), the damping rate of the quasiparticle is expressed as
\[
\tilde{\Gamma}_k^{(f)} = z \tilde{\alpha}_{\alpha,k}^{(f)} \Gamma_f,
\]
where \( \Gamma_f \) is defined as \( \Gamma \equiv -\text{Im} \tilde{G}_{k\alpha}^{(f)}(\mu) > 0 \) in Eq. (72).

Hence, by using Eq. (95) as the Green function for quasiparticles, the ground-state properties of \( \sigma_{xx}, \sigma_{xy}, H \), and the Hall coefficient will be discussed in the next Sect. on the basis of the exactly-derived formulas, Eq. (39) and Eq. (50).

As shown in Ref. 17, by calculating the vertex correction in the self energy and the total current consistently for the conductivity in the clean limit at finite temperatures, the total current \( J_{k\alpha} \) has a finite value without diverging because of the presence of the Umklapp process in the periodic lattice in Eq. (23). In the present framework for the ground state (\( T = 0 \)), we consider the self energy with the impurity scattering as in Eq. (69), which is consequently expressed as Eq. (72). As for the total current, the present framework corresponds to approximating the resultant \( J_{k\alpha} \) at \( \nu_{k\alpha} \) in Eq. (21).

The validity of this framework at least within approximating \( J_{k\alpha} \) as \( \nu_{k\alpha} \) is confirmed by comparing it with the finite-\( U \) result based on the Fermi-liquid theory in Sect. 2, which will be shown below (see also Appendix).

4.2 Numerical Results

On the basis of the theoretical framework described in the previous Sect., we calculate the conductivity in the periodic Anderson model on the square lattice. We consider the nearest-neighbor hopping for conduction electrons on the square lattice and the energy band is given by \( \epsilon_k = -2[\cos(k_x) + \cos(k_y)] \). As a typical parameter for heavy electrons, we set \( t = 1, V = 0.3, U = \infty \) at the filling \( n = 7/4 \). Hereafter, the transfer of conduction electrons is taken to be the energy unit of the parameters in the Hamiltonian, Eq. (73). The imaginary part of the f-electron self energy is set to be \( \Gamma = 10^{-3} \) in Eq. (98) as a typical value. We solve the mean-field equations self-consistently at \( T = 0 \) in the several system sizes for \( N = L_x^2 \) with \( L_x = 112, 800, 1200, 1600, 1920, \) and 2240. Below we will show the results calculated on the lattice sites with \( L_x = 1200 \) unless otherwise noted.

4.2.1 f-electron number per site and the characteristic energy

Figure 2 shows the \( \xi_f \) dependence of the f-electron number per site, \( n_f \). As \( \xi_f \) increases, the crossover from the Kondo regime with \( n_f = 1 \) in the deep-\( \xi_f \) regime to the valence-fluctuation regime with \( n_f < 1 \) in the shallow-\( \xi_f \) region occurs in the ground state.

The characteristic energy scale of the present system, which is given by the hybridization gap \( \Delta_{hyb} \), is defined by the energy gap between the bottom of the upper hybridized band and the top of the lower hybridized band of quasiparticles:
\[
\Delta_{hyb} = \tilde{E}_{k\alpha}^{(c)} - \tilde{E}_{k\alpha}^{(f)}.
\]

Since we consider the filling of \( n = 7/4 \) less than half filling, the Fermi level is located at the lower hybridized band. The Kondo temperature \( T_K \), which is the characteristic energy scale of the heavy-electron system, is defined as the energy difference between the renormalized f level and the Fermi level \( T_K = \xi_f - \mu \) in the present mean-field framework. The inset of Fig. 2 shows that \( \Delta_{hyb} \) (solid line) roughly corresponds to \( T_K \) (dashed line), both of which well scale for \( \xi_f \leq 0 \).

To visualize the Fermi surface at \( n = 7/4 \), we plot the spectral function \( A_{\alpha\beta}(k,\epsilon) \equiv -\frac{1}{2} \text{Im} \tilde{G}_{k\alpha}^{(f)}(\epsilon) \) for \( \alpha = - \) and \( \epsilon = \mu \) in Fig. 3. Here we show the contour plot for \( \xi_f = -4.0 \) as a
typical case calculated in the \( N = 112 \times 112 \) lattice sites.

### 4.2.2 Diagonal conductivity

By using the mean-field solutions, the conductivity is calculated on the basis of Eq. (39) at \( T = 0 \). The \( \epsilon_\ell \) dependence of \( \sigma_{xx} \) is shown in Fig. 4. In the deep-\( \epsilon_\ell \) region, as \( \epsilon_\ell \) increases, \( \sigma_{xx} \) shows a gradual increase which can be seen as almost constant behavior, while \( \sigma_{xx} \) shows a sharp increase in the shallow-\( \epsilon_\ell \) region for \( \epsilon_\ell \geq 0 \). The inset shows the \( \epsilon_\ell \)-level dependence of the resistivity \( \rho_{xx} = 1/\sigma_{xx} \).

To analyze the mechanism, we plot \( \sigma_{xx}^{(0)} \) in Fig. 4, which is defined by

\[
\sigma_{xx}^{(0)} = \frac{2e^2}{(2\pi)^2} \sum_{\mathbf{k} \mathbf{k}'} \frac{(v_{\mathbf{k}'}^{(0)2} (a_{\mathbf{k}' \mathbf{k}}^{cc})^2)}{|\nabla E_{\mathbf{k}}^{(0)2}} |\mathbf{F}_{\mathbf{k}}^{x}|, \tag{100}
\]

with \( \mathbf{F}_{\mathbf{k}}^{x} = \frac{1}{2\pi} \). Here, the summation is taken over the Fermi wave vector \( \mathbf{k}_F \) and \( |\mathbf{A}| \) is the length between each next \( \mathbf{k}_F \) point. This is the two-dimensional version of Eq. (59) in the lattice space. We see that the result almost coincides with \( \sigma_{xx}^{(0)} \). This indicates that \( \sigma_{xx}^{(0)} \) in Eq. (40) gives the dominant contribution to \( \sigma_{xx} \) in Eq. (39) and the analysis with the small \( \Gamma_{k} \) in Eq. (55) is applicable to the parameter regime shown in Fig. 4. Since the velocity of the lower hybridized band \( v_{k}^{-} = v_{k}^{0} a_{\mathbf{k} \mathbf{k}'}^{cc} \) [see Eq. (43)], Eq. (100) can be expressed as

\[
\sigma_{xx}^{(0)} = \frac{2e^2}{(2\pi)^2} \sum_{\mathbf{k} \mathbf{k}'} \frac{(v_{\mathbf{k}'}^{(0)2} (a_{\mathbf{k}' \mathbf{k}}^{cc})^2)}{|\nabla E_{\mathbf{k}}^{(0)2}} |\mathbf{F}_{\mathbf{k}}^{x}|. \tag{101}
\]

This implies that the ratio of the conduction-electron weight factor \( a_{\mathbf{k} \mathbf{k}'}^{cc} \), and the damping rate \( \Gamma_{k}^{x} \) determines the behavior of \( \sigma_{xx}^{(0)} \). This gives essentially the same form as Eq. (16), which was formulated on the basis of the Fermi-liquid theory,\(^{17}\) as shown in Appendix. This indicates the validity of the present formalism.

In order to clarify the \( \epsilon_\ell \) dependence of \( \Gamma_{k}^{x} \) from Eq. (98) in detail, we plot in Fig. 5 the \( \epsilon_\ell \) dependence of the renormalization factor \( z \) and the f-electron weight factor which is averaged over the Fermi surface

\[
\langle \tilde{a}_{\mathbf{k} \mathbf{k}'}^{f} \rangle_{av} \equiv \frac{1}{N_{\mathbf{k} \mathbf{k}'}} \sum_{\mathbf{k} \mathbf{k}'} \tilde{a}_{\mathbf{k} \mathbf{k}'}^{f}, \tag{102}
\]

with \( N_{\mathbf{k} \mathbf{k}'} \) being the number of the \( \mathbf{k}_F \) points. As \( \epsilon_\ell \) increases, \( \langle \tilde{a}_{\mathbf{k} \mathbf{k}'}^{f} \rangle_{av} \) is kept to be almost 1 up to \( \epsilon_\ell \sim 1 \) and sharply decreases to zero for \( \epsilon_\ell \geq 1 \).

The renormalization factor \( z \) approaches zero in the deep-\( \epsilon_\ell \) limit due to strong correlation effect on f electrons with \( n_{f} \rightarrow 1 \) (see Fig. 2). As \( \epsilon_\ell \) increases, \( z \) increases gradually. The damping rate \( \Gamma_{k}^{x} \) given by the multiplication of \( \tilde{a}_{\mathbf{k} \mathbf{k}'}^{f} \) and \( z \) in Eq. (98) is averaged over the Fermi surface

\[
\langle \tilde{\Gamma}_{\mathbf{k}}^{x} \rangle_{av} = \frac{1}{N_{\mathbf{k} \mathbf{k}'}} \sum_{\mathbf{k} \mathbf{k}'} \tilde{\Gamma}_{\mathbf{k}}^{x}, \tag{103}
\]

which shows a peak structure around \( \epsilon_\ell \sim 2 \) as shown in Fig. 5. An important result here is that \( \langle \tilde{\Gamma}_{\mathbf{k}}^{x} \rangle_{av} \) is suppressed compared to \( \Gamma = 10^{-3} \) in all the \( \epsilon_\ell \) region since in both the large-\( \epsilon_\ell \) and small-\( \epsilon_\ell \) limits \( \langle \tilde{\Gamma}_{\mathbf{k}}^{x} \rangle_{av} \) approaches zero and the peak value is bounded by the small \( \Gamma \).

Figure 6 shows the \( \epsilon_\ell \) dependence of the conduction-electron weight factor averaged over the Fermi surface

\[
\langle \tilde{a}_{\mathbf{k} \mathbf{k}'}^{cc} \rangle_{av} \equiv \frac{1}{N_{\mathbf{k} \mathbf{k}'}} \sum_{\mathbf{k} \mathbf{k}'} \tilde{a}_{\mathbf{k} \mathbf{k}'}^{cc}. \tag{104}
\]

In Fig. 6, \( \langle \tilde{\Gamma}_{\mathbf{k}}^{x} \rangle_{av} \) is also re-plotted for comparison. As \( \epsilon_\ell \) increases, \( \langle \tilde{a}_{\mathbf{k} \mathbf{k}'}^{cc} \rangle_{av} \) increases gradually in the deep-\( \epsilon_\ell \) region, while it shows a sharp increase around \( \epsilon_\ell \sim 1 \). The gradual increase in \( \langle \tilde{a}_{\mathbf{k} \mathbf{k}'}^{cc} \rangle_{av} \) and \( \langle \tilde{\Gamma}_{\mathbf{k}}^{x} \rangle_{av} \) in the deep-\( \epsilon_\ell \) region gives rise to cancellation of the effect of the mass renormalization\(^{17}\) in Eq. (101), which causes the almost constant \( \epsilon_\ell \) dependence of \( \sigma_{xx}^{(0)} \). However, as \( \epsilon_\ell \) increases to reach the shallow-\( \epsilon_\ell \) region, \( \epsilon_\ell \geq 0 \), i.e., so-called the ‘valence-fluctuation’ regime, the cancellation does not work, where \( \tilde{a}_{\mathbf{k} \mathbf{k}'}^{cc} \) increases sharply.
while $\bar{\Gamma}_k$ remains small. This imbalance is the reason why $\sigma_{xx}$ shows a sharp increase in the valence-fluctuation regime for $\varepsilon_f \gtrsim 0$ in Fig. 4. This gives a natural explanation for the pressure dependence of the residual resistivity frequently observed in the Ce-based compounds and Yb-based compounds. The pressure dependence of the conductivity will be discussed in detail in Sect. 4.2.7.

The above result is obtained by using constant $\Gamma$ in Eq. (72). As noted below Eq. (71), $\langle \tilde{\sigma}^{\text{eff}} \rangle_{0} N(\mu)$ can be expressed essentially by the bare quantities, which is on the order of $O(\pi v^2 N(\mu))^{-1}$. Hence, $\Gamma$ defined in Eq. (72) has only weak $\varepsilon_f$ dependence. However, as shown in Fig. 5, the quantities related to renormalization factor, $\bar{\Gamma}$ and $\tilde{\sigma}^{\text{eff}}$, have strong $\varepsilon_f$ dependence, which give the main contribution to the remarkable change of $\sigma_{xx}$ when $\varepsilon_f$ varies from the Kondo regime to the valence-fluctuation regime. Hence, present treatment using constant $\Gamma$ is considered to capture the essence of the transport phenomena. As for the hybridization dependence, we have also performed the calculations of the $\varepsilon_f$ dependence of $\sigma_{xx}$ by inputting several values of $\Gamma$ and confirmed that the main conclusion above does not change as far as the renormalized damping rate is far smaller than the hybridization gap. The dependence and the $\Gamma$ dependence will be discussed in Sect. 4.2.6 and Sect. 4.2.7, respectively.

### 4.2.3 Hall conductivity

The $\varepsilon_f$ dependence of the Hall conductivity is shown in Fig. 7. The Hall conductivity $\sigma_{xy}/H$ is calculated by using Eq. (50) at $T = 0$. As $\varepsilon_f$ increases, in the deep-$\varepsilon_f$ region $\sigma_{xy}/H$ gradually increases, which can be seen as almost constant behavior, while it shows a sharp increase in the shallow-$\varepsilon_f$ region for $\varepsilon_f \gtrsim 0$.

To analyze the mechanism, we plot $\sigma_{xy}^{(0)}/H$ in Fig. 7, which is defined by

$$\frac{\sigma_{xy}^{(0)}}{H} = \frac{-2 \varepsilon_f^3}{(2\pi)^2} \sum_{k-k'} \frac{\left(\left|v_{k'}\right|^2 \frac{\partial_v}{\partial \varepsilon} \left(\tilde{\sigma}^{\text{eff}}_{k-k'}\right)^3}{\left|\nabla E_k\right|^2} \left(\tilde{\Gamma}_k\right)^2 |\Delta k|}$$

with the same notation as Eq. (100). This is the two-dimensional version of Eq. (63) in the lattice system. We see that the result almost coincides with $\sigma_{xy}/H$. This indicates that $\sigma_{xy}/H$ in Eq. (51) dominantly contributes to $\sigma_{xy}/H$ in Eq. (50) and the analysis by the small $\bar{\Gamma}_k = \frac{1}{\bar{\Gamma}}$ in Eq. (58) is applicable to the parameter regime shown in Fig. 7. By using the velocity of the lower hybridized band, $\nu_{k} = \nabla E_k = v_{k}^{\prime} v_{k}^{\text{eff}}$, Eq. (105) can be expressed as

$$\frac{\sigma_{xy}^{(0)}}{H} = \frac{-2 \varepsilon_f^3}{(2\pi)^2} \sum_{k-k'} \frac{\left|v_{k'}\right|^2 \frac{\partial_v}{\partial \varepsilon} \left(\tilde{\sigma}^{\text{eff}}_{k-k'}\right)^3}{\left|\nu_{k'}\right|^2 \left|\Delta k\right| \bar{\Gamma}_k^3}$$

In the right hand side, $(\tilde{\sigma}^{\text{eff}}_{k-k'}/\bar{\Gamma}_k^3)$ appears, which implies that the ratio $\tilde{\sigma}^{\text{eff}}_{k-k'}/\bar{\Gamma}_k^3$ determines the behavior of $\sigma_{xy}^{(0)}/H$. As shown in Fig. 6, in the deep-$\varepsilon_f$ region, $\tilde{\sigma}^{\text{eff}}_{k-k'}/\bar{\Gamma}_k$ increases gradually, while it shows a sharp increase in the shallow-$\varepsilon_f$ region for $\varepsilon_f \gtrsim 0$. Namely, cancellation of the effect of the mass

![Fig. 5](image-url) (Color online) The $\varepsilon_f$ dependence of the $\Gamma$-electron weight factor $(\tilde{\sigma}^{\text{eff}}_{k-k'})_{0}$ (dashed line) and the renormalization factor $\tilde{\Gamma}$ (dash-dotted line) for $t = 1$, $V = 0.3$, and $U = \infty$ at $\tilde{n} = 7/4$ with $\Gamma = 10^{-3}$ is shown in the right axis, which is calculated in the $N = 1200 \times 1200$ lattice sites. The $\varepsilon_f$ dependence of the imaginary part of the self energy $(\tilde{\Gamma}_{k})_{0}$ is also plotted (solid line) in the left axis.

![Fig. 6](image-url) (Color online) The $\varepsilon_f$ dependence of the conduction-electron weight factor $(\tilde{\sigma}^{\text{eff}}_{k-k'})_{0}$ (dashed line, right axis) and the imaginary part of the selfenergy $(\tilde{\Gamma}_{k})_{0}$ (solid line, left axis) is shown, which is calculated for $t = 1$, $V = 0.3$, and $U = \infty$ at $\tilde{n} = 7/4$ with $\Gamma = 10^{-3}$ in the $N = 1200 \times 1200$ lattice sites.

![Fig. 7](image-url) (Color online) The $\varepsilon_f$ dependence of the conductivity $\sigma_{xy}/H$ (solid line) and $\sigma_{xy}^{(0)}/H$ (dashed line) for $t = 1$, $V = 0.3$, and $U = \infty$ at $\tilde{n} = 7/4$ with $\Gamma = 10^{-3}$ is shown in the left axis, which is calculated in the $N = 1200 \times 1200$ lattice sites. We set $\varepsilon = 1$. 

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enhancement, i.e., \( \tilde{\alpha}_{\tilde{R}}^{\text{cc}}/\Gamma_{\tilde{R}} \approx 1 \), causes the almost constant behavior of \( \sigma_{xy}/H \) in the deep-\( \epsilon_f \) region and the imbalance, i.e., \( \tilde{\alpha}_{\tilde{R}}^{\text{cc}}/\Gamma_{\tilde{R}} \gg 1 \), makes the sharp increase in \( \sigma_{xy}/H \) in the valence-fluctuation regime for \( \epsilon_f \geq 0 \) in Fig. 7.

### 4.2.4 Hall coefficient

The \( \epsilon_f \) dependence of the Hall coefficient is shown in Fig. 8. Here we set \( \epsilon = 1 \). The Hall coefficient \( R_H = \sigma_{xy}/(H\sigma_{xx}^2) \) is calculated using Eqs. (39) and (50) and shows a slight decrease as a function of \( \epsilon_f \), exhibiting almost constant behavior. Namely, the sharp increase in \( \sigma_{xy}/H \) in the valence-fluctuation regime for \( \epsilon_f \geq 0 \) in Fig. 4 and Fig. 7, respectively, cancel out each other in \( R_H \). To analyze this cancellation which occurs even in the valence-fluctuation regime, we use Eq. (100) and (105) in Fig. 8. We see that \( R_H^{(0)} \) also exhibits almost constant behavior. This is understood from expressions Eq. (100) and Eq. (105) since the factors of \( \tilde{\alpha}_{\tilde{R}}^{\text{cc}}/\Gamma_{\tilde{R}} \) which appear in both \( \sigma_{xx}^{(0)} \) and \( \sigma_{xy}^{(0)}/H \) cancel out in \( R_H^{(0)} \). The close agreement between \( R_H \) and \( R_H^{(0)} \) indicates that the cancellation of the factors of \( \tilde{\alpha}_{\tilde{R}}^{\text{cc}}/\Gamma_{\tilde{R}} \) actually occurs in \( R_H \) as was shown for the isotropic free-electrons in Eq. (68).

To figure out the filling dependence of \( R_H \), we calculate \( \sigma_{xx} \) and \( \sigma_{xy}/H \) for \( 1 \leq \tilde{n} < 2 \) plausible to the heavy-electron state since system sizes and extrapolate \( R_H \) to the bulk limit, \( N = L_x^2 \to \infty \). Figure 9 shows \( R_H \) vs. \( 1/N \) for \( \epsilon_f = -4.0 \) at \( \tilde{n} = 1, 6/5, 7/5, 8/5, 7/4, \) and \( 9/5 \). The system sizes used for the extrapolation are \( N = L_x^2 \) with \( L_x = 1200, 1600, 1920, \) and 2240.

The \( \tilde{n} \) dependence of \( R_H \) in the bulk limit is shown in Fig. 10. Note that the error bar by the least-square fit done for the system-size extrapolation is attached to each filled circle. The error bars are within the symbol sizes and invisible, indicating that the size system dependence does not matter in the \( N \geq 1200 \) lattice sites. Here we also plot the Hall coefficient expressed by the hole density as \( R_{\text{hole}} = \sigma_{xy} / \varrho \) with \( \varrho_{\text{hole}} = 2 - \tilde{n} \) by a dashed line (Note that we set \( \epsilon = 1 \)). We can see that \( R_H \) approaches \( R_{\text{hole}} \) as \( \tilde{n} \) approaches half filling, \( \tilde{n} = 2 \). However, \( R_H \) approaches zero as \( \tilde{n} \) approaches 1, which shows a clear deviation from the dashed line. These results indicate that near the quarter filling, i.e., for \( 1 \leq \tilde{n} \leq 1.6 \), \( R_H \) is not expressed simply by the hole density as \( 1/\varrho_{\text{hole}} \).

### 4.2.5 Curvature of the Fermi surface and Hall conductivity and Hall coefficient

To understand the reason why \( R_H \) does not follow the simple relation \( R_H = 1/(\varrho_{\text{hole}}\epsilon) \), we analyze \( \sigma_{xy}/H \) from the view-
point of the curvature of the Fermi surface. In the single-band system constituted of a single orbital, it has been shown that \( \sigma_{xy}/H \) can be expressed by the angle between \( \vec{v}_k \) and the \( k_x \) axis within the Boltzmann transport theory\(^{12-14} \) and the theory considering the vertex corrections.\(^{24} \) In the present system, there exist two orbitals of \( \Gamma \) and conduction electrons, which form the lower and upper hybridized bands. Since the Fermi level is located at the lower hybridized band, the system is regarded as the single-band system at \( T = 0 \) in the small-\( \Gamma_k \) limit.

At sufficiently low temperatures in the small damping rate, \( \sigma_{xy}/H \) in Eq. (51) dominantly contributes to \( \sigma_{xy}/H \) in Eq. (50). Let us write Eq. (57) in the original form like Eq. (50) as

\[
\sigma_{xy}/H = -\frac{e^3}{2V_0} \sum_{k_{\sigma}} \frac{\partial f(\tilde{E}_k)}{\partial \tilde{E}_k} A_{xy}(\mathbf{k}) \frac{2}{4(\Gamma_k)^2}.
\]

(107)

Here, by Eq. (43), the velocity of the lower hybridized band \( \vec{v}_k^- = \nabla \tilde{E}_k^- \) in the present system for Eq. (73) is written as

\[
\vec{v}_k^- = \vec{v}^{\alpha} \vec{k} \equiv \vec{v}_k^\alpha.
\]

(108)

Now we apply the formalism shown in Ref. 24 to Eq. (107). Here we describe it up to Eq. (116) below as the self-contained explanation although it was originally published in Ref. 24 [see Eq. (22) in Ref. 24].

For the subsequent discussion, we rewrite Eq. (107) as follows

\[
\sigma_{xy}/H = -\frac{e^3}{2V_0} \sum_{k_{\sigma}} \frac{\partial f(\tilde{E}_k)}{\partial \tilde{E}_k} A_{xy}(\mathbf{k}) \frac{2}{4(\Gamma_k)^2}.
\]

(109)

by introducing

\[
A_{xy}(\mathbf{k}) \equiv \vec{v}_k^\alpha \left( \frac{\partial \vec{v}_k^\alpha}{\partial k_x} - \vec{v}_k^\alpha \frac{\partial \vec{v}_k^\alpha}{\partial k_y} \right).
\]

(110)

As shown in Ref. 20 [see Eq. (3.21) in Ref. 20], this can be rewritten in a simpler form as

\[
\sigma_{xy}/H = -\frac{e^3}{4V_0} \sum_{k_{\sigma}} \frac{\partial f(\tilde{E}_k)}{\partial \tilde{E}_k} A_{xy}(\mathbf{k}) \frac{2}{4(\Gamma_k)^2},
\]

where \( A_{xy}(\mathbf{k}) \) is defined as

\[
A_{xy}(\mathbf{k}) = A_{-xy}(\mathbf{k}) + A_{+xy}(\mathbf{k}).
\]

(112)

This can be expressed as\(^{24} \)

\[
A_{-xy}(\mathbf{k}) = \vec{v}_k^\alpha (\vec{\epsilon}_k \times \vec{\epsilon}_k) \nabla \vec{v}_k^\alpha - \vec{v}_k^\alpha (\vec{\epsilon}_k \times \vec{\epsilon}_k) \nabla \vec{v}_k^\alpha,
\]

(113)

\[
\left[ \vec{v}_k^\alpha \right] = \vec{v}_k^\alpha \left( \frac{\partial \vec{v}_k^\alpha}{\partial k} \right),
\]

(114)

where \( k_{\parallel} \) is the component of \( \vec{k} \) along the vector \( \vec{\epsilon}_k' = (\vec{\epsilon}_k \times \vec{\epsilon}_k')/|\vec{\epsilon}_k'| \), and tangential to the Fermi surface at \( \mathbf{k} \) since \( \vec{v}_k^\alpha \) is perpendicular to the Fermi surface. In Eq. (115), \( \theta_{\parallel-k} \) is the angle between \( \vec{v}_k^\alpha \) and the \( k_x \) axis.

By applying the similar derivation used in Eq. (63) to Eq. (111), \( \Sigma_{\parallel-k} \) can be expressed by the line integral along the Fermi surface in the present two-dimensional system. Then we have

\[
\sigma_{xy}/H = \frac{e^3}{4(2\pi)^2} \int_{FS} dk_\parallel |\vec{v}_k^\alpha| \left( \frac{d\theta_{\parallel-k}(\mathbf{k})}{dk_\parallel} \right)^2 \frac{2}{4(\Gamma_k)^2},
\]

(116)

where the \( \mathbf{k} \) point moves counterclockwise along the Fermi surface in this line integral. Note that by Eq. (108) the mass renormalization factors appear as \( \left( |\vec{v}_k^\alpha|/\tilde{E}_k \right)^2 \) in the integrand, which cancel out in the deep-\( \epsilon_F \) region as noted in Eq. (106).

To visualize the Fermi surface, we plot the spectral function \( A_{\alpha}(\mathbf{k}, \epsilon) \equiv -ImG^{\alpha R}(\epsilon)/\pi \) for \( \alpha = - \) and \( \epsilon = \mu \) at (a) \( \bar{n} = 1 \), (b) 6/5, (c) 7/5, (d) 8/5, and (e) 9/5 for \( t = 1 \), \( V = 0.3 \), \( \epsilon_F = -4.0 \), and \( U = \infty \) with \( \Gamma = 10^{-3} \) calculated in the \( N = 112 \times 112 \) lattice sites. (f) The velocity of the lower hybridized band \( \vec{v}_k^- \) on the Fermi surface \( k = k_F \). (g) The relation among \( k_F \), \( k_{F_{hole}} \), and \( Q = (\pi, \pi) \). \( k_F = Q + k_{F_{hole}} \). (h) The path for the line integral Eq. (117) along the Fermi surface.

Fig. 11. (Color online) The contour plot of the spectral function \( A_{\alpha}(\mathbf{k}, \epsilon) \equiv -ImG^{\alpha R}(\epsilon)/\pi \) at (a) \( \bar{n} = 1 \), (b) 6/5, (c) 7/5, (d) 8/5, and (e) 9/5 for \( t = 1 \), \( V = 0.3 \), \( \epsilon_F = -4.0 \), and \( U = \infty \) with \( \Gamma = 10^{-3} \) is the same as those in Fig. 9 and the results calculated in the \( N = 112 \times 112 \) lattice sites are shown.

At quarter filling, \( \bar{n} = 1 \), we see that \( \theta_{\parallel-k}(\mathbf{k}) \) for example on the first quadrant does not change, since \( \vec{v}_k^\alpha \) is perpendicular to the Fermi surface, which makes \( \theta_{\parallel-k}(\mathbf{k}) \) to be kept to be \( \pi/4 \). This gives rise to \( d\theta_{\parallel-k}(\mathbf{k})/dk_\parallel = 0 \) in Eq. (116). Hence, it turns out that \( \sigma_{xy}/H \) and \( R_{H} \) as well become zero at \( \bar{n} = 1 \) at least for the small-\( \Gamma_k \) limit. Actually, \( R_{H} \) at \( \bar{n} = 1 \) in Figs. 9 and 10
is shown to be almost zero although the spectral function is broadened near $k = (0, \pi)$ and $(\pi, 0)$ in Fig. 11(a) because of the finite damping rate $\Gamma_{f}^{-1}$.

The reason why the sign of $\sigma_{xy}/H$ and the resultant $R_H$ become positive for $1 < \bar{n} < 2$ can be also understood from expression Eq. (116). As illustrated in Fig. 11(f), the angle $\theta_{\bar{n}}(k)$ becomes smaller as $k$ moves along the Fermi surface. Namely, $d\theta_{\bar{n}}(k)/dk_{\parallel} < 0$ in Eq. (116) makes the sign of $\sigma_{xy}/H$ be positive, and hence the positive Hall coefficient appears, $R_H > 0$.

Furthermore, the reason why $R_H$ approaches $1/(2 - \bar{n})e$ as $\bar{n}$ approaches half filling, 2, in Fig. 10 can be also understood on the basis of Eq. (116). As $\bar{n}$ approaches $\bar{n} = 2$, the form of the Fermi surface for holes approaches the circle around $k = (\pi, \pi)$ as shown in Fig. 11(e). Hence, it is convenient to introduce the variable transformation $k_F = Q + k_{hole}$ with a constant shift $Q = (\pi, \pi)$ in Eq. (116), as shown in Fig. 11(g). Then, Eq. (116) is expressed as

$$\sigma_{xy}/H = \frac{e^3}{4(2\pi)^2} \int_{FS} dk_{\parallel} |\bar{\nu}_F|^2 \left( \frac{d\theta_{\bar{n}}(k)}{dk_{\parallel}^{hole}} \right) \frac{2}{4(\Gamma_F^2)^2},$$

(117)

When the Fermi surface is a circle, the integration can be easily performed as follows: Since the line integral in Fig. 11(h) is performed clockwise, the negative sign appears as $d\theta_{\bar{n}}(k)/dk_{\parallel}^{hole} = -1/k_{F}^{hole}$. By using $\bar{\nu}_F dk_{\parallel}^{hole} = 2\pi k_F$, we obtain

$$\sigma_{xy}/H = \frac{e^3}{4(2\pi)^2} 2\pi k_F^{hole} \left( \frac{1}{k_F^{hole}} \right) \frac{1}{(\Gamma_F^2)^2}.$$  

(118)

From Eq. (59) applied to the two-dimensional system, it can be shown that $\sigma_{xx}$ for the hole Fermi surface with a circle shape is expressed as

$$\sigma_{xx} = \frac{e^2}{2\pi} k_F^{hole} \frac{1}{2\Gamma_F^2}.$$  

(119)

By Eqs. (118) and (119), the Hall coefficient is obtained as

$$R_H = \frac{\sigma_{xy}}{H \sigma_{xx}^{1/2}} = \frac{1}{\bar{n}_{hole} e},$$

(120)

where the hole density is given by $\bar{n}_{hole} = (k_F^{hole})^2/(2\pi)$ in the two-dimensional system. Then it is understandable that $R_H$ is expressed by the hole density as $1/(\bar{n}_{hole} e)$ with $\bar{n}_{hole} \equiv 2 - \bar{n}$ as $\bar{n}$ approaches half filling, $\bar{n} = 2$, in Fig. 10.

4.2.6 Damping-rate dependence

So far, we have presented the results for the damping rate $\Gamma = 10^{-3}$ [see Eq. (72)] as a typical case. In this Subsect., we discuss the $\Gamma$ dependence.

Figure 12 shows the $\epsilon_f$ dependence of the conductivity $\sigma_{xy}$ for $t = 1$, $V = 0.3$, and $U = \infty$ at $\bar{n} = 7/4$ with (a) $\Gamma = 10^{-2}$, (b) $10^{-3}$, and (c) $10^{-4}$ calculated in the $N = 1200 \times 1200$ lattice sites. Almost constant behavior in the deep-$\epsilon_f$ regime, i.e., Kondo regime, and sharp increase in the shallow-$\epsilon_f$ regime, i.e., valence-fluctuation regime appears in every case, although absolute value of $\sigma_{xx}$ increases. As analyzed in Eq. (101), $\sigma_{xx}$ is proportional to $\Gamma^{-1}$, which can be seen by comparing Fig. 12(b) with Fig. 12(c). However, the relation $\sigma_{xx} \propto \Gamma^{-1}$ does not seem to hold simply between Fig. 12(a) and Fig. 12(b). This indicates that the case of Fig. 12(a) cannot be regarded as the small-$\Gamma$ regime where the analysis based on Eq. (101) is valid. This point will be more clearly seen when we calculate the Hall coefficient $R_H$, which will be discussed in Fig. 14 below.

Figure 13 shows the $\epsilon_f$ dependence of the Hall conductivity $\sigma_{xy}/H$ for (a) $\Gamma = 10^{-2}$, (b) $10^{-3}$, and (c) $10^{-4}$. Almost constant behavior in the Kondo regime and sharp increase in the valence-fluctuation regime appears in every case. The relation $\sigma_{xy}/H \propto \Gamma^{-2}$, which is shown in Eq. (106), seems to hold between Figs. 13(b) and 13(c) but not between Figs. 13(a) and 13(b). As noted above, this is due to the fact that $\Gamma = 10^{-2}$ cannot be regarded as small $\Gamma$.

Figure 14 shows the $\epsilon_f$ dependence of the Hall coefficient $R_H$ for $V = 0.3$ at $\bar{n} = 7/4$ for a series of damping rates due to impurity scattering; $\Gamma = 10^{-4}$ (dashed line), $\Gamma = 10^{-3}$ (solid line), and $\Gamma = 10^{-2}$ (dash-dotted line), which are calculated...
in the $N = 1200 \times 1200$ lattice sites. Almost constant $\sigma_f$ dependence, $R_H \approx 1/(\bar{\rho}_{\text{hole}}e) = 4/e$, appears for $\Gamma = 10^{-4}$ and $\Gamma = 10^{-3}$. However, for $\Gamma = 10^{-2}$, $R_H$ shows a visible deviation from the constant behavior.

To quantify the magnitude of the damping rate, in the inset of Fig. 14 we plot the $\epsilon_f$ dependence of the ratio of the damping rate averaged over the Fermi surface ($\tilde{\Gamma}_{E_{f}}^{\text{av}}$ defined by Eq. (103) to $\Delta_{\text{hyb}}$ defined by Eq. (99)). These results indicate that when the damping rate becomes comparable to about 10% of the hybridization gap, the treatment of the small $\tilde{\Gamma}_{k}$ discussed in Sect. 3.2 and also using Eqs. (100) and (105) are not justified. Namely, the contributions from the energies distant from the Fermi energy in Eq. (40) and Eq. (51) become relevant to $\sigma_{xx}$ and $\sigma_{xy}/H$, respectively. For example, the downward deviation of $R_H$ with $\Gamma = 10^{-2}$ seen in the deep-$\epsilon_f$ region in Fig. 14 reflects the tendency that the electron-like curvature of the $k$ points in the $\epsilon < \mu$ region of the lower hybridized band gives contributions with negative sign in $\sigma_{xy}/H$.

Hence, in the case that strong impurity scattering and/or high impurity density as well as the extraordinarily-strong correlation gives rise to a large damping rate which exceeds 10% of the hybridization gap, $R_H$ is not expressed simply by the hole density as $1/(\bar{\rho}_{\text{hole}}e)$ even near the half filling at $T = 0$. It is noted that not only the contributions distant from the Fermi energy to $\sigma_{xx}$ in Eq. (40) and $\sigma_{xy}$ in Eq. (51) but also the contributions other than the lower hybridized band are considered to play a significant role in $\sigma_{xx}$ and $\sigma_{xy}$ in such a case.

### 4.2.7 Hybridization dependence and pressure dependence in Ce- and Yb-based compounds

When pressure is applied to the Ce-based compounds, the anions surrounding the Ce$^{3+}$ ion approach the tail of the wavefunction of the 4f electron at the Ce site. This causes increase in the crystalline-electronic-field (CEF) level, i.e., $\sigma_f$ increases. When pressure is applied to the Yb-based compounds, the negative ions surrounding the Yb$^{3+}$ ion approach, which also makes the 4f-electron level at the Yb site increase. Since Yb$^{3+}$ contains 4f$^3$ electrons, the hole picture is applied to the periodic Anderson model for the Yb-based systems. Hence, applying pressure makes the 4f-hole level $\epsilon_f$ decrease in Eq. (1).

In both the Ce- and Yb-based systems, the hybridization strength between $f$ and conduction electrons is also expected to increase in general. In this subsection, we examine the hybridization dependence of the conductivity, the Hall conductivity, and the Hall coefficient.

In Fig. 15, we show $\sigma_f$ dependence of $\sigma_{xx}$ for $V = 0.3$ (solid line), 0.4 (dashed line) and 0.5 (dashed-dotted line) with $\Gamma = 10^{-3}$, which is calculated in the $N = 1200 \times 1200$ lattice sites. We see that $\sigma_{xx}$ shifts to larger values as $V$ increases. As analyzed below Eq. (101), main contribution to $\sigma_{xx}$ comes from $\tilde{\sigma}_{xx}^{\text{hyb}}/\tilde{\Gamma}_{xx}$ at the Fermi level. To clarify how hybridization strength affects this quantity, we plot the $\epsilon_f$ dependence of $\tilde{\Gamma}_{xx}$ (solid line) and $\tilde{\Gamma}_{xy}$ (dashed line) for $V = 0.3$, 0.4 and 0.5 in Fig. 16. The result shows that the weight factor of conduction electrons $\tilde{\sigma}_{xx}^{\text{hyb}}/\tilde{\Gamma}_{xx}$ shifts to larger values remarkably as $V$ increases while the damping rate of quasiparticles $\tilde{\Gamma}_{xx}^{\text{av}}$ shows no marked enhancement. This can be understood from Eq. (98). Since the renormalized damping rate is expressed as multiplication of the renormalization factor $z$ and the f-electron weight factor $\bar{\sigma}_{xx}^{\text{hyb}}$, as $V$ increases, increase in $z$ and decrease in $\bar{\sigma}_{xx}^{\text{hyb}}$ causes cancellation, giving rise to no remarkable enhancement of $\tilde{\Gamma}_{xx}$. On the other hand, $\tilde{\sigma}_{xy}^{\text{av}}/\tilde{\Gamma}_{xx}$ increases as $V$ increases since the weight of conduction electrons at the Fermi level increases by $c$-$f$ hybridization as understandable from Eq. (91). Hence, it turns out that hybridization makes $\tilde{\sigma}_{xy}^{\text{hyb}}/\tilde{\Gamma}_{xx}$ increase, which results in increase in $\sigma_{xx}$ in Fig. 15.

As for the Hall conductivity, the $\epsilon_f$ dependence of $\sigma_{xy}/H$ for $V = 0.3$ (solid line), 0.4 (dashed line), and 0.5 (dash-dotted line) with $\Gamma = 10^{-3}$ is shown in Fig. 17, which is calculated in the $N = 1200 \times 1200$ lattice sites. As $V$ increases,
Fig. 16. (Color online) The $\epsilon_f$ dependence of the conduction-electron weight factor $\langle \tilde{\gamma}^c_{k_0} \rangle_{av}$ (dashed line, right axis) and the imaginary part of the selfenergy $\tilde{\Gamma}^c_{k_0}$ (solid line, left axis) for $V = 0.3$, 0.4 and 0.5 at $t = 1$, $U = \infty$, $\bar{n} = 7/4$ with $\Gamma = 10^{-3}$ calculated in the $N = 1200 \times 1200$ lattice.

Fig. 17. (Color online) The $\epsilon_f$ dependence of the Hall conductivity for $V = 0.3$ (solid line), 0.4 (dashed line) and 0.5 (dash-dotted line) at $t = 1$, $U = \infty$, $\bar{n} = 7/4$ with $\Gamma = 10^{-3}$ calculated in the $N = 1200 \times 1200$ lattice.

$\sigma_{xy}/H$ shifts to larger values, similarly to the case of $\sigma_{xx}$. This can be understood from Eq. (106). As analyzed below Eq. (106), main contribution to $\sigma_{xy}/H$ comes from $(\tilde{\gamma}^c_{k_0}/\tilde{\gamma}^c_{k})^2$ at the Fermi level. As shown in Fig. 16, $\tilde{\gamma}^c_{k_0}/\tilde{\Gamma}^c_{k}$ increases as $V$ increases, which causes increase in $\sigma_{xy}/H$.

In Fig. 18, we plot the $\epsilon_f$ dependence of the Hall coefficient $R_H$ for a series of hybridization strength: $V = 0.3$ (solid line), $V = 0.4$ (dashed line), and $V = 0.5$ (dash-dotted line) with $\Gamma = 10^{-3}$, which are calculated in the $N = 1200 \times 1200$ lattice sites. The result shows that even in the cases of $V = 0.4$ and $V = 0.5$ with increased hybridizations, the $\epsilon_f$ dependence of $R_H$ remains almost the same as that for $V = 0.3$. This is because the factors $\tilde{\gamma}^c_{k_0}/\tilde{\Gamma}^c_{k}$ in $\sigma_{xx}$ and $\sigma_{xy}/H$ are canceled out each other in the expression of $R_H = \frac{\sigma_{xy}}{\sigma^2_{xx}}$, as discussed in Sect. 4.2.4. This can be also understood from the results shown in Fig. 14. When $V$ increases, the hybridization gap $\Delta_{\text{hyb}}$ increases while $\langle \tilde{\Gamma}^c_{k_0} \rangle_{av}$ shows minor change as shown in Fig. 16. Hence, the ratio $\langle \tilde{\Gamma}^c_{k_0} \rangle_{av}/\Delta_{\text{hyb}}$ decreases. Then, the larger $V$ makes the treatment of the small $\tilde{\Gamma}^c_{k}$ works better in the calculations of $\sigma_{xx}, \sigma_{xy}/H$, and $R_H$, which reproduces the almost constant $\epsilon_f$ dependence of $R_H$.

In the Ce-based compounds, applying pressure makes $\epsilon_f$ and $V$ increase in general. From the results shown in Figs. 4 and 13, and Figs. 7 and 15, $\sigma_{xx}$ and $\sigma_{xy}/H$ show gradual increase in the Kondo (deep-$\epsilon_f$) regime and sharp increase in the valence-fluctuation (shallow-$\epsilon_f$) regime as pressure increases. On the other hand, from the results shown in Figs. 8 and 16, almost unchanged $R_H$ appears irrespective of the Kondo or valence-fluctuation regime under pressure as far as the system stays in the Fermi liquid. Hence, frequently observed behavior in the Ce-based compounds where the residual resistivity decreases gradually in the Kondo regime and drops sharply in the valence-fluctuation regime as pressure increases is naturally explained by the mechanism shown here.

In the Yb-based compounds, on the other hand, applying pressure makes $V$ increase while $\epsilon_f$ in the hole picture decrease in general. Hence, pressure dependence of $\sigma_{xx}$ and $\sigma_{xy}/H$ depends on which factor is more effective. In case that the residual resistivity increases sharply in the valence-fluctuation regime and changes to the monotonic increase in the Kondo regime as pressure increases, it indicates that the effect of the $\epsilon_f$ dependence gives major contribution. In case that both effects of decreasing $\epsilon_f$ and increasing $V$ are canceled each other, almost unchanged $\sigma_{xx}$ and $\sigma_{xy}/H$ as well as $R_H$ are expected to appear under pressure.

5. Summary

We have derived exact formulas for $\sigma_{xx}$ and $\sigma_{xy}$ in the periodic Anderson model for $U = 0$, which give general expressions of the conductivities in the two-orbital systems with arbitrary band dispersions for $T = 0$ as well as finite temperatures. On the basis of the theoretical framework for the Fermi liquid based on these formulas, we have studied the groundstate properties of the diagonal and Hall conductivities and

\[ \sigma_{xy}/H = C \langle \tilde{\gamma}^c_{k_0}/\tilde{\Gamma}^c_{k} \rangle \]

\[ \sigma_{xx} = C \langle \tilde{\gamma}^c_{k_0}/\tilde{\Gamma}^c_{k} \rangle \]
the Hall coefficient in the periodic Anderson model with electron correlations on the square lattice, taking into account the effect of the weak local impurity scattering. The results obtained for the typical case where the Fermi level is located at the lower-hybridized band for the filling of $1 \leq n < 2$ with the small damping rate are summarized as follows:

In the deep-$\epsilon_f$ region where $n_{\text{f}} \geq 0.8$, i.e., the Kondo regime, almost constant-$\epsilon_f$ dependence of $\sigma_{xx}$ and $\sigma_{xy}/H$ appears as a result of the cancellation of the mass renormalization factors. On the other hand, in the shallow-$\epsilon_f$ region, i.e., the valence-fluctuation regime with $n_{\text{f}} \leq 0.8$, a sharp increase in $\sigma_{xx}$ and $\sigma_{xy}/H$ appears as $\epsilon_f$ increases. This is because the cancellation of the renormalization factors does not occur in the valence-fluctuation regime where the conduction-electron weight factor rapidly increases as $\epsilon_f$ increases while the $f$-electron damping rate remains to be suppressed.

On the contrary, the Hall coefficient $R_{xy}$ shows an almost constant $\epsilon_f$ dependence in the shallow-$\epsilon_f$ region as well as in the deep-$\epsilon_f$ region. This is because the renormalization factors expressed as the ratio of the conduction-electron weight factor to the damping rate for $f$ electrons completely cancel out in the expression of $R_{xy}$. It is shown that $R_{xy}$ is expressed as $\frac{1}{n_{\text{hole}}} \approx 2 \bar{n}$ as $\bar{n}$ approaches the half filling, $\bar{n} = 2$, while $R_{xy}$ approaches zero as $\bar{n}$ approaches the quarter filling, $\bar{n} = 1$. The reason is shown to be naturally understood from the curvatures of the Fermi surface.

We confirmed that the above conclusions hold at least for the small damping rate for $f$ electrons where it is less than about 10% of the hybridization gap, which roughly corresponds to the Kondo temperature. It is also confirmed that for the small damping rate the $c$-$f$ hybridization dependence gives minor effects on the $\epsilon_f$ dependence of $R_{xy}$.

In this paper, we have concentrated on the ground-state properties of the typical periodic Anderson model for the Fermi liquid. Theoretically, it has been shown that the magnetically ordered phase generally appears in the deep-$\epsilon_f$ region with $n_{\text{f}}$ being close to 1 in Eq. (1) if the counter effects such as the magnetic frustration are irrelevant. In the systems where the inter-orbital Coulomb repulsion between the $f$ electron and the conduction electron which contributes to the energy band located at the Fermi level has a certain magnitude, the quantum critical point (QCP) of the valence transition appears in the ground-state phase diagram. As the magnitude of the $c$-$f$ hybridization decreases, the QCP of the magnetic transition approaches the QCP of the valence transition and finally coincide each other where the enhanced critical valence fluctuation suppresses the magnetic order giving rise to the first-order magnetic transition.

When we discuss the transport properties near the QCP of the phase transition such as the valence transition, the magnetic transition, the magnetic fluctuation and the critical valence fluctuation should be taken into account. Indeed, it was shown theoretically that near the QCP of the valence transition in the dirty system, the residual resistivity is enhanced considerably, which explains the measurements in the CeCu$_2$Ge$_2$, CeCu$_2$Si$_2$, and CeCu$_2$(Si$_{1-x}$Ge$_x$)$_2$ systems. Hence, when the system approaches the QCP, such effects of the critical fluctuations give rise to additional effects on the results presented in this paper.

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Appendix: Renormalization factors in conductivity

In this Appendix, we show that the theoretical framework in Sect. 4.1 gives essentially the same analytic structure of the conductivity formulated on the basis of the Fermi-liquid theory in Sect. 2. While we consider the case of $\epsilon_{k}^f = \epsilon_f$ and $V_{k} = V$ in Eq. (1) as discussed in Sect. 4.1. Let us start with the first line of Eq. (16):

$$\sigma_{xx}^{(1)} = \frac{2e^2}{V_0} \sum_{\mathbf{k}} \int_{-\infty}^\infty \frac{d\epsilon}{\pi} \left( \frac{\partial f(\epsilon)}{\partial \epsilon} \right) \left| G_{\mathbf{k}}^{\text{eff}}(\epsilon) \right|^2 v_{\mathbf{k}}(\epsilon) J_\mathbf{k}(\epsilon).$$

For $\Gamma_{\mathbf{k}}^{f} \ll T$, $\left| G_{\mathbf{k}}^{\text{eff}}(\epsilon) \right|^2$ is evaluated as

$$\left| G_{\mathbf{k}}^{\text{eff}}(\epsilon) \right|^2 \approx 2\pi i \left( \frac{\sigma_{xx}}{\Gamma_{\mathbf{k}}^{f}} \right)^2 \frac{\delta(\epsilon - E_{\mathbf{k}}^{xx})}{i\Gamma_{\mathbf{k}}^{f}}.$$  \hspace{1cm} (A.2)

When the vertex correction in the total current is ignored in Eq. (21), the current is given by $J_{\mathbf{k}}(\epsilon) = v_{\mathbf{k}}(\epsilon)$. Then Eq. (A.1) leads to

$$\sigma_{xx}^{(1)} = \frac{e^2}{V_0} \sum_{\mathbf{k}} \left( \frac{\partial f(E_{\mathbf{k}}^{xx})}{\partial E_{\mathbf{k}}^{xx}} \right) \left( \frac{\sigma_{xx}}{\Gamma_{\mathbf{k}}^{f}} \right)^2 \left| v_{\mathbf{k}}(E_{\mathbf{k}}^{xx}) \right|^2.$$  \hspace{1cm} (A.3)

By using Eq. (11) and Eq. (17), the relation $\left( \frac{\sigma_{xx}}{\Gamma_{\mathbf{k}}^{f}} \right)^2 \left| v_{\mathbf{k}}(E_{\mathbf{k}}^{xx}) \right|^2 = \left( \alpha_{\mathbf{k}}^{xx} \right)^2 v_{\mathbf{k}}^{0,2}$ holds. Hence, at sufficiently-low temperatures, $T \approx 0$, Eq. (A.3) is expressed as

$$\sigma_{xx}^{(1)} = \frac{e^2}{V_0} \sum_{\mathbf{k}} \delta(E_{\mathbf{k}}^{xx} - \mu) \left( \frac{\sigma_{xx}}{\Gamma_{\mathbf{k}}^{f}} \right)^2 \left| v_{\mathbf{k}}^{0,2} \right|^2.$$  \hspace{1cm} (A.4)

Since the factor $\left( \frac{\sigma_{xx}}{\Gamma_{\mathbf{k}}^{f}} \right)^{-1}$ arises from the delta function, $\delta(E_{\mathbf{k}}^{xx} - \mu)$ [see Eq. (101)], the factor $\frac{\sigma_{xx}}{\Gamma_{\mathbf{k}}^{f}}$ finally appears in Eq. (A.4). This is the same as Eq. (101). This confirms the validity of the framework described in Sect. 4.1.

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