Many-body effects on the resistivity of a multiorbital system
beyond Landau’s Fermi-liquid theory

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I review many-body effects on the resistivity of a multiorbital system beyond Landau’s Fermi-liquid (FL) theory. Landau’s FL theory succeeds in describing electronic properties of some correlated electron systems at low temperatures. However, the behaviors deviating from the temperature dependence in the FL, non-FL-like behaviors, emerge near a magnetic quantum-critical point. These indicate the importance of many-body effects beyond Landau’s FL theory. Those effects in multiorbital systems have been little understood, although their understanding is important to deduce ubiquitous properties of correlated electron systems and characteristic properties of multiorbital systems. To improve this situation, I formulate the resistivity of a multiorbital Hubbard model using the extended Eliashberg theory and adopt this method to the inplane resistivity of quasi-two-dimensional paramagnetic ruthenates in combination with the fluctuation-exchange approximation including the current vertex corrections arising from the self-energy and Maki-Thompson four-point vertex function. The results away from and near the antiferromagnetic quantum-critical point reproduce the temperature dependence observed in Sr$_2$RuO$_4$ and Sr$_2$Ru$_{0.975}$Ti$_{0.025}$O$_4$, respectively. I highlight the importance of not only the momentum and the temperature dependence of the damping of a quasiparticle but also its orbital dependence in discussing the resistivity of correlated electron systems.

Keywords: many-body effects; non-Fermi-liquid-like behaviors; ruthenates; $t_{2g}$ orbital; nearly magnetic metal; fluctuation-exchange approximation; current vertex correction.

1. Introduction

Landau’s Fermi-liquid (FL) theory can describe electronic properties of some correlated electron systems at low temperatures. In this theory, low-energy excitations are described by quasiparticles (QPs), i.e. electrons in a self-consistent field of surrounding electrons due to electron correlation. Also, the interactions between QPs, described by the Landau parameters, are independent of temperature. Due to these two properties, the temperature dependence of physical quantities in low-$T$ region are governed by the temperature dependence of the Fermi distribution function, and the corrections due to electron correlation, the mass enhancement and the FL correction, are independent of temperature. As a result, thermodynamic or magnetic or transport quantities show the same temperature dependence as those of the free electron system in low-$T$ region, and the difference is the coefficient due
to the mass enhancement or the FL correction or both. For example, the specific heat is proportional to $T$, and the coefficient is renormalized by the mass enhancement; the spin susceptibility is independent of temperature, and the coefficient is renormalized by the mass enhancement and the FL correction.

The original Landau phenomenological theory can be justified by microscopic perturbation theory with several imposed conditions. One of the basic assumptions, the one-to-one correspondence, becomes valid if the QP damping is much smaller than temperature considered (i.e., the QP lifetime, the inverse of the QP damping, is very long). Actually, the single-particle spectral function near the Fermi level becomes delta-function-type in the coherent limit \[ \gamma_*^{\alpha}(k)/T \to 0 \text{ for all Fermi momenta}, \]

Here we consider only the coherent part, \[ G_\alpha^{(R)}(k) = z_\alpha^{\alpha}(k) \frac{\gamma_*^{\alpha}(k)}{[\epsilon - \xi_*^{\alpha}(k)]^2 + \gamma_*^{\alpha}(k)^2} \to z_\alpha^{\alpha}(k) \delta(\epsilon - \xi_*^{\alpha}(k)). \] (1)

In addition, the other basic assumption about the Landau parameters becomes valid if the reducible four-point vertex functions and mass enhancement factor are independent of temperature. Note, first, that the Landau parameter is proportional to the product of the reducible four-point vertex function and the square root of the four mass enhancement factors; second, that the four-point vertex function describes the multiple scattering of an electron and a hole; third, that all reducible diagrams can be split into two parts by removing a pair of the retarded and advanced single-particle Green’s functions, while all irreducible diagrams cannot be done by using that removing.

In contrast to successful description in the paramagnetic (PM) phase of Sr$_2$RuO$_4$, Landau’s FL theory fails in describing electronic properties of other PM ruthenates near a magnetic quantum-critical point (QCP). For example, in Sr$_2$Ru$_{0.075}$Ti$_{0.025}$O$_4$, located near an antiferromagnetic (AF) QCP, the spin susceptibility shows the Curie-Weiss-like temperature dependence and the in-plane resistivity, $\rho_{ab}$, shows the $T$-linear dependence, deviating from the FL-type $T^2$ dependence; the characteristic wave vectors of this AF QCP, $Q_{IC-AF} = (\frac{2\pi}{3}, \frac{2\pi}{3})$ and its symmetrically equivalent ones, are the same as the wave vectors of the most strongly enhanced spin fluctuation in Sr$_2$RuO$_4$. Also, in Ca$_{2-x}$Sr$_x$RuO$_4$ around $x = 0.5$, located near a ferromagnetic QCP, the Curie-Weiss-like temperature
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dependence of the spin susceptibility and $T^{1.4}$ dependence of $\rho_{ab}$ are observed.\cite{12}

Since such non-FL-like behaviors are observed in other systems near a magnetic QCP\cite{13} or a Mott transition\cite{14}, where many-body effects generally become very important, these experimental facts indicate the necessity of both considering how the basic assumptions of Landau’s FL theory are violated and discussing many-body effects beyond Landau’s FL theory in a more elaborate theory.

So far, there are two candidates for the origin of such non-FL-like behaviors.

One is bad metal\cite{15,16} due to local correlation enhanced near a Mott transition. If the low-energy excitations can be satisfactorily described by using only low-order Taylor series of the self-energy in terms of frequency, the coherent part of the single-particle Green’s function plays dominant roles in discussing electronic properties. However, if there are some non-negligible contributions from the higher-order Taylor series, the incoherent part also becomes important. Such case is realized in a PM metallic phase near the Mott transition due to the formation of the upper and lower Hubbard peaks, arising from enhanced local correlation\cite{17,18}. Since perturbation theory can treat the coherent part appropriately and its treatment of the incoherent part is insufficient,\cite{17} perturbation theory is unsuitable in the latter case. Instead, the latter case can be well described in dynamical-mean-field theory (DMFT) since the DMFT can take account of the frequency dependence of the self-energy nonperturbatively.\cite{15,16} Actually, several non-FL-like behaviors are obtained in the DMFT near the Mott transition as a result of the $T$-linear unrenormalized QP damping and the temperature-dependent mass enhancement factor\cite{20,21}. [In this paper, I define the unrenormalized QP damping as the QP damping divided by the mass enhancement factor.] These results indicate the importance of nonperturbative effects of local correlation near the Mott transition.

Note that Hund’s metal\cite{22,23} is classified as the bad metal since the non-FL-like behaviors in the Hund’s metal arise from local spin fluctuation enhanced near a Mott transition, although there is a crucial difference between the Hund’s rule coupling dependence of the critical value of the intraorbital Coulomb interaction for the Mott transition at half-filling and non-half-filling\cite{23}.

The other is nearly magnetic metal\cite{24,25,26,27} due to spatial correlation enhanced near a magnetic QCP. If a system is located far away from a magnetic QCP, all scattering processes are independent of temperature. However, if the system approaches the QCP, several characteristic scattering processes of the QCP show the strong temperature-dependent enhancement\cite{28}. For example, in case near a stripe-type AF QCP the scattering processes mediated by AF spin fluctuations with $q = (\pi, \pi)$ and its symmetrically equivalent ones are strongly enhanced as decreasing temperature.\cite{28} Such strong temperature-dependent enhancement leads to the strong temperature dependence of the reducible four-point vertex function whose momentum is characterized by the QCP. Thus, the basic assumption of Landau’s FL theory about the Landau parameters is violated only for the characteristic momenta of spin fluctuation enhanced near the QCP\cite{28}. Also, the basic assump-
tion about the QP damping is violated for the characteristic momenta due to the formation of hot spot, arising from enhanced spin fluctuation; at the hot spot, the QP damping does not become much smaller than temperature considered. For example, in case near the stripe-type AF QCP, the QP dampings at the momenta connected by the nesting vector \( q = (\pi, \pi) \) and its symmetrically equivalent ones are more strongly enhanced than those at the other momenta due to the enhancement of the corresponding AF spin fluctuations. These two violations suggest the necessity of discussing electronic properties near a magnetic QCP in the microscopic perturbation theory beyond Landau's FL theory. Actually, fluctuation-exchange (FLEX) approximation reproduces several non-FL-like behaviors due to the hot-spot structure of the QP damping or the Curie-Weiss-like temperature dependence of spin fluctuations or both. As explained in Sect. 2.3, this approximation can take account of spatial correlation beyond a mean-field theory and describe electronic properties of a metallic phase at low temperatures for moderately strong electron correlation satisfactorily. In contrast to case near the Mott transition, the DMFT is inappropriate to describe electronic properties near a magnetic QCP since the DMFT neglects spatial correlation completely. These results indicate powerfulness of the microscopic perturbation theory and the importance of temperature-dependent spatial correlation near a magnetic QCP.

With the backgrounds explained above, I studied electronic structure and magnetic and transport properties of some quasi-two-dimensional (quasi-2D) PM ruthenates near and away from the AF QCP in the FLEX approximation with Maki-Thompson (MT) current vertex correction (CVC) for the \( t_{2g} \)-orbital Hubbard model on a square lattice and succeeded in reproducing several experimental results of \( \text{Sr}_2\text{Ru}_{0.075}\text{Ti}_{0.025}\text{O}_4 \) and \( \text{Sr}_2\text{RuO}_4 \). Thus, the non-FL-like behaviors in \( \text{Sr}_2\text{Ru}_{0.075}\text{Ti}_{0.025}\text{O}_4 \) can be understood as the nearly magnetic metal near the AF QCP. Moreover, since the results away from the AF QCP about the orbital dependence of the mass enhancement are in better agreement with the experiment in \( \text{Sr}_2\text{RuO}_4 \) than those of the DMFT, electronic properties of ruthenates at low temperatures except a few cases near the Mott transition may be better described in the microscopic perturbation theory than in the DMFT.

In this paper, I review part of the above previous study and show some new results. In Sect. 2, I explain the microscopic theory used for analyzing \( \rho_{ab} \) of some quasi-two-dimensional (quasi-2D) PM ruthenates. In Sect. 3, I show the results about many-body effects on \( \rho_{ab} \) of the ruthenates near and away from the AF QCP in the FLEX approximation with or without the MT CVC or without all the CVCs. In Sect. 4, I summarize the results and draw some conclusions.

Due to the limit of space, I do not consider the Aslamasov-Larkin (AL) CVC, which is the other CVC in the FLEX approximation; its detailed derivation and effects are going to be discussed elsewhere.
2. Method

In this section, I explain an effective model of some quasi-2D ruthenates, briefly review the formal derivation of the resistivity of a multiorbital Hubbard model in a PM metallic phase, and formulate the microscopic perturbation theory used to calculate the resistivity. The more detailed explanations about those derivation and formulation are going to be given elsewhere.43

In the following, I use the unit $\hbar = c = e = \mu_B = k_B = 1$, set the coordinates $x$, $y$, and $z$ in the directions of the Ru–O bonds of RuO$_6$ octahedra, and label the $d_{xz}$, $d_{yz}$, and $d_{xy}$ orbitals as 1, 2, and 3, respectively.

2.1. Effective model for some quasi-2D ruthenates

I explain an effective model to describe electronic properties of some quasi-2D ruthenates without the rotation or the tilting of RuO$_6$ octahedra.44

Before introducing the effective model, I briefly explain several basic electronic properties. Some ruthenates whose crystal structures are 214-type such as Sr$_2$RuO$_4$ or 327-type such as Sr$_3$Ru$_2$O$_7$ are categorized into quasi-2D $t_{2g}$-orbital systems. For simplicity, we focus on Sr$_2$RuO$_4$; the following properties remain qualitatively the same in other metallic ruthenates.12,45 First, the inplane resistivity is about $10^{-3}$ times as small as the out-of-plane resistivity at low temperatures,46 and the almost cylindrical Fermi surface (FS) is observed in the de Haas–van Alphen measurement.36 These indicate quasi-2D electronic conduction. Moreover, according to several density-functional calculations in local-density approximation (LDA), conducting bands near the Fermi level are formed by the antibonding bands of the Ru $t_{2g}$ and the O $2p$ orbitals, and the $t_{2g}$ orbitals mainly contribute to the density-of-states (DOS) near the Fermi level. Since the topology of the FS obtained in the LDA qualitatively agrees with experiments, the $t_{2g}$ orbitals play dominant roles in discussing electronic properties at low temperatures.

With the above background, I assume that the electronic structure obtained in the LDA for Sr$_2$RuO$_4$ is a good starting point to consider many-body effects beyond a mean-field approximation, and I use a $t_{2g}$-orbital Hubbard model on a square lattice as the effective model. Thus, the Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$ with

$$\hat{H}_0 = \sum_{k} \sum_{a,b=1}^{3} \sum_{s=\uparrow,\downarrow} \epsilon_{ab}(k) \hat{c}^\dagger_{kas} \hat{c}_{kbs},$$

and

$$\hat{H}_{\text{int}} = \frac{1}{4} \sum_{j} \sum_{a,b,c,d=1}^{3} \sum_{s_1,s_2,s_3,s_4=\uparrow,\downarrow} U_{abcd} s_1 s_2 s_3 s_4 \hat{c}^\dagger_{jasa} \hat{c}^\dagger_{jdsb} \hat{c}_{jcsa} \hat{c}_{jbs} + U' \sum_{j} \sum_{a=1}^{3} \sum_{b < a} \hat{n}_{ja} \hat{n}_{jb}$$

$$- J_H \sum_{j} \sum_{a=1}^{3} \sum_{b < a} (2 \hat{s}_{ja} \cdot \hat{s}_{jb} + \frac{1}{2} \hat{n}_{ja} \hat{n}_{jb}) + J' \sum_{j} \sum_{a=1}^{3} \sum_{b \neq a} \hat{c}^\dagger_{ja} \hat{c}^\dagger_{ja} \hat{c}_{jb} \hat{c}_{jb}. \tag{3}$$
where $\epsilon_{ab}(\mathbf{k})$ is the energy dispersions, measuring from the chemical potential, $\mu$, $U$, $U'$, $J_{H}$, and $J'$ are intraorbital Coulomb interaction, interorbital Coulomb interaction, Hund’s rule coupling, and pair hopping term, $\hat{n}_{a} \equiv n_{a} = \sum_{s} \hat{n}_{jas} = \sum_{s} \hat{c}_{jas}^{\dagger} \hat{c}_{jas}$ and $\hat{s}_{ja} = \frac{1}{2} \sum_{s,s'} \epsilon_{jasa}^{\dagger} \sigma_{ss'} \hat{c}_{jas}^{\dagger} \hat{c}_{jas'}$ with the Pauli matrices $\sigma_{ss'}$. Since I do not consider the effects of the rotation and the tilting, we focus on electronic properties of Sr$_{2}$RuO$_{4}$ and some doped Sr$_{2}$RuO$_{4}$ without these distortions. Note that the rotation is present in Ca$_{2-x}$Sr$_{x}$RuO$_{4}$ around $x = 0.144$.

By considering some symmetrically possible hopping processes and the difference between the crystalline-electric-field energies of the $d_{xy}$ and $d_{xz/yz}$ orbitals, $\Delta_{2g}$, we can construct the tight-binding model whose parameters are chosen so as to reproduce the results in the LDA for Sr$_{2}$RuO$_{4}$.

$$\epsilon_{11}(\mathbf{k}) = - \frac{\Delta_{2g}}{3} - 2t_{1} \cos k_{x} - 2t_{2} \cos k_{y} - \mu,$$
$$\epsilon_{12}(\mathbf{k}) = \epsilon_{21}(\mathbf{k}) = 4t' \sin k_{x} \sin k_{y},$$
$$\epsilon_{22}(\mathbf{k}) = - \frac{\Delta_{2g}}{3} - 2t_{2} \cos k_{x} - 2t_{1} \cos k_{y} - \mu,$$
$$\epsilon_{33}(\mathbf{k}) = \frac{2\Delta_{2g}}{3} - 2t_{3}(\cos k_{x} + \cos k_{y}) - 4t_{4} \cos k_{x} \cos k_{y} - \mu,$$

and otherwise $\epsilon_{ab}(\mathbf{k}) = 0$. $\mu$ is chosen so that the electron number per a site, $n_{e}$, is fixed. For the actual calculations, $\mu$ is determined by the bisection method using

$$n_{e} = \frac{2}{N} \sum_{\mathbf{k}} \sum_{\alpha} f(\epsilon_{\alpha}(\mathbf{k})) + \frac{2T}{N} \sum_{\mathbf{k}} \sum_{m} \sum_{a=1}^{3} \left[ G_{aa}(\mathbf{k}, i\omega_{m}) - G_{aa}^{0}(\mathbf{k}, i\omega_{m}) \right].$$

where the second term becomes zero without the interaction terms. Here $\epsilon_{\alpha}(\mathbf{k})$ is

$$\epsilon_{\alpha}(\mathbf{k}) = \sum_{a,b=1}^{3} (U_{k}^{0})_{\alpha a} \epsilon_{ab}(\mathbf{k}) (U_{k}^{0})_{b\alpha},$$

$f(\epsilon)$ is the Fermi distribution function, $G_{ab}(\mathbf{k}, i\omega_{m})$ is the noninteracting single-particle Green’s function with fermionic Matsubara frequency, $\omega_{m} = \pi T (2m + 1)$,

$$G_{ab}^{0}(\mathbf{k}, i\omega_{m}) = \sum_{\alpha} (U_{k}^{0})_{\alpha a} \frac{1}{i\omega_{m} - \epsilon_{a}(\mathbf{k})} (U_{k}^{0})_{b\alpha},$$

and $G_{ab}(\mathbf{k}, i\omega_{m})$ is the single-particle Green’s function whose determination is explained in Sect. 2.3. In Eq. (8), we put the chemical potentials in $f(\epsilon_{\alpha}(\mathbf{k}))$. 

![Fig. 1. (a) Band structure, (b) FS, and (c) DOS for $\hat{H}_{0}$ whose parameters are chosen so as to reproduce the results in the LDA for Sr$_{2}$RuO$_{4}$.](image)
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$G_{aa}(k, i\omega_n)$, and $G_{aa}^0(k, i\omega_n)$ the same to reduce the numerical error arising from the cut-off frequency. To reproduce the electronic structure obtained in the LDA, I set $(t_1, t_2, t_3, t_4, t', \Delta_{t_{2g}}) = (0.675, 0.09, 0.45, 0.18, 0.03, 0.13)$ (eV) and $n_e = 4$. Actually, we see from Fig. 1 that the total bandwidth, the topology of each FS sheet, and the location of the van Hove singularity of the $d_{xy}$ orbital agree with the LDA result. The total bandwidth is about 4 eV; the FS consists of the quasi-1D hole-like $\alpha$ and electron-like $\beta$ sheets of the $d_{xz/yz}$ orbital and the quasi-2D electron-like $\gamma$ sheet of the $d_{xy}$ orbital, and the $\gamma$ sheet is located nearer to the inner sheet in $k_x = k_y$ or $k_x = -k_y$ line than in the experiment; the van Hove singularity is located above the Fermi level. Also, the occupation numbers of the $d_{xz/yz}$ and the $d_{xy}$ orbital, being $n_{xz/yz} = 1.38$ and $n_{xy} = 1.25$, are consistent with the LDA values.

Then, I set $J' = J_H$, $U' = U - 2J_H$, and $J_H = \frac{U}{8}$, use $U$ as a parameter, and treat the effects of interactions in the FLEX approximation with or without the MT CVC or without all the CVCs; its detail is explained in Sect. 2.3.

Finally, we remark on suitability neglecting the spin-orbit coupling of Ru ions for discussing many-body effects on the resistivity. A density-functional calculation for Sr$_2$RuO$_4$ within local-spin-density approximation shows that the coupling constant is 0.167 eV, and that the main effect on the electronic structure is the weak mixing between the bands of the $d_{xz/yz}$ and the $d_{xy}$ orbital around $k = (\frac{2\pi}{3}, \frac{2\pi}{3})$ and its symmetrically equivalent ones. This effect will not qualitatively change the results shown in Sect. 3 since this coupling constant is smaller than the main terms in $\hat{H}$ and that weak mixing will lead to small changes of the momentum dependence and value of the spin susceptibility from those without the spin-orbit coupling. Thus, I think that neglecting the spin-orbit coupling is suitable for qualitative discussions about many-body effects on the resistivity.

2.2. Extended Éliashberg theory for the resistivity of a multiorbital Hubbard model in a PM metallic phase

I briefly review the formal derivation of the resistivity of a multiorbital Hubbard model in a PM metallic phase. We first derive an exact expression of the longitudinal conductivity, the inverse of the resistivity, in the presence of electron correlation within the linear-response theory. Then, we rewrite this exact expression in terms of the four-point vertex function by using the three-point vector vertex function. Due to difficulty solving the exact expression, we derive an approximate expression by using the most-divergent-term approximation introduced by Éliashberg.

To discuss the resistivity within the linear-response theory, we use the Kubo formula for the longitudinal conductivity, $\sigma_{\nu\nu}$ ($\nu = x, y$), in $\omega$-limit and $\omega \tau_{\text{trans}} \ll 1$ with $\tau_{\text{trans}}$ being the transport relaxation time, which is of the order of magni-
K tex function, we can carry out the analytic continuation of the analytic properties of the single-particle Green's function and four-point relaxation compared with ω tdistribution.

For example, such importance of the inequality of ω q distribution. Also, the value of observables due to the screening induced by the modulations of the charge currents can be obtained by the dynamical and uniform field (i.e., lim ω→0). Thus, the analytic continuation of necessary to calculate σ

σνν = 2 lim ω→0 q→0 1 T 0 iω dτ e iωτ (T Jνν (τ) Jνν (0)) = 2 lim ω→0 q→0 1 T 0 iω dτ e iωτ (vνν) T ω k (vνν) cd (T τ k) ε k a ε k c ε k' b ε k' d)

where ˜Kνν (0, ω) is obtained by the analytic continuation of ˜Kνν (iΩ)₂

Kabcd (k, k'; iΩ) = − δk, k' T × Gc (k, iεm+n) Gd (k, iεm)

where Γ (k, iω m, k', iω m'; iΩ) = Γ ABCD (k, iω m, k', iω m; iΩ) is the reducible four-point vertex function. Thus, the analytic continuation of Kabcd (k, k'; iΩ) is necessary to calculate σνν.

Before the analytic continuation of Kabcd (k, k'; iΩ), I remark on the important physical meanings of limω→0 limq→0 and ω τ trans ≪ 1. The order of limω→0 and limq→0 is very important in discussing transport properties since the observable currents can be obtained by the dynamical and uniform field (i.e., limω→0 limq→0) but the static and non-uniform field (i.e., limq→0) does not cause any observable currents due to the screening induced by the modulations of the charge distribution. Also, the value of ω τ trans is very important since the adiabatic condition ω τ trans ≪ 1 means the realization of local equilibrium due to the rapid relaxation compared with ω−1, a typical time scale of the field; as a result of that relaxation, the electronic transports are governed mainly by the QPs near the Fermi level. For example, such importance of the inequality of ω τ trans is seen from the difference between the zero and the first sound.

Replacing T ∑m and T² ∑m,m' in Eq. (13) by the corresponding contour integrals and doing several straightforward calculations with attention to the analytic properties of the single-particle Green’s function and four-point vertex function, we can carry out the analytic continuation of Kabcd (k, k'; iΩ). As a
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result, \( \tilde{\rho}_{\nu\nu}^{(R)}(0, \omega) \) is given by

\[
\tilde{\rho}_{\nu\nu}^{(R)}(0, \omega) = -\frac{1}{N} \sum_{k, k'} \sum_{\{a\}} \langle v_{kA}\rangle \langle v_{k'A}\rangle_{cd} \times \int_{-\infty}^{\infty} \frac{d\epsilon}{4\pi i} \left[ \tanh \frac{\epsilon}{2T} K_{1;abcd}^{(R)}(k, k'; \epsilon; \omega) \\
+ \left( \tanh \frac{\epsilon + \omega}{2T} - \tanh \frac{\epsilon}{2T} \right) K_{2;abcd}^{(R)}(k, k'; \epsilon; \omega) \\
- \tanh \frac{\epsilon + \omega}{2T} K_{3;abcd}^{(R)}(k, k'; \epsilon; \omega) \right],
\]

where \( K_{l;abcd}^{(R)}(k, k'; \epsilon; \omega) \) is

\[
K_{l;abcd}^{(R)}(k, k'; \epsilon; \omega) = g_{l;acdb}(k; \omega) \delta_{k,k'} + \int_{-\infty}^{\infty} \frac{d\epsilon'}{4\pi i} \sum_{\{A\}} \sum_{\{A'\}} g_{l;aABb}(k; \omega) \times J_{l';\{A\}}(k, k'; \omega) g_{l';CBdD}(k'; \omega),
\]

with \( g_{l;acdb}(k; \omega) \) being

\[
g_{1;acdb}(k; \omega) = \Gamma_{11;\{A\}}(k, k'; \omega),
\]

and

\[
g_{3;acdb}(k; \omega) = \Gamma_{13;\{A\}}(k, k'; \omega),
\]

and \( J_{l';\{A\}}(k, k'; \omega) \) being

\[
J_{11;\{A\}}(k, k'; \omega) = \tanh \frac{\epsilon'}{2T} \Gamma_{11;\{A\}}(k, k'; \omega) + \coth \frac{\epsilon' - \epsilon}{2T} \left[ \Gamma_{11;\{A\}}(k, k'; \omega) - \Gamma_{11;\{A\}}(k, k'; \omega) \right],
\]

\[
J_{12;\{A\}}(k, k'; \omega) = \left( \tanh \frac{\epsilon + \omega}{2T} - \tanh \frac{\epsilon'}{2T} \right) \Gamma_{12;\{A\}}(k, k'; \omega),
\]

\[
J_{13;\{A\}}(k, k'; \omega) = -\tanh \frac{\epsilon + \omega}{2T} \Gamma_{13;\{A\}}(k, k'; \omega) - \coth \frac{\epsilon + \epsilon'}{2T} \left[ \Gamma_{13;\{A\}}(k, k'; \omega) - \Gamma_{13;\{A\}}(k, k'; \omega) \right],
\]

\[
J_{21;\{A\}}(k, k'; \omega) = \tanh \frac{\epsilon'}{2T} \Gamma_{21;\{A\}}(k, k'; \omega),
\]

\[
J_{22;\{A\}}(k, k'; \omega) = \left( \coth \frac{\epsilon' - \epsilon}{2T} - \tanh \frac{\epsilon'}{2T} \right) \Gamma_{22;\{A\}}(k, k'; \omega) + \left( \coth \frac{\epsilon + \epsilon'}{2T} - \coth \frac{\epsilon' - \epsilon}{2T} \right) \Gamma_{22;\{A\}}(k, k'; \omega) + \left( \tanh \frac{\epsilon' + \epsilon}{2T} - \coth \frac{\epsilon' + \epsilon}{2T} \right) \Gamma_{22;\{A\}}(k, k'; \omega),
\]

\[
J_{23;\{A\}}(k, k'; \omega) = -\tanh \frac{\epsilon + \omega}{2T} \Gamma_{23;\{A\}}(k, k'; \omega),
\]
Fig. 2. The connection between the additional subscripts of the four-point vertex function and the relations among \((\epsilon', \epsilon'', \omega)\) of that function.

\[
J_{31;\{A\}}(k, k'; \omega) = \tanh \frac{\epsilon'}{2T} \Gamma_{31-I;\{A\}}(k, k'; \omega) \\
+ \coth \frac{\epsilon + \epsilon' + \omega}{2T} \left[ \Gamma_{31-II;\{A\}}(k, k'; \omega) - \Gamma_{31-I;\{A\}}(k, k'; \omega) \right], 
\]

(25)

\[
J_{32;\{A\}}(k, k'; \omega) = \left( \tanh \frac{\epsilon' + \omega}{2T} - \tanh \frac{\epsilon'}{2T} \right) \Gamma_{32;\{A\}}(k, k'; \omega), 
\]

(26)

and

\[
J_{33;\{A\}}(k, k'; \omega) = - \tanh \frac{\epsilon' + \omega}{2T} \Gamma_{33-I;\{A\}}(k, k'; \omega) \\
- \coth \frac{\epsilon' - \epsilon}{2T} \left[ \Gamma_{33-II;\{A\}}(k, k'; \omega) - \Gamma_{33-I;\{A\}}(k, k'; \omega) \right]. 
\]

(27)

In Eq. (15), I have not explicitly written whether the frequency integral is the principal integral or not; the integrals containing hyperbolic cotangent are the principal ones. Also, in Eqs. (19)–(27) the additional subscript of the four-point vertex function such as 12 represents the relations among its three frequency variables, as shown in Fig. 2. Since \(J_{W';\{a\}}(k, k'; \omega)\) is determined by the Bethe-Salpeter equation,

\[
J_{W';\{a\}}(k, k'; \omega) = J_{W;\{a\}}(k, k'; \omega) + \sum_{l''=1}^{3} \frac{1}{N} \sum_{l''} \sum_{\{A\}} \int_{-\infty}^{\infty} \frac{d\epsilon''}{2\pi T} J_{W'';\{a\}}(k, k''; \omega) \\
\times g_{l'';ABCD}(k'', \omega) J_{W';\{a\}}^{(1)}(k'', k'; \omega), 
\]

(28)

and \(J_{W';\{a\}}^{(1)}(k, k'; \omega)\) is obtained by the method explained in Sect. 2.3, we can exactly calculate \(\sigma_{\nu\nu}\) from Eqs. (11), and (14)–(28) in principle.

Then, to rewrite Eq. (14) in a more compact form, we use the three-point vector vertex function instead of the four-point vertex function. The three-point vertex function in Matsubara-frequency representation is defined as

\[
\sum_{A,B} G_{AA}(k + q, i\epsilon_{m+n}) A_{\nu;AB}(k, i\epsilon_{m}; q, i\epsilon_{n}) G_{BB}(k, i\epsilon_{m}) \\
= \int_{0}^{T-1} d\tau e^{i\epsilon_{m+n}\tau} \int_{0}^{T-1} d\tau' e^{-i\epsilon_{m}\tau'} \langle T_{\nu} \hat{c}_{k+q}(\tau) \hat{J}_{-q\nu}(\tau') \hat{c}_{k}^{\dagger} \rangle. 
\]

(29)
Since the analytic continuation of the three-point vertex function can be carried out\cite{14} in a similar way to that used for $K_{abcd}(k, k'; i\Omega)$, we obtain the three-point vector vertex function in real-frequency representation,

$$\Lambda_{\nu;1;cd}(k; q) = \langle v_{k\nu} \rangle_{ab} + \frac{1}{N} \sum_k \sum_{(A)} \sum_{l=1}^{3} \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}J_{ll'}^{(A)}(k; k'; q)$$

$$\times g_{l';CA\nu}(k'; q)(v_{k\nu})_{AB}.$$ \hspace{1cm} (30)

Here the additional subscript of the three-point vector vertex function, $l$, denotes the conditions about its $\epsilon$ and $\omega$: $l = 1$ denotes $\text{Im}\epsilon > 0$ and $\text{Im}\epsilon + \text{Im}\omega > 0$; $l = 2$ denotes $\text{Im}\epsilon < 0$ and $\text{Im}\epsilon + \text{Im}\omega > 0$; $l = 3$ denotes $\text{Im}\epsilon < 0$ and $\text{Im}\epsilon + \text{Im}\omega < 0$. Combining Eqs. (11) and (15) with Eq. (30), we can rewrite $\tilde{K}_{\nu\nu}^{(R)}(0, \omega)$ as

$$\tilde{K}_{\nu\nu}^{(R)}(0, \omega) = -\frac{1}{N} \sum_k \sum_{(A)} \langle v_{k\nu} \rangle_{ba} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi}$$

$$\times \left[ \tanh \frac{\epsilon}{2T} g_{1;1;cd}(k; \omega)\Lambda_{\nu;1;cd}(k; \omega)$$

$$+ \left( \tanh \frac{\epsilon + \omega}{2T} - \tanh \frac{\epsilon}{2T} \right) g_{2;1;cd}(k; \omega)\Lambda_{\nu;2;cd}(k; \omega)$$

$$- \tanh \frac{\epsilon + \omega}{2T} g_{3;1;cd}(k; \omega)\Lambda_{\nu;3;cd}(k; \omega) \right].$$ \hspace{1cm} (31)

Since the exact expression is difficult to solve, we use the most-divergent-term approximation\cite{20} based on the properties\cite{20} of the product of the single-particle Green’s functions in the limit $q \equiv (\mathbf{q}, \omega) \to 0$ in the presence of the QP peak. This is correct in the FL and remains appropriate in a correlated metallic system where perturbation expansion is satisfactory. As explained in Sect. 1, applicability of the FL theory differs from that of a microscopic perturbation theory. The microscopic perturbation theory is satisfactory to describe electronic properties of a correlated electron system if perturbation expansion has a good convergence or becomes an asymptotic expansion. Let us recall, first, that a well approximate partial sum can be constructed even if its convergence is not good; second, that perturbation expansion becomes an asymptotic expansion near a phase transition.

Before proceeding with the formal derivation of $\sigma_{\nu\nu}$, we remark on the property\cite{20} of a pair of the single-particle Green’s functions in the limit $q \to 0$. When the QP peak exists and the QP damping is much smaller than $T$ (i.e., cold-spot-type), only $G_{\nu\nu}^{(R)}(k + \frac{\mathbf{q}}{2}, \mathbf{q} + \frac{\mathbf{q}}{2})G_{\nu\nu}^{(A)}(k - \frac{\mathbf{q}}{2}, \mathbf{q} - \frac{\mathbf{q}}{2})$ gives the most singular term being inversely proportional to the QP damping due to the merging of the poles of these Green’s functions in $q \to 0$; the others, the retarded-retarded and the advanced-advanced pair, become the higher order terms. In this discussion, we have considered only the contribution from the coherent part of the single-particle Green’s function since the incoherent part does not lead to such singular term in $q \to 0$. Also, I have used $\lim_{x \to a^+} \frac{1}{x - a^+} = \lim_{x \to a^+} \frac{1}{2} = -2\pi i \delta(x - a)$ since the QP damping at momenta near the Fermi level is assumed to be negligible at low temperatures. The singular contribution from the hot spot is less important than that from the cold spot since the QP damping at the hot spot remains non-negligible.
even on the Fermi level. Since the existence of the QP peak and cold-spot-type QP damping is appropriate at least for several momenta in a metallic phase near a magnetic QCP[57] or a Mott transition,[58] the leading terms in \( g_{1;acdb}(k;\omega) \) with respect to the QP damping or \( \omega \) at low temperatures and frequencies are given by

\[
g_{1;acdb}(k;\omega) \sim \sum_{\alpha,\beta} u_{ac;db}(k) \frac{z_\alpha(k)z_\beta(k)}{\epsilon - \xi_\alpha^*(k) + i0+|\epsilon - \xi_\beta^*(k) + i0+|},
\]

(32)

and

\[
g_{2;acdb}(k;\omega) \sim 2\pi i \sum_{\alpha,\beta} u_{ac;db}(k) \frac{z_\alpha(k)z_\beta(k)\delta(\epsilon - \xi_\alpha^*(k))}{\omega - \xi_\alpha^*(k) + \xi_\beta^*(k) + i[\gamma_\alpha^*(k) + \gamma_\beta^*(k)]},
\]

(33)

where \( u_{ac;db}(k) = (U_k)_{ac}(U_k^\dagger)_{db}(U_k^\dagger)_{\beta\alpha} \) with \( (U_k)_{aa} \) being the unitary matrix to obtain the QP bands [not equal to \( (U_k^\dagger)_{aa} \)]. Thus, the most divergent terms in the coherent limit arise from \( g_{2;acdb}(k;\omega) \) at cold spots.

Using the above property, we obtain an approximate expression of \( \sigma_{\nu\nu} \) where we consider only the most divergent terms with respect to the QP damping in the coherent limit. To use the most-divergent-term approximation,[53] we introduce two quantities, \( J_{\nu l';\{a\}}^{(0)}(k, k'; \omega) \) and \( \Lambda_{\nu l';\{a\}}^{(0)}(k; \omega) \), which are irreducible with respect to only a retarded-advanced pair of the single-particle Green’s functions,

\[
J_{\nu l';\{a\}}^{(0)}(k, k'; \omega) = J_{\nu l';\{a\}}^{(1)}(k, k'; \omega) + \sum_{l'' \neq 2} \frac{1}{N} \sum_{k''} \sum_{\{A\}} \int_{-\infty}^{\infty} \frac{d\nu''}{2\pi i} J_{\nu l'';ab}^{(0)}(k, k''; \omega)
\times g_{\nu'';CABD}(k'', \omega) J_{\nu l';ABCD}(k'', k', \omega),
\]

(35)

and

\[
\Lambda_{\nu l';\{a\}}^{(0)}(k; \omega) = (v_{\nu l'})_{ab} + \sum_{\{A\}} \frac{1}{N} \sum_{k''} \int_{-\infty}^{\infty} \frac{d\nu''}{2\pi i} J_{\nu l'';ab}^{(0)}(k, k''; \omega)
\times g_{\nu'';CABD}(k'', \omega) (v_{\nu l'})_{AB}.
\]

(36)

Using these two quantities with Eqs. (20), (22), (24) and (26) and the exchange symmetry of the four-point vertex function among its momentum and frequency variables, we can rewrite Eq. (31) as

\[
\tilde{K}_{\nu\nu}^{(R)}(0, \omega) = -\frac{1}{N} \sum_k \sum_{\{a\}} (v_{\nu l'})_{ba} \int_{-\infty}^{\infty} \frac{d\epsilon}{4\pi i} \left[ \tanh \frac{\epsilon}{2T} g_{1;acdb}(k;\omega) \Lambda_{\nu l';1;cd}^{(0)}(k;\omega)
\right.
\]

\[
-\tanh \frac{\epsilon + \omega}{2T} \Lambda_{\nu l';2;cd}^{(0)}(k;\omega)
\left. - \frac{1}{N} \sum_k \sum_{\{a\}} \Lambda_{\nu l';3;cd}^{(0)}(k;\omega) \int_{-\infty}^{\infty} \frac{d\epsilon}{4\pi i} \left( \tanh \frac{\epsilon + \omega}{2T} - \tanh \frac{\epsilon}{2T} \right) \right]
\times g_{2;acdb}(k;\omega) \Lambda_{\nu l';2;cd}^{(0)}(k;\omega).
\]

(37)

At this stage, this expression remains exact. Then, since only the second term in Eq. (37) contains a retarded-advanced pair and the leading term with respect to
\[ \omega \text{ comes from } (\tanh \frac{\epsilon - \omega}{2T} - \tanh \frac{\epsilon}{2T}) \approx \frac{2\omega}{\beta} (\frac{\partial f(\epsilon)}{\partial \epsilon}), \] we can obtain an approximate expression of \( \sigma_{\nu\nu} \) in the most-divergent-term approximation,

\[ \sigma_{\nu\nu} = \frac{2}{N} \sum_{k} \sum_{\{a\} = 1}^{3} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \Lambda_{\nu;2;ba}(k;0)g_{2;2;cd}(k;0)\Lambda_{\nu;2;cd}(k;0) \left( -\frac{\partial f(\epsilon)}{\partial \epsilon} \right). \]  

From this and Eq. (33), we can show that \( \sigma_{\nu\nu} \) is inversely proportional to the unrenormalized QP damping \( \Sigma_{\nu;2;ba}(k;0) \) and \( \Lambda_{\nu;2;cd}(k;0) \) in Eq. (38) are determined as follows. By combining Eq. (36) with the Ward identity, \( \Lambda_{\nu;2;ba}(k;0) \) is given by

\[ \Lambda_{\nu;2;ba}(k;0) = (v_{k\nu})_{ba} + \frac{\partial \text{Re} \Sigma_{ba}(A)}{\partial k_{\nu}}. \]  

In the present model, \( \text{Re} \Sigma_{ba}(A)(k) = \text{Re} \Sigma_{ba}(R)(k) \) holds due to the even-parity and the time-reversal symmetry. Since \( J_{22;\{a\}}(k,k';0) = J_{22;\{a\}}(k,k';0) \) is satisfied due to Eqs. (20), (26), and (35), \( \Lambda_{\nu;2;cd}(k;0) \) is given by

\[ \Lambda_{\nu;2;cd}(k;0) = \Lambda_{\nu;2;cd}(k;0) + \frac{1}{N} \sum_{k'} \sum_{\{A\}} \int_{-\infty}^{\infty} \frac{d\epsilon}{4\pi} J_{22;\{a\}}(k,k';0) \times g_{2;2;AB}(k',0) \Lambda_{\nu;2;cd}(k';0). \]  

Thus, the present theory takes account of the CVCs due to the self-energy and four-point vertex function, neglected in the relaxation approximation.

2.3. **FLEX approximation with the MT CVC for a multiorbital Hubbard model in a PM phase**

To calculate the resistivity, I use the FLEX approximation with or without the MT CVC or without all the CVCs in a PM phase. I first explain the FLEX approximation for a multiorbital Hubbard model in a PM phase. Next, I derive the irreducible four-point vertex function in this approximation; as described in Sect. 1, I consider only the MT term and neglect the AL term. Then, I show the Bethe-Salpeter equation for the current by using the MT term as the kernel of the CVC. I also remark on the numerical treatment of the principal integral appearing in that CVC. Finally, I discuss applicability of this method.

I determine several single-particle or two-particle quantities using the FLEX approximation in a PM phase where only the electron-hole scattering processes of the bubble and the ladder diagrams are considered as the Luttinger-Ward functional, \( \Phi_{\text{LW}}[G] \). Since that is a conserving approximation based on the free energy expressed in terms of the single-particle Green’s function, we can determine single-particle or two-particle quantities by using \( \Phi_{\text{LW}}[G] \) and its functional derivative. Since constructing \( \Phi_{\text{LW}}[G] \) is equivalent to constructing the effective interaction, where the same kinds of the diagrams are considered, and the latter is easier, we formulate the FLEX approximation by the latter procedure as follows.
First, considering the electron-hole scattering processes of the bubble and the ladder diagrams for $H_{\text{int}}$, we obtain the effective interaction in the FLEX approximation,

$$V_{abcd}^{s_1s_2s_3s_4}(\mathbf{q}, i\Omega_n) = \frac{1}{2} \left[ U_{abcd}^C - \sum_{\{A\}} U_{abAB}^C \chi_{ABCD}(\mathbf{q}, i\Omega_n) U_{CDcd}^C \right] \sigma_{s_1s_2}^0 \sigma_{s_3s_4}^0$$

$$- \frac{1}{2} \left[ U_{abcd}^S + \sum_{\{A\}} U_{abAB}^S \chi_{ABCD}^S(\mathbf{q}, i\Omega_n) U_{CDcd}^S \right] \sigma_{s_1s_2} \cdot \sigma_{s_3s_4},$$

with

$$\chi_{abcd}^S(\mathbf{q}, i\Omega_n) = \chi_{abcd}(\mathbf{q}, i\Omega_n) + \sum_{\{A\}} \chi_{abAB}(\mathbf{q}, i\Omega_n) U_{ABCD}^S \chi_{CDcd}^S(\mathbf{q}, i\Omega_n),$$

$$\chi_{abcd}^C(\mathbf{q}, i\Omega_n) = \chi_{abcd}(\mathbf{q}, i\Omega_n) - \sum_{\{A\}} \chi_{abAB}(\mathbf{q}, i\Omega_n) U_{ABCD}^C \chi_{CDcd}^C(\mathbf{q}, i\Omega_n),$$

and

$$\chi_{abcd}(\mathbf{q}, i\Omega_n) = -\frac{T}{N} \sum_{\mathbf{k}} \sum_m G_{ac}(\mathbf{k} + \mathbf{q}, i\omega_{m+n}) G_{db}(\mathbf{k}, i\omega_m).$$

Here we introduce the bare four-point vertex functions in spin and charge sector,

$$U_{abcd}^S = U_{abcd}^{\uparrow\downarrow} - U_{abcd}^{\uparrow\uparrow} = \left\{ \begin{array}{ll} U & \text{for } a = b = c = d \\ J_H & \text{for } a = b \neq c = d \\ U' & \text{for } a = c \neq b = d \\ J' & \text{for } a = d \neq b = c \end{array} \right.,$$

and

$$U_{abcd}^C = U_{abcd}^{\uparrow\downarrow} + U_{abcd}^{\downarrow\uparrow} = \left\{ \begin{array}{ll} U & \text{for } a = b = c = d \\ 2U' - J_H & \text{for } a = b \neq c = d \\ -U' + 2J_H & \text{for } a = c \neq b = d \\ J' & \text{for } a = d \neq b = c \end{array} \right.,$$

where $U_{abcd}^{s's'}$ is $U_{abcd}^{s's'} \equiv U_{abcd}^{s's'}$ and the spin-flipping term, $U_{abcd}^{s's'}$ for $s \neq s'$, satisfies $U_{abcd}^{\uparrow\downarrow \downarrow \uparrow} = -U_{abcd}^{\uparrow\uparrow \downarrow \downarrow} = -U_{abcd}^{s's'}$. Also, we neglect the vertex corrections to the susceptibilities in spin and charge sector; its effects are discussed later. Then, the single-particle Green’s function is determined by the Dyson equation,

$$G_{ab}(\mathbf{k}, i\omega_m) = G_{ab}^0(\mathbf{k}, i\omega_m) + \sum_{A,B} G_{ab}^0(\mathbf{k}, i\omega_m) \Sigma_{AB}(\mathbf{k}, i\omega_m) G_{BA}(\mathbf{k}, i\omega_m),$$

with the self-energy given by

$$\Sigma_{ac}(\mathbf{k}, i\omega_m) = \frac{T}{N} \sum_{\mathbf{q}} \sum_n \sum_{b,d} V_{abcd}(\mathbf{q}, i\Omega_n) G_{bd}(\mathbf{k} - \mathbf{q}, i\omega_{m-n}),$$
where

\[
V_{abcd}(q, i\Omega_n) = -V_{abcd}^{\uparrow\uparrow\uparrow\uparrow}(q, i\Omega_n) - V_{abcd}^{\uparrow\uparrow\downarrow\downarrow}(q, i\Omega_n) - \sum_{\{A\}} U_{aAbB}^{\uparrow\downarrow\uparrow\downarrow}(q, i\Omega_n) U_{CdDd}^{\uparrow\uparrow\downarrow\downarrow}
\]

\[
= \frac{3}{2} \left[ U_{abcd}^S + \sum_{\{A\}} U_{abAB}^S \chi_{ABCD}(q, i\Omega_n) U_{CDcd}^S \right]
\]

\[
+ \frac{1}{2} \left[ -U_{abcd}^C + \sum_{\{A\}} U_{abAB}^C \chi_{ABCD}(q, i\Omega_n) U_{CDcd}^C \right]
\]

\[
- \sum_{\{A\}} U_{aAbB}^{\uparrow\downarrow\uparrow\downarrow}(q, i\Omega_n) U_{CdDd}^{\uparrow\downarrow\uparrow\downarrow}.
\] (49)

The last term in Eq. (49) is introduced to exclude the double counting of the topologically equivalent term in the self-energy. Solving Eqs. (42)–(44) and (47)–(49) with Eqs. (8), (10), (45) and (46) selfconsistently by iteration, we can determine the single-particle and the two-particle quantities in the FLEX approximation.

It should be noted that the partial inclusion of mode-mode couplings for fluctuations, the interactions between fluctuations at different momenta, through the self-energy improves some unrealistic results obtained in the random-phase approximation, although the susceptibilities are determined by the random-phase approximation-type (but renormalized) equations. For example, in the FLEX approximation\(^{28,29,61,65}\), the value of \(U\) for a magnetic transition becomes about 2 eV, the momentum dependence of the mass enhancement and FS deformation are taken into account, and the Curie-Weiss-like temperature dependence of the spin susceptibility is obtained near a magnetic QCP. In particular, the final improvement is powerful to describe electronic properties near a magnetic QCP.

We also determine the irreducible four-point vertex function in the FLEX approximation in keeping conservation laws\(^{31}\). In a conserving approximation, the irreducible four-point vertex function is given by\(^{28,31,63}\)

\[
\Gamma^{(1)}_{abcd}(k, i\omega_m, k', i\omega_{m'}; q, i\Omega_n) = \frac{\delta \Sigma_{ab}(k, i\omega_m) \delta \Sigma_{cd}(k', i\omega_{m'})}{\delta G_{cd}(k', i\omega_{m'})}.
\] (50)

For the actual calculations, we first calculate the right-hand side at \(q = 0\) and \(\Omega_n = 0\) and then label momentum and frequency transfers correctly as the scattering process between the initial state consisting of an electron of orbital \(b\) with \((k, i\omega_m)\) and a hole of orbital \(d\) with \((k', i\omega_{m'})\) and the final state consisting of an electron of orbital \(a\) with \((k + q, i\omega_{m+n})\) and a hole of orbital \(c\) with \((k' + q, i\omega_{m'+n})\). After several straightforward calculations\(^{13}\) by using Eqs. (48)–(50), we obtain the irreducible four-point vertex function in the FLEX approximation, which is the sum of the MT and the AL term\(^{13}\). In this paper, I consider only the MT term,

\[
\Gamma^{(1)}_{abcd}(k, i\omega_m, k', i\omega_{m'}; q, i\Omega_n) = V_{abcd}(k - k', i\omega_m - i\omega_{m'}).
\] (51)

This treatment will be sufficient for a qualitative discussion about many-body effects on \(\rho_{ab}\) since the CVC of the AL term gives the higher order contribution compared with that of the MT term\(^{29}\). I have checked the validity of this statement by
calculating the main terms of the AL CVC [43]. Since it is necessary to calculate $J^{(1)}_{22;cdCD}(k, k'; 0)$ in Eq. (40), we need to carry out the analytic continuation of Eq. (51) in region 22-II, region 22-III, and region 22-IV. Carrying out the analytic continuation [43] of the MT term and using Eq. (23), we obtain

$$J^{(1)}_{22;cdCD}(k, k'; 0) = 2i \left( \coth \frac{\epsilon - \epsilon'}{2T} + \tanh \frac{\epsilon'}{2T} \right) \text{Im} V^{(R)}_{cCdD}(k - k').$$

(52)

Substituting Eq. (52) into Eq. (40), we obtain the Bethe-Salpeter equation for the current in the FLEX approximation with the MT CVC in a PM phase,

$$\Lambda^{(0)}_{\nu;2;cd}(k; 0) = \Lambda^{(0)}_{\nu;2;cd}(k) + \frac{1}{N} \sum k' \sum_{\langle A \rangle} \int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \left( \coth \frac{\epsilon - \epsilon'}{2T} + \tanh \frac{\epsilon'}{2T} \right) \times \text{Im} V^{(R)}_{cCdD}(k - k') g_{2;CABD}(k'; 0) \Lambda^{(0)}_{\nu;2;AB}(k'; 0).$$

(53)

We see the roles of the MT CVC are similar to those of the backflow correction [2].

Finally, I discuss applicability of the FLEX approximation with the MT CVC. Before discussing applicability, I explain how to treat the principal integral in Eq. (53) for the numerical calculations. Since both the numerator and denominator of the term containing $\coth \frac{\epsilon - \epsilon'}{2T}$ in the MT CVC become zero simultaneously at $\epsilon' = \epsilon$ due to $\text{Im} V^{(R)}_{abcd}(q, 0) = 0$, the principal integral can be calculated as follows:

$$\int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \coth \frac{\epsilon - \epsilon'}{2T} \text{Im} V^{(R)}_{cCdD}(k - k') g_{2;CABD}(k'; 0) \Lambda^{(0)}_{\nu;2;AB}(k; 0)
= \int \frac{d\epsilon'}{2\pi} \coth \frac{\epsilon - \epsilon'}{2T} \text{Im} V^{(R)}_{cCdD}(k - k') g_{2;CABD}(k'; 0) \Lambda^{(0)}_{\nu;2;AB}(k; 0)
- \frac{\Delta^{(2)} T}{2\pi} \frac{\partial}{\partial \epsilon'} \left[ (e^{\epsilon'} - 1) \text{Im} V^{(R)}_{cCdD}(k - k') g_{2;CABD}(k'; 0) \Lambda^{(0)}_{\nu;2;AB}(k'; 0) \right]_{\epsilon' = \epsilon},$$

(54)

where the first term contains the contributions other than $\epsilon' = \epsilon$.

Actually, the FLEX approximation is suitable to describe the electronic structure at low temperatures for moderately strong electron correlation. In a single-orbital Hubbard model on a square lattice [30], [32], the imaginary-time dependence of the single-particle Green’s function at several momenta in the FLEX approximation shows satisfactory (but not perfect) agreement with that in the quantum-Monte-Carlo calculation at $U$ being a half of the bandwidth; the agreement becomes better near the AF QCP than away from the AF QCP. Since the similar agreement will hold even in a multi-orbital Hubbard model on the same lattice and the FLEX approximation can treat the coherent part of the electronic spectrum satisfactorily [19], the electronic structure in metallic phases of the present model at low temperatures will be well described by the FLEX approximation at least qualitatively.

In contrast, the FLEX approximation becomes unsuitable at high temperatures or near a Mott transition for strong electron correlation. This is because local
correlation plays important roles in such cases \cite{15,16}, and the effects of local correlation on the electronic spectrum are smeared out in the FLEX approximation \cite{19}.

Then, the magnetic properties at low temperatures for moderately strong electron correlation will be appropriately described by the FLEX approximation if the dominant correlation of the system is spin fluctuation whose largest contribution comes from a non-degenerate orbital. Due to neglecting the vertex corrections to the susceptibilities, the enhancement of spin fluctuation arising from electron correlation is overestimated in the FLEX approximation compared with the enhancement of charge or orbital fluctuation. Actually, in a two-degenerate-orbital Hubbard model on a square lattice at small \((J_H/U)\) near an AF QCP, the AL vertex correction to the susceptibilities causes the enhancement of orbital fluctuation \cite{66}. However, I think that in the present model the FLEX approximation is sufficient to describe the magnetic properties at least qualitatively since the \(d_{xy}\) orbital gives the largest contribution to spin fluctuation \cite{29}; in this case, even if the MT and the AL vertex correction to the susceptibilities are considered beyond the FLEX approximation, the magnetic properties will not qualitatively change and these corrections will modify the values of the susceptibilities since orbital fluctuation enhanced due to the AL term does not dominate over spin fluctuation. Actually, the strongest enhancement of spin fluctuation at \(Q_{IC-AF}\) in the FLEX approximation \cite{29} away from and near the AF QCP agrees with the experiments in \(\text{Sr}_2\text{RuO}_4\) \cite{10} and \(\text{Sr}_2\text{Ru}_{0.075}\text{Ti}_{0.025}\text{O}_4\) \cite{7}.

Moreover, if the vertex corrections to the current arising from the self-energy and four-point vertex function due to electron correlation are added to the FLEX approximation, this method is suitable to describe the transport properties of a metallic phase due to low-frequency external field satisfying \(\omega \tau_{\text{trans}} \ll 1\) at low temperatures. In contrast to case of the vertex corrections to the susceptibilities, the vertex corrections to the current are essential for discussing the transport properties \cite{2,59} since the CVCs are vital to satisfy conservation laws and conservation laws play significant roles in transport phenomena. For example, the importance of the treatment holding conservation laws is known for a system without the lattice (e.g., the electron gas): only if the CVCs due to electron correlation are correctly taken into account, we can obtain the correct results such as the absence both of the resistivity \cite{58} and of the renormalization of the Drude weight \cite{57} and electron cyclotron frequency \cite{68}. Also, the CVCs due to electron correlation are important in a system with the lattice since these CVCs are necessary to obtain the correct effects of electron correlation on the transport coefficients in the presence of the Umklapp scattering \cite{59,67,69}. Another example showing the importance of the CVCs is the emergence of the Curie-Weiss-like temperature dependence of the Hall coefficient near the AF QCP due to the MT CVC in the FLEX approximation in the single-orbital Hubbard model on a square lattice \cite{28}. In addition to the treatment holding conservation laws, the satisfactory treatment of the coherent part in the FLEX approximation is powerful to describe the transport properties of a metallic phase.
due to the low-frequency external field. This is because the dominant contributions to the response induced by that external field at low temperatures come from the contributions near the Fermi level as a result of the energy derivative of the Fermi distribution function in the response function. Furthermore, this powerfulness of the FLEX approximation will hold even near a Mott transition since it is shown in the DMFT \cite{21} for a single-orbital Hubbard model that the transport properties in $\omega \tau_{\text{trans}} \ll 1$ are well described in the approximation where only the coherent part is considered. Thus, the FLEX approximation with the MT CVC is satisfactory to describe the transport properties of metallic phases of the present model at low temperatures. Actually, this method \cite{29} near and away from the AF QCP reproduced the temperature dependence of several transport properties of Sr$_2$RuO$_4$ \cite{37,38} and Sr$_3$Ru$_{0.775}$Ti$_{0.225}$O$_4$ \cite{39}, as pointed out in Sect. 1.

3. Results

In this section, I show the results of $\rho_{ab} = \sigma_{xx}^{-1}$ of some quasi-2D PM ruthenates in the FLEX approximation with or without the MT CVC or without all the CVCs. In particular, we focus on the effects of the self-energy and MT four-point vertex function due to electron correlation and the role of each $t_{2g}$ orbital.

I carried out the numerical calculations as follows. I set the $64 \times 64$ meshes of the Brillouin zone and 2048 Matsubara frequencies and used the fast Fourier transformation with the zero padding method \cite{70}. I obtained the single-particle Green’s function, self-energy, and MT four-point vertex function in the FLEX approximation by solving Eqs. (42)–(44) and (47)–(49) with Eqs. (8), (10), (45) and (46) by iteration, where I assumed that convergence is reached when the difference between the self-energies before and after certain iteration is less than $10^{-4}$. To obtain the quantities as a function of real frequency, I used the Padé approximation \cite{71} using the quantities at the lowest four Matsubara frequencies. The real-frequency integrations are approximated by the integrations with the interval 0.0025 eV and the upper and lower values 0.2 and $-0.2$ eV. The current was determined by solving Eq. (53) by iteration, where the convergence condition was assumed to be that the difference between the currents before and after certain iteration is less than $10^{-4}$. 

Fig. 3. Momentum dependence of the static spin susceptibility, $\chi^S(q,0) = \sum_{a,b} \chi^S_{aab}(q,0)$, for several temperatures at $U = (a) 1.8$ and (b) 2.1 eV, and (c) temperature dependence of $\chi^S(Q_{\text{IC-AF}},0)$ at $U = 1.8$ and 2.1 eV.
In the following, I consider cases at \( U = 1.8 \) and 2.1 eV as cases away from and near the AF QCP, respectively. These correspondences are because of the Pauli-PM temperature dependence of the spin susceptibility at \( U = 1.8 \) eV and the Curie-Weiss-like temperature dependence of the spin susceptibility at \( q = Q_{IC-AF} \) at \( U = 2.1 \) eV [see Figs. 3(a)–3(c)]. The latter is characteristic of a magnetic QCP and causes the strong temperature dependence of the Landau parameters with momentum transfer \( Q_{IC-AF} \) through the temperature dependence of the reducible four-point vertex function. The choice of \( U \) is reasonable since the value estimated experimentally in Sr\(_2\)RuO\(_4\) is about 2 eV\(^7\)

As explained below in detail, there are three main results: (i) \( \rho_{ab} \) of some quasi-2D PM ruthenates without the rotation and the tilting of RuO\(_6\) octahedra is determined almost by the conductions of the \( d_{xz/yz} \) orbital due to the smaller unrenormalized QP dampings of the \( d_{xz/yz} \) orbital than those of the \( d_{xy} \) orbital; (ii) The crossover between the \( T \)-linear and the \( T^2 \) dependence of \( \rho_{ab} \) occurs away from the AF QCP at about \( T = 0.008 \) eV due to the temperature dependence of the unrenormalized QP dampings of the \( d_{xz/yz} \) orbital; (iii) The \( T \)-linear \( \rho_{ab} \) emerges near the AF QCP due to the hot-spot structure of the QP dampings of the \( d_{xz/yz} \) orbital at \( k = Q_{IC-AF} \) and its symmetrically equivalent ones.

### 3.1. Case away from the AF QCP

I begin with the temperature dependence of \( \rho_{ab} \) at \( U = 1.8 \) eV in Fig. 4. Three cases in that figure are defined as follows: in case MT CVC, the CVCs arising from the self-energy and MT four-point vertex function are included; in case No MT CVC, the CVC arising from the self-energy is included; in case No all CVCs, which is equivalent to the relaxation-time approximation\(^6\), all the CVCs are neglected. There are three main remarks about Fig. 4. First, in all the three cases, decreasing temperature causes the crossover from the \( T \)-linear dependence to the \( T^2 \) dependence at about \( T = 0.008 \) eV. The \( T^2 \) dependence at low temperatures is more
clearly seen from the inset of Fig. 4. Second, the value of \( \rho_{ab} \) in case No all CVCs at each temperature is largest in the three cases. Third, the value of \( \rho_{ab} \) increases from that in case No MT CVC when the MT CVC is included. The first remark indicates that the CVCs little affect on the power of the temperature dependence of the resistivity. The second indicates that the value of the resistivity is overestimated in the relaxation-time approximation. The third indicates that the MT CVC enhances the resistivity as a result of the reduction of the current, which is similar to the effect of the backflow correction. Thus, the effects of the CVCs on the resistivity just change its value.

Then, to understand the role of each \( t_{2g} \) orbital, I analyze the orbital-decomposed \( \sigma_{xx} \) at \( U = 1.8 \) eV. The orbital-decomposed \( \sigma_{xx} \) for the \( d_{xz}/yz \) and the \( d_{xy} \) orbital are obtained by replacing \( \sum_{a}^{3} \) in Eq. (38) by \( \sum_{a}^{2} \) and \( \sum_{a}^{3} \), respectively. Those components are sufficient in the present model since the intraorbital components are much larger than the interorbital components due to the large intraorbital hopping integrals compared with the interorbital ones. We see from Figs. 5(a)–5(c) that the dominant contributions to the total of \( \sigma_{xx} \) come from the component of the \( d_{xz} \) orbital, and that the component of the \( d_{xy} \) orbital is less than 10% of the total. Due to the rotational symmetry of the system, in case of \( \sigma_{yy} \), the component of the \( d_{yz} \) orbital gives the dominant contributions. Thus, the inplane transport is governed mainly by the conductions of the \( d_{xz}/yz \) orbital.
The above orbital-dependent transport arises from the smaller unrenormalized QP dampings of the \( d_{xz/yz} \) orbital than those of the \( d_{xy} \) orbital since \( \sigma_{\nu\nu} \) is inversely proportional to the unrenormalized QP damping, as explained in Sect. 2.2. Actually, we see from Fig. 6(a) that the unrenormalized QP dampings of the \( d_{xz/yz} \) orbital are smaller. The similar orbital dependence holds at the other temperatures.

Also, we see from Figs. 6(b) and 6(c), respectively, that the QP dampings of the \( d_{xz/yz} \) orbital remain the cold spot, and that the temperature dependence of the unrenormalized QP damping of the \( d_{xz/yz} \) orbital at \( k = Q_{1C-AF} \) changes from \( T^2 \) to \( T \)-linear at about \( T = 0.008 \) eV. Thus, the latter is the origin of the crossover of the power of the temperature dependence of \( \rho_{ab} \) at about \( T = 0.008 \) eV.

### 3.2. Case near the AF QCP

I turn to the temperature dependence of \( \rho_{ab} \) at \( U = 2.1 \) eV in the three cases, considered in Sect. 3.1. From Fig. 7 we see that the \( T \)-linear \( \rho_{ab} \) emerges in all the three cases. We also see the similar effects of the CVCs on the value of \( \rho_{ab} \) to those at \( U = 1.8 \) eV, the overestimation in the relaxation-time approximation (i.e., case No all CVCs) and the increase from the value in case No MT CVC due to the MT CVC. The first result indicates that the emergence of the \( T \)-linear \( \rho_{ab} \) near the AF QCP arises from the temperature dependence of the unrenormalized QP damping. Furthermore, those results and the corresponding results at \( U = 1.8 \) eV suggest that the effects of the self-energy and MT four-point vertex function on the value of \( \rho_{ab} \) and power of the temperature dependence of \( \rho_{ab} \) are ubiquitous.

Also, comparing Fig. 7 with Fig. 4 we see electron correlation enhances the value of \( \rho_{ab} \) at each temperature. This is due to an increase in the unrenormalized QP dampings of the \( d_{xz/yz} \) orbital with increasing \( U \) [e.g., see Figs. 6(a) and 6(b)].

Then, in a similar way to that used at \( U = 1.8 \) eV, I analyze the role of each \( t_{2g} \) orbital at \( U = 2.1 \) eV. Figures 9(a)–9(c) show the temperature dependence of the total and orbital-decomposed components of \( \sigma_{xx} \) at \( U = 2.1 \) eV in the three cases.
Fig. 8. Momentum dependence of (a) the unrenormalized QP damping and (b) the QP damping for each $t_{2g}$ orbital at $(U, T) = (2.1, 0.01)\, \text{eV}$, and (c) the unrenormalized QP damping of the $d_{xz/yz}$ orbital at $k = Q_{IC-AF}$ against $T^0.5$ at $U = 2.1\, \text{eV}$. The dashed lines in panel (b) denotes $T = 0.01\, \text{eV}$.

Fig. 9. Temperature dependence of the total and orbital-decomposed components of $\sigma_{xx}$ at $U = 2.1\, \text{eV}$ in (a) case MT CVC, (b) case No MT CVC, and (c) case No all CVCs. The definition of each orbital-decomposed $\sigma_{xx}$ is described in the main text in Sect. 3.1.

The orbital-dependent transport holds even near the AF QCP: the conduction of the $d_{xz/yz}$ orbital mainly contribute to the inplane transport. Its mechanism is the same as that at $U = 1.8\, \text{eV}$, i.e. the smaller unrenormalized QP dampings of the $d_{xz/yz}$ orbital than those of the $d_{xy}$ orbital [see Fig. 8(a)]. Thus, this orbital-dependent transport is characteristic in some quasi-2D PM ruthenates.

Moreover, we find from Figs. 8(b) and 8(c), respectively, that the QP damping of the $d_{xz/yz}$ orbital at $k = Q_{IC-AF}$ becomes the hot spot, and that the temperature dependence of the unrenormalized QP damping of the $d_{xz/yz}$ orbital at $k = Q_{IC-AF}$ is roughly proportional to $T^0.5$. Since such $T^0.5$ dependence near the hot spot causes the $T$-linear dependence of the average of the unrenormalized QP dampings for states along the FS, the origin of the $T$-linear $\rho_{ab}$ near the AF QCP is the hot-spot structure of the QP dampings of the $d_{xz/yz}$ orbital at momenta connected each other by the characteristic spin fluctuations of this AF QCP.

4. Conclusions

In summary, I reviewed many-body effects of $\rho_{ab}$ of the quasi-2D PM ruthenates away from and near the AF QCP in the FLEX approximation with or without the MT CVC or without all the CVCs.

The temperature dependence of $\rho_{ab}$ away from and near the AF QCP agree with experiments of Sr$_2$RuO$_4$ [57] and Sr$_2$Ru$_{0.075}$Ti$_{0.025}$O$_4$ [58], respectively: in case
away from the AF QCP, the crossover between the $T$-linear and the $T^2$ dependence at about $T = 0.008$ eV and the $T^2$ dependence at low temperatures are obtained; in case near the AF QCP, the $T$-linear dependence even at low temperatures is obtained. Here the main effect of the Ti substitution on the temperature dependence of $\rho_{ab}$ is assumed to be pushing the system nearer the AF QCP than Sr$_2$RuO$_4$.

The obtained results reveal some important aspects of many-body effects on the resistivity of correlated electron systems. First, the overestimation of the value of $\rho_{ab}$ in the relaxation-time approximation and the back-flow-like effect of the MT CVC on the value of $\rho_{ab}$ are ubiquitous. It is also ubiquitous that the power of the temperature dependence of the resistivity is determined by the temperature dependence of the momentum- and orbital-dependent unrenormalized QP damping. The similar results have been obtained in a single-orbital Hubbard model on a square lattice. Moreover, the $T$-linear resistivity near the AF QCP is similar to that obtained in those previous studies. However, I emphasize that the criticality of the resistivity, the power of its temperature dependence, does not always connect with the criticality of spin fluctuation enhanced near a magnetic QCP in multiorbital systems, while these are always the same in single-orbital systems. This characteristic property comes from the facts that the orbital whose unrenormalized QP damping is small mainly contributes to the resistivity, and that the main orbital of the characteristic spin fluctuation of a magnetic QCP has the large unrenormalized QP damping. Since the momentum, the temperature, and the orbital dependence of the damping of a QP (i.e., the unrenormalized QP damping or the QP damping) are overlooked in Landau’s FL theory and such momentum dependence is overlooked in the DMFT, the obtained results highlight their importance in discussing the resistivity of correlated electron systems.

I close this paper with several remarks about the remaining issues. First, it is necessary to study the transport properties of other ruthenates using the method I used and discuss the similarities and differences. In particular, the study for a quasi-2D ruthenate near a ferromagnetic QCP is highly desirable to understand the similarities and differences between many-body effects and role of each $t_{2g}$ orbital near the AF and the ferromagnetic QCP. Also, it is important to analyze the transport properties of 3D ruthenates since comparison of the results in quasi-2D and 3D ruthenates leads to a deep understanding of the dimensionality. Other remaining issues are the applications to other correlated electron systems such as transition-metal oxides, organic conductors, CeCoIn$_5$, and UPt$_3$ since these studies are important to deduce ubiquitous properties of correlated electron systems and characteristic properties of multiorbital systems. Then, it is intriguing to study the transport properties in a superconducting phase by extending the present method in a PM phase since in some cases the CVCs arising from not only spin fluctuations but also superconducting fluctuations play important roles. Furthermore, another remaining issue is to clarify the role of each $t_{2g}$ orbital in the thermal transport in the superconducting phase of Sr$_2$RuO$_4$ on
the basis of the method where the orbital dependence of the damping of a QP is satisfactorily considered. This is because the combination of my result[29] and several previous studies[81,82] suggest the existence of the difference between the main orbitals of the inplane transport and the superconductivity; if this is correct, we should pay attention to the effects of the orbital-dependent damping of a QP on the thermal transport[20] for correct understanding of the experimental results.

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