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Theory of multicomponent Fermi liquid: General formulas for susceptibilities and applications to periodic Anderson models

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We treat the multicomponent fermion system (MCFS) in which several distinct types of fermions interact and hybridize mutually. For the most general MCFS we reconstruct and unify the Fermi-liquid theory for the susceptibility: (a) We obtain the dynamical susceptibility $\chi(q,\Omega)$ on the basis of the Kubo formula, in a form where the identity of the original local basis and its relation to the quasiparticle (qp) band basis are transparent; (b) we obtain the isothermal static uniform susceptibility χ_T by Luttinger's procedure; and then (c) we present the explicit identities showing that $\chi(q\rightarrow 0, \Omega\equiv 0)$ coincides with χ_T, provided that the magnetization is conserved; in addition to the mathematical origin, we give a physical interpretation of the singular behavior of $\chi(q,\Omega)$ for small (q,Ω). In the latter part of this paper, three kinds of periodic Anderson models (PAM's) are considered as examples of MCFS's: (i) the SU(N) PAM, (ii) a doubly degenerate PAM with different g values for the c and f electrons, and (iii) an orbitally degenerate PAM with different degeneracies for the c and f electrons. The qp and non-qp parts of the susceptibility are obtained separately, and we find that the non-qp parts of these models behave completely differently from each other. This diversity of the behavior of the non-qp parts depending on the details of the model suggests a possible resolution of the Wilson-ratio problem of the heavy-fermion systems posed by Anderson and others.

I. INTRODUCTION

Electrons in several crystalline compounds containing an actinide or lanthanide element form the heavy Fermi liquid;[1] in other words, they behave as if they are weakly interacting degenerate fermions with a mass much greater than the electron mass in vacuum.[2] For example, the static uniform susceptibility χ and the temperature-linear coefficient of the specific heat, γ, of these materials are very large and roughly proportional to each other. The strong repulsive interaction between the bare f electrons on the same site is consumed mainly to make the quasiparticle (qp) heavy. The residual interaction plays only a secondary role such as to affect the material-dependent ratio between χ and γ, which is called the Wilson ratio.

The periodic Anderson model (PAM) is believed to contain the essence of the heavy-fermion systems and is widely used in the literature.[3] In the PAM there exist two distinct types of the electrons: the c and f electrons. The f electrons are localized, and between them on the same site acts a strong repulsive interaction. The c electrons wander from site to site with some bare transfer-matrix element, while the c-c and c-f interactions are neglected. However, the c and f electrons are hybridized. Thus the real qp is composed both of the c and f electrons and has the characteristics of the heavy fermion.

In the PAM the f-f repulsive interaction is assumed to be large. Nonetheless, the perturbation expansion in this interaction is useful, because the experimentally observed Fermi-liquid property can be reproduced by making a small number of hypotheses. We refer to these hypotheses in a bundle as the Fermi-liquid hypothesis (FLH). Although we cannot deduce the validity of the FLH starting from the Hamiltonian, we can justify its use *a posteriori*, taking in advance that the PAM should show the Fermi-liquid property. Once the FLH is made, we can relate the phenomenological parameters, such as the qp mass and qp interaction, with microscopically definable objects, such as the self-energy and the vertex parts; eventually, we can predict some correlation among different observable quantities. This helps us to make a clear and unified vision on the heavy-fermion systems. Thus it is worthwhile considering the PAM under the FLH. Let us review a few problems which have been resolved and are to be resolved about the PAM under the FLH.

First, Yamada and Yosida derived,[4] by Luttinger's procedure,[5] a formula for the isothermal static uniform susceptibility χ_T of the SU(2) PAM, where both of the c and f electrons have only the spin-$\frac{1}{2}$ degeneracy. Their formula is expressed with the bare c and f electron density of states and the field derivative of the f-electron self-energy on the Fermi surface. However, this type of formula cannot be extended to the other more complicated PAM's, because Luttinger's procedure is applicable only when the magnetization is conserved. Yamada and coworkers[6,7] made a mistake in applying the procedure to the PAM where the magnetization is not conserved owing to the orbital moment; then they realized the mistake and have made some trials to overcome the difficulty and to derive a similar formula for the more elaborate model than the SU(2) PAM, but they have not fully succeeded yet.[8,9] Therefore, at this point, we would like to clarify the range of the applicability of this type of formula, and then we would like to derive the most general formula being valid in that whole range.

Second, Yip[10] considered the dynamical susceptibility $\chi(q,\Omega)$, starting from the Kubo formula. He treated a PAM which is slightly more general than the SU(2) PAM, but is still very simple. He succeeded in reformulating the theory in a form where one can see the identities of the original local c and f electrons. Yip's formalism is very neat, but heavily depends on the special simplicity of his PAM Hamiltonian; a disadvantage of his formalism is that an extension to the more general models is impossible. On the other hand, there is earlier work by Jones and McClure[11] on the multicomponent Fermi liquid, whose formalism does not rely upon any special simplicity of the system; however, it is formulated on the qp-band basis throughout, and so the information on the original local basis is completely lost, or such a problem was not in their mind from the beginning. Therefore, at this point, we would like to construct a general formalism which is applicable to the wider range of models and simultaneously retains the identities of the fermions with respect to the original local basis.

Finally, Yip applied his formalism to the SU(2) PAM and obtain a formula for χ^k, the k limit (i.e., the usual static limit) of $\chi(q,\Omega)$; then he complained[12] that he could not show the equivalence between his formula for χ^k and Yamada and Yosida's formula for χ_T. In principle, these two static uniform susceptibilities may be different, but it is commonly believed that they would coincide. The correctness of Luttinger's procedure leaves no room for doubt when the magnetization is conserved, while the approach from the Kubo formula is more general. Thus, at this point, we encounter a fundamental theoretical problem whether χ^k and χ_T are really equivalent or not, at least in the Fermi liquid.

As described in the previous paragraphs, starting from a few questions concerning the simple PAM's, we have arrived at the point where we must develop a simple and systematic way to treat the general multicomponent fermion system (MCFS): The MCFS is a fermion system in which there locally exist several distinct types of fermions whose mutual hybridization and interaction may be complicated in general. The PAM is a simple kind of MCFS.

In summary, what we would like to perform are (i) to reformulate the Fermi-liquid theory for the general MCFS in a form where the relation between the qp-band basis and the original local basis is transparent; (ii) to apply Luttinger's procedure to the same general MCFS and derive the general formula for χ_T, while examining carefully where the conservation property is used; and (iii) to investigate as generally as possible the question about the equivalence between χ^k and χ_T. The former part of this paper (Secs. II–V) is devoted to these problems.

Then, in Sec. VI, our formalism is applied to the PAM's. Generally, the low-frequency and long-wavelength susceptibility is divided into the qp and non-qp parts. In the first of the three models we consider, the non-qp part does not exist. In the remaining two models, it does exist. However, the behaviors of the non-qp part of these two models are significantly different. These results suggest that the character of the non-qp part is very sensitive to the details of the model, and this makes it very difficult to estimate it by theoretical analyses. In connection with this problem, there has been some controversy on the origin of the smallness of the observed Wilson ratio of the heavy-fermion systems.[13–17] The more elaborate introduction to this subject is deferred until the general formalism and the example calculations are completed. In Sec. VII we review the foregoing arguments in the literature and reveal the origin of the controversy; then we propose a possible resolution. Although it is not completely satisfactory, I believe that our discussion will contribute to deepen one's understanding and will serve as a step toward a true resolution of the problem.

II. MULTICOMPONENT FERMION SYSTEM

In reformulating the theory for the susceptibility of the Fermi liquid in a form applicable to the most general MCFS, we try to classify the results as clear as possible into the three categories: (i) the general results free from the FLH, (ii) the consequences of the FLH, and (iii) the consequences both of the conservation property and FLH. This section is devoted to the results of the first category.

A. Model

1. Hamiltonian

We consider the most general MCFS, which we assume to have ν components locally. The creation operators at a lattice point r are denoted as

$$\hat{\psi}^\dagger(r)=(\hat{\psi}_1^\dagger(r),\hat{\psi}_2^\dagger(r),\ldots,\hat{\psi}_\nu^\dagger(r)) . \tag{2.1}$$

The Hamiltonian is of the form

$$\hat{H}=\hat{H}_0+\hat{U} , \tag{2.2}$$

with

$$\begin{aligned}\hat{H}_0&=\sum_{r_1,r_2} E_{ij}(r_1,r_2)\hat{\psi}_i^\dagger(r_1)\hat{\psi}_j(r_2)=\sum_k E_{ij}(k)\hat{\psi}_i^\dagger(k)\hat{\psi}_j(k)\\&=\sum_{r_1,r_2}\hat{\psi}^\dagger(r_1)E(r_1,r_2)\hat{\psi}(r_2)=\sum_k\hat{\psi}^\dagger(k)E_k\hat{\psi}(k) ,\end{aligned} \tag{2.3}$$

$$\begin{aligned}\hat{U}&=\tfrac{1}{2}\sum_{i,j,l,m}\sum_{r_1,\ldots,r_4} U_{lm}^{ij}(r_1,r_2,r_3,r_4)\hat{\psi}_l^\dagger(r_1)\hat{\psi}_j^\dagger(r_2)\hat{\psi}_m(r_3)\hat{\psi}_i(r_4)\\&=\frac{1}{2N_{\text{sys}}}\sum_{i,j,l,m}\sum_{k,p,q} U_{lm}^{ij}(k,p,q)\hat{\psi}_l^\dagger(p)\hat{\psi}_j^\dagger(q)\hat{\psi}_m(q-k)\hat{\psi}_i(p+k) ,\end{aligned} \tag{2.4}$$

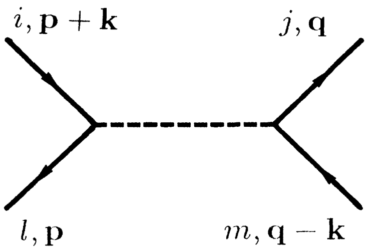

FIG. 1. Two-body interaction vertex $U^{ij}_{lm}(k,p,q)$.

where we assume the translational invariance of the system,

$$E_{ij}(r_1,r_2)=E_{ij}(r_1-r_2,0)\ , \tag{2.5}$$

$$U^{ij}_{lm}(r_1,r_2,r_3,r_4)=U^{ij}_{lm}(r_1-r_4,r_2-r_4,r_3-r_4,0)\ , \tag{2.6}$$

so that the spatial Fourier transforms of E_{ij} and U^{ij}_{lm} have only one and three independent variables, respectively. The Fourier transform is denoted by the same symbol and distinguished by its argument throughout this paper. If we further restrict the two-body interaction to be velocity independent, like the Coulomb interaction or the spin-spin exchange, then it reduces to

$$U^{ij}_{lm}(r_1,r_2,r_3,r_4)=U^{ij}_{lm}(r_1-r_2)\delta(r_1-r_4)\delta(r_2-r_3)\ , \tag{2.7}$$

and the spatial Fourier transform will depend on only one variable as $U^{ij}_{lm}(k)$. The system size (the number of the lattice points) is denoted by $N_{\rm sys}$. The convention of the indices of the two-body interaction is shown in Fig. 1.

In this paper, many ν-dimensional objects such as vectors, matrices, and tensors appear, as well as some objects of reduced dimensions. To avoid the proliferation of symbols, we use the same symbol for these objects and for their elements; they are distinguished by the appearance of indices. For example, in (2.3), $\hat\psi$ represents a ν-dimensional column vector, $\hat\psi^\dagger$ a row vector, and $\hat\psi_i,\hat\psi_j^\dagger$ their elements; E,E_k are matrices and E_{ij} their elements.

2. *Magnetization*

We define a scalar local one-body quantity $\hat m(r)$ and its summation over the system $\hat M$ as

$$\hat m(r)=\hat\psi^\dagger(r)M\hat\psi(r)=\sum_i \mu_i\hat\psi_i^\dagger(r)\hat\psi_i(r)\ , \tag{2.8}$$

$$\hat M=\sum_r \hat m(r)=\sum_k \hat\psi^\dagger(k)M\hat\psi(k)=\hat m(q=0)N_{\rm sys}\ , \tag{2.9}$$

where, by a proper choice of a local basis, the matrix M is assumed to be diagonal without loss of generality. The coupling of our system to the external scalar field $h(r,t)$ is assumed to be prescribed by

$$\hat H_{\rm ext}(t)=-\sum_r \hat m(r)h(r,t) \tag{2.10}$$

$$=-\sum_q \int d\Omega\, e^{i(qr-\Omega t)}\hat m(-q)h(q,\Omega)\ . \tag{2.11}$$

If the external field is static and uniform, the above reduces to

$$\hat H_{\rm ext}=-h\hat M\ . \tag{2.12}$$

We set the equilibrium statistical average of $\hat m(r)$ under no external field to be zero for simplicity:

$$\langle \hat m(r)\rangle_0=0\ . \tag{2.13}$$

We call $\hat m(r)$ and $\hat M$ the local and total magnetization for short. Accordingly, μ_i is called the magnetic moment of the ith fermion, and the linear response function of these quantities to the external fields is referred to simply as the susceptibility.

B. Single-particle Green's functions

Most of the results in the remaining of this section are probably familiar to the readers, except for the matrix or tensor character of the Green's functions and related objects. The results are itemized rather routinely for the completeness of the derivations and proofs in the subsequent development. However, please appreciate the A-matrix representation of the single-particle Green's function given in Sec. II B 4; this representation proves to be very useful in the following development of the theory for the multicomponent Fermi liquid.

1. *Definition*

The single-particle Matsubara Green's function (or temperature Green's function) is defined by[18]

$$\mathcal{G}_k(\tau-\tau')=-\langle \mathrm{T}_\tau\hat\psi(k,-i\tau)\hat\psi^\dagger(k,-i\tau')\rangle_0\ , \tag{2.14}$$

which is a $\nu\times\nu$ matrix. Written explicitly, the elements are

$$[\mathcal{G}_k(\tau-\tau')]_{ij}=-\langle \mathrm{T}_\tau\hat\psi_i(k,-i\tau)\hat\psi_j^\dagger(k,-i\tau')\rangle_0\ , \tag{2.15}$$

where $\langle\ \rangle_0$ denotes the equilibrium statistical average for a given chemical potential μ and a given temperature $T=\beta^{-1}$, under no external field [(A1) with $h=0$]; T_τ is the usual τ-ordering operator, and the time dependence of a quantum operator in the Heisenberg representation is given by

$$\hat O(t)=e^{i(\hat H-\mu\hat N)t}\hat O e^{-i(\hat H-\mu\hat N)t}\ . \tag{2.16}$$

The Fourier frequency transform of $\mathcal{G}_k(\tau)$ is defined by

$$\mathcal{G}_k(i\omega_n)=\int_0^\beta d\tau\exp(i\omega_n\tau)\mathcal{G}_k(\tau)\ , \tag{2.17}$$

where $\omega_n=(2n+1)\pi/\beta$, with n an integer. The analytic continuations[19] of $\mathcal{G}_k(i\omega_n)$ from the upper and lower complex planes to the real axis are denoted by $G_k^A(\omega)$ and $G_k^R(\omega)$, respectively.

2. *Spectral representation*

With the spectral weight function matrix $\rho_k(x)$ given by (B1) the single-particle Green's functions are expressed as

$$\mathcal{G}_k(i\omega_n)=\int dx\frac{\rho_k(x)}{i\omega_n-x} \tag{2.18}$$

and

$$\left.\begin{matrix} G_k^R(\omega) \\ G_k^A(\omega) \end{matrix}\right\} = \int dx \frac{\rho_k(x)}{(\omega \pm i0^+)-x} = \mathrm{P}\int dx \frac{\rho_k(x)}{\omega - x} \mp i\pi\rho_k(\omega) \ . \tag{2.19}$$

The range of the integration over x extends from $-\infty$ to ∞. Since ρ_k is Hermitian, $G_k^R(\omega)$ and $G_k^A(\omega)$ are Hermitian conjugate. Thus we can write

$$\rho_k(\omega) = -\frac{1}{2\pi i}[G_k^R(\omega) - G_k^A(\omega)] = \frac{1}{\pi}\mathrm{Im}G_k^A(\omega) \ . \tag{2.20}$$

The symbols Re and Im before a matrix denote the Hermitian and anti-Hermitian parts of the matrix, which are Hermitian by themselves. From the spectral representation (2.19), we can deduce that

$$\mathrm{Re}(G_k^R) \to 1/\omega \quad \text{and} \quad \mathrm{Im}(G_k^A) \to o(1/\omega) \quad \text{as } |\omega| \to \infty \ . \tag{2.21}$$

The spectral weight function of the single-particle Green's function is positive semidefinite and is sometimes referred to as the *density of states*. Nevertheless, it is quite different from the *quasiparticle density of states*, which will be defined later in the context of the Fermi-liquid hypothesis.

3. *Self-energy*

The self-energy Σ_k relates the true Green's function $\mathcal{G}_k$ defined above and the noninteracting Green's function

$$\mathcal{G}_k^0(i\omega_n) = (i\omega_n + \mu - E_k)^{-1} \tag{2.22}$$

through the Dyson equation (Fig. 2):

$$\mathcal{G}_k = \mathcal{G}_k^0 + \mathcal{G}_k^0 \Sigma_k \mathcal{G}_k \ . \tag{2.23}$$

Solving it, we obtain

$$\mathcal{G}_k(i\omega_n) = [(i\omega_n + \mu) - E_k - \Sigma_k(i\omega_n)]^{-1} \ . \tag{2.24}$$

The analytic continuations of $\Sigma_k(i\omega_n)$ are similarly defined and denoted by $\Sigma_k^A(\omega)$ and $\Sigma_k^R(\omega)$, which are Hermitian conjugate to each other. Note that the positive semidefiniteness of $\mathrm{Im}G_k^A(\omega) = \pi\rho_k(\omega)$ leads to the positive semidefiniteness of $\mathrm{Im}\Sigma_k^A(\omega)$.

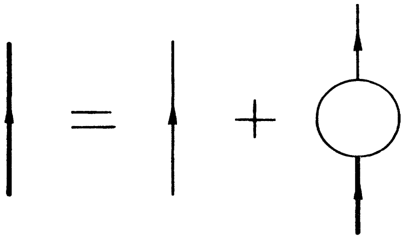

FIG. 2. Circle is the self-energy. The thin and thick lines are the noninteracting and exact single-particle Green's functions respectively.

4. *A-matrix representation*

The explicit form of the Green's-function matrix depends on the fermion basis we choose. If we go from basis to basis by unitary transformations, the elements of the Green's function will transform accordingly. However, the positions of the singular points as a function of the complex frequency variable are independent of the choice of the basis. Thus it is convenient if we can factorize the Green's function into two parts such that one part contains the singularity but is independent of the basis and another part transforms according to the choice of the basis but is free from the singularity. This purpose is achieved as follows.

The inverse of the Green's function is diagonalized by a similar transformation as[20]

$$\mathcal{P}_k^{-1}(\zeta)[(\zeta+\mu) - E_k - \Sigma_k(\zeta)]\mathcal{P}_k(\zeta) = \begin{bmatrix} \zeta+\mu-\mathcal{L}_{k1}(\zeta) & & \\ & \ddots & \\ & & \zeta+\mu-\mathcal{L}_{k\nu}(\zeta) \end{bmatrix} \ . \tag{2.25}$$

Taking the inverse of the both sides and multiplying them by $\mathcal{P}_k$ and $\mathcal{P}_k^{-1}$ from the left and right, respectively, we can rewrite the Green's function as

$$\mathcal{G}_k(\zeta) = \sum_{\alpha=1}^{\nu} \frac{\mathcal{A}_{k\alpha}(\zeta)}{\zeta+\mu-\mathcal{L}_{k\alpha}(\zeta)} \ , \tag{2.26}$$

where

$$\mathcal{A}_{k\alpha}(\zeta) = \mathcal{P}_k(\zeta) e^{(\alpha)} \mathcal{P}_k^{-1}(\zeta) \tag{2.27}$$

and

$$(e^{(\alpha)})_{\beta\gamma} = \delta_{\beta\alpha}\delta_{\alpha\gamma} \ . \tag{2.28}$$

Thus the Green's function can be written as a sum of the product of the two factors: The one factor $[\zeta+\mu-\mathcal{L}_{k\alpha}(\zeta)]^{-1}$ contains a singularity and is invariant under the transformation of the fermion basis, and the other factor $\mathcal{A}_{k\alpha}(\zeta)$ does not contain a singularity and transforms according to the choice of the fermion basis. Let us call (2.26) the A-matrix representation of the single-particle Green's function in this paper. The A matrix satisfies several useful identities, which is shown later, and plays an important role throughout this paper.

Finally, let us note that, since $\mathrm{Im}\Sigma_k^A$ is positive semidefinite,

$$\mathrm{Im}L_{k\alpha}^A(\omega) \geq 0 \ , \tag{2.29}$$

where $L_{k\alpha}^A(\omega)$ is the analytic continuation of $\mathcal{L}_{k\alpha}(i\omega_n)$.

5. *Under static uniform field*

When we consider the isothermal static uniform susceptibility or a kind of Ward identity, we need $\mathcal{G}_k$ defined under a static uniform field h. In this case, $\hat{H}_{\mathrm{tot}} = \hat{H} - h\hat{M}$ is used in place of $\hat{H}$; thus the matrix E_k in the one-body part of the Hamiltonian is replaced by

$$E_k(h) \equiv E_k - hM \ , \tag{2.30}$$

and the average $\langle\ \rangle_0$ is replaced by $\langle\ \rangle_h$ of (A1). As a result, all of $\mathcal{G}_k$, Σ_k, $\mathcal{A}_{k\alpha}$, and $\mathcal{L}_{k\alpha}$ depend on h. However, since the context will reveal which case we consider, the parameter h is usually suppressed.

C. Two-particle Green's functions

1. Definition

The two-particle temperature Green's function we need is the following:

$$\mathcal{K}(q,i\Omega_l)=\int_0^\beta d\tau \exp(i\Omega_l\tau)\mathcal{K}(q,\tau)\ , \tag{2.31}$$

where

$$\mathcal{K}(q,\tau-\tau')=N_{\rm sys}\langle \mathrm{T}_\tau \hat{m}(q,-i\tau)\hat{m}(-q,-i\tau')\rangle_0\ , \tag{2.32}$$

and $\Omega_l=2l\pi/\beta$, with l an integer. The analytic continuation[19] of the above from the upper complex plane to the real axis is denoted by $K^R(q,\Omega)$.

2. Spectral representation

With the spectral weight function $w(q,x)$ given by (B3), the two-particle Green's functions are expressed as

$$\mathcal{K}(q,i\Omega_l)=\int\frac{dx}{\pi}\,\frac{w(q,x)}{x-i\Omega_l} \tag{2.33}$$

and

$$K^R(q,\Omega)=\int\frac{dx}{\pi}\,\frac{w(q,x)}{x-\Omega-i0^+}\ . \tag{2.34}$$

The formula (2.33) is originally derived for $l\neq 0$, but is also applicable to $l=0$ with some care. The formula (2.34) is valid for all Ω, including $\Omega=0$.

One must be very careful, however, that there is no straightforward connection between $\mathcal{K}(q,0)$ and $K^R(q,0)$, because $K^R(q,\Omega)$ is obtained from $\mathcal{K}(q,i\Omega_l)$ with $l\geq 1$; no information about $\mathcal{K}(q,0)$ is contained in $K^R(q,\Omega)$. Hence $\mathcal{K}(q,0)$ is different from $K^R(q,0)$ in general. I would like to emphasize this fact here, because it is sometimes misunderstood in the literature.

3. Vertex parts

The complete vertex part Γ relates the two-particle Green's function and the single-particle Green's functions as

$$\mathcal{K}=-M(\mathcal{G}\otimes\mathcal{G})M-M(\mathcal{G}\otimes\mathcal{G})\Gamma(\mathcal{G}\otimes\mathcal{G})M\ . \tag{2.35}$$

In this and the following symbolic equations, the integrations or the summations over internal frequencies and crystal momenta are implicit, as well as the summations over the local fermion indices; Γ is a tensor of the form

$$[\Gamma(k,k',\omega,\omega';q,\Omega)]^{ij}_{lm}\ , \tag{2.36}$$

and $\mathcal{G}\otimes\mathcal{G}$ a tensor of the form

$$(\mathcal{G}\otimes\mathcal{G})^{ij}_{lm}(k,\omega;q,\Omega)=[\mathcal{G}_{k+q}(i\omega_n+i\Omega)]_{ji}[\mathcal{G}_k(i\omega_n)]_{lm}\ . \tag{2.37}$$

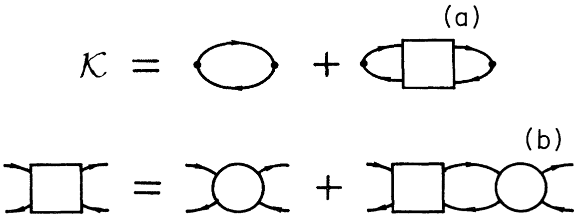

FIG. 3. Square represents Γ and the circle Γ_0.

The fermion indices run from 1 to ν; thus these tensors have ν^4 elements (ν is the number of the local fermion components). As a Feynman diagram, (2.35) is expressed as in Fig. 3(a).

The vertex part Γ is obtained with the (bare-particle-hole) irreducible vertex part Γ_0 through the Bethe-Salpeter equation, symbolically as

$$\Gamma=\Gamma_0+\Gamma(\mathcal{G}\otimes\mathcal{G})\Gamma_0 \tag{2.38}$$

and diagramatically as in Fig. 3(b).

4. Decomposition

We separate $\mathcal{G}\otimes\mathcal{G}$ into two parts as

$$\mathcal{G}\otimes\mathcal{G}=Q+\varphi\ , \tag{2.39}$$

where the equality of $Q+\varphi$ to $\mathcal{G}\otimes\mathcal{G}$ is allowed to be an abstract one such that it has meaning only after proper analytical continuation and does not have one-to-one correspondence for each discrete frequency variable. With the same abstractness, we define Γ_1 as

$$\Gamma_1=\Gamma_0+\Gamma_0\varphi\Gamma_1\ ; \tag{2.40}$$

then it holds that

$$\Gamma=\Gamma_1+\Gamma_1 Q\Gamma\ . \tag{2.41}$$

With these quantities, we can decompose $\mathcal{K}$ as

$$\mathcal{K}=-M\varphi(1+\Gamma_1\varphi)M-M(1+\varphi\Gamma_1)(Q+Q\Gamma Q)(1+\Gamma_1\varphi)M\ . \tag{2.42}$$

At present, the separation into Q and φ is arbitrary, and so is the decomposition of $\mathcal{K}$. Only after introducing the Fermi-liquid hypothesis and defining the concept of the quasiparticle, they will acquire appropriate physical meaning and corresponding mathematical property.

D. Susceptibility

1. Dynamical susceptibility

Let us consider the linear response of the dynamical average [defined by (A4)] of the local magnetization, $m(r,t)=\langle\hat{m}(r)\rangle(t)$, to the external field $h(r,t)$. In the Fourier component,

$$\delta m(q,\Omega)=\chi(q,\Omega)h(q,\Omega)\ . \tag{2.43}$$

We refer to this proportionality constant $\chi(q,\Omega)$ as the dynamical susceptibility. By the Kubo formula,[21] it is given by

$$\chi(q,\Omega)=\int dt\, e^{i(\Omega+i0^+)t}\chi(q,t)\ , \tag{2.44}$$

where

$$\chi(q,t-t')=iN_{\mathrm{sys}}\langle[\hat{m}(q,t),\hat{m}(-q,t)]\rangle_0\Theta(t-t')\ . \tag{2.45}$$

By rewriting $\chi(q,\Omega)$ in the spectral form, we can see that $\chi(q,\Omega)$ can be identified with $K^R(q,\Omega)$:

$$\chi(q,\Omega)\equiv K^R(q,\Omega)\ , \tag{2.46}$$

and since the spectral weight function $w(q,x)$ is real, (2.34) leads to

$$\mathrm{Im}\chi(q,\Omega)=w(q,\Omega)\ , \tag{2.47}$$

$$\mathrm{Re}\chi(q,\Omega)=\mathrm{P}\int\frac{dx}{\pi}\,\frac{w(q,x)}{x-\Omega}\ . \tag{2.48}$$

The last equation is the celebrated Kramers-Kronig relation.

It must be noticed here that $\chi(q,\Omega)$ may have singular behavior for $(q,\Omega)\approx(0,0)$: The two kinds of static uniform limits,

$$\chi^k=\lim_{q\to 0}\,[\,\lim_{\Omega\to 0}\chi(q,\Omega)]\ , \tag{2.49}$$

$$\chi^\omega=\lim_{\Omega\to 0}\,[\,\lim_{q\to 0}\chi(q,\Omega)]\ , \tag{2.50}$$

are different in general. We call them the k and ω limits, respectively.

2. *Isothermal static uniform susceptibility*

Under a static uniform field h, the total magnetization is given by

$$M_{\mathrm{tot}}(h)=\langle\hat{M}\rangle_h=\sum_k\langle\hat{\psi}^\dagger(k)M\hat{\psi}(k)\rangle_h\ , \tag{2.51}$$

where

$$\langle\hat{\psi}^\dagger(k)M\hat{\psi}(k)\rangle_h=\frac{1}{\beta}\sum_n\exp(i\omega_n 0^+)\mathrm{Tr}[M\mathcal{G}_k(i\omega_n)]\ . \tag{2.52}$$

The isothermal static uniform susceptibility (per site) is defined as

$$\chi_T=\frac{1}{N_{\mathrm{sys}}}\left[\frac{\partial M_{\mathrm{tot}}}{\partial h}\right]_{h=0}\ . \tag{2.53}$$

It can be rewritten as

$$\chi_T=\frac{1}{N_{\mathrm{sys}}}\int_0^\beta\langle\hat{M}(-i\tau)\hat{M}\rangle_0\ . \tag{2.54}$$

From this we can see that

$$\chi_T=\mathcal{K}(q=0,\,i\Omega_l=0)\ , \tag{2.55}$$

where $\mathcal{K}$ is the two-particle temperature Green's function (2.31).

3. *Static uniform susceptibilities χ^k, χ^ω, and χ_T*

So far, three kinds of the static uniform susceptibilities are defined, but the relations among them have not been clarified yet. As mentioned in Sec. II C 2, the relation between $\chi(0,0)=K^R(0,0)$ and $\chi_T=\mathcal{K}(0,0)$ is not trivial, or more precisely, $\chi(0,0)$ is not well defined in general. It is easy to make an example such that

$$\chi^\omega\neq\chi_T\ . \tag{2.56}$$

In fact, if $\hat{M}$ is conserved, $\chi^\omega=0$, while χ_T is a positive constant. On the other hand, there is no general proof of

$$\chi^k=\chi_T\ . \tag{2.57}$$

In the following we obtain formulas for both $\chi(q,\Omega)$ and χ_T separately under the Fermi-liquid hypothesis. The formulas are useful by themselves, yet the interrelation between them is not so trivial; this makes one feel uneasy to use them. One of the purposes of this paper is to give the identities, which show explicitly that the equality (2.57) holds for any multicomponent Fermi liquid, provided that $\hat{M}$ is conserved.

III. FERMI-LIQUID HYPOTHESIS

Those hypotheses on the regularities of the self-energy and the vertex parts which are required for the formation of the Fermi liquid are summarized for completeness. The novel thing is only that the renormalized A matrix $A^*_{k\alpha}$ replaces the residue of the qp pole in the usual theory.[5,22–24] Thus, after noting it, most readers can skip to the next section.

A. Fermi surface, quasiparticle, and self-energy

We will take the following hypotheses as our starting point and will make no argument for their plausibility.

Hypothesis 1. For an arbitrary k, $\mathrm{Im}\Sigma^A_k$ is infinitesimally small at $(\omega,T)=(0,0)$, and

$$\mathrm{Im}L^A_{k\alpha}(\omega,T)=0^+ + C_{k\alpha}\omega^2+D_{k\alpha}T^2+o(\omega^2,T^2)\ , \tag{3.1}$$

for $(\omega,T)\approx(0,0)$, where $C_{k\alpha}$ and $D_{k\alpha}$ are some positive constants.

In general, we know only that $\mathrm{Im}L^A_{k\alpha}\geq 0$ [Eq. (2.29)]. However, the above hypothesis states that both $\mathrm{Im}L^A_{k\alpha}$ and $\mathrm{Im}(\partial L^A_{k\alpha}/\partial\omega)$ will vanish at $(\omega,T)=(0,0)$. Hence this hypothesis restricts the behavior of the self-energy very strongly.

The Fermi surface (FS) in k space is defined as a set of points which satisfy[5]

$$\mu-\mathrm{Re}L^A_{k\alpha}(0,0)=0\ , \tag{3.2}$$

for each band index α. In the usual case, Eq. (3.2) has solution points k only for a small number of bands, if any. These small number of bands will have the FS and quasiparticles (qp's). If Eq. (3.2) does not have solution points k, neither the FS nor the qp exists and the system does not exhibit any Fermi-liquid character.[1] Thus we assume our second hypothesis.

Hypothesis 2. The FS does exist.

The qp energy measured from the chemical potential, $E^*_{k\alpha}-\mu$, is defined as the solution of

$$\omega+\mu-\mathrm{Re}L^A_{k\alpha}(\omega,0)=0 \ . \tag{3.3}$$

The qp velocity $v^*_{k\alpha}$ is defined by

$$v^*_{k\alpha}=\frac{dE^*_{k\alpha}}{dk} \ . \tag{3.4}$$

The wave-function renormalization factor $Z_{k\alpha}$ for k on the FS is defined as

$$Z_{k\alpha}=\tilde{Z}_{k\alpha}(0,0) \ , \tag{3.5}$$

where

$$\tilde{Z}_{k\alpha}(\omega,T)=\left[1-\frac{\partial}{\partial\omega}L^A_{k\alpha}\right]^{-1} \ . \tag{3.6}$$

By (3.1), $Z_{k\alpha}$ is real. Our additional assumption is

Hypothesis 3. The wave-function renormalization factor $Z_{k\alpha}$ and qp velocity $v^*_{k\alpha}$ are finite (neither zero nor infinite) on the FS.

We further assume our fourth hypothesis.

Hypothesis 4. As a function of (k,ω,T), $L^A_{k\alpha}$ is satisfactorily smooth such that $C_{k\alpha}$, $D_{k\alpha}$, $E^*_{k\alpha}$, $v^*_{k\alpha}$, and $Z_{k\alpha}$ are regular for k near the FS, as well as $\tilde{Z}_{k\alpha}(\omega,T)$ being regular for $(\omega,T)\approx(0,0)$.

For T sufficiently *low* and k sufficiently *near* the FS, the real part $\mathcal{E}^*_{k\alpha}$ and the imaginary part $\gamma^*_{k\alpha}$ of the complex solution of

$$\zeta+\mu-L^A_{k\alpha}(\zeta,T)=0 \tag{3.7}$$

are given by[25]

$$\mathcal{E}^*_{k\alpha}=E^*_{k\alpha} \ , \tag{3.8}$$

$$\gamma^*_{k\alpha}=Z_{k\alpha}\mathrm{Im}L^A_{k\alpha}(E^*_{k\alpha}-\mu,T) \ , \tag{3.9}$$

in the lowest order of $E^*_{k\alpha}-\mu$ and T; in this case, $\mathcal{E}^*_{k\alpha}$ can be used in place of $E^*_{k\alpha}$. To what extent T should be *low* and to what extent k should be *near* the FS are elucidated in the following.

B. Conditions on temperature and external field

In addition to the above hypotheses, which are necessary for the system to behave as the Fermi liquid, some additional conditions on the temperature and external field must be satisfied in order for the Fermi-liquid theory to give a good description of the response of the system. Using the energy scales T_0 and ε_0 defined later, the conditions can be stated as follows: The temperature T must be low such that

$$T\le T_0 \ , \tag{3.10}$$

and the frequency and wavelength of the external field $h(q,\Omega)$ must be sufficiently low and long such that

$$\Omega\ll\varepsilon_0, \quad q\cdot v^*_{k\alpha}\ll\varepsilon_0 \ . \tag{3.11}$$

Insofar as these conditions be satisfied, the values of T_0 and ε_0 do not enter into the final results of the Fermi-liquid theory.

The energy T_0 is the upper bound of T such that

$$Z_{k\alpha}D_{k\alpha}T^2\ll T \ , \tag{3.12}$$

and such that one can find an energy scale ε_0 simultaneously satisfying the following three conditions:

$$Z_{k\alpha}C_{k\alpha}(\varepsilon_0)^2\ll T \tag{3.13}$$

and

$$T\ll\varepsilon_0 \ , \tag{3.14}$$

$$\int\frac{d^3k}{(2\pi)^3}\Theta(\varepsilon_0-|E^*_{k\alpha}-\mu|)\ll 1 \ . \tag{3.15}$$

The value of T_0 depends on $C_{k\alpha}, D_{k\alpha}, Z_{k\alpha}$ and the shape of the FS, and in turn they depend on the details of the system; thus it is usually difficult to estimate T_0 by theory from the microscopic model. Nonetheless, the important thing is that such a temperature scale T_0 always exists under our hypotheses, however small it might be.

Under the conditions (3.10) and (3.11), the qp's excited by the thermal fluctuation or by the external field are restricted in the k-space region near the FS satisfying

$$|E^*_{k\alpha}-\mu|\le\varepsilon_0 \ , \tag{3.16}$$

and in this region of k space, the qp's are well defined in the sense that the damping $\gamma^*_{k\alpha}$ given by (3.9) is smaller than the temperature or qp energy.

The conditions (3.14) combined with (3.15) represent that T_0 is lower than the degeneracy temperature of the fermion system, which is often expressed as $T_0\ll E_F$ in the literature, where E_F is meant to be the energy of the qp on the FS measured from the bottom of the band and is used as a characteristic energy scale of the system to be compared with the temperature. However, we have intentionally avoided using E_F. It must be noted that E_F cannot have any definite meaning in the interacting case, because the bottom of the band is not well defined; moreover, even in the noninteracting case, E_F cannot serve as a characteristic energy of the band, except for those featureless bands such as the parabolic band.

C. Single-particle Green's functions

Owing to hypothesis 1, at $(\omega,T)=(0,0)$, both of the analytic continuations of $\mathcal{A}_{k\alpha}(i\omega_n,T)$ become Hermitian and coincide with each other. Let us denote this by $A_{k\alpha}$:

$$A_{k\alpha}\equiv\mathcal{A}_{k\alpha}(\zeta=\pm i0^+,\ T=0) \ . \tag{3.17}$$

By multiplying $Z_{k\alpha}$, let us define the renormalized A matrix as

$$A^*_{k\alpha}\equiv Z_{k\alpha}A_{k\alpha} \ . \tag{3.18}$$

Then, provided that the condition (3.10) is satisfied, the advanced and retarded single-particle Green's functions can be expressed as

$$\left.\begin{matrix} G_k^R(\omega) \\ G_k^A(\omega) \end{matrix}\right\} = \sum_\alpha \frac{A_{k\alpha}^* \Theta(\varepsilon_0 - |E_{k\alpha}^* - \mu|)}{\omega + \mu - E_{k\alpha}^* \mp i\gamma_{k\alpha}^*} + \left\{\begin{matrix} G_k^R(\omega) \\ G_k^A(\omega) \end{matrix}\right\}_{\text{incoherent}} . \tag{3.19}$$

The first term is nonzero only for k near the Fermi surface, while the second incoherent term will vanish for k near the Fermi surface.

In the zero temperature limit, $\gamma_{k\alpha}^*$ can be replaced with 0^+; as a result, the spectral weight function matrix can be written as

$$\rho_k(\omega) = \sum_\alpha A_{k\alpha}^* \delta(\omega + \mu - E_{k\alpha}^*) \Theta(\varepsilon_0 - |E_{k\alpha}^* - \mu|) + \rho_k'(\omega) . \tag{3.20}$$

Although the residual term $\rho_k'(\omega)$ due to the incoherent term of (3.19) is nonzero for general ω's, it will vanish at $\omega = 0$. Thus we obtain

$$\rho_k(0) = \sum_\alpha A_{k\alpha}^* \delta(\mu - E_{k\alpha}^*) . \tag{3.21}$$

D. Two-particle Green's functions

Now we can decompose $\mathcal{G} \otimes \mathcal{G}$ into the near part Q and the far part φ, where Q stems from the product of only the coherent parts of the single-particle Green's function, while φ includes at least one incoherent part. Then the qp irreducible vertex part Γ_1 can be defined through (2.40). Following Leggett,[24] we assume that, in evaluating $K^R(q,\Omega)$ under the condition of (3.10) and (3.11), the several analytic continuations of Γ_1 can be replaced with a single tensor $\Gamma^\omega(k,k';\omega,\omega';q,\Omega)$, which is regular for $\omega,\omega' \le \varepsilon_0$ and (k,k') satisfying (3.16). As a result, the near part can be identified with[26]

$$Q(k,\omega;q,\Omega) = -\sum_\alpha \Delta_{k\alpha}(q,\Omega) \delta(\mu - E_{k\alpha}^*) \delta(\omega) (A_{k\alpha}^* \otimes A_{k\alpha}^*) , \tag{3.22}$$

where

$$\Delta_{k\alpha}(q,\Omega) \equiv \frac{q \cdot v_{k\alpha}^*}{q \cdot v_{k\alpha}^* - \Omega} \delta(\mu - E_{k\alpha}^*) . \tag{3.23}$$

The near part Q is singular for $(q,\Omega) \approx (0,0)$; in particular, the ω limit vanishes:

$$Q^\omega(k,\omega) \equiv \lim_{\Omega \to 0} \lim_{q \to 0} Q(k,\omega;q,\Omega) = 0 . \tag{3.24}$$

On the other hand, the far part φ can be replaced with a regular function of (q,Ω). Since $\Gamma^\omega(k,k',\omega,\omega';q,\Omega)$ contains no near part, it can be identified with the ω limit of the full vertex part and its dependence on (q,Ω) can be neglected:

$$\Gamma^\omega(kk',\omega\omega') = \lim_{\Omega \to 0} \lim_{q \to 0} \Gamma(k,k',\omega,\omega';q,\Omega) . \tag{3.25}$$

There is generally a close relation between the self-energy and vertex part, and the statement on the regularity of the vertex part in this paragraph seems to be consistent with our hypotheses on the self-energy. Nonetheless, I am not sure of the mathematically rigorous derivation of the statement on the vertex part from the hypotheses on the self-energy. Therefore, I must take this as an additional hypothesis.

Hypothesis 5. The vertex parts have the regular property stated above.

As a result, in the zero-temperature limit and, for our purpose of evaluating the reactive part of the susceptibility, the sum over the discrete frequency variable can be replaced by the integration over the continuous imaginary frequency variable; eventually, by the Wick rotation of the path of integration, the whole formalism can be identified with the zero-temperature one.

We refer to hypotheses 1–5 as the Fermi-liquid hypothesis (FLH) as a bundle in this paper.

IV. IDENTITIES

Here we collect the identities we need in the following argument. Before listing them, a few notational conventions are made here. Owing to hypothesis 1, $\Sigma_k^A(\omega)$ and $\Sigma_k^R(\omega)$ and their derivatives are Hermitian and coincide at $(\omega,T)=(0,0)$. So we omit the superscript A or R in most cases where they are evaluated at the origin in the zero temperature. Similarly, the analytic continuations of $\mathcal{P}_k(\zeta)$ coincide at $(\omega,T)=(0,0)$ and become unitary; we denote this by P_k:

$$P_k \equiv \mathcal{P}_k(\zeta = \pm i0^+, T=0) . \tag{4.1}$$

A. Identities on the A matrix

The Hermitian matrix $A_{k\alpha}$ defined by (2.27) and (3.17) satisfies the following identities:

$$\mathrm{Tr} A_{k\alpha} = 1 , \tag{4.2}$$

$$(A_{k\alpha})^2 = A_{k\alpha} , \tag{4.3}$$

$$A_{k\alpha} \left[1 - \frac{\partial \Sigma_k}{\partial \omega} \right] A_{k\alpha} = (Z_{k\alpha})^{-1} A_{k\alpha} , \tag{4.4}$$

$$A_{k\alpha} \left[M - \frac{\partial \Sigma_k}{\partial h} \right] A_{k\alpha} = -\frac{\partial L_{k\alpha}^A}{\partial h} A_{k\alpha} . \tag{4.5}$$

From these identities it can be deduced that

$$(Z_{k\alpha})^{-1} = \mathrm{Tr} \left[\left[1 - \frac{\partial \Sigma_k}{\partial \omega} \right] A_{k\alpha} \right] , \tag{4.6}$$

$$-\left[\frac{\partial L_{k\alpha}^A}{\partial h} \right] = \mathrm{Tr} \left[\left[M - \frac{\partial \Sigma_k}{\partial h} \right] A_{k\alpha} \right] . \tag{4.7}$$

For arbitrary $\nu \times \nu$ matrices B and C, it holds that

$$(P_k^{-1} B P_k)_{\alpha\alpha} = \mathrm{Tr}(B A_{k\alpha}) \tag{4.8}$$

and

$$\mathrm{Tr}(A_{k\alpha}BA_{k\alpha}C)=\mathrm{Tr}(A_{k\alpha}B)\mathrm{Tr}(A_{k\alpha}C)\ . \tag{4.9}$$

The sum of all $A_{k\alpha}$ will become the unit matrix

$$\left[\sum_{\alpha=1}^{\nu} A_{k\alpha}\right]_{ij}=\delta_{ij}\ . \tag{4.10}$$

B. Identities free from conservation

By differentiating the defining equation of the quasiparticle energy [Eq. (3.3)], we obtain

$$\frac{\partial E^*_{k\alpha}}{\partial h}=Z_{k\alpha}\left[\frac{\partial L^A_{k\alpha}}{\partial h}\right]\ . \tag{4.11}$$

The vertex parts satisfy

$$(1+\varphi\Gamma^{\omega})(1+Q\Gamma)=1+(Q+\varphi)\Gamma\ . \tag{4.12}$$

The field derivative of the self-energy is related to the vertex part by a Ward identity[27] as

$$M[1+(Q^k+\varphi)\Gamma^k]=M-\frac{\partial\Sigma}{\partial h}\ . \tag{4.13}$$

All of the above identities are general ones free from the conservation property.

C. Identities based on conservation

The identities which stem from the conservation of $\hat{M}$ are collected in the following. If $\hat{M}$ is conserved,

$$\mathcal{K}(q=0,i\Omega_l)=0\ , \tag{4.14}$$

for all $l\neq 0$. Therefore,

$$\chi(q=0,\Omega)\equiv K^R(q=0,\Omega)=0\ , \tag{4.15}$$

for all Ω, including $\Omega=0$. In particular,

$$\chi^{\omega}=0\ . \tag{4.16}$$

In the zero-temperature limit,

$$\sum_k\frac{1}{\beta}\sum_n \exp(i\omega_n 0^+)\mathrm{Tr}\left[M\frac{\partial\Sigma_k}{\partial\zeta}\mathcal{G}_k\right]_{\zeta=i\omega_n}=0\ . \tag{4.17}$$

Note that we need only the *weak* conservation to obtain this identity (see Appendix C). The frequency derivative of the self-energy multiplied by the matrix M can be related to the vertex part by a Ward identity:

$$M(1+\varphi\Gamma^{\omega})=M\left[1-\frac{\partial\Sigma}{\partial\omega}\right]\ . \tag{4.18}$$

Multiplying (4.18) by Q and using (3.22), (4.4), and the definition of $A^*_{k\alpha}$ in (3.18), we obtain

$$M(1+\varphi\Gamma^{\omega})Q=-\sum_{\alpha}\mu_\alpha\Delta_{k\alpha}(q,\Omega)\delta(\mu-E^*_{k\alpha})\delta(\omega)A^*_{k\alpha}\ . \tag{4.19}$$

Comparing this with the definition of $\rho_k(0)$ in (3.21), one can find that (4.19) is reduced, in the k limit, to

$$-M(1+\varphi\Gamma^{\omega})Q^k=M\rho_k(0)\delta(\omega)\ . \tag{4.20}$$

D. Specific heat

In this paper we concentrate on the susceptibility and do not discuss the other experimentally obtainable quantities. However, we make a brief exception here.

It is proved by Luttinger[5] that the temperature-linear coefficient of the specific heat, γ, is given by[28]

$$\gamma=\frac{\pi^2}{3}(k_B)^2\mathcal{N}^*_{\mathrm{tot}}\ , \tag{4.21}$$

where the total qp density of states, $\mathcal{N}^*_{\mathrm{tot}}$, is given by

$$\mathcal{N}^*_{\mathrm{tot}}=\sum_{k,\alpha}\delta(\mu-E^*_{k\alpha})\ . \tag{4.22}$$

Let us define

$$\rho^*_k(0)=\sum_{\alpha}A_{k\alpha}\delta(\mu-E^*_{k\alpha})\ , \tag{4.23}$$

which differs from $\rho_k(0)$ in that $A^*_{k\alpha}=Z_{k\alpha}A_{k\alpha}$ is replaced by $A_{k\alpha}$. Then we can rewrite $\mathcal{N}^*_{\mathrm{tot}}$ as

$$\mathcal{N}^*_{\mathrm{tot}}=\sum_k \mathrm{Tr}[\rho^*_k(0)]\ , \tag{4.24}$$

where we use (4.2). Alternatively, from (3.21) and (4.6), we can rewrite $\mathcal{N}^*_{\mathrm{tot}}$ as

$$\mathcal{N}^*_{\mathrm{tot}}=\sum_k \mathrm{Tr}\left[\left[1-\frac{\partial\Sigma_k}{\partial\omega}\right]\rho_k(0)\right]\ . \tag{4.25}$$

Be careful that, since $Z_{k\alpha}$ may be very small, the qp density of states, $\rho^*_k(0)$, and the bare-particle density of states, $\rho_k(0)$, are completely different quantities.

Now let us return to our main theme, the linear response to the external field, which we refer to simply as the susceptibility.

V. SUSCEPTIBILITIES
OF THE MULTICOMPONENT FERMI LIQUID

First, utilizing the Luttinger's method,[5] we derive an expression for χ_T of the general multicomponent Fermi liquid [Eq. (5.17)] and rewrite it in a form reminiscent of the one by Yamada and Yosida[4] for the spin susceptibility of the SU(2) PAM [Eq. (5.21)]. Next, we obtained $\chi(q,\Omega)$ based on the Kubo formula and express the qp interaction function with the vertex part represented in the original local basis. Finally, we show that $\chi^k=\chi_T$ at three levels: (i) The explicit transformation form χ^k to χ_T is performed, by using the identities presented in the previous section, under the assumption that $\hat{M}$ is conserved; then (ii) a more formal mathematical origin, which is free from the conservation of $\hat{M}$, is discussed; and finally (iii) a physical interpretation is given for the characteristic (q,Ω) dependence of $\chi(q,\Omega)$.

A. Isothermal static uniform susceptibility

1. General expression

We must note, from the outset, that Luttinger's method is efficient only when $\hat{M}$ is conserved. If $\hat{M}$ is not conserved, the procedure breaks at the very first stage. It is regrettable that there is no way to escape from this breakdown. I would like to emphasize it here, because this fact is sometimes forgotten even by experts of this method.[6,7]

First, we proceed as far as possible without using the conservation of $\hat{M}$, in order to reveal where the difficulty arises when $\hat{M}$ is not conserved. The trace in (2.52) can be rewritten as

$$\mathrm{Tr}[M\mathcal{G}_k(\zeta)]=X_k(\zeta)+Y_k(\zeta)+C_k^1(\zeta)+C_k^2(\zeta)\ , \tag{5.1}$$

where

$$X_k(\zeta)=\frac{\partial}{\partial\zeta}\mathrm{Tr}[M\ln(-\mathcal{G}_k^{-1})]\ , \tag{5.2}$$

$$Y_k(\zeta)=\mathrm{Tr}\left[M\frac{\partial\Sigma_k}{\partial\zeta}\mathcal{G}_k\right]\ , \tag{5.3}$$

$$C_k^1(\zeta)=\mathrm{Tr}\left[\mathcal{P}_k\frac{\partial\mathcal{P}_k^{-1}}{\partial\zeta}\mathcal{G}_k[\mathcal{G}_k^{-1},M]\right]\ , \tag{5.4}$$

$$C_k^2(\zeta)=\mathrm{Tr}\left[\mathcal{P}_k\frac{\partial\mathcal{P}_k^{-1}}{\partial\zeta}[\ln(-\mathcal{G}_k^{-1}),M]\right]\ . \tag{5.5}$$

The frequency summation of the first term $X_k(\zeta)$ can be transformed, in the zero-temperature limit, into a very attractive form:

$$\frac{1}{\beta}\sum_n \exp(i\omega_n)X_k(i\omega_n) \tag{5.6}$$

$$=\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{0}d\omega\frac{\partial}{\partial\omega}\mathrm{Tr}\{M\ln[E_k-\mu+\Sigma_k^A(\omega)-\omega]\} \tag{5.7}$$

$$=\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\{M\ln[E_k-\mu+\Sigma_k^A(\omega=0)]\} \tag{5.8}$$

$$=\frac{1}{\pi}\sum_\alpha \mu_{k\alpha}\arg[L_{k\alpha}^A(\omega=0)-\mu] \tag{5.9}$$

$$=\sum_\alpha \mu_{k\alpha}\Theta(\mu-E_{k\alpha}^*)\ , \tag{5.10}$$

where, in the second step, we use (2.21); in the final step, we employ hypothesis 1. The quantity $\mu_{k\alpha}$, which depends on the external field in general, is defined by

$$\mu_{k\alpha}(h)\equiv(P_k^{-1}MP_k)_{\alpha\alpha} \tag{5.11}$$

$$=\mathrm{Tr}[MA_{k\alpha}(h)]\ , \tag{5.12}$$

where, in the second step, we use (4.8).

Thus the total magnetization can be written as

$$M_{\mathrm{tot}}(h)=\sum_{k,\alpha}\mu_{k\alpha}(h)\Theta(\mu-E_{k\alpha}^*(h))+M_{\mathrm{rc}}(h)\ , \tag{5.13}$$

where $M_{\mathrm{rc}}(h)$ is the residual correction due to the terms Y_k, C_k^1, and C_k^2. Hence χ_T is obtained as

$$\chi_T\equiv\frac{1}{N_{\mathrm{sys}}}\left[\frac{\partial M_{\mathrm{tot}}}{\partial h}\right]=\chi_P+\chi_V+\frac{1}{N_{\mathrm{sys}}}\left[\frac{\partial M_{\mathrm{rc}}}{\partial h}\right]\ , \tag{5.14}$$

$$\chi_P=\frac{1}{N_{\mathrm{sys}}}\sum_{k,\alpha}\left[-\frac{\partial E_{k\alpha}^*}{\partial h}\right]\mu_{k\alpha}\delta(\mu-E_{k\alpha}^*)\ , \tag{5.15}$$

$$\chi_V=\frac{1}{N_{\mathrm{sys}}}\sum_{k,\alpha}\left[\frac{\partial\mu_{k\alpha}}{\partial h}\right]\Theta(\mu-E_{k\alpha}^*)\ . \tag{5.16}$$

All the quantities are evaluated at $h=0$. We call χ_P the Pauli term and χ_V the Van Vleck term in this paper, whereas this terminology is not universal in the literature.

The Van Vleck term cannot be expressed by the qp's, because the formula (5.16) includes an integration over k far apart from the Fermi surface, where the concept of the qp does not exist. Therefore, it is very difficult or practically impossible to discuss the general property of this term; it differs case by case depending on the details of the system.

What is worse, any further simplification or even a gross estimation of the term $(\partial M_{\mathrm{rc}}/\partial h)$ is impossible in general. Thus Luttinger's method is useless, unless $\hat{M}$ is conserved.

2. *Luttinger's expression*

If $\hat{M}$ is conserved, M commutes with $\mathcal{G}_k$. Then C_k^1 and C_k^2 are simply zero. Furthermore, by identity (4.17), the summation of Y_k over both of the frequency and wave vector will vanish. In addition, the $\mu_{k\alpha}$'s become independent of h and k; they coincide with the elements of the diagonal matrix M. Thus we obtain χ_T as

$$\chi_T=\frac{1}{N_{\mathrm{sys}}}\sum_{k,\alpha}\left[-\frac{\partial E_{k\alpha}^*}{\partial h}\right]\mu_\alpha\delta(\mu-E_{k\alpha}^*)\ . \tag{5.17}$$

The Van Vleck term and residual correction term do not exist when $\hat{M}$ is conserved. Here I would like to claim that we need only the *weak* conservation of $\hat{M}$ in deriving the above expression, whereas Luttinger's original derivation for the spin susceptibility seems to require the *strong* conservation of the spin (see Appendix C).

3. *Yamada and Yosida's expression*

Utilizing the above result of Luttinger [Eq. (5.17)] and the equation

$$\det[\omega+\mu-E_k(h)-\mathrm{Re}\Sigma_k^A(\omega)]=0\ , \tag{5.18}$$

the roots of which determine the qp-band dispersion $E_{k\alpha}^*-\mu$, Yamada and Yosida[4] express the spin susceptibility of the SU(2) periodic Anderson model in terms of the spectral weight function and field derivative of the self-energy. We derive a similar expression for our more general model. For this purpose it is easier to start from (5.8):

$$\chi_T = \frac{1}{N_{\mathrm{sys}}} \sum_k \frac{1}{\pi} \frac{\partial}{\partial h} \mathrm{Im}\,\mathrm{Tr}\{M \ln[E_k(h) - \mu + \Sigma_k^A(\omega=0)]\} \tag{5.19}$$

$$= \frac{1}{N_{\mathrm{sys}}} \sum_k \mathrm{Im}\,\mathrm{Tr} \left[M \left[M - \frac{\partial \Sigma_k^A(0)}{\partial h} \right] \frac{1}{\pi} G_k^A(0) \right] \tag{5.20}$$

$$= \frac{1}{N_{\mathrm{sys}}} \sum_k \mathrm{Tr} \left[M \left[M - \frac{\partial \Sigma_k^A(0)}{\partial h} \right] \rho_k(0) \right] , \tag{5.21}$$

where, in the last step, we use the formula (2.20) and $\mathrm{Im}\Sigma_k^A(0)=0$. Let us note that the conservation of $\hat{M}$ plays a crucial role again in the above transformation: The differentiation of the logarithm of the matrix can be done in such a simple manner as in the above, because M commutes with the argument of the logarithm.

Finally, in order to confirm the consistency with Luttinger's expression (5.17), let us make a further transformation: Using (3.21) and (4.7), Eq. (5.21) is transformed as

$$\chi_T = \frac{1}{N_{\mathrm{sys}}} \sum_{k\alpha} \mathrm{Tr} \left[M \left[M - \frac{\partial \Sigma_k^A(0)}{\partial h} \right] A_{k\alpha} \right] Z_{k\alpha} \delta(\mu - E_{k\alpha}^*) \tag{5.22}$$

$$= \frac{1}{N_{\mathrm{sys}}} \sum_{k\alpha} \mu_\alpha \left[- Z_{k\alpha} \left[\frac{\partial L_{k\alpha}^A}{\partial h} \right] \right] \delta(\mu - E_{k\alpha}^*) \; . \tag{5.23}$$

By identity (4.11), this reduces to (5.17). Thus the consistency is confirmed, or (5.17) is proved by an alternative way.

B. Dynamical susceptibility

We restrict ourselves to the low temperature, low frequency, and long wavelength in the sense described in Sec. III B.

1. *Expected phenomenology*

Let us first present the equations to be derived: The qp part of $\chi(q,\Omega)$ is expected to be obtained as follows.[29,30] Under the external field $h(r,t)$, the space-time-dependent qp energy $\mathcal{E}_{k\alpha}^*(r,t)$ is given by

$$\mathcal{E}_{k\alpha}^*(r,t) = E_{k\alpha}^* - \mu_{k\alpha}^* h(r,t) + \sum_{k',\beta} f_{\alpha\beta}(k,k') \delta n_{k'\beta}(r,t) \; , \tag{5.24}$$

where $E_{k\alpha}^*$ is the qp energy in zero field, $\mu_{k\alpha}^*$ the effective moment of the qp, $f_{\alpha\beta}(k,k')$ the Landau qp interaction function, and $\delta n_{k\alpha}(r,t)$ the deviation of the qp distribution function from $\Theta(\mu - E_{k\alpha}^*)$. In the collisionless regime, $n_{k\alpha}$ is governed by

$$\left[\frac{\partial}{\partial t} + \frac{dr}{dt} \frac{\partial}{\partial r} + \frac{dk}{dt} \frac{\partial}{\partial k} \right] n_{k\alpha}(r,t) = 0 \; , \tag{5.25}$$

with

$$\frac{dr}{dt} = v_{k\alpha}^* , \quad \frac{dk}{dt} = \frac{\partial \mathcal{E}_{k\alpha}^*}{\partial r} \; . \tag{5.26}$$

Combining these and taking the Fourier transform, δn satisfies the following linearized Landau-Boltzmann kinetic equation to the first order in h:

$$(\Omega - q \cdot v_{k\alpha}^*) \delta n_{k\alpha}(q,\Omega) = q \cdot v_{k\alpha}^* \delta(\mu - E_{k\alpha}^*) \left[-\mu_{k\alpha}^* h(q,\Omega) + \sum_{k',\beta} f_{\alpha\beta}(k,k') \delta n_{k'\beta}(q,\Omega) \right] , \tag{5.27}$$

which can be solved as

$$\frac{\delta n_{k\alpha}(q,\Omega)}{h(q,\Omega)} = \Delta_{k\alpha}(q,\Omega) \mu_{k\alpha}^* - \Delta_{k\alpha}(q,\Omega) \sum_{k',\beta} S_{\alpha\beta}(k,k';q,\Omega) \Delta_{k'\beta}(q,\Omega) \mu_{k'\beta}^* \; , \tag{5.28}$$

with

$$S_{\alpha\beta}(k,k';q,\Omega) = f_{\alpha\beta}(k,k') - \sum_{k'',\gamma} f_{\alpha\gamma}(k,k'') \Delta_{k''\gamma}(q,\Omega) S_{\gamma\beta}(k'',k';q,\Omega) \; , \tag{5.29}$$

where $\Delta_{k\alpha}(q\Omega)$ is defined in (3.23). Since the local magnetization is given by

$$\delta m(r,t)=\sum_{k,\alpha}\mu^*_{k\alpha}\delta n_{k\alpha}(r,t)\ , \tag{5.30}$$

the dynamical susceptibility

$$\chi(q,\Omega)=\frac{\delta m(q,\Omega)}{h(q,\Omega)}=\sum_{k\alpha}\mu^*_{k\alpha}\frac{\delta n_{k\alpha}(q,\Omega)}{h(q,\Omega)} \tag{5.31}$$

is obtained as

$$\chi_{\text{qp}}(q,\Omega)=\sum_{k,\alpha}(\mu^*_{k\alpha})^2\Delta_{k\alpha}(q,\Omega)-\sum_{k,k'}\sum_{\alpha,\beta}\mu^*_{k\alpha}\Delta_{k\alpha}(q,\Omega)S_{\alpha\beta}(k,k';q,\Omega)\Delta_{k'\beta}(q,\Omega)\mu^*_{k'\beta}\ . \tag{5.32}$$

The above derivation of Eqs. (5.29) and (5.32) is purely phenomenological. In the following, however, we can derive the equations logically and can reveal what $\mu^*_{k\alpha}$ and $f_{\alpha\beta}(k,k')$ are at all.

2. Decomposition

Applying the decomposition of $\mathcal{G}\otimes\mathcal{G}$ defined in Sec. III D to (2.42) and (2.41), we obtain

$$\chi(q,\Omega)=\chi_{\text{nqp}}+\chi_{\text{qp}}(q,\Omega)\ , \tag{5.33}$$

where

$$\chi_{\text{nqp}}=-M\varphi(1+\Gamma^{\omega}\varphi)M\ , \tag{5.34}$$

$$\chi_{\text{qp}}=-M(1+\varphi\Gamma^{\omega})(Q+Q\Gamma Q)(1+\Gamma^{\omega}\varphi)M\ , \tag{5.35}$$

and

$$\Gamma=\Gamma^{\omega}+\Gamma^{\omega}Q\Gamma\ . \tag{5.36}$$

The non-qp part χ_{nqp} is smooth for small (q,Ω), and so we can replace (q,Ω) by (0,0) and take it as a constant, as the notation implies. The qp part χ_{qp} is singular for $(q,\Omega)\approx(0,0)$:

$$\chi^{\omega}_{\text{qp}}\equiv\chi_{\text{qp}}(q\equiv 0,\ \Omega\rightarrow 0)=0\ , \tag{5.37}$$

$$\chi^{k}_{\text{qp}}\equiv\chi_{\text{qp}}(q\rightarrow 0,\ \Omega\equiv 0)>0\ . \tag{5.38}$$

Finally, note that, because of these limiting behavior of χ_{qp}, the ω limit of the dynamical susceptibility χ^{ω} coincides with the non-qp part:

$$\chi^{\omega}=\chi_{\text{nqp}}\ . \tag{5.39}$$

3. Quasiparticle part

By virtue of identity (4.9), the intermediate tensor product including Q given by (3.22) over the local-basis indices can be decoupled into the matrix product over the qp-band indices. For example, the tensor product in $\Gamma^{\omega}Q\Gamma$,

$$\begin{aligned}[\Gamma^{\omega}(A^*_{k\alpha}\otimes A^*_{k\alpha})\Gamma]^{ij}_{lm}&=(\Gamma^{\omega})^{ir}_{lt}(A^*_{k\alpha}\otimes A^*_{k\alpha})^{rs}_{tu}(\Gamma)^{sj}_{um}\\&=(\Gamma^{\omega})^{ir}_{lt}(A^*_{k\alpha})_{sr}(A^*_{k\alpha})_{tu}(\Gamma)^{sj}_{am}\ ,\end{aligned} \tag{5.40}$$

can be decoupled as

$$[(\Gamma^{\omega})^{ir}_{lt}(A^*_{k\alpha})_{tr}]\times[(A^*_{k\alpha})_{us}(\Gamma)^{sj}_{um}] \tag{5.41}$$

$$=[(\Gamma^{\omega}A^*_{k\alpha})\times(A^*_{k\alpha}\Gamma)]^{ij}_{lm}\ , \tag{5.42}$$

and there remains the summation over the qp-band index.[31]

Now, substitute (3.22) into (5.35) and (5.36), and then apply the above technique. This yields exactly the expected formulas (5.32) and (5.29) with the quantities defined as follows:[32]

$$\mu^*_{k\alpha}=M(1+\varphi\Gamma^{\omega})A^*_{k\alpha}\ , \tag{5.43}$$

$$f_{\alpha\beta}(k,k')=A^*_{k\alpha}\Gamma^{\omega}(k,k')A^*_{k'\beta}\ , \tag{5.44}$$

$$S_{\alpha\beta}(k,k';q,\Omega)=A^*_{k\alpha}\Gamma(k,k';q,\Omega)A^*_{k'\beta}\ . \tag{5.45}$$

Thus we accomplish giving a microscopic foundation to the phenomenology given in Sec. V B 1, while relating the phenomenological parameters to the microscopically definable quantities.

If $\hat{M}$ is conserved, the results are simplified further as follows. From (5.39) and (4.16), it is deduced that

$$\chi_{\text{nqp}}(0,0)=0\ . \tag{5.46}$$

Thus the low-frequency and long-wavelength response to the external field is completely determined by the qp's near the Fermi surface with dispersion $E^*_{k\alpha}$. In addition, we can show that the qp effective moment $\mu^*_{k\alpha}$ is not renormalized at all in this case: Substituting (4.18) into (5.43) and using (4.4), we obtain

$$\mu^*_{k\alpha}=\text{Tr}(MA_{k\alpha})=\mu_{\alpha}\ . \tag{5.47}$$

Therefore, the qp, which is a very complex object if defined with respect to the bare particle, couples to the external field exactly the same as the bare particle. Note that this rather fortunate result is due to the conservation of $\hat{M}$. In general, the coupling of the qp to the external field may be very complicated, as well as there being a complication due to the existence of the non-qp part.

4. Advantage of our formalism

Jones and MaClure[11] have already derived the above result, working on the qp-band basis throughout. The vertex part in their representation is given in our formulation as

$$\Gamma^{\omega}_{\alpha\beta}(k,k')\equiv A_{k\alpha}\Gamma^{\omega}(k,k')A_{k'\beta}\ , \tag{5.48}$$

which is related to $f_{\alpha\beta}$ as

$$f_{\alpha\beta}(k,k')=Z_{k\alpha}\Gamma^{\omega}_{\alpha\beta}(k,k')Z_{k'\beta} \; . \tag{5.49}$$

Although the final result is the same, as it must be so, the formulation of ours with the A matrix has the following advantage compared with that of Jones and MaClure: The identity of the original local basis is made to be transparent as well as its relation to the qp-band basis.

The information connecting the local basis with the qp-band basis is contained in the matrix $A^*_{k\alpha}$ defined by (2.27), (3.17), and (3.18). Written explicitly, for example,

$$f_{\alpha\beta}(k,k')=\sum_{i,j,l,m}(A^*_{k\alpha})_{ij}[\Gamma^{\omega}(k,k')]^{il}_{jm}(A^*_{k'\beta})_{ml} \; . \tag{5.50}$$

Here, recalling that the indices i,j,l,m are the local-basis indices, our purpose of relating the qp-band basis and the original local basis is completely achieved. Although we admit that expressions such as (5.50) are not so elucidating in general, most of the elements of Γ^{ω} will vanish and an expression such as (5.50) will become neat and useful on some occasions.

Furthermore, the factor $Z_{k\alpha}$, which is originally defined in the qp-band basis by (3.5) and (3.6), can also be expressed in the original local basis through (4.6). The matrix $A_{k\alpha}$, whose trace is unity, gives the constitution of the qp in the αth band of the wave number k with respect to the original local basis. Yip[10] has partly attained the same purposes as ours; he has succeeded in reformulating the Fermi-liquid theory retaining the identity of the c and f electrons for one of the simplest periodic Anderson models (PAM's). However, his method depends heavily on the special simplicity of his PAM Hamiltonian. On the contrary, my formulation and results accomplish the same purpose in a form independent of any specific character of the Hamiltonian.

C. χ^k, χ^{ω}, and χ_T

As we have seen, the behavior of $\chi(q,\Omega)$ based on the Kubo formula is singular for $(q,\Omega)\approx(0,0)$. For example, if $\hat{M}$ is conserved, $\chi^{\omega}=0$, while $\chi^k>0$. From this, one could expect that the static uniform susceptibility one obtains experimentally should be identified with the k limit χ^k and it would coincide with χ_T. Nonetheless, this is not trivial in principle. In fact, Yip complains that he cannot see the equivalence between his χ^k and Yamada and Yosida's χ_T for the spin susceptibility of the SU(2) PAM. The same complaint can be posed on our more general formula for χ_T and χ^k; they are considerably different at first sight. Thus let us investigate the relation between our χ^k and χ_T.

1. Explicit derivation of $\chi^k=\chi_T$ for conserved magnetization

Below, we show explicitly that the k limit of $\chi(q,\Omega)$ based on the Kubo formula can be reduced to χ_T obtained by Luttinger's method, for the most general multicomponent Fermi liquid (MCFL), under the condition that the magnetization is conserved:

$$\chi^k=\chi^k_{\mathrm{qp}} \tag{5.51}$$

$$=-M(1+\varphi\Gamma^{\omega})(Q^k+Q^k\Gamma Q^k)(1+\Gamma^{\omega}\varphi)M \tag{5.52}$$

$$=-M(1+\varphi\Gamma^{\omega})(1+Q^k\Gamma)Q^k(1+\Gamma^{\omega}\varphi)M \tag{5.53}$$

$$=-M[1+(Q^k+\varphi)\Gamma]Q^k(1+\Gamma^{\omega}\varphi)M \tag{5.54}$$

$$=-\left[M-\frac{\partial\Sigma}{\partial h}\right]Q^k(1+\Gamma^{\omega}\varphi)M \tag{5.55}$$

$$=\sum_k \mathrm{Tr}\left[M\left[M-\frac{\partial\Sigma_k(0)}{\partial h}\right]\rho_k(0)\right] \tag{5.56}$$

$$=\chi_T \; . \tag{5.57}$$

In the above transformations, we use successively the fact that the non-qp part vanishes [Eq. (5.46)], the definition of the qp part [Eq. (5.35)], identity (4.12), a Ward identity (4.13), identity (4.20), and our formula for χ_T [Eq. (5.21)].

This resolves positively the question posed by Yip that his χ^k for the SU(2) PAM seems different from χ_T of Yamada and Yosida, in the most general form applicable to any conserved quantity of any MCFL.

2. Mathematical origin

In the above transformation, the condition that $\hat{M}$ is conserved has been crucial; yet we expect that the equivalence $\chi^k=\chi_T$ holds more generally. Below is a sketch of the mathematical origin of this equivalence at a more general but less rigorous level.

The neighboring two poles of the first order at $E^*_{k+q}-\mu-i\Omega_l$ and at $E^*_k-\mu$, which appears in $K^R(q,\Omega)=\chi(q,\Omega)$ [see (3.22)], yield the following factor, under the operation $(\beta)^{-1}\sum_n\sum_k$ and after the analytic continuation $i\Omega_l\rightarrow\Omega+i0^+$:

$$\frac{1}{i\omega_n+i\Omega_l+\mu-E^*_{k+q}}\,\frac{1}{i\omega_n+\mu-E^*_k}$$
$$\sim\frac{f(E^*_{k+q})-f(E^*_k)}{E^*_{k+q}-E^*_k-\Omega}\delta(\omega)$$
$$=\frac{-q\cdot v^*_k}{q\cdot v^*_k-\Omega}\delta(\mu-E^*_k)\delta(\omega) \; , \tag{5.58}$$

where $f(x)$ is the Fermi distribution function

$$f(x)=\frac{1}{e^{\beta(x-\mu)}+1} \; , \tag{5.59}$$

whose derivative reduces to the δ function in the zero-temperature limit:

$$\frac{df}{dx}=-\delta(\mu-x) \; . \tag{5.60}$$

On the other hand, the single pole of the second order at $E^*_k-\mu$, which appears in $\mathcal{H}(q=0,i\Omega_l=0)=\chi_T$, yields the following factor:

$$\frac{1}{(i\omega_n+\mu-E^*_k)^2}\sim-\delta(\mu-E^*_k)\delta(\omega) \; . \tag{5.61}$$

The k limit of (5.58) coincides with (5.61), while the ω limit of (5.58) vanishes. Thus the k limit of $K^R(q,\Omega)$ coincides with $\mathcal{K}(q=0, i\Omega_l=0)$.

In fact, the summation over ω_n must be performed after multiplying extra factors, such as $\Gamma^{\omega}(\omega,\omega')$ and $\hat{Z}(\omega)$. However, with our Fermi-liquid hypothesis, such factors are expected to be satisfactorily well behaved. Hence the above consideration on the poles exhausts the mathematical origin of the equivalence between χ^k and χ_T of the Fermi liquid.

3. Physical interpretation

Let me make a digression departing from the Fermi liquid and present a physical interpretation of the characteristic behavior of $\chi(q,\Omega)$ for $(q,\Omega)\approx(0,0)$, which seems to be valid beyond the case of the Fermi liquid.

The trouble in the Kubo formula is that, since the statistical density operator develops adiabatically and there is no outer magnetic-moment bath, the system cannot respond to the uniform field if the total magnetization of the system is conserved. Therefore, let us think of the following *gedanken* experiment in which the external field is nearly uniform but not completely uniform.

First, we abruptly apply an external field $h(r)$ of the spatial profile depicted in Fig. 4(a). Then the magnetic moment $m(r)$ will grow and eventually stop changing; the final profile of $m(r)$ would be like the one depicted in Fig. 4(b). By $\tau_{\text{relax}}(l_{\text{ext}})$, we denote the time for this to take place. We expect the final ratio of $m(r_0)/h(r_0)$ would be equal to χ_T, because the outer region can play a role of the bath of the magnetic moment as well as the thermal energy.

Now let us assume that $\hat{M}$ is conserved; then all the magnetic moments appearing in this region of linear size l_{ext} must come from the outer region by the flow through the boundary. Therefore, $\tau_{\text{relax}}(l_{\text{ext}})$ is a limitlessly increasing function of l_{ext}.

Next, we make the external field oscillate with a period τ_{ext}. If the oscillation is too rapid or, more quantitatively, if

$$\tau_{\text{ext}} \ll \tau_{\text{relax}}(l_{\text{ext}}) \ , \qquad (5.62)$$

then $m(r,t)$ cannot follow the external field, and hence the response to the external field is to be zero. On the other hand, if the oscillation is slow enough, i.e.,

$$\tau_{\text{ext}} \gg \tau_{\text{relax}}(l_{\text{ext}}) \ , \qquad (5.63)$$

then $m(r,t)$ can follow the external field; the ratio $m(r_0,t)/h(r_0,t)$ is expected to be independent of time t and again equal to χ_T.

Finally, we apply the external field $h(r,t)\propto e^{i(qr-\Omega t)}$. Then we can make the following replacements:

$$l_{\text{ext}} = 2\pi/|q| \ , \qquad (5.64)$$

$$\tau_{\text{ext}} = 2\pi/\Omega \ . \qquad (5.65)$$

If we take the limit $|q|\to 0$ first (the ω limit), condition (5.62) is realized, because $\tau_{\text{relax}}(l_{\text{ext}})$ becomes infinite, as mentioned above; thus the ω limit of $\chi(q,\Omega)$ will vanish.

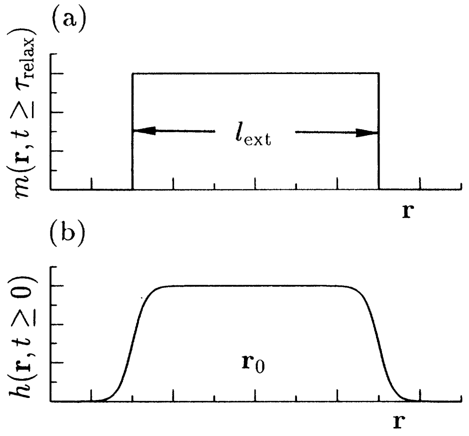

FIG. 4. Spatial profile of $h(r)$ and $m(r)$ in the *gedanken* experiment.

On the contrary, if we take the limit $\Omega\to 0$ first (the k limit), τ_{ext} becomes infinite, and hence condition (5.63) is fulfilled; thus the k limit of $\chi(q,\Omega)$ will coincide with χ_T.

On the other hand, for the unconserved part of the magnetization, $\tau_{\text{relax}}(l_{\text{ext}})$ is expected to become constant, independent of l_{ext} for sufficiently large l_{ext}. Therefore, condition (5.63) is always realized as $\Omega\to 0$. Thus this part of $\chi(q,\Omega)$ is insensitive to the order of the two limits.

The digression ends here. We return to the susceptibility of the Fermi liquid. Before proceeding to some example calculations on the periodic Anderson models, let us make one more and final general consideration, this time on how to make approximations in our Fermi-liquid theory, in particular, on what is called the random-phase approximation (RPA).

D. Susceptibilities in the RPA

One inevitably uses some approximations in calculating the values of the susceptibilities. In order to preserve the Ward identities or the other identities deduced from the conservation property, and hence in order to make applicable the general theory developed by using these identities, such as the one given in the former part of this paper, we must be careful to retain the consistency between the self-energy and vertex part in approximating them. The simplest approximation satisfying this consistency is the one in which the self-energy and irreducible vertex part are approximated by the diagrams in Figs. 5 and 6. In other words, the single-particle Green's function is approximated by the self-consistent Hartree-Fock approximation, while the two-particle Green's function by the random-phase approximation: The diagrams

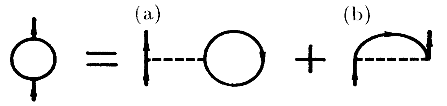

FIG. 5. Self-energy in the RPA. The thick line represents the full single-particle Green's function.

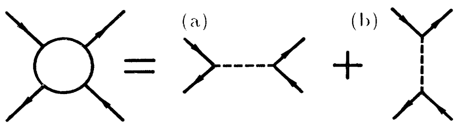

FIG. 6. Irreducible vertex part in the RPA.

contributing to the susceptibility are depicted in Fig. 7. We refer to this set of approximations simply as the RPA in this paper.

In the RPA the self-energy and, hence, the transformation matrix $\mathcal{P}_k$ are independent of the frequency variable. Therefore, the terms Y_k, C_k^1, and C_k^2 in (5.1) will automatically vanish, and so $M_{rc}=0$. Thus χ_T^{RPA} is given by

$$\chi_T^{RPA}=\chi_P^{RPA}+\chi_V^{RPA} , \tag{5.66}$$

$$\chi_P^{RPA}=\frac{1}{N_{sys}}\sum_{k,\alpha}\left[-\frac{\partial E_{k\alpha}^*}{\partial h}\right]\mu_{k\alpha}\delta(\mu-E_{k\alpha}^*) , \tag{5.67}$$

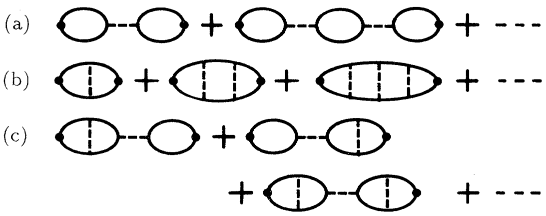

FIG. 7. Three types of diagrams contributing to the RPA susceptibility: (a) the bubble type ones, (b) the ladder type ones, and (c) the mixed ones.

$$\chi_V^{RPA}=\frac{1}{N_{sys}}\sum_{k,\alpha}\left[\frac{\partial \mu_{k\alpha}}{\partial h}\right]\Theta(\mu-E_{k\alpha}^*) . \tag{5.68}$$

The field derivative of $E_{k\alpha}^*$ and $\mu_{k\alpha}$ can be obtained as follows: Since $Z_{k\alpha}=1$ in the RPA, (4.7) and (4.11) reduce to

$$-\frac{\partial E_{k\alpha}^*}{\partial h}=\mathrm{Tr}\left[\left[M-\frac{\partial \Sigma^{RPA}}{\partial h}\right]A_{k\alpha}\right] . \tag{5.69}$$

Starting from (5.12), we can deduce[33]

$$\frac{\partial \mu_{k\alpha}}{\partial h}=\sum_{\beta(\neq\alpha)}\frac{1}{E_{k\beta}^*-E_{k\alpha}^*}\mathrm{Tr}\left[\left[M-\frac{\partial \Sigma^{RPA}}{\partial h}\right](A_{k\alpha}MA_{k\beta}+A_{k\beta}MA_{k\alpha})\right] . \tag{5.70}$$

On the other hand, we can naturally decompose the dynamical susceptibility into the qp and non-qp parts by separating $\mathcal{G}\otimes\mathcal{G}$ into Q and φ as

$$Q(k,\omega;q,\Omega)=\sum_{\alpha}\mathcal{G}_{k+q}^{(\alpha)}(i\omega_n+i\Omega_l)\otimes\mathcal{G}_k^{(\alpha)}(i\omega_n) , \tag{5.71}$$

$$\varphi(k,\omega;q,\Omega)=\sum_{\substack{\alpha,\beta\\(\alpha\neq\beta)}}\mathcal{G}_{k+q}^{(\beta)}(i\omega_n+i\Omega_l)\otimes\mathcal{G}_k^{(\alpha)}(i\omega_n) , \tag{5.72}$$

where $\mathcal{G}_k^{(\alpha)}$ is the summand of (2.26):

$$\mathcal{G}_k^{(\alpha)}(\zeta)=\frac{A_{k\alpha}}{\zeta+\mu-E_{k\alpha}^*} . \tag{5.73}$$

Note that the A matrix is independent of the frequency variable in the RPA.

Although $\chi_V=\chi_{nqp}$ when $\hat{U}=0$, they do not coincide in the RPA. Substitute (5.69) and (5.70) into (5.67) and (5.68), and then apply identity (4.13); this reveals that

$$\chi_P^{RPA}=-MQ^k[1+\Gamma^k(Q^k+\varphi)]M , \tag{5.74}$$

$$\chi_V^{RPA}=-M\varphi[1+\Gamma^k(Q^k+\varphi)]M . \tag{5.75}$$

Comparing these formulas with (5.34) and (5.35), we can understand well why χ_P and χ_V are not equivalent to χ_{qp} and χ_{nqp}. The origin of the inequivalence is that $\partial\Sigma/\partial h$ and thus χ_V include the diagrams which vanish in the ω limit.

At this point you might think that what is wrong is our terminology, and think that we should simply call χ_{qp} and χ_{nqp} the Pauli and Van Vleck terms (actually, this terminology is sometimes used). What I would like to emphasize here is that the naive definition of the Pauli and Van Vleck terms cannot be extended easily when $\hat{U}\neq 0$ if one considers only the isothermal static uniform susceptibility as in Sec. V A. On the other hand, the decomposition of the dynamical susceptibility $\chi(q,\Omega)$ into the qp and non-qp parts will never be obscured because of their characteristic dependence on (q,Ω). This ends the part of the general formalism.

VI. PERIODIC ANDERSON MODEL

In this section we apply the general formalism we have constructed thus far to three kinds of the periodic Anderson models.

The first PAM we consider is the so-called SU(N) PAM, which is widely used in the $1/N$ expansion and which includes, as a special case ($N=2$), the simplest PAM in which the c and f electrons have only the spin-$\frac{1}{2}$ degeneracy. For this SU(N) PAM, we derive formulas for χ_T and $\chi(q,\Omega)$. The resultant formulas are only simple and rather trivial generalizations of the ones obtained by Yamada and Yosida[4] and Yip,[10] respectively, for the SU(2) PAM. My emphasis here is on the utility of our formalism, which enables one to reach the final desired

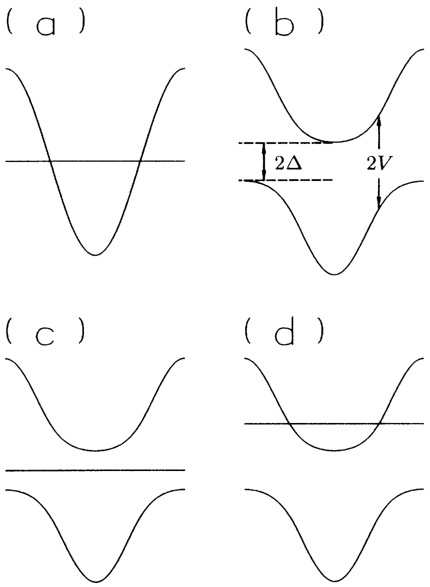

FIG. 8. Schematic band structure of the PAM's: (a) unhybridized c band and f level(s) ($V=0$), (b) hybridized band of the DD PAM, (c) hybridized band of the OD PAM ($U=0$), and (d) Hartree-Fock band of the OD PAM ($U\neq 0$).

results far more easily and simply.

In the second model, the spins of the c and f electrons are allowed to have different g values, while the degeneracy of the spin is retained to be 2; we call this model the doubly degenerate (DD) PAM. In the third model, which we call the orbitally degenerate (OD) PAM, the c and f electrons have different degeneracies. In these two models, the magnetization is not conserved, and hence the non-qp part of the susceptibility exists, in contrast with the SU(N) PAM. Thus we carefully obtain the qp and non-qp parts separately, although the treatment is restricted in the RPA. The schematic band structures of the DD and OD PAM's are illustrated in Figs. 8(b) and 8(c); in the former no band or level remains in the hybridization gap, while some remain in the latter. As a result, the non-qp parts of these two models show completely different character as a function of the hybridization between the c and f electrons and as a function of the Coulomb repulsion between the f electrons. The results of these example calculations are found to be helpful in discussing the Wilson-ratio problem in the next section.

A. SU(N) periodic Anderson model

1. *Model*

The SU(N) PAM is defined as follows. The electron has $2\times N$ components locally:

$$\hat{\psi}^\dagger(r)=(\hat{\psi}^\dagger_{(-J)}(r),\hat{\psi}^\dagger_{(-J+1)}(r),\ldots,\hat{\psi}^\dagger_J(r)) \ , \tag{6.1}$$

$$\hat{\psi}^\dagger_\lambda(r)=[\hat{c}^\dagger_\lambda(r),\hat{f}^\dagger_\lambda(r)] \ , \tag{6.2}$$

where $N=2J+1$, with N an integer, and the flavor λ takes the values from $-J$ to J. The $2N\times 2N$ matrix E_k in the one-body part of the Hamiltonian can be decomposed into the direct sum of N pieces of 2×2 matrices $E_{k\lambda}$:

$$E_k\equiv E_{k(-J)}\oplus E_{k(-J+1)}\oplus\cdots\oplus E_{kJ} \tag{6.3}$$

$$=\begin{bmatrix} E_{\mathbf{k}(-J)} & & \\ & \ddots & \\ & & E_{kJ}\end{bmatrix} , \tag{6.4}$$

where

$$E_{k\lambda}=\begin{bmatrix}\varepsilon_k & V_k^* \\ V_k & E_k^f\end{bmatrix} . \tag{6.5}$$

The two-body part of the Hamiltonian is of the form

$$\hat{U}=\frac{1}{2N_{\text{sys}}}\sum_{\lambda,\lambda'}\sum_{k,p,q}U(k,p,q)\hat{f}^\dagger_\lambda(p)\hat{f}^\dagger_{\lambda'}(q)\times\hat{f}_{\lambda'}(q-k)\hat{f}_\lambda(p+k) \ . \tag{6.6}$$

The local magnetization is defined as[34]

$$\hat{m}(r)=\sum_\lambda\lambda\hat{\psi}^\dagger_\lambda(r)\begin{bmatrix}g & 0\\ 0 & g\end{bmatrix}\hat{\psi}_\lambda(r) \ ; \tag{6.7}$$

i.e., the $2N\times 2N$ matrix M is given by

$$M=\mu_{(-J)}\mathbb{1}\oplus\mu_{(-J+1)}\mathbb{1}\oplus\cdots\oplus\mu_J\mathbb{1} \ , \tag{6.8}$$

where $\mathbb{1}$ is the 2×2 unit matrix and $\mu_\lambda=g\lambda$.

In order to apply the $1/N$ expansion, $E_{k\lambda}$ must be independent of the flavor λ, and it is desirable that $U(k,p,q)=U$ (where U is a constant). However, we do not need these restrictions in deriving the general expression of the susceptibility below. In addition, we can take μ_λ arbitrary, departing from the SU(N) symmetry.

The important assumptions for us are only that the c and f electrons have the same degeneracy and that both the hybridization and two-body interaction conserve the magnetic moment. The additional assumption which makes the results considerably simple is that the two-body interaction acts only between the f electrons.

2. *Susceptibility*

Because of the conservation of the magnetization, the self-energy and spectral weight function can be decomposed into a direct sum such as E_k and M as

$$\Sigma_k=\Sigma_{k(-J)}\oplus\Sigma_{k(-J+1)}\oplus\cdots\oplus\Sigma_{kJ} \ , \tag{6.9}$$

$$\rho_k=\rho_{k(-J)}\oplus\rho_{k(-J+1)}\oplus\cdots\oplus\rho_{kJ} \ . \tag{6.10}$$

Since the interaction is only between the f electrons, the self-energy matrix has only the f-f element:

$$\Sigma_{k\lambda}=\begin{bmatrix}0 & 0\\ 0 & \Sigma^f_{k\lambda}\end{bmatrix} , \tag{6.11}$$

while all the elements of the spectral weight function are finite in general:

$$\rho_{k\lambda}=\begin{bmatrix}\rho^{c}_{k\lambda} & \rho^{cf}_{k\lambda}\\ \rho^{fc}_{k\lambda} & \rho^{f}_{k\lambda}\end{bmatrix} . \tag{6.12}$$

Substituting these to the general formula (5.21) for χ_T, it is easy to obtain the result

$$\chi_T=\frac{1}{N_{\text{sys}}}\sum_{k,\sigma}\left[(\mu_\lambda)^2\rho^{c}_{k\lambda}(0)\right.$$
$$\left.+\left[(\mu_\lambda)^2-\mu_\lambda\frac{\partial\Sigma^{f}_{k\lambda}(0)}{\partial h}\right]\rho^{f}_{k\lambda}(0)\right] . \tag{6.13}$$

The off-diagonal terms of $\rho_{k\lambda}$ do not appear in the above expression owing to the special simplicity of the two-body interaction of the present model.

Now let us assume that the Fermi surface lies wholly in the lower bands. Then we need only the renormalized A matrix for the lower bands (we use the symbol a^{α}_{k} instead of $A^{*}_{k\alpha}$ in the following and reserve the subscript for the flavor index),

$$a_k^{-}=a^{-}_{k(-J)}\oplus a^{-}_{k(-J+1)}\oplus\cdots\oplus a^{-}_{kJ} , \tag{6.14}$$

and so let us denote the elements of $a^{-}_{k\lambda}$ simply (without an index of the lower band) as

$$a^{-}_{k\lambda}=\begin{bmatrix}a^{c}_{k\lambda} & a^{cf}_{k\lambda}\\ a^{fc}_{k\lambda} & a^{f}_{k\lambda}\end{bmatrix} . \tag{6.15}$$

Similarly, the qp interaction function f has elements only between the lower bands, and so we denote it simply, without indices of the lower band, as $f_{\lambda\lambda'}(k,k')$. This $f_{\lambda\lambda'}(k,k')$ can be expressed with the elements of $a^{-}_{k\lambda}$ and vertex part $\Gamma^{\omega}(k,k')$.

Out of the $(2N)^4$ elements of the vertex parts Γ, N^4 terms will be identically zero, because the c electrons do not interact:

$$[\Gamma^{\omega}(k,k')]^{(c\lambda_1)(c\lambda_2)}_{(c\lambda_3)(c\lambda_4)}=0 . \tag{6.16}$$

In the expression of the susceptibility, only the following elements will appear:

$$\Gamma^{\omega}_{f}(k,k';\lambda,\lambda')\equiv[\Gamma^{\omega}(k,k')]^{(f\lambda)(f\lambda')}_{(f\lambda)(f\lambda')} . \tag{6.17}$$

Using this, we can write the qp interaction function as

$$f_{\lambda\lambda'}(k,k')=a^{f}_{k\lambda}a^{f}_{k'\lambda'}\Gamma^{\omega}_{f}(k,k';\lambda,\lambda') . \tag{6.18}$$

Because of the conservation, the magnetic moments are not renormalized: The qp of the flavor λ has the same effective moment μ_λ as the bare particle. In addition, the non-qp part of the dynamical susceptibility does not exist, again because of the conservation. Therefore, now that we have obtained the interaction function and effective moment of the qp's, we can completely determine the dynamical susceptibility for low frequencies and long wavelengths.

We will not pursue further simplifications as a result of the spatial isotropy or the spherical symmetry, which is incompatible with the lattice translational symmetry.

The results corresponding to (6.13) and (6.18) for the SU(2) PAM have already been obtained by Yamada and Yosida[4] and Yip,[10] respectively. The advantage of our formalism is that similar final results can be obtained much more easily and systematically as above.

B. Doubly degenerate PAM

1. Model

In order to make the simplest example in which the non-qp part of the susceptibility exists, we modify the SU(2) PAM as allowing the spin of the c and f electrons to have different g values:

$$\hat{m}(r)=\sum_{\sigma}\sigma\hat{\psi}^{\dagger}_{\sigma}(r)\begin{bmatrix}g^{c} & 0\\ 0 & g^{f}\end{bmatrix}\hat{\psi}_{\sigma}(r) \tag{6.19}$$

$$=\sum_{\sigma}\sigma[g^{c}\hat{c}^{\dagger}_{\sigma}(r)\hat{c}_{\sigma}(r)+g^{f}\hat{f}^{\dagger}_{\sigma}(r)\hat{f}_{\sigma}(r)] , \tag{6.20}$$

while keeping the degeneracy to be twofold, i.e., $\sigma=\pm\frac{1}{2}$, which are sometimes denoted by ↑ and ↓. In addition, we assume, for simplicity, that the bare transfer to the f electron is zero and that the hybridization between the c and f electrons and the repulsive interaction between the f electrons are on site:

$$E^{f}_{k}=E^{f} , \tag{6.21}$$

$$V_k=V , \tag{6.22}$$

$$\hat{U}=\frac{U}{2}\sum_{\substack{\sigma,\sigma'\\(\sigma\neq\sigma')}}\sum_{r}\hat{f}^{\dagger}_{\sigma}(r)\hat{f}_{\sigma}(r)\hat{f}^{\dagger}_{\sigma'}(r)\hat{f}_{\sigma'}(r) \tag{6.23}$$

$$=\frac{U}{2N_{\text{sys}}}\sum_{\sigma,\sigma'}\sum_{k,p,q}\hat{f}^{\dagger}_{\sigma}(p)\hat{f}^{\dagger}_{\sigma'}(q)\hat{f}_{\sigma'}(q-k)\hat{f}_{\sigma}(p+k) , \tag{6.24}$$

where we set V real positive without loss of generality.

The existence of the non-qp part of the susceptibility is manifested in Fig. 9: The magnetization appears linearly as a function of h, although the Fermi level lies in the

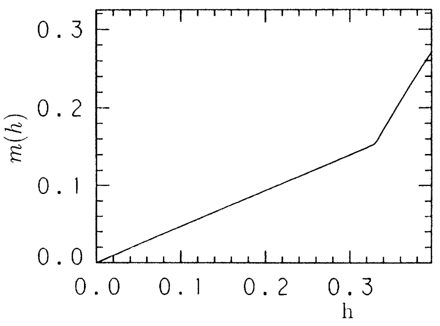

FIG. 9. Magnetization as a function of h calculated for the band structure described in Fig. 10 with $D=1.0$ and $\Delta=0.1$ at $U=0$ for $g^{c}=2.0$ and $g^{f}=0.5$. The Fermi level is assumed to lie at the center of the band gap when $h=0$. The analytic expression is given in Appendix D. The bend in the curve is due to the field induced metal-insulator transition. $D=1.0$ $\bar{V}=0.5$, and thus $\Delta\approx0.2$.

band gap.

Whereas we refer to σ as the spin, it should not be taken literally. This model can be seen as a simplified version of the model considered by Hanzawa, Yosida, and Yamada[8] and Yamada and Nakano,[9] in which the degeneracy of the f electron is reduced to 2 by a strong spin-orbit coupling and crystalline field.

2. *Green's function in the RPA*

The self-energy has only the f-f element $\Sigma^f_{k\sigma}$. In the RPA described in Sec. V D, it is independent of k and coincides with the number of f electrons per site with the opposite spin multiplied by U, which is the contribution from the diagram of Fig. 5(a); the diagram of Fig. 5(b) is irrelevant in this model, because the f electrons with the same spin do not interact at all owing to the on siteness of our simplified two-body interaction. In the following we treat the Green's function in zero field only. In zero field the self-energy becomes independent of σ:

$$\Sigma^f_{k\sigma}=\tfrac{1}{2}n_f U \;, \tag{6.25}$$

where n_f is the number of f electrons per site. Thus let us make $\sum^f_{k\sigma}$ absorbed in E^f, by redefining E^f. In addition, let us take this redefined E^f as the origin of energy: $E^f=0$.

With these preparations the single-particle Green's function in the RPA in zero field is obtained as follows. It can be written in a block-diagonal form as

$$\mathcal{G}_k=\mathcal{G}_{k\downarrow}\otimes\mathcal{G}_{k\uparrow} \;. \tag{6.26}$$

The block-diagonal element $\mathcal{G}_{k\sigma}$ is given by

$$\mathcal{G}_{k\sigma}=\mathcal{G}^{(-)}_{k\sigma}+\mathcal{G}^{(+)}_{k\sigma} \;, \tag{6.27}$$

where

$$\mathcal{G}^{(\pm)}_{k\sigma}(\zeta)=\frac{a^{\pm}_{k\sigma}}{\zeta+\mu-E^{\pm}_k} \;. \tag{6.28}$$

The energy dispersions of the upper and lower bands, $E^{\pm}_k$, are

$$E^{\pm}_k=\tfrac{1}{2}\{\varepsilon_k\pm[(\varepsilon_k)^2+4V^2]^{1/2}\} \;. \tag{6.29}$$

The explicit forms of the A matrices are given below.

Now let us assume that the Fermi surface lies wholly in the lower bands; in this case $a^-_{k\sigma}$ is more important. Thus we denote the c-c and f-f elements of $a^-_{k\sigma}$ simply by a^c_k and a^f_k. Then the explicit calculation shows that the off-diagonal elements can also be expressed with these a^c_k and a^f_k, and the final form of $a^-_{k\sigma}$ is obtained as[35]

$$a^-_{k\sigma}=\begin{bmatrix} a^c_k & -(a^c_k a^f_k)^{1/2} \\ -(a^c_k a^f_k)^{1/2} & a^f_k \end{bmatrix} , \tag{6.30}$$

where the diagonal elements are given by

$$a^c_k=\frac{(E^-_k)^2}{(E^-_k)^2+V^2}\equiv a^c(E^-_k) \;, \tag{6.31}$$

$$a^f_k=\frac{V^2}{(E^-_k)^2+V^2}\equiv a^f(E^-_k) \;. \tag{6.32}$$

Note that, in this approximation, the k dependence of the elements is only through the band energy (of the lower band), as the notation of the right-hand sides implies.

Although it is of less importance, we also need $a^+_{k\sigma}$ when calculating the quantities such as the qp interaction function, qp effective moment, and non-qp part of the susceptibility. Using the same a^c_k and a^f_k, the matrix $a^+_{k\sigma}$ can be written as

$$a^+_{k\sigma}=\begin{bmatrix} a^f_k & +(a^c_k a^f_k)^{1/2} \\ +(a^c_k a^f_k)^{1/2} & a^c_k \end{bmatrix} . \tag{6.33}$$

Be careful that, in the above expression, the c-c element is a^f_k and vice versa; this happens because we make the notation so that the expression for $a^-_{k\sigma}$ would be natural. It is instructive to check that these A matrices satisfy the identities presented in Sec. IV A.

The decomposition of $\mathcal{G}\otimes\mathcal{G}$ into Q and φ is done according to the scheme given in Sec. V D:

$$Q=\mathcal{G}^{(-)}\otimes\mathcal{G}^{(-)} \;, \tag{6.34}$$

$$\varphi=\mathcal{G}^{(+)}\otimes\mathcal{G}^{(-)}+\mathcal{G}^{(-)}\otimes\mathcal{G}^{(+)} \;. \tag{6.35}$$

The term $\mathcal{G}^{(+)}\otimes\mathcal{G}^{(+)}$ is redundant under our assumption that the Fermi level lies in the lower bands.

3. *Static uniform susceptibility in the RPA*

In this model, owing to the on siteness of the two-body interaction, the diagrams in Figs. 7(b) and 7(c) will never appear. Thus the irreducible vertex part of Fig. 6(b) can be neglected completely. In the RPA all of the internal frequency and wave-vector summations can be performed independently; the following two summations over k will appear after the frequency summation:

$$\tfrac{1}{2}\mathcal{N}_{\text{tot}}\equiv\sum_k \delta(\mu-E^-_k) \;, \tag{6.36}$$

$$\mathcal{R}\equiv\sum_k \frac{2a^c_k a^f_k}{E^+_k-E^-_k}\Theta(\mu-E^-_k) \;. \tag{6.37}$$

The first one is the density of states per spin at the Fermi level, coming from the term $-Q^k$. The second one is coming from the term $-\varphi$.

The ω limit of the vertex part is of the form (6.17) with λ replaced by σ, and it is independent of the k's in the RPA. They are given by

$$\Gamma^{\omega}_f(\sigma=\sigma')=\frac{-U\mathcal{R}U}{1-(U\mathcal{R})^2} \;, \tag{6.38}$$

$$\Gamma^{\omega}_f(\sigma\neq\sigma')=\frac{U}{1-(U\mathcal{R})^2} \;. \tag{6.39}$$

The non-qp part of the susceptibility is obtained as

$$\chi^{\text{RPA}}_{\text{nqp}}=2\left[\frac{1}{2}\right]^2(g^f-g^c)^2\frac{\mathcal{R}}{1-U\mathcal{R}}=\frac{\chi^0_{\text{nqp}}}{1-U\mathcal{R}} \;, \tag{6.40}$$

where the factor $2(\frac{1}{2})^2$ comes from $\sum_\sigma \sigma^2$ (our convention is $\sigma=\pm\frac{1}{2}$). The superscript 0 on χ^0_{nqp} means $U=0$. The effective moment of the qp on the Fermi surface is

$$\mu^{*}_{k\sigma}=\sigma g^{*} \tag{6.41}$$

$$\equiv\sigma\left[g^{c}a^{c}+\left[g^{f}+(g^{f}-g^{c})\frac{U\mathcal{R}}{1-U\mathcal{R}}\right]a^{f}\right], \tag{6.42}$$

where a^c and a^f without argument are evaluated at the Fermi level: $a^c=a^c(\mu)$ and $a^f=a^f(\mu)$. The effective g value g^* is renormalized, varying from $g^0=g^c a^c+g^f a^f$ with U. If $g^c=g^f=g$, however, we can see that $g^*=g$ as well as $\chi^{\rm RPA}_{\rm nqp}=0$; this is in accordance with the general remark that the effective moment is not renormalized and the $\chi_{\rm nqp}$ does not exist if $\hat{\mathcal{M}}$ is conserved.

In the expression of $\chi^{\rm RPA}_{\rm qp}$, only the following combination of the interaction function multiplied by $\mathcal{N}_{\rm tot}$ appears:

$$F^{a}\equiv(a^{f})^{2}[\Gamma^{\omega}_{f}(\sigma=\sigma')-\Gamma^{\omega}_{f}(\sigma\neq\sigma')]\tfrac{1}{2}\mathcal{N}_{\rm tot} \tag{6.43}$$

$$=(a^{f})^{2}\frac{-U}{1-U\mathcal{R}}\left[\frac{1}{2}\mathcal{N}_{\rm tot}\right]. \tag{6.44}$$

With this parameter, the qp part of the susceptibility (in the k limit) is expressed as

$$\chi^{\rm RPA}_{\rm qp}=\left[\frac{1}{2}g^{*}\right]^{2}\frac{\mathcal{N}_{\rm tot}}{1+F^{a}}. \tag{6.45}$$

If one prefers the form in which the enhancement factor will appear only in front of the f-electron density of states, one can rewrite (6.45) as

$$\chi^{\rm RPA}_{\rm qp}=(\tfrac{1}{2}g^{*})^{2}[\mathcal{N}_{c}+(1+\chi^{f}_{\rm enh})\mathcal{N}_{f}], \tag{6.46}$$

where

$$\mathcal{N}_{c}=a^{c}\mathcal{N}_{\rm tot},\quad \mathcal{N}_{f}=a^{f}\mathcal{N}_{\rm tot}, \tag{6.47}$$

and

$$\chi^{f}_{\rm enh}=-F^{a}[a^{f}(1+F^{a})]^{-1}$$

$$=\frac{\frac{1}{2}\mathcal{N}_{f}U}{1-U(\frac{1}{2}a^{f}\mathcal{N}_{f}+\mathcal{R})}. \tag{6.48}$$

Nonetheless, one must be careful not to give too much physical interpretation to expressions such as (6.46), because such a rewriting is not unique and nor is the meaning of $\chi^{f}_{\rm enh}$ clear. If and only if $g^c=g^f=g$, it is given by

$$\chi^{f}_{\rm enh}=\frac{1}{g\sigma}\left[\frac{\partial\Sigma^{f}_{k\sigma}}{\partial h}\right]_{\rm RPA}. \tag{6.49}$$

4. *Constant density of states for the conduction band*

Now let us further assume that the density of states of the conduction band ε_k is constant with width $2D$ and symmetric about $E^f=0$ (Fig. 10). Then the parameters appearing in the preceding expressions of the RPA susceptibilities are evaluated as follows. The density of states per spin is

$$\tfrac{1}{2}\mathcal{N}_{\rm tot}=\frac{1}{2D}\left[\frac{\mu^{2}+V^{2}}{\mu^{2}}\right], \tag{6.50}$$

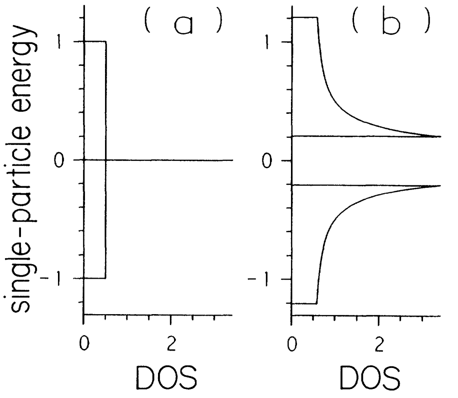

FIG. 10. (a) Symmetric and constant c-electron density of states and f-electron level. (b) Density of states after hybridization. $D=1.0$, $V=0.5$, and thus $\Delta\approx0.2$.

and the c- and f-electron weights are

$$a^{c}(\mu)=\frac{\mu^{2}}{\mu^{2}+V^{2}},\quad a^{f}(\mu)=\frac{V^{2}}{\mu^{2}+V^{2}}. \tag{6.51}$$

The k summation (6.37) can be performed as

$$\mathcal{R}=\frac{1}{2D}\left[\frac{V^{2}-\mu^{2}}{\mu^{2}+V^{2}}+\frac{D}{(D^{2}+4V^{2})^{1/2}}\right]. \tag{6.52}$$

By the way, I would like to emphasize again the fact that the decomposition of the susceptibility into the qp and non-qp parts can easily be obscured if one considers only the static uniform susceptibility; in fact, one can rewrite $\chi^{0}_{\rm nqp}=\chi^{0}_{V}$ as

$$\chi^{0}_{V}=2\left[\frac{1}{2}\right]^{2}(g^{f}-g^{c})^{2}a^{c}a^{f}\mathcal{N}_{\rm tot}+O\left[\left[\frac{V}{D}\right]^{2}\right], \tag{6.53}$$

where χ^{0}_{V} seems to be proportional to the density of states at the Fermi level: It cannot be distinguished from the qp part in this respect. Only through the characteristic dependence on (q,Ω) can the identities of the qp and non-qp contributions be established without ambiguity.

Besides, it must be noted that, even if V becomes small and hence the gap Δ between the upper and lower bands becomes very small, $\chi^{0}_{\rm nqp}$ does not grow large, but remains almost constant: The factor $a^c a^f\mathcal{N}_{\rm tot}\approx\mathcal{R}$ in (6.53) is equal to $(1/D)[V^2/(\mu^2+V^2)]\approx1/D$, as long as $V/D<1$ and $n_f\approx1$. The origin of why $\mathcal{R}$ remains small is as follows: First, because of the conservation of the wave number, the energy denominator of (6.37) does not become small in most of the k space, although the gap Δ becomes small [see Fig. 8(b)]. Second, the interband matrix element [the numerator of (6.37)] is small in most of the k space.

Let us return to the RPA susceptibility. Some results are depicted for $V/D=0.3$, $g^c/g^f=4.0$, and $n_f=0.9$. The renormalizations of $\chi_{\rm nqp}$ and g^* are small [Figs. 11(b) and 11(c)], while $\chi_{\rm qp}$ is much enhanced in the usual RPA manner [Fig. 11(a)]. Thus the ratio of $\chi_{\rm qp}$ and $\chi_{\rm nqp}$, which is already small at $U=0$, becomes smaller at finite

U's. Therefore, in the whole range of U where $\chi_{\mathrm{qp}}^{\mathrm{RPA}}$ remains finite, χ_{nqp} is negligible.

However, we must be careful that the above behavior of χ_{nqp} is specific to this model. The behavior of χ_{nqp} varies from model to model. In the next subsection, we consider a different kind of PAM, in which χ_{nqp} will behave in a completely different way.

C. Orbitally degenerate PAM

1. Model

As a final example, we consider a PAM which has a band structure as schematically shown in Fig. 8(c) when $U=0$: The unmixed f-electron levels are left in the gap after the hybridization.

The f electron is assumed to have the orbital degeneracy of $2L+1$ in addition to spin-$\frac{1}{2}$ degeneracy, while the c electron has only spin-$\frac{1}{2}$ degeneracy; so the total number of local fermion components is $2(2L+2)$:

$$\hat{\psi}^{\dagger}(r)=(\hat{\psi}_{\downarrow}^{\dagger}(r),\hat{\psi}_{\uparrow}^{\dagger}(r)) \tag{6.54}$$

is $2(2L+2)$ dimensional, and

$$\hat{\psi}_{\sigma}^{\dagger}=(\hat{c}_{\sigma}^{\dagger},\hat{f}_{(-L)\sigma}^{\dagger},\hat{f}_{(-L+1)\sigma}^{\dagger},\ldots,\hat{f}_{m\sigma}^{\dagger},\ldots,\hat{f}_{L\sigma}^{\dagger}) \tag{6.55}$$

is $(2L+2)$ dimensional. It is assumed that all the f electrons of spin σ are hybridized with the c electron of the same spin σ by a common matrix element $V(2L+1)^{-1/2}$ independent of k and m:

$$E_k=E_{k\downarrow}\oplus E_{k\uparrow}\ ,$$
$$E_{k\sigma}=\begin{bmatrix}\varepsilon_k & V\mathsf{u}^T\\ V\mathsf{u} & E^f\mathsf{I}\end{bmatrix}\ , \tag{6.56}$$

where u is the $(2L+1)$-dimensional row vector, whose transpose u^T is given by

$$\mathsf{u}^T=(2L+1)^{-1/2}(1,1,\ldots,1)\ , \tag{6.57}$$

and I is the $(2L+1)$-dimensional unit matrix

$$\mathsf{I}=\begin{bmatrix}1 & & \\ & \ddots & \\ & & 1\end{bmatrix}\ . \tag{6.58}$$

The two-body interaction is assumed to be only between the f electrons on the same site:

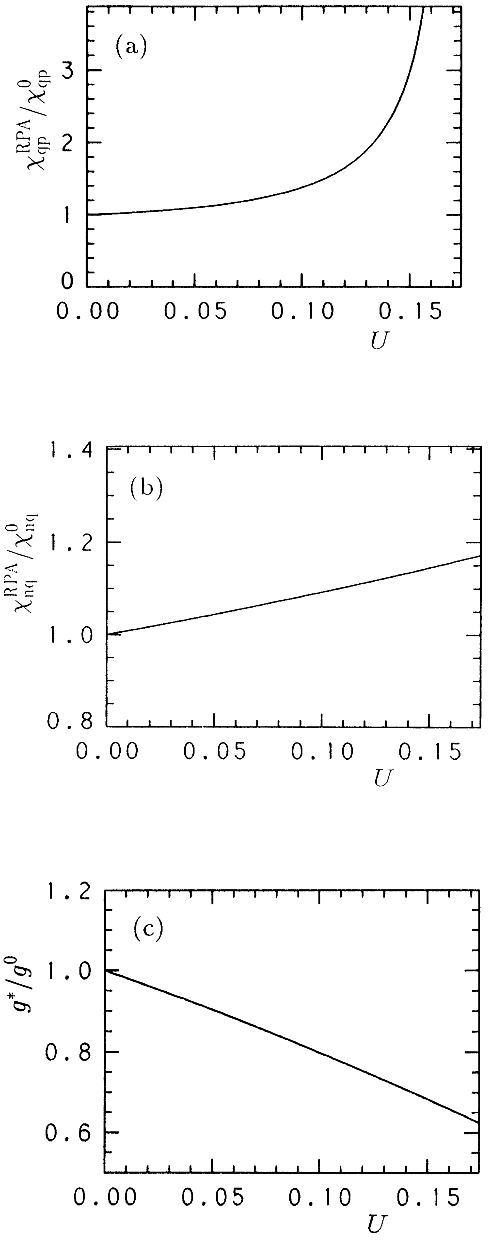

FIG. 11. Renormalization of (a) the qp part of the susceptibility, (b) the non-qp part of the susceptibility, and (c) the qp effective moment of the DD PAM in the RPA for $V/D=0.3$, $g^c/g^f=4.0$, and $n_f=0.9$.

$$\hat{U}=\frac{U}{2}\sum_{\substack{m,m'\\(m\neq m')}}\sum_{\substack{\sigma,\sigma'\\(\sigma\neq\sigma')}}\sum_{r}\hat{f}_{m\sigma}^{\uparrow}(r)\hat{f}_{m\sigma}(r)\hat{f}_{m'\sigma'}^{\dagger}(r)\hat{f}_{m'\sigma'}(r) \tag{6.59}$$

$$=\frac{U}{2N_{\mathrm{sys}}}\sum_{m,m'}\sum_{\sigma,\sigma'}\sum_{k,p,q}\hat{f}_{m\sigma}^{\dagger}(p)\hat{f}_{m'\sigma'}^{\dagger}(q)\hat{f}_{m'\sigma'}(q-k)\hat{f}_{m\sigma}(p+k)\ . \tag{6.60}$$

The magnetization is assumed to be given by

$$\hat{m}(r)=\hat{\psi}^{\dagger}(r)M\hat{\psi}(r)=\hat{s}(r)+\hat{l}(r)\ , \tag{6.61}$$

where

$$M=S+L\ , \tag{6.62}$$

$$\hat{s}(r)=\hat{\psi}^{\dagger}(r)S\hat{\psi}(r)=g^s\sum_{\sigma}\sigma\hat{\psi}_{\sigma}^{\dagger}(r)\hat{\psi}_{\sigma}(r)\ , \tag{6.63}$$

and

$$\hat{l}(r)=\hat{\psi}^{\dagger}(r)L\hat{\psi}(r)=g^{l}\sum_{m,\sigma} m\hat{f}^{\dagger}_{m\sigma}(r)\hat{f}_{m\sigma}(r)\ . \tag{6.64}$$

The matrices M,S,L are $2(2L+2)$ dimensional, σ takes the values $\pm\frac{1}{2}$, and m takes the values from $-L$ to L.

The assumption that the hybridization matrix element is independent of m and k contradicts the physical meaning of the spin and orbit. Therefore, although we call σ the spin and m the orbit, it cannot be taken literally. This model should be regarded simply as a model for a model in which the unmixed f bands (levels) remain in the hybridization gap as a result of the different degeneracies of the c and f electrons. (Some results of an alternative choice of the hybridization matrix element are given in Appendix E.)

2. Green's function in the RPA

The single-particle Green's function in the RPA is the direct sum of $\mathcal{G}_{k\sigma}$ as in the previous DD PAM, but the block diagonal elements $\mathcal{G}_{k\sigma}$ has an additional term, $\mathcal{G}^{(0)}_{k\sigma}$, in contrast to the previous model, representing the unmixed f levels:

$$\mathcal{G}_{k\sigma}=\mathcal{G}^{(-)}_{k\sigma}+\mathcal{G}^{(+)}_{k\sigma}+\mathcal{G}^{(0)}_{k\sigma}\ , \tag{6.65}$$

where

$$\mathcal{G}^{(\pm)}_{k\sigma}(\zeta)=\frac{a^{\pm}_{k\sigma}}{\zeta+\mu-E^{\pm}_{k}}\ , \tag{6.66}$$

$$\mathcal{G}^{(0)}_{k\sigma}(\zeta)=\frac{b_k}{\zeta+\mu-\frac{1}{2}n_f U}\ , \tag{6.67}$$

with the A matrices

$$a^{-}_{k\sigma}=\begin{bmatrix} a^{c} & -(a^{c}a^{f})^{1/2}\mathrm{u}^{T} \\ -(a^{c}a^{f})^{1/2}\mathrm{u} & a^{f}\mathrm{W} \end{bmatrix}\ , \tag{6.68}$$

$$a^{+}_{k\sigma}=\begin{bmatrix} a^{f} & +(a^{c}a^{f})^{1/2}\mathrm{u}^{T} \\ +(a^{c}a^{f})^{1/2}\mathrm{u} & a^{c}\mathrm{W} \end{bmatrix}\ , \tag{6.69}$$

$$b_k=\begin{bmatrix} 0 & \cdots 0 \cdots \\ \vdots & \\ 0 & \mathrm{I}-\mathrm{W} \\ \vdots & \end{bmatrix}\ . \tag{6.70}$$

The $(2L+2)$-dimensional matrix b_k is the sum of the A matrices over all of the unmixed bands, and W is the following $(2L+1)$-dimensional matrix:

$$\mathrm{W}=\frac{1}{2L+1}\begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix}\ . \tag{6.71}$$

The constants a^{c}, a^{f}, and $E^{\pm}_{k}$ are given by the same formulas as (6.31), (6.32), and (6.29) in the previous model; in fact, we have normalized u by $(2L+1)^{-1/2}$ in order for them to be given by the same formulas. As in the previous model, the notation is such that the elements of $a^{-}_{k\sigma}$ seem to be natural, since we consider only the case in which the Fermi level lies in the lower bands.

Note that, even after the redefinition of E^{f}, which removes the self-energy from the denominator of $\mathcal{G}^{(\pm)}_{k\sigma}$, (a half of) the self-energy $\frac{1}{2}n_f U$ remains in the denominator of $\mathcal{G}^{(0)}_{k\sigma}$. This is in contrast to the previous DD PAM. The reason is that the f electrons in the unmixed bands feel the Coulomb repulsion from all the f electrons in the lower bands of both spins, while the f electron of a spin in the lower band feels the repulsion from only the f electron of the different spin. This happens because we can recombine *locally* the f electrons into those which are mixed with the c electrons and those which are not mixed, owing to the somewhat artificial assumption that the hybridization matrix element is independent of k and m. A more realistic choice of the hybridization matrix elements may alter this aspect of the model. (For another possible choice of the hybridization matrix, see Appendix E.) However, since our object is only to present a model whose χ_{nqp} have a different character from that of the previous model and to show the variety of the behavior of χ_{nqp}, let us continue to concentrate on this specific and somewhat artificial model.

It is often convenient to use Green's functions represented in the recombined local basis mentioned above in evaluating the diagrams. It is one of the superiorities of our A-matrix representation of $\mathcal{G}_k$ that we can easily move from basis to basis including such an intermediate basis, as well as the original local basis and qp-band basis. By this local transformation $\hat{f}_{m\sigma}(r)\rightarrow\hat{f}_{\tilde{m}\sigma}(r)$, the two-body interaction and matrix S are invariant, while

$$E_{k\sigma}\rightarrow\tilde{E}_{k\sigma}=\begin{bmatrix} \begin{bmatrix} \varepsilon_k & V \\ V & E^{f} \end{bmatrix} & 0 \\ 0 & \begin{bmatrix} E^{f} & & \\ & \ddots & \\ & & E^{f} \end{bmatrix} \end{bmatrix}\ , \tag{6.72}$$

$$a^{-}_{k\sigma}\rightarrow\tilde{a}^{-}_{k\sigma}=\begin{bmatrix} \begin{bmatrix} a^{c} & -(a^{c}a^{f})^{1/2} \\ -(a^{c}a^{f})^{1/2} & a^{f} \end{bmatrix} & 0 \\ 0 & 0 \end{bmatrix}\ , \tag{6.73}$$

$$a^{+}_{k\sigma}\rightarrow\tilde{a}^{+}_{k\sigma}=\begin{bmatrix} \begin{bmatrix} a^{f} & +(a^{c}d^{f})^{1/2} \\ +(a^{c}a^{f})^{1/2} & a^{c} \end{bmatrix} & 0 \\ 0 & 0 \end{bmatrix}\ , \tag{6.74}$$

$$b_k\rightarrow\tilde{b}_k=\begin{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} & 0 \\ 0 & \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} \end{bmatrix}\ , \tag{6.75}$$

$$L\rightarrow\tilde{L}\ . \tag{6.76}$$

The explicit form of $\tilde{L}$ is complicated, but we do not need (or do not use) it.

The decomposition $\mathcal{G}\otimes\mathcal{G}=Q+\varphi=Q+\varphi_{(a)}+\varphi_{(b)}$ is done as

$$Q=\mathcal{G}^{(-)}\otimes\mathcal{G}^{(-)}\ , \tag{6.77}$$

$$\varphi_{(a)}=\mathcal{G}^{(+)}\otimes\mathcal{G}^{(-)}+\mathcal{G}^{(-)}\otimes\mathcal{G}^{(+)}\ , \tag{6.78}$$

$$\varphi_{(b)}=\mathcal{G}^{(0)}\otimes\mathcal{G}^{(-)}+\mathcal{G}^{(-)}\otimes\mathcal{G}^{(0)}\ . \tag{6.79}$$

In contrast to the previous DD PAM, both of the irreducible vertex parts in Figs. 6(a) and 6(b) are relevant. Therefore, all three types of diagrams in Fig. 7 might contribute to the susceptibility. Fortunately, however, the diagrams of the type shown in Fig. 7(c) will completely vanish owing to the special simplicity of our model, which can be easily seen if one uses the recombined basis. Thus the evaluation of the RPA susceptibility in the following is considerably simplified.

3. Static uniform susceptibility in the RPA

Now that we have determined the A matrices, the remaining work is not difficult to perform. After the frequency summation, the k summation

$$\mathcal{S}=\sum_k \frac{a_k^f}{\frac{1}{2}n_f U-E_k^-} \tag{6.80}$$

will appear from $-\varphi_{(b)}$, as well as $\frac{1}{2}\mathcal{N}_{\rm tot}$ and $\mathcal{R}$ given by (6.36) and (6.37) from $-Q$ and $-\varphi_{(a)}$. In the following we restrict ourselves to the symmetric constant density of states for the conduction band [Fig. 10(b)]. Then, after the k summation, we obtain

$$\mathcal{S}=\frac{1}{U}-\frac{1}{U^2}\frac{1}{(\frac{1}{2}n_f)^2}\frac{V^2}{2D}\ln\left[\frac{|E_{\min}|}{|\mu|}\frac{|\mu|+\frac{1}{2}n_f U}{|E_{\min}|+\frac{1}{2}n_f U}\right]\ , \tag{6.81}$$

where the bottom of the lower band, $E_{\min}$, is

$$E_{\min}=\tfrac{1}{2}[-D-(D^2+4V^2)^{1/2}]\ , \tag{6.82}$$

and a half of the f-electron number per site is

$$\frac{1}{2}n_f=\frac{V^2}{2D}\left[\frac{1}{|\mu|}-\frac{1}{|E_{\min}|}\right]\ . \tag{6.83}$$

The matrix L out of $M=S+L$ does not contribute to the effective moment of the qp, and only the diagrams of Fig. 7(a) contribute to $\chi_{\rm qp}$:

$$\chi_{\rm qp}^{\rm RPA}=-M(1+\varphi\Gamma^\omega)(Q^k+Q^k\Gamma Q^k)(1+\Gamma^\omega\varphi)M \tag{6.84}$$

$$=-S(Q^k+Q^k\Gamma Q^k)S \tag{6.85}$$

$$=\left[\frac{1}{2}g^s\right]^2\frac{\mathcal{N}_{\rm tot}}{1+F^a}\ . \tag{6.86}$$

The Fermi-liquid parameter F^a and total density of states at the Fermi level, $\mathcal{N}_{\rm tot}$, are given by the same formulas as (6.44) and (6.50).

To $\chi_{\rm nqp}$, only L and the diagrams of Fig. 7(b) contribute;

$$\chi_{\rm nqp}^{\rm RPA}=-M(\varphi+\varphi\Gamma^\omega\varphi)M \tag{6.87}$$

$$=-L(\varphi_{(b)}+\varphi_{(b)}\Gamma^\omega\varphi_{(b)}L \tag{6.88}$$

$$=\frac{L(L+1)(g^l)^2}{3}\frac{4\mathcal{S}}{1-U\mathcal{S}}\ , \tag{6.89}$$

where the factor $L(L+1)/3$ comes from $\sum_m m^2/(2L+1)$.

Let us now consider the meaning of $\mathcal{S}$ and $\mathcal{S}/(1-U\mathcal{S})$ in the above equation. If we had approximated the single-particle Green's function in the Hartree-Fock approximation, but inconsistently and erroneously had approximated the irreducible vertex part Γ_0 as zero, then we would have obtained $\chi_{\rm nqp}$ as proportional to $\mathcal{S}$ (without denominator). The integral $\mathcal{S}$ represents the non-qp contribution evaluated for the Hartree-Fock band of Fig. 8(d) as the noninteracting band. Thus it varies as $1/U$ for large U, which is completely incorrect. Owing to the correction due to the vertex part, it has regained the correct order. The correct limiting behaviors are given by the following:

$$\chi_{\rm nqp}^{\rm RPA}\to\chi_{\rm nqp}^0[B_1+O(1/U)]\quad\text{as } U\to\infty\ , \tag{6.90}$$

$$\chi_{\rm nqp}^{\rm RPA}\to\chi_{\rm nqp}^0[1-UB_2+O(U^2)]\quad\text{as } U\to 0\ , \tag{6.91}$$

where

$$B_1=\frac{|E_{\min}|-|\mu|}{|E_{\min}|+|\mu|}\frac{2}{\ln(|E_{\min}|/|\mu|)}\ , \tag{6.92}$$

$$B_2=\frac{D}{3V^2}\left[\frac{1}{2}n_f\right]^2\frac{|E_{\min}|-|\mu|}{|E_{\min}|+|\mu|}\ , \tag{6.93}$$

and

$$\chi_{\rm nqp}^0=\frac{L(L+1)(g^l)^2}{3}4\mathcal{S}_0\ , \tag{6.94}$$

with

$$\mathcal{S}_0=\frac{1}{2D}\left[\frac{V^2}{|\mu|^2}-\frac{V^2}{|E_{\min}|^2}\right]\ . \tag{6.95}$$

Let me once again emphasize that the distinction between $\chi_{\rm qp}$ and $\chi_{\rm nqp}$ is obscured if one considers only the static uniform susceptibility and metamorphosizes it too much; in fact, the above $\chi_{\rm nqp}^0$ can be transformed as

$$\chi_{\rm nqp}^0=\frac{L(L+1)(g^l)^2}{3}a^f\mathcal{N}_{\rm tot}+O\left[\left[\frac{V}{D}\right]^2\right]\ . \tag{6.96}$$

Adding this and $\chi_{\rm qp}^0=(\frac{1}{2}g^s)^2\mathcal{N}_{\rm tot}$, we obtain, neglecting $O((V/D)^2)$,

$$\chi_{\rm qp}^0+\chi_{\rm nqp}^0=\left[\frac{1}{2}g^s\right]^2\mathcal{N}_c+\left[\left[\frac{1}{2}g^s\right]^2+\frac{L(L+1)(g^l)^2}{3}\right]\mathcal{N}_f\ . \tag{6.97}$$

In this formula the missing contribution to the qp effective moment from the orbital moment seems to be completely recovered; this formula gives an incorrect im-

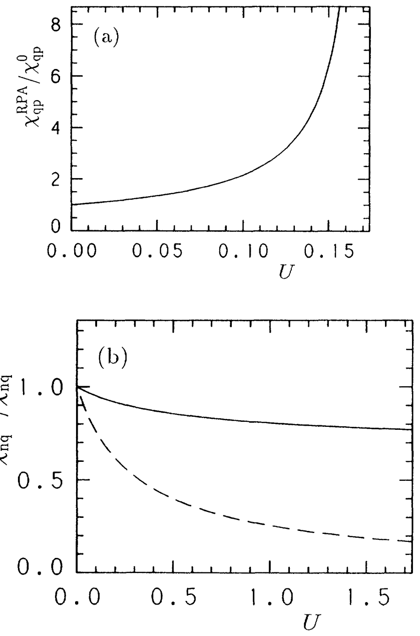

FIG. 12. Renormalization of (a) the qp part and (b) the non-qp part of the RPA susceptibility of the OD PAM for $V/D=0.3$ and $n_f=0.9$. The dashed line in (b) decreases as $1/U$, which is the one calculated without the vertex correction.

pression that the term $L(L+1)(g^l)^2/3$ should be included in the effective moment of the qp. Note that, in contrast to the previous model, χ_{nqp}^0 grows roughly in proportion to V^{-2} similarly as χ_{qp}^0, because the factor a^c is not multiplied: Compare (6.96) and (6.53).

Now let us turn to the numerical results. The dependence of $\chi_{\mathrm{qp}}^{\mathrm{RPA}}$ and $\chi_{\mathrm{nqp}}^{\mathrm{RPA}}$ on U is depicted in Fig. 12 for $n_f=0.9$. As U increases, $\chi_{\mathrm{qp}}^{\mathrm{RPA}}$ is enhanced in the usual RPA manner [Fig. 12(a)], while $\chi_{\mathrm{nqp}}^{\mathrm{RPA}}$ decreases slowly [Fig. 12(b), in which the range of U is taken far beyond the stable region of $\chi_{\mathrm{qp}}^{\mathrm{RPA}}$ in illustration of the asymptotic behavior of (6.90)].

In this model the ratio of χ_{nqp} and χ_{qp}, which is appreciable at $U=0$, decreases as a function of U, but remains the same order: The Coulomb interaction between the f electrons reduces the importance of the non-qp part, yet the reduction is not complete.

VII. WILSON RATIO

A. General

We define the *observed* Wilson ratio as

$$R_{\mathrm{obs}} \equiv \frac{1}{\langle \mu_{\mathrm{eff}}^2 \rangle} \frac{\chi}{\mathcal{N}_{\mathrm{tot}}^*} , \tag{7.1}$$

where χ is the observed static uniform susceptibility, $\mathcal{N}_{\mathrm{tot}}^*$ the qp density of states at the Fermi level deduced from the observed temperature-linear coefficient of the specific heat by the relation (4.21), and $\langle \mu_{\mathrm{eff}}^2 \rangle$ is the qp effective moment, which must be obtained theoretically.

If $\hat{M}$ is conserved, the non-qp contribution to χ does not exist, i.e., $\chi=\chi_{\mathrm{qp}}$. At the same time, the effective moment of the qp is not renormalized; so there is no ambiguity in the theoretical evaluation of $\langle \mu_{\mathrm{eff}}^2 \rangle$. Thus R_{obs} can be directly related to the Fermi-liquid parameter, which is an average of some combination of the qp interaction function $f_{\alpha\beta}(k,k')$ over the Fermi surface (FS). For example, in our DD PAM with $g^c=g^f$ [i.e., in the SU(2) PAM] and in the RPA, R_{obs} is given by

$$R_{\mathrm{obs}} = \frac{1}{1+F^a} . \tag{7.2}$$

For the spin susceptibility of the isotropic single-component Fermi liquid, R_{obs} is given by the same formula as the above, where F^a is a simple combination of the coefficients of the spherical harmonic expansion of $f_{\alpha\beta}(k,k')$ multiplied by the total qp density of states at the Fermi level. In anisotropic systems and beyond the RPA, the relation between R_{obs} and $f_{\alpha\beta}(k,k')$ becomes more complicated. Yet it can be given by the same formula as the above; in this case, F^a stands for a complicated weighted average of $f_{\alpha\beta}(k,k')$ over the FS. Anyway, R_{obs} conveys us some knowledge about the interaction between the qp's if $\hat{M}$ is conserved.

On the contrary, if $\hat{M}$ is not conserved, R_{obs} cannot be related to the Fermi-liquid parameter directly, because the susceptibility contains necessarily χ_{nqp}, and at the same time, the effective moment of the qp is inevitably renormalized. What is related to $f_{\alpha\beta}(k,k')$ directly is

$$R_{\mathrm{qp}} = \frac{1}{\langle \mu_{\mathrm{qp}}^2 \rangle} \frac{\chi_{\mathrm{qp}}}{\mathcal{N}_{\mathrm{tot}}^*} , \tag{7.3}$$

where $\langle \mu_{\mathrm{qp}}^2 \rangle$ stands for an average of the renormalized qp moment over the FS. However, we can neither extract χ_{qp} logically from an observed value of the static uniform χ nor predict the value of $\langle \mu_{\mathrm{qp}}^2 \rangle$ theoretically. Therefore, we cannot obtain R_{qp} from the experimental data if $\hat{M}$ is not conserved. This conclusion is somewhat pessimistic, yet is unavoidable.

Nonetheless, there has been a strong desire to extract some information about the Fermi-liquid parameter of the PAM's or the heavy-fermion systems where $\hat{M}$ is not conserved. The problem has been discussed by Anderson and others, yet there has been no consensus. In the following we first review their discussion, taking our OD PAM as an example; then we seek for a possible resolution. In preparation, let us further define

$$R_{\mathrm{nqp}} = \frac{1}{\langle \mu_{\mathrm{nqp}}^2 \rangle} \frac{\chi_{\mathrm{nqp}}}{\mathcal{N}_{\mathrm{tot}}^*} , \tag{7.4}$$

where

$$\langle \mu_{\mathrm{nqp}}^2 \rangle = \langle \mu_{\mathrm{eff}}^2 \rangle - \langle \mu_{\mathrm{qp}}^2 \rangle . \tag{7.5}$$

Then R_{obs} can be rewritten as

$$R_{\mathrm{obs}} = \frac{\langle \mu_{\mathrm{qp}}^2 \rangle}{\langle \mu_{\mathrm{eff}}^2 \rangle} R_{\mathrm{qp}} + \frac{\langle \mu_{\mathrm{nqp}}^2 \rangle}{\langle \mu_{\mathrm{eff}}^2 \rangle} R_{\mathrm{nqp}} . \tag{7.6}$$

B. Orbitally degenerate PAM

Let us refer back to Eq. (6.97), an expression for the static uniform susceptibility of our OD PAM at $U=0$. If one would try to define $R_{\rm obs}$ such that it reduces to unity when $U=0$, one should set

$$\langle \mu_{\rm eff}^2 \rangle = (\tfrac{1}{2} g^s)^2 + \tfrac{1}{3} L(L+1)(g^l)^2 , \tag{7.7}$$

which coincides with the effective moment deduced from the high-temperature Curie law.[36] (In this section we neglect $\mathcal{N}_c$, taking it as much smaller than $\mathcal{N}_f$.) However, the qp effective moment is [see (6.86)]

$$\langle \mu_{\rm qp}^2 \rangle = (\tfrac{1}{2} g^s)^2 , \tag{7.8}$$

and the other term is due to the non-qp contribution [see (6.96)]

$$\langle \mu_{\rm nqp}^2 \rangle = \tfrac{1}{3} L(L+1)(g^l)^2 . \tag{7.9}$$

Thus the effective moment of the qp is severely quenched compared with the high-temperature value given by (7.7).

The observed Wilson ratio is less than unity in the existing heavy-fermion systems.[37] It might be taken as direct evidence for the Fermi-liquid parameter being positive, if one does not realize the difference between $R_{\rm obs}$ and $R_{\rm qp}$.

In the Letter by Zou and Anderson (ZA),[13] they calculated $\langle \mu_{\rm qp}^2 \rangle$, finding that it is much less than $\langle \mu_{\rm eff}^2 \rangle$. (Their calculation is, of course, based on a more realistic model, but what will happen is independent of the details of the model; our oversimplified model is sufficient to illustrate their results.) Then they argued that $\langle \mu_{\rm eff}^2 \rangle$ in (7.1) must be replaced by $\langle \mu_{\rm qp}^2 \rangle$, and they defined

$$R_{\rm ZA} \equiv \frac{1}{\langle \mu_{\rm qp}^2 \rangle} \frac{\chi}{\mathcal{N}_{\rm tot}^*} = \frac{\langle \mu_{\rm eff}^2 \rangle}{\langle \mu_{\rm qp}^2 \rangle} R_{\rm obs} . \tag{7.10}$$

The factor $\langle \mu_{\rm eff}^2 \rangle / \langle \mu_{\rm qp}^2 \rangle$ is considerably greater than unity according to their calculation (as in our OD PAM result). Therefore, $R_{\rm ZA} > 1$, even though $R_{\rm obs} < 1$. They took this evidence for the Fermi-liquid parameter being negative; ZA identified $R_{\rm ZA}$ with $R_{\rm qp}$, by neglecting $\chi_{\rm nqp}$.

However, this identification is incorrect. In fact, from (7.6) and (7.10), it is deduced that

$$R_{\rm ZA} = R_{\rm qp} + \frac{\langle \mu_{\rm nqp}^2 \rangle}{\langle \mu_{\rm qp}^2 \rangle} R_{\rm nqp} . \tag{7.11}$$

Thus the largeness of $R_{\rm ZA}$ does not necessarily mean the largeness of $R_{\rm qp}$, unless the second term is negligible. Note that ZA's calculation is actually at $U=0$; the effect of U is presumed to be incorporated by the use of a renormalized value for V. In such a calculation, the second term of (7.11) is large: $\langle \mu_{\rm nqp}^2 \rangle / \langle \mu_{\rm qp}^2 \rangle$ is large and $R_{\rm nqp}$ is of the same order with $R_{\rm qp}$. Thus, as a calculation at $U=0$, ZA's result was incorrect as pointed out by many authors[14–16] and as admitted by Anderson and Zou[17] themselves.

Furthermore, Zhang and Lee[14] argued that $R_{\rm obs} < 1 \Longrightarrow R_{\rm qp} < 1$ as follows. They inferred two possibilities for the effect of U on $R_{\rm nqp}$.

Possibility 1. $R_{\rm nqp} \approx R_{\rm qp}$.

Possibility 2. $R_{\rm nqp} \approx 1$.

In the first case, (7.6) reduces to $R_{\rm qp} \approx R_{\rm obs}$. In the second case, (7.6) reduces to

$$R_{\rm qp} \approx 1 + \frac{\langle \mu_{\rm eff}^2 \rangle}{\langle \mu_{\rm qp}^2 \rangle} (R_{\rm obs} - 1) . \tag{7.12}$$

In both cases, $R_{\rm obs} < 1 \Longrightarrow R_{\rm qp} < 1$. Their deduction is correct at all; nonetheless, there is a room for doubt in their assumption.

Anderson and Zou[17] criticized this point: they proposed the following.

Possibility 3. $R_{\rm nqp} \approx 0$.

Hence they asserted that $R_{\rm qp} \approx R_{\rm ZA}$ in reality [see (7.11)] and that their former argument for the smallness of the observed Wilson ratio need not be changed essentially. Their reasoning for the above possibility is that the qp mass enhancement, i.e., the renormalization of V, is not effective to the enhancement of $\chi_{\rm nqp}$. Seeing our Eqs. (5.34) and (5.35) and noting that the mass enhancement is solely embedded in Q, it is not astonishing even if $R_{\rm nqp}$ is somewhat smaller than $R_{\rm qp}$, whereas we cannot be sure of such a quantitative affirmation as possibility 3.

Aeppli and Varma[15] argue that $\chi_{\rm nqp}$ is also affected by U in the same order as $\chi_{\rm qp}$ by exploiting a sum rule. Their argument seems reasonable. Nonetheless, it is only an order estimation; it is not surprising even if the enhancements of $\chi_{\rm qp}$ and $\chi_{\rm nqp}$ due to U are different by a numerical factor.

Now let me propose another possibility.

Possibility 4. $R_{\rm nqp} \not\approx 0$ but $R_{\rm nqp} < 1$.

In other words, the enhancement of $\chi_{\rm nqp}$ is of the same order as that of the qp specific-heat mass, but smaller by a numerical factor. In a sense this proposal is a reconciliation of Anderson and Zou's and Aeppli and Varma's. My proposal is as vague and abstract as theirs, so that one may think it too tricky. Nonetheless, whether $R_{\rm qp} < 1$ or not is such a subtle problem which depends on this tricky numerical factor.

For example, let us tentatively set $\langle \mu_{\rm qp}^2 \rangle : \langle \mu_{\rm eff}^2 \rangle = 1{:}5$, which is realized by putting $g^s = 2g^l$ and $L=3$ in our OD PAM. In addition, let us tentatively set $R_{\rm qp} = 1.5$ and $R_{\rm nqp} = 0.3$; our OD PAM in the RPA allows that $R_{\rm qp} > 1$ and at the same time $R_{\rm nqp} < 1$. Then (7.6) is evaluated as $R_{\rm obs} = 0.54$. Thus possibility 4 combined with a large ratio between $\langle \mu_{\rm qp}^2 \rangle$ and $\langle \mu_{\rm nqp}^2 \rangle$ can lead to $R_{\rm qp} > 1$ even if $R_{\rm obs} < 1$.

Although possibility 4, which favors negative F^a, is proposed, the true intention of mine is not to insist that $R_{\rm qp} > 1$ or $F^a < 0$. Possibility 4 lacks a quantitative physical background as well as the other possibilities. Furthermore, our OD PAM in the RPA does not support the above values $R_{\rm qp} = 1.5$ and $R_{\rm nqp} = 0.3$; these values are chosen only for an illustration.

What our results in the RPA suggest, instead and in actual, is that there can be a variety of behaviors of $\chi_{\rm nqp}$, depending on the details of the model. If we make the model more realistic by incorporating the crystalline field and spin-orbit coupling, the Hartree-Fock band would change somewhat and thus $\chi_{\rm nqp}$ might change considerably; we cannot predict which one is realized out of possibilities 1–4. Therefore, my conclusion is simply that we have no ability to obtain $R_{\rm qp}$ or F^a from experiment by theory.

Finally, let me comment on the two alternative approaches which might be used to discuss the present problem, but, in fact, would not work efficiently. The first one is the renormalized-parameter theories, which are obtained by unsophisticated approximations in some sophisticated methods[38–40] such as the slave-boson theory, the $1/N$ expansion, or the Gutzwiller projection method. In these theories there is no legal procedure to define the qp part of the response function, as well as the fact that those unsophisticated approximations are as unreliable as our RPA. Thus these theories are incapable of treating the problem of F^a.

The second one is the sophisticated band calculation. While the band calculation preserves the symmetry of the real materials well, it is nothing but a somewhat elaborate but incomplete version of the Hartree-Fock approximation. When one tries to calculate the susceptibility based on a band calculation result, one must take into account the correction due to the vertex parts. (Recall that, in our OD PAM, the Hartree-Fock band without the vertex correction gives unphysical results.) However, as the method of the band calculation becomes intricate and the model used in the band calculation becomes complicated, it becomes more and more a formidable task to treat the vertex correction consistently with the way the electron-electron interaction is treated in the band calculation. Thus, although the band calculation might be valuable for the determination of the Fermi surface, it is not efficient, at least, in the estimation of the non-qp part of the response function.

What we can affirm with confidence is only that the static uniform susceptibility is large if the specific-heat mass is large, because there is always a conserved part of the magnetization. This is trivial from the first. Alas, we cannot know what is not trivial at present.

VIII. CONCLUSION

In this paper we have reformulated the Fermi-liquid theory for the dynamical susceptibility $\chi(q,\Omega)$ based on the Kubo formula with sufficient systematics and generality as applicable to the most general form of the multicomponent Fermion system. The long-wavelength and low-frequency response can be divided into the quasiparticle (qp) and non-qp parts; the qp part can be described by a natural extension of Landau's phenomenological formula for the Fermi liquid. An advantage of our formalism is that the relation of the qp-band basis to the original local basis is transparent.

Luttinger's procedure to obtain the isothermal static uniform susceptibility χ_T has been examined with a similar systematics and generality. We have carefully clarified where the conservation property is required in the procedure and recognized the difficulty in applying it to the systems where the magnetization is not conserved. It has been also emphasized that there is no simple way of extending the concept of the Pauli and Van Vleck terms to the interacting case if one considers only χ_T, which is in contrast to the fact that the qp and non-qp parts of the dynamical susceptibility are well defined even for the interacting Fermi liquid. On the other hand, if the magnetization is conserved, a compact general formula for χ_T has been obtained.

We have presented explicit identities which shows $\chi^k=\chi_T$, while $\chi^\omega=0$, provided that the magnetization is conserved, where χ^k and χ^ω are the k limit (the usual static limit) and the ω limit of the dynamical susceptibility. In addition, we have given a physical interpretation of the difference of χ^k and χ^ω. Thus we have unified the two seemingly distinct Fermi-liquid approaches for the static uniform susceptibility, in the most general form applicable to any conserved quantity of any multicomponent Fermi liquid.

By applying the above general formalism to the three kinds of the periodic Anderson models, we have found great variety of the behavior of the non-qp part of the susceptibility. It has been shown to be possible, in principle, that the Fermi-liquid parameter F^a is negative even if the observed Wilson ratio is less than unity. However, our more unfeigned and a bit regrettable conclusion is that it is impossible to estimate the value of F^a theoretically or experimentally in practice at present.

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APPENDIX A: STATISTICAL AVERAGES

The equilibrium statistical average of a quantum observable under a static uniform external field h for a temperature $T=\beta^{-1}$ and a chemical potential μ is given by

$$\langle \hat{O} \rangle_h \equiv \mathrm{tr}(\hat{\rho}_h \hat{O}) , \tag{A1}$$

where the equilibrium density operator is

$$\hat{\rho}_h(T,\mu) \equiv e^{-\beta(\hat{H}-h\hat{M}-\mu\hat{N})}/Z_h(T,\mu) , \tag{A2}$$

and the grand partition function is

$$Z_h = \mathrm{tr}(e^{-\beta(\hat{H}-h\hat{M}-\mu\hat{N})}) , \tag{A3}$$

with $\hat{N}$ the total number operator.

The dynamical statistical average of a quantum observable under the space-time-dependent external field given by (2.11) is defined as

$$\langle \hat{O} \rangle(t) \equiv \mathrm{tr}[\hat{\rho}(t)\hat{O}] , \tag{A4}$$

where the time dependence of the density operator is governed by

$$i\frac{\partial}{\partial t}\hat{\rho}(t)=[\hat{H}_{\rm tot}(t)-\mu\hat{N},\hat{\rho}(t)]\ , \tag{A5}$$

with the initial condition

$$\lim_{t\to-\infty}\hat{\rho}(t)=\hat{\rho}_0\ , \tag{A6}$$

where $\hat{\rho}_0$ is given by (A2) with $h=0$.

APPENDIX B: SPECTRAL WEIGHT FUNCTIONS

The spectral weight function (matrix) $\rho_k(\omega)$ of the single-particle Green's function is given by

$$[\rho_k(\omega)]_{ij}=\sum_{a,b}\langle a|\hat{\psi}_i(k)|b\rangle\langle b|\hat{\psi}_j^\dagger(k)|a\rangle \times(e^{-\beta E_a}+e^{-\beta E_b})\delta(\omega-(E_b-E_a))/Z_0\ , \tag{B1}$$

where $|a\rangle$ and E_a are an eigenpair pair of $\hat{H}-\mu\hat{N}$, and satisfies the sum rule

$$\int d\omega[\rho_k(\omega)]_{ij}=\langle[\hat{\psi}_i(k),\hat{\psi}_j^\dagger(k)]\rangle_0=\delta_{ij}\ . \tag{B2}$$

The spectral weight function $w(q,\omega)$ of the two-particle Green's function is given by

$$w(q,\omega)=\pi(1-e^{-\beta\omega})S(q,\omega)\ , \tag{B3}$$

where

$$S(q,\omega)=\int\frac{dt}{2\pi}e^{i\omega t}\langle\hat{m}(q,t)\hat{m}(-q,0)\rangle_0 \tag{B4}$$

$$=N_{\rm sys}\sum_{a,b}\langle a|\hat{m}(q)|b\rangle\langle b|\hat{m}(-q)|a\rangle \times e^{-\beta E_a}\delta(\omega-(E_b-E_a))/Z_0\ . \tag{B5}$$

At $q=0$, they satisfy the sum rules

$$\int d\omega\, w(0,\omega)=\frac{1}{N_{\rm sys}}\langle[\hat{M},\hat{M}]\rangle_0=0\ , \tag{B6}$$

$$\int d\omega\, S(0,\omega)=\frac{1}{N_{\rm sys}}\langle\hat{M}\hat{M}\rangle_0\ , \tag{B7}$$

$$\int\frac{d\omega}{\pi}\ \frac{w(0,\omega)}{\omega}=\mathcal{K}(0,0)=\chi_T\ , \tag{B8}$$

$$\mathrm{P}\int\frac{d\omega}{\pi}\ \frac{w(0,\omega)}{\omega}=K^R(q\equiv0,\ \Omega\to0)=\chi^\omega\ . \tag{B9}$$

Be careful with the last two formulas. The principal-part integral is defined as

$$\mathrm{P}\int\equiv\lim_{\epsilon\to0^+}\left[\int_{-\infty}^{-\epsilon}+\int_{+\epsilon}^{+\infty}\right]\ . \tag{B10}$$

In (B8), first the limit $\epsilon\to0^+$ is taken and then the limit $q\to0$; in (B9), the order of the two limits is reversed. Explicit formulas for the right-hand sides of (14) and (15) are as follows:

$$\chi^\omega=\frac{1}{Z_0N_{\rm sys}}\sum_{\substack{a,b\\(E_a\neq E_b)}}\langle a|\hat{M}|b\rangle\langle b|\hat{M}|a\rangle\frac{e^{-\beta E_a}-e^{-\beta E_b}}{E_a-E_b}\ , \tag{B11}$$

$$\chi_T=\chi^\omega+\frac{\beta}{Z_0N_{\rm sys}}\sum_{\substack{a,b\\E_a=E_b}}\langle a|\hat{M}|b\rangle\langle b|\hat{M}|a\rangle e^{-\beta E_a}\ . \tag{B12}$$

APPENDIX C: PROOF OF (4.17) UNDER *WEAK* CONSERVATION

By the *(weak)* conservation of $\hat{M}$, we mean that $[\hat{M},\hat{H}]=0$ and therefore

$$\mu_i+\mu_m=\mu_l+\mu_j\ , \tag{C1}$$

at each two-body interaction vertex (Fig. 1), as well as M commutes with E_k. On the other hand, by the *strong* conservation, we mean that there is a further restriction at each two-body interaction vertex such that either

$$(\mu_i,\mu_m)=(\mu_j,\mu_l)\ \text{ or }\ (\mu_i,\mu_m)=(\mu_l,\mu_m)\ . \tag{C2}$$

We sketch the proof of (4.17) under the weak conservation of $\hat{M}$, which is a slight modification of the argument given in Sec. IV of Luttinger and Ward (LW).[41] First, note that M, Σ_k, and $\mathcal{G}_k$ are simultaneously diagonalizable because of the weak conservation; we denote the diagonal elements of the latter as Σ_{ki} and $\mathcal{G}_{ki}$, respectively. Thus, by a partial integration, the left-hand side of (4.17) can be rewritten as

$$\frac{-1}{2\pi i}\sum_{k,i}\mu_iJ_{ki} \tag{C3}$$

with

$$J_{ki}=\int_C d\zeta\,\Sigma_{ki}(\zeta)\frac{\partial\mathcal{G}_{ki}}{\partial\zeta}\ , \tag{C4}$$

where the contour of integration is the same as that of LW. If we further assume the *strong* conservation, each of J_{ki} vanishes independently by a similar argument to the one given in Sec. IV of Luttinger.[5] But this does not hold generally under only the weak conservation. Nonetheless, the sum of all the J_{ki}'s vanishes as a whole. The only change we need compared to the argument of LW is that a factor of the following form appears instead of the left-hand side of Eq. (64) in LW:

$$\left[\sum_{i=1}^4\mu_i\frac{\partial}{\partial\zeta_i}\right]\delta(\zeta_1+\zeta_2-\zeta_3-\zeta_4)\ . \tag{C5}$$

This factor reduces to zero because of (C1). Therefore, (C3) yields nothing, and thus (4.17) is proved under the weak conservation.

APPENDIX D: $m(h)$ OF THE DD PAM

The expression for the magnetization per site at $T=0$ under a static uniform field, $m(h)=M(h)/N_{\rm sys}$, is given for $U=0$ and $\mu=0$ (i.e., for the noninteracting case, where the Fermi level lies in the gap when $h=0$).

(i) For $0\le h\le h_1$,

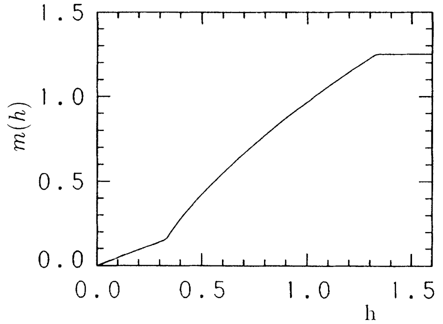

FIG. 13. Magnetization per site of the DD PAM with $D=1.0$ and $\Delta=0.1$ at $U=0$ and $\mu=0$ for $g^c=2.0$ and $g^f=0.5$.

$$m(h)=\frac{\mu_1}{2D}\{[(D+\mu_1 h)^2+4V^2]^{1/2} -[(D-\mu_1 h)^2+4V^2]^{1/2}\} . \tag{D1}$$

(ii) For $h_1 \le h \le h_2$,

$$m(h)=\mu_2+\frac{\mu_1}{2D}[(D+\mu_1 h)^2+4V^2]^{1/2} \tag{D2}$$

$$+\frac{1}{2D}\left[\frac{1}{4}[(g^c)^2-(g^f)^2+2g^c g^f]h-\frac{2V^2}{h}\right] . \tag{D3}$$

(iii) For $h_2 \le h$,

$$m(h)=\mu_2 , \tag{D4}$$

where

$$\mu_1=\tfrac{1}{2}(g^f-g^c) , \tag{D5}$$

$$\mu_2=\tfrac{1}{2}(g^f+g^c) , \tag{D6}$$

and

$$h_1=\frac{1}{g^c g^f}\{-Dg^f+[(Dg^f)^2+4g^c g^f V^2]^{1/2}\} , \tag{D7}$$

$$h_2=\frac{1}{g^c g^f}\{Dg^f+[(Dg^f)^2+4g^c g^f V^2]^{1/2}\} . \tag{D8}$$

The $m(h)$ curve on the whole range of h is depicted in Fig. 13.

APPENDIX E: ANOTHER OD PAM

Another orbitally denigrate PAM is considered: We assume that the hybridization matrix element is of the form

$$V_{km}=\sqrt{4\pi/(2L+1)}VY_L^m(k/|k|) , \tag{E1}$$

where $Y_L^m(k/|k|)$ is the usual spherical harmonics. For the same noninteracting band as the OD PAM of Sec. VI C 3 and in the same RPA, we obtain the susceptibilities as follows: the qp part is

$$\chi_{\mathrm{qp}}^{\mathrm{RPA}}=\left[\frac{1}{2}g^s\right]^2\frac{\mathcal{N}_{\mathrm{tot}}}{1+F^*} , \tag{E2}$$

where F^* is given by (6.44) with U replaced by

$$U^*=U/(2L+1) . \tag{E3}$$

The non-qp part is

$$\chi_{\mathrm{nqp}}^{\mathrm{RPA}}=\frac{L(L+1)(g^l)^2}{3}\frac{4\mathcal{S}_0}{1-U^*\mathcal{S}_0} , \tag{E4}$$

where $\mathcal{S}_0$ is given by (6.95).

The main difference between this OD PAM and the one in the text lies in the fact that the f electrons cannot be recombined *locally* into those which hybridize with the c electron and those which do not. As a result, (i) the term $\frac{1}{2}n_f U$ vanishes from the denominator of $\mathcal{G}_{k\sigma}^{(0)}$, and (ii) the elements of the matrix W become dependent on k and σ differently. As long as $n_f \approx 1$ and $V/D<1$,

$$U^*\mathcal{S}_0 \approx -F^* \approx \tfrac{1}{2}\mathcal{N}_{\mathrm{tot}}U^* . \tag{E5}$$

Thus, as opposed to the model in the text, both $\chi_{\mathrm{qp}}^{\mathrm{RPA}}$ and $\chi_{\mathrm{nqp}}^{\mathrm{RPA}}$ are enhanced, while the enhancement of $\chi_{\mathrm{nqp}}^{\mathrm{RPA}}$ is slightly smaller than that of $\chi_{\mathrm{nqp}}^{\mathrm{RPA}}$.

The above results have already been obtained in the limit of $V/D \to 0$ by Yamada *et al.*[6] In their calculation, however, the condition $V/D \ll 1$ is used in the intermediate steps, and hence the origin of the terms is obscured, and their result cannot be applicable unless $V/D \ll 1$.

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[25] Here we use that $\mathrm{Re}[L^A_{k\alpha}(\omega,T)-L^A_{k\alpha}(\omega,0)]$ is $O(T^2)$. If one fixes the total number of the fermions rather than the chemical potential μ, then μ varies with T; however, the variation of μ is expected to be $O(T^2)$, and thus (3.8),(3.9) are valid in the lowest order in this case, too.

[26] If the distinct bands of the indices α and β degenerate, the cross term proportional to $A^*_{k\alpha}\otimes A^*_{k\beta}$ has the similar singularity and must be included in the near part.

[27] In this paper the term "Ward identity" is used as the generic name for any relation between the self-energy and vertex parts.

[28] The Boltzmann constant k_B is suppressed except here.

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[30] L. D. Landau, Zh. Eksp. Teor. Fiz. **35**, 143 (1959) [Sov. Phys. JETP **8**, 101 (1959)].

[31] In order for the following argument to work, it is necessary either that the cross terms mentioned in Ref. 26 do not exist or that the contribution from these terms will vanish by some symmetry reason or others. The latter holds in the examples treated in this paper.

[32] By hypothesis 5, we can set $\omega=\omega'=0$ in $f_{\alpha\beta}$ and $S_{\alpha\beta}$.

[33] The summand vanishes as $E^*_{k\beta}\to E^*_{k\alpha}$, and there is no fear of divergence.

[34] It is assumed that the direction of the external field is fixed, and only the magnetization along that direction is considered; thus the magnetization is treated as a scalar quantity.

[35] Note that (6.30) is different from Eq. (2.13) of Yip (Ref. 10). His result for the off-diagonal element is not precise enough, because the phase factor in front of the square root is not determined; the factor depends on the phase of V_k and whether the Fermi surface lies in the upper or lower band. In our choice of the real positive V and the lower band, the correct factor is -1, as written in (6.30).

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