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Fermi Liquid Theory on the Basis of the Periodic Anderson Model with Spin-Orbit Coupling and Crystalline Field

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In order to discuss the normal-state properties of heavy-fermion systems, the Fermi liquid theory is developed on the basis of the periodic Anderson model with arbitrary spin-orbit coupling and crystalline field. For the unperturbed ($U=0$) case, the electronic band structure is determined; then the expressions of T-linear coefficient of specific heat and magnetic susceptibility are derived. For $U\neq 0$, the general expressions for T-linear coefficient of specific heat and magnetization are derived. However, the expression for magnetic susceptibility cannot generally be brought into such a usual form that includes only the quantities on the Fermi surface because of the existence of off-diagonal elements of f-electron self-energy. Therefore, the susceptibility is calculated in the special case that only the lowest Kramers doublet is taken into account.

§ 1. Introduction

Heavy fermions are characterized by the large values of the T-linear coefficient (γ) of specific heat, magnetic susceptibility (χ) and the T-square coefficient (A) of resistivity. The values of γ and χ observed in Ce and U metallic compounds are 10^{2-3} times larger than those in ordinary metals, and the values of A are more than 10^4 times larger.[1] These heavy-fermion behaviors are understood most naturally by the Fermi liquid theory which starts from the unperturbed hybridized-band states between localized f electrons and conduction electrons and then includes the Coulomb repulsion between f electrons.[2),3)] The first paper[2)] is concerned with the orbitally-non-degenerate case, and in the second[3)] the orbital degeneracy of f electrons is included. In order to understand the heavy-fermion behaviors of real metallic compounds more precisely, it is necessary to take the spin-orbit coupling and the crystal field into consideration. The purpose of the present paper is to extend the Fermi liquid theory[2),3)] to the most general case including the spin-orbit coupling and the crystal field for f electrons.

The periodic Anderson Hamiltonian constructed by localized f-electron states with Coulomb repulsion U, conduction-electron states of plane waves and hybridizations between them is considered:

$$H=\sum_{\boldsymbol{k}\sigma}\varepsilon_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}^{\dagger}c_{\boldsymbol{k}\sigma}+\sum_{iMM'}E_{MM'}f_{iM}^{\dagger}f_{iM'}+\frac{U}{2}\sum_{iM\neq M'}f_{iM}^{\dagger}f_{iM}f_{iM'}^{\dagger}f_{iM'}$$
$$+\frac{1}{\sqrt{N}}\sum_{iM\boldsymbol{k}\sigma}(V_{\boldsymbol{k}M\sigma}e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}f_{iM}^{\dagger}c_{\boldsymbol{k}\sigma}+V_{\boldsymbol{k}M\sigma}^{*}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i}c_{\boldsymbol{k}\sigma}^{\dagger}f_{iM}). \tag{1}$$

Here, $c_{\boldsymbol{k}\sigma}^{\dagger}$ is the creation operator of conduction electron in the plane wave state with wavevector $\boldsymbol{k}$ and spin σ, whose wave function and energy are given by

$$|\boldsymbol{k}\sigma\rangle=\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\chi_\sigma=\frac{4\pi}{\sqrt{\Omega}}\sum_{l=0}^{\infty}i^l j_l(kr)\sum_{m=-l}^{l}Y_l^{m*}(\theta_k,\varphi_k)Y_l^m(\theta_r,\varphi_r)\chi_\sigma\,, \tag{2}$$

$$\varepsilon_{k\sigma}=\varepsilon_k-\sigma\mu_B H\,. \tag{3}$$

Here, χ_σ is the spin function, $j_l(kr)$ is the spherical Bessel function, $Y_l^m(\theta,\varphi)$ is the spherical harmonic and Ω is the volume of the crystal. H is the magnitude of the external magnetic field applied along z-axis, μ_B is the Bohr magneton, and $\sigma=1$ for up-spin and $\sigma=-1$ for down. $f_{iM}^\dagger$ is the creation operator of f electron at site i in the eigenstate of spin-orbit coupling and crystal field, which is denoted by M. The eigenstate is expressed as

$$|iM\rangle=R_{nl}(|\boldsymbol{r}-\boldsymbol{R}_i|)\sum_{m\sigma}a_{lm\sigma}^M Y_l^m(\theta_{r-R_i},\varphi_{r-R_i})\chi_\sigma\,, \tag{4}$$

where R_{nl} is the radial part in which $n=4$ and $l=3$ for Ce ion, and $a_{lm\sigma}^M$ is the Clebsch-Gordan coefficient. The f-electron energy with off-diagonal elements of the Zeeman term is given by

$$E_{MM'}=E_M\delta_{MM'}-\langle M|(l_z+2s_z)|M'\rangle\mu_B H\,. \tag{5}$$

The third term of Eq. (1) represents the on-site Coulomb repulsion between f electrons, $U>0$, and the fourth term represents the mixing between f electron and conduction electron. The mixing matrix element is given as

$$V_{kM\sigma}=\sqrt{4\pi}\sum_m a_{lm\sigma}^M Y_l^m(\theta_k,\varphi_k)V_{knl}\,, \tag{6}$$

$$V_{knl}=(-i)^l\sqrt{\frac{4\pi}{\Omega}}\int_0^\infty j_l(kr)V(r)R_{nl}(r)r^2dr\,, \tag{7}$$

where $V(r)$ is the effective potential for electrons. In this paper, the Fermi liquid theory is developed by taking the $U=0$ case as the unperturbed state. For that purpose, it is convenient to rewrite the Hamiltonian (1) as

$$H=\sum_{k\sigma}\varepsilon_{k\sigma}c_{k\sigma}^\dagger c_{k\sigma}+\sum_{kMM'}E_{MM'}f_{kM}^\dagger f_{kM'}+\sum_{kM\sigma}(V_{kM\sigma}f_{kM}^\dagger c_{k\sigma}+V_{kM\sigma}^* c_{k\sigma}^\dagger f_{kM})$$
$$+\frac{U}{2N}\sum_{kk'qMM'}f_{k-qM}^\dagger f_{k'+qM'}^\dagger f_{k'M'}f_{kM} \tag{8}$$

by introducing the Bloch state of f electron as

$$f_{kM}=\frac{1}{\sqrt{N}}\sum_i e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}f_{iM}\,. \tag{9}$$

In this paper the T-linear coefficient of specific heat and the magnetic susceptibility are derived. In § 2, the electronic band structures are determined for the unperturbed ($U=0$) case. In § 3, the magnetic susceptibility for $U=0$ is calculated, which corresponds to the generalization of the results for the case of strong spin-orbit coupling limit derived in Ref. 4). The perturbed ($U\neq0$) case is treated in § 4, in which the T-linear coefficient of specific heat is derived but the magnetic susceptibility can be calculated only in the case where the lowest Kramers doublet of f-electron state is

relevant. The reason why it is difficult to calculate the susceptibility for general cases is discussed in § 4. Concluding remarks are made in the last section.

§ 2. Electronic band structure and density of states for non-interacting case ($U=0$)

In this section we derive the electronic band structure of the $U=0$ non-interacting case as the unperturbed state of the Fermi liquid theory. In the absence of magnetic field ($H=0$), the Green's functions of conduction electrons and f electrons are given by

$$G^c_{\boldsymbol{k}\sigma\sigma}(\omega)=A_{\boldsymbol{k}\bar{\sigma}}(\omega)/[A_{\boldsymbol{k}\sigma}(\omega)A_{\boldsymbol{k}\bar{\sigma}}(\omega)-B_{\boldsymbol{k}\sigma}(\omega)B_{\boldsymbol{k}\bar{\sigma}}(\omega)]\,, \tag{10}$$

$$G^c_{\boldsymbol{k}\bar{\sigma}\sigma}(\omega)=B_{\boldsymbol{k}\bar{\sigma}}(\omega)/[A_{\boldsymbol{k}\sigma}(\omega)A_{\boldsymbol{k}\bar{\sigma}}(\omega)-B_{\boldsymbol{k}\sigma}(\omega)B_{\boldsymbol{k}\bar{\sigma}}(\omega)]\,, \tag{11}$$

$$G^f_{\boldsymbol{k}MM'}(\omega)=\frac{\delta_{MM'}}{\omega-E_M}+\sum_{\sigma\sigma'}\frac{V_{\boldsymbol{k}M\sigma}}{\omega-E_M}G^c_{\boldsymbol{k}\sigma\sigma'}(\omega)\frac{V^*_{\boldsymbol{k}M'\sigma'}}{\omega-E_{M'}}\,, \tag{12}$$

where $\bar{\sigma}=-\sigma$ and

$$A_{\boldsymbol{k}\sigma}(\omega)=\omega-\varepsilon_{\boldsymbol{k}}-\sum_M\frac{|V_{\boldsymbol{k}M\sigma}|^2}{\omega-E_M}\,, \tag{13}$$

$$B_{\boldsymbol{k}\sigma}(\omega)=\sum_M\frac{V^*_{\boldsymbol{k}M\sigma}V_{\boldsymbol{k}M\bar{\sigma}}}{\omega-E_M}\,. \tag{14}$$

Note that the Hamiltonian (8) is diagonal with respect to $\boldsymbol{k}$ and M in the case $U=0$ and $H=0$.

In the case that localized f-electron states have the Kramers degeneracy as for Ce^{3+}, $B_{\boldsymbol{k}\sigma}$ always vanishes as proved in the following. The time-reversal operation, denoted by the operator K, on the state $|iM\rangle$ of Eq. (4) gives its counterpart of the Kramers doublet, denoted by $|i\bar{M}\rangle$, with a phase factor which has no physical significance. Using the relations that $K(\psi\chi_\uparrow)=\psi^*\chi_\downarrow$, $K(\psi\chi_\downarrow)=-\psi^*\chi_\uparrow$ and $Y_l^{m*}(\theta_{\boldsymbol{k}},\varphi_{\boldsymbol{k}})=(-)^mY_l^{-m}(\theta_{\boldsymbol{k}},\varphi_{\boldsymbol{k}})$, we obtain

$$a^{\bar{M}}_{l-m\uparrow}=e(-)^{m+1}a^M_{lm\downarrow}\,,\quad a^{\bar{M}}_{l-m\downarrow}=e(-)^ma^M_{lm\uparrow}\,. \qquad (e=1 \text{ or } -1) \tag{15}$$

Note that the Clebsch-Gordan coefficients are taken to be real. From Eqs. (6), (15) and $E_M=E_{\bar{M}}$, $B_{\boldsymbol{k}\uparrow}(\omega)$ of Eq. (14) is calculated as

$$\begin{aligned}B_{\boldsymbol{k}\uparrow}(\omega)&=\frac{1}{2}\sum_M\frac{V^*_{\boldsymbol{k}M\uparrow}V_{\boldsymbol{k}M\downarrow}+V^*_{\boldsymbol{k}\bar{M}\uparrow}V_{\boldsymbol{k}\bar{M}\downarrow}}{\omega-E_M}\\&=2\pi|V_{knl}|^2\sum_M\frac{1}{\omega-E_M}\sum_{mm'}(a^M_{lm\uparrow}a^M_{lm'\downarrow}Y_l^{m*}Y_l^{m'}+a^{\bar{M}}_{l-m'\uparrow}a^{\bar{M}}_{l-m\downarrow}Y_l^{-m'*}Y_l^{-m})\\&=2\pi|V_{knl}|^2\sum_M\frac{1}{\omega-E_M}\sum_{mm'}(a^M_{lm\uparrow}a^M_{lm'\downarrow}-a^M_{lm'\downarrow}a^M_{lm\uparrow})Y_l^{m*}Y_l^{m'}=0\,.\end{aligned}$$

In the same way, $B_{\boldsymbol{k}\downarrow}(\omega)=0$.

In the case $U=0$ and $H=0$, therefore, the Green's functions are written by

$$G^c_{\boldsymbol{k}\sigma\sigma}(\omega)=1/A_{\boldsymbol{k}\sigma}(\omega)\,, \tag{16}$$

$$G^f_{kMM}(\omega)=\frac{1}{\omega-E_M}+\sum_\sigma\frac{|V_{kM\sigma}|^2}{(\omega-E_M)^2}G^c_{k\sigma\sigma}(\omega)\,. \tag{17}$$

It is shown that

$$\begin{aligned}|V_{kM\sigma}|^2+|V_{k\bar{M}\sigma}|^2&=|V_{kM\sigma}|^2+|V_{kM\bar{\sigma}}|^2\\&=4\pi|V_{knl}|^2\sum_{mm'}(a^M_{lm\sigma}a^M_{lm'\sigma}+a^M_{lm\bar{\sigma}}a^M_{lm'\bar{\sigma}})\,Y_l^{m*}(\theta_k,\varphi_k)\,Y_l^{m'}(\theta_k,\varphi_k)\\&\equiv 2I_{kM}\,,\end{aligned} \tag{18}$$

which is independent of σ and the same as $2I_{k\bar{M}}$. Therefore, we obtain

$$G^c_{k\sigma\sigma}(\omega)=1/A_k(\omega)\,, \tag{19}$$

$$G^f_{kMM}(\omega)=\frac{1}{\omega-E_M}+\frac{2I_{kM}}{(\omega-E_M)^2A_k(\omega)}\,, \tag{20}$$

where

$$A_k(\omega)=\omega-\varepsilon_k-\sum_M\frac{I_{kM}}{\omega-E_M}\,, \tag{21}$$

which is independent of σ, so that we drop the subscript σ. The Green's functions of Eqs. (19) and (20) have the same pole at $\omega=E^*_{kn}$ which is an eigenvalue of the hybridized band and determined by

$$A_k(E^*_{kn})=E^*_{kn}-\varepsilon_k-\sum_M\frac{I_{kM}}{E^*_{kn}-E_M}=0\,, \tag{22}$$

where the subscript n is assigned to the different eigenvalues. Corresponding eigenstates are given by

$$|\boldsymbol{k}n\sigma^*\rangle=\frac{1}{\sqrt{A_k'(E^*_{kn})}}\left[c^\dagger_{k\sigma}+\sum_M\frac{V_{kM\sigma}}{E^*_{kn}-E_M}f^\dagger_{kM}\right]|0\rangle\,, \tag{23}$$

where $|0\rangle$ is the vacuum state and

$$A_k'(E^*_{kn})=\left.\frac{dA_k(\omega)}{d\omega}\right|_{\omega=E^*_{kn}}=1+\sum_M\frac{I_{kM}}{(E^*_{kn}-E_M)^2}=\frac{d\varepsilon_k}{dE^*_{kn}}\,. \tag{24}$$

Furthermore, $G^f_{kMM}(\omega)$ has another pole at $\omega=E_M$. Residues of $G^c_{k\sigma\sigma}(\omega)$ and $G^f_{kMM}(\omega)$ are given by

$$z^c_{k\sigma}(E^*_{kn})=\frac{1}{A_k'(E^*_{kn})}=\left[1+\sum_M\frac{I_{kM}}{(E^*_{kn}-E_M)^2}\right]^{-1}\,, \tag{25}$$

$$z^f_{kM}(E^*_{kn})=\frac{2I_{kM}}{(E^*_{kn}-E_M)^2}z^c_{k\sigma}(E^*_{kn})\,, \tag{26}$$

$$z^f_{kM}(E_M)=1-\frac{2I_{kM}}{\sum_{M'\in\{E_{M'}=E_M\}}I_{kM'}}\qquad\text{for}\quad I_{kM}\neq 0\,, \tag{27}$$

$$z^f_{kM}(E_M)=1 \qquad \text{for} \quad I_{kM}=0\,. \tag{28}$$

Here it should be noted that $z^c_{k\sigma}(E^*_{kn})$ is independent of σ and

$$z^c_{k\sigma}(E^*_{kn})+\frac{1}{2}\sum_M z^f_{kM}(E^*_{kn})=1\,. \tag{29}$$

Introducing the Green's function of the electron in the hybridized-band state by

$$G^*_{kn\sigma}(\omega)=1/(\omega-E^*_{kn})\,, \tag{30}$$

we can rewrite the Green's functions of c- and f-electrons as

$$G^c_{k\sigma\sigma}(\omega)=\sum_n z^c_{k\sigma}(E^*_{kn})G^*_{kn\sigma}(\omega)\,, \tag{31}$$

$$G^f_{kMM}(\omega)=\sum_n z^f_{kM}(E^*_{kn})G^*_{kn\sigma}(\omega)+z^f_{kM}(E_M)/(\omega-E_M)\,. \tag{32}$$

Now we discuss how the electronic band structures are obtained. We put aside the exceptional case of some I_{kM} vanishing which we will discuss later.

If there are no degeneracies but the Kramers one, the residues at any E_M for $\boldsymbol{k}$ (Eq. (27)) vanish and Eq. (22) gives the whole band energies: The number of E^*_{kn} becomes $N_f/2+1$. Here, N_f denotes the degeneracy of the local f-electron states, and $N_f/2$ corresponds to the number of the Kramers doublets. In such a case, the whole bands are obtained to have dispersion.

If some f level including the state M has further degeneracy besides the Kramers one, a fraction of the state M mixes with the conduction-electron states to construct the hybridized bands, and the remaining part stays at the original energy E_M with the weight of Eq. (27). The total weight of the remaining unhybridized parts of the f level (named lth level) is calculated from Eq. (27) as $\sum_{M\in l\text{th level}} z^f_{kM}(E_M)=N_{fl}-2$ where N_{fl} is the degeneracy of the level. These remaining parts, of course, form dispersionless bands at the original energy.

An exceptional case that $I_{kM}=0$ occurs, for example, for $\boldsymbol{k}$ parallel to one of the crystal axes for the cubic Γ_7 doublet. In such a case the Γ_7 state is outside of the mixing problem solved by Eq. (22), but joins the band formation by connecting continuously to a solution of Eq. (22) for $I_{kM}\neq 0$.

A simplicity of Eq. (22) to be solved appears for the spherically symmetric case that only the spin-orbit coupling is considered. Using the expressions of Clebsch-Gordan coefficients

$$a^M_{lm\sigma}=-\sigma\sqrt{\frac{l+1/2-j_{1z}\sigma}{2l+1}}\,\delta_{m,j_{1z}-1/2\sigma} \qquad \text{for} \quad M\colon j_1=l-\frac{1}{2},\ j_{1z}\,, \tag{33}$$

$$a^M_{lm\sigma}=\sqrt{\frac{l+1/2+j_{2z}\sigma}{2l+1}}\,\delta_{m,j_{2z}-1/2\sigma} \qquad \text{for} \quad M\colon j_2=l+\frac{1}{2},\ j_{2z}\,, \tag{34}$$

and the relations $\sum_{m=-l}^{l}|Y_l^m(\theta,\varphi)|^2=(2l+1)/4\pi$, $\sum_{m=-l}^{l} m|Y_l^m(\theta,\varphi)|^2=0$, we obtain

$$\sum_{M=j_1,-j_1}^{j_1,j_1} I_{kM}=l|V_{knl}|^2=\frac{2j_1+1}{2}|V_{knl}|^2\,, \tag{35}$$

$$\sum_{M=j_2,-j_2}^{j_2,j_2} I_{kM}=(l+1)|V_{knl}|^2=\frac{2j_2+1}{2}|V_{knl}|^2 . \tag{36}$$

Therefore, Eq. (22) is rewritten as

$$E^*_{kn}-\varepsilon_k-\frac{l|V_{knl}|^2}{E^*_{kn}-E_{j_1}}-\frac{(l+1)|V_{knl}|^2}{E^*_{kn}-E_{j_2}}=0 , \tag{37}$$

which does not depend on the direction of $\boldsymbol{k}$, thereby leading to an expected result that the whole bands are spherical. The degree of Eq. (37) with respect to E^*_{kn} becomes three, giving three hybridized bands with twofold degeneracy. The prefactors of $|V_{knl}|^2$ are equal to half of the degeneracy of the corresponding spin-orbit levels. It means that the effective mixing matrices are enhanced by the square root of half of the degeneracy. This fact can be seen straightforwardly if one compares Eq. (37) for the single-level case of infinite E_{j_2} or $E_{j_1}=E_{j_2}$ with the corresponding equation for the orbitally nondegenerate case in which the prefactor equals one.

In the present paper, we consider the case that the total number of f- and c-electrons per f-site is less than two and the lowest band is a hybridized one denoted by E^*_{k0}, so that only the lowest band of E^*_{k0} is partially-filled and the other bands are unoccupied. In this case, the T-linear coefficient of the specific heat is given by

$$\gamma=\frac{2\pi^2}{3}k_B{}^2\sum_k \delta(\mu-E^*_{k0}) , \tag{38}$$

where k_B is the Boltzmann constant and μ is the Fermi energy. This is proportional to the density of states at the Fermi energy, which is rewritten using Eq. (29) as

$$\sum_k \delta(\mu-E^*_{k0})=\sum_k\left[z^c_{k\sigma}(E^*_{k0})+\frac{1}{2}\sum_M z^f_{kM}(E^*_{k0})\right]\delta(\mu-E^*_{k0}) . \tag{39}$$

By denoting the density of states of the original conduction band per spin as $\rho(\varepsilon_k)$, the summation over wavevector is replaced by

$$\sum_k=\int\frac{d\Omega_k}{4\pi}\int\rho(\varepsilon_k)d\varepsilon_k=\int\frac{d\Omega_k}{4\pi}\int\rho(\varepsilon_k)\frac{d\varepsilon_k}{dE^*_{k0}}dE^*_{k0} , \tag{40}$$

where $d\Omega_k=\sin\theta_k d\theta_k d\varphi_k$. Noting Eq. (24), we have

$$\sum_k \delta(\mu-E^*_{k0})=\int\frac{d\Omega_k}{4\pi}\rho(\varepsilon_k{}^\mu)+\sum_M\int\frac{d\Omega_k}{4\pi}\rho(\varepsilon_k{}^\mu)\frac{I_{kM}}{(\mu-E_M)^2} , \tag{41}$$

where

$$\varepsilon_k{}^\mu=\mu-\sum_M\frac{I_{kM}}{\mu-E_M} . \tag{42}$$

The first term of Eq. (41) corresponds to the density of states of conduction electrons, which coincides with that of the original conduction band for a constant density of states, and the second term to that of f electrons.

§ 3. Susceptibility for $U=0$

To derive the expression of magnetic susceptibility, we must solve the equation for $H\neq 0$

$$A_{k\sigma}(\omega)A_{k\bar{\sigma}}(\omega)-B_{k\sigma}(\omega)B_{k\bar{\sigma}}(\omega)=0 \tag{43}$$

to obtain the eigenvalues up to the order of H^2. Here $A_{k\sigma}(\omega)$ and $B_{k\sigma}(\omega)$ are obtained as

$$A_{k\sigma}(\omega)=\omega-\varepsilon_k-a_k(\omega)+\sigma[1+b_k(\omega)]h-c_k(\omega)h^2+O(h^3)\,, \tag{44}$$

$$B_{k\sigma}(\omega)=-d_{k\sigma}(\omega)h+O(h^2)\,, \tag{45}$$

where $h=\mu_B H$ and

$$a_k(\omega)=\sum_M \frac{|V_{kM\sigma}|^2}{\omega-E_M}\,, \tag{46}$$

$$b_k(\omega)=\sigma\sum_{MM'}\frac{V^*_{kM\sigma}\langle M|(l_z+2s_z)|M'\rangle V_{kM'\sigma}}{(\omega-E_M)(\omega-E_{M'})}\,, \tag{47}$$

$$c_k(\omega)=\sum_{MM'M''}\frac{V^*_{kM\sigma}\langle M|(l_z+2s_z)|M'\rangle\langle M'|(l_z+2s_z)|M''\rangle V_{kM''\sigma}}{(\omega-E_M)(\omega-E_{M'})(\omega-E_{M''})}\,, \tag{48}$$

$$d_{k\sigma}(\omega)=\sum_{MM'}\frac{V^*_{kM\sigma}\langle M|(l_z+2s_z)|M'\rangle V_{kM'\bar{\sigma}}}{(\omega-E_M)(\omega-E_{M'})}\,. \tag{49}$$

It is easily shown that $a_k(\omega)$, $b_k(\omega)$, $c_k(\omega)$ and $d_{k\sigma}(\omega)d_{k\bar{\sigma}}(\omega)=|d_{k\sigma}(\omega)|^2\equiv e_k(\omega)$ are independent of σ. Therefore, Eq. (43) is reduced to

$$\omega=\varepsilon_k+a_k(\omega)-\sigma\sqrt{[1+b_k(\omega)]^2+e_k(\omega)}\,h+c_k(\omega)h^2+O(h^3)\,. \tag{50}$$

We define the solutions of (50) for σ by $E^*_{k\sigma n}$, and consider the case that only the lowest bands $n=0$ are occupied as in the previous section. From the expressions of the total number of electrons and the energy of the ground state

$$N_e=\sum_{k\sigma}\theta(\mu-E^*_{k\sigma 0})\,, \tag{51}$$

$$E_0=\sum_{k\sigma}E^*_{k\sigma 0}\theta(\mu-E^*_{k\sigma 0})\,, \tag{52}$$

the susceptibility is obtained as

$$\chi=\chi_P+\chi_V\,, \tag{53a}$$

$$\chi_P=\sum_{k\sigma}\left[\frac{\partial E^*_{k\sigma 0}}{\partial H}\right]^2_{H=0}\delta(\mu-E^*_{k0})\,, \tag{53b}$$

$$\chi_V=-\sum_{k\sigma}\left.\frac{\partial^2 E^*_{k\sigma 0}}{\partial H^2}\right|_{H=0}\theta(\mu-E^*_{k0})\,. \tag{53c}$$

The first term χ_P may be called the Pauli term which gives rise to a usual Pauli susceptibility, and the second χ_V the Van Vleck term. The contribution from χ_V is crucial when the orbital degeneracy is considered. Differentiating Eq. (50) by h, we have

$$\left.\frac{\partial\omega}{\partial h}\right|_{h=0}=-\sigma\frac{\sqrt{[1+b_k(\omega)]^2+e_k(\omega)}}{1-a_k'(\omega)}, \tag{54}$$

$$\left.\frac{\partial^2\omega}{\partial h^2}\right|_{h=0}=\frac{1}{1-a_k'(\omega)}\left[\frac{\partial}{\partial\omega}\left\{\frac{[1+b_k(\omega)]^2+e_k(\omega)}{1-a_k'(\omega)}\right\}+2c_k(\omega)\right], \tag{55}$$

where $a_k'(\omega)=\partial a_k(\omega)/\partial\omega$. Noting that $1-a_k'(E^*_{kn})$ is just the same as $A_k'(E^*_{kn})$ of Eq. (24), and replacing the summation over $\boldsymbol{k}$ by the integration as Eq. (40), we have

$$\chi_P=2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\rho(\varepsilon_k{}^{\mu})\frac{[1+b_k(\mu)]^2+e_k(\mu)}{A_k'(\mu)}, \tag{56}$$

$$\begin{aligned}\chi_V&=-2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\int_{-D^*}^{\mu}dE^*_{k0}\rho(\varepsilon_k^{E^*_{k0}})\left[\frac{d}{dE^*_{k0}}\left\{\frac{[1+b_k(E^*_{k0})]^2+e_k(E^*_{k0})}{A_k'(E^*_{k0})}\right\}+2c_k(E^*_{k0})\right]\\&=-2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\rho(\varepsilon_k{}^{\mu})\frac{[1+b_k(\mu)]^2+e_k(\mu)}{A_k'(\mu)}\\&\quad+2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\rho(\varepsilon_k{}^{-D^*})\frac{[1+b_k(-D^*)]^2+e_k(-D^*)}{A_k'(-D^*)}\\&\quad+2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\int_{-D^*}^{\mu}dE^*_{k0}\left.\frac{d\rho(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=\varepsilon_k^{E^*_{k0}}}\{[1+b_k(E^*_{k0})]^2+e_k(E^*_{k0})\}\\&\quad-4\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\int_{-D^*}^{\mu}dE^*_{k0}\rho(\varepsilon_k^{E^*_{k0}})c_k(E^*_{k0}),\end{aligned} \tag{57}$$

where $-D^*$ is the lowest value of E^*_{k0} and

$$\varepsilon_k^{E^*_{k0}}=E^*_{k0}-\sum_M\frac{I_{kM}}{E^*_{k0}-E_M}. \tag{58}$$

The Pauli term χ_P is entirely cancelled by the first term of χ_V, Eq. (57). If we consider the case that the conduction-band width is much larger than the mixing matrix elements, which is relevant for the heavy-fermion systems, we have $A_k'(-D^*)=1$, $b_k(-D^*)=0$ and $e_k(-D^*)=0$. Then, we obtain

$$\begin{aligned}\chi&=2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\rho(\varepsilon_k{}^{-D^*})-4\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\int_{-D^*}^{\mu}dE^*_{k0}\rho(\varepsilon_k^{E^*_{k0}})c_k(E^*_{k0})\\&\quad+2\mu_B{}^2\int\frac{d\Omega_k}{4\pi}\int_{-D^*}^{\mu}dE^*_{k0}\left.\frac{d\rho(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=\varepsilon_k^{E^*_{k0}}}\{[1+b_k(E^*_{k0})]^2+e_k(E^*_{k0})\}.\end{aligned} \tag{59}$$

The fiirst term is the contribution from the conduction electrons, and the second is that from the f electrons. The third term is a correction which vanishes if the density of states of the original conduction band is constant. Here we assume the density of

states and the mixing integral to be constant: $\rho(\varepsilon_k)=\rho_0$; $|V_{knl}|^2=V^2$, then we obtain

$$\chi=2\mu_B{}^2\rho_0+\mu_B{}^2\rho_0 V^2\sum_{MM'}\frac{|\langle M|(l_z+2s_z)|M'\rangle|^2}{(\mu-E_M)(\mu-E_{M'})}, \tag{60a}$$

where

$$\langle M|(l_z+2s_z)|M'\rangle=\sum_{m\sigma}(m+\sigma)a^M_{lm\sigma}a^{M'}_{lm\sigma}. \tag{60b}$$

Here we have used Eqs. (48), (4), (6) and the orthonormalities of $|iM\rangle$, R_{nl} and Y_l^m. It should be noted that the expression of f-electron part is essentially the same as that for the Ce-impurity case derived in Ref. 5). This simple feature results from the assumptions of constant density of states and constant mixing.

We now calculate the susceptibility in the case of only the spin-orbit coupling considered. Using Eqs. (33) and (34), we have

$$\chi=2\mu_B{}^2\rho_0+\frac{2}{3}\mu_B{}^2\rho_0\left[\frac{g_{j_1}^2 j_1(j_1+1)}{(\mu-E_{j_1})^2}\left\{\frac{2j_2+1}{2}V^2\right\}+\frac{g_{j_2}^2 j_2(j_2+1)}{(\mu-E_{j_2})^2}\left\{\frac{2j_2+1}{2}V^2\right\}\right.$$
$$\left.+\frac{2l(l+1)/(2l+1)}{(\mu-E_{j_1})(\mu-E_{j_2})}V^2\right]. \tag{61}$$

Note that $j_1=l-1/2$, $g_{j_1}=2l/(2l+1)$; $j_2=l+1/2$, $g_{j_2}=(2l+2)/(2l+1)$. If $E_{j_1}=E_{j_2}=E$, we have

$$\chi=2\mu_B{}^2\rho_0+2\mu_B{}^2\rho_0\frac{(2l+1)V^2}{(\mu-E)^2}+\frac{2}{3}\mu_B{}^2\rho_0 l(l+1)\frac{(2l+1)V^2}{(\mu-E)^2}. \tag{62}$$

§ 4. Specific heat and susceptibility for full Hamiltonian ($U\neq 0$)

In the case that the Coulomb repulsion between f electrons is included, we can introduce the self-energy of f electron by $\Sigma_{kMM'}(\omega)$, then determine the Green's functions by

$$\hat{P}_k\hat{G}_k=\hat{1}_{N_f+2}, \tag{63a}$$

$$\hat{P}_k=\begin{pmatrix}\omega\hat{1}_{N_f}-\hat{E}-\hat{\Sigma}_k & \hat{v}_{k\uparrow} & \hat{v}_{k\downarrow}\\ \hat{v}^\dagger_{k\uparrow} & \omega-\varepsilon_{k\uparrow} & 0\\ \hat{v}^\dagger_{k\downarrow} & 0 & \omega-\varepsilon_{k\downarrow}\end{pmatrix}, \tag{63b}$$

$$\hat{G}_k=\begin{pmatrix}\hat{G}_k{}^f & \hat{G}^{fc}_{k\uparrow} & \hat{G}^{fc}_{k\downarrow}\\ \hat{G}^{cf}_{k\uparrow} & G^c_{k\uparrow\uparrow}(\omega) & G^c_{k\uparrow\downarrow}(\omega)\\ \hat{G}^{cf}_{k\downarrow} & G^c_{k\downarrow\uparrow}(\omega) & G^c_{k\downarrow\downarrow}(\omega)\end{pmatrix}\ (=\hat{P}_k{}^{-1}). \tag{63c}$$

$\hat{P}_k$ and $\hat{G}_k$ are $(N_f+2)\times(N_f+2)$ matrices. $\hat{1}_{N_f+2}$ and $\hat{1}_{N_f}$ denote the unit matrices of rank N_f+2 and N_f, respectively. These are simply written by $\hat{1}$ in the following. $\hat{E}$, $\hat{\Sigma}_k$ and $\hat{G}_k{}^f$ are $N_f\times N_f$ matrices whose MM' components are given by $E_{MM'}$, $\Sigma_{kMM'}(\omega)$ and $G^f_{kMM'}(\omega)$, respectively. $\hat{v}_{k\sigma}$ and $\hat{G}^{fc}_{k\sigma}$ are N_f-dimensional column vectors whose M component are given by $V_{kM\sigma}$ and $G^{fc}_{kM\sigma}(\omega)$, and $\hat{v}^\dagger_{k\sigma}$ and $\hat{G}^{cf}_{k\sigma}$ are the row vectors.

The determinant of $\hat{P}_k$ is expressed as

$$|\hat{P}_k|=\begin{vmatrix} \omega\hat{1}-\hat{E}-\hat{\Sigma}_k-\dfrac{\hat{v}_{k\sigma}\hat{v}^{\dagger}_{k\sigma}}{\omega-\varepsilon_{k\sigma}} & \dfrac{\hat{v}_{k\bar{\sigma}}}{\omega-\varepsilon_{k\bar{\sigma}}} \\ \hat{v}^{\dagger}_{k\bar{\sigma}} & \end{vmatrix}(\omega-\varepsilon_{k\sigma})$$

$$=\left|\omega\hat{1}-\hat{E}-\hat{\Sigma}_k-\sum_{\sigma}\frac{\hat{v}_{k\sigma}\hat{v}^{\dagger}_{k\sigma}}{\omega-\varepsilon_{k\sigma}}\right|(\omega-\varepsilon_{k\uparrow})(\omega-\varepsilon_{k\downarrow})\,, \tag{64}$$

where $\hat{v}_{k\sigma}\hat{v}^{\dagger}_{k\sigma}$ is the $N_f\times N_f$ matrix (tensor) whose MM' component is given by $V^{*}_{kM\sigma}V_{kM'\sigma}$. Therefore, if we define the $N_f\times N_f$ matrix

$$\hat{F}_k=\omega\hat{1}-\hat{E}-\hat{\Sigma}_k-\sum_{\sigma}\frac{\hat{v}_{k\sigma}\hat{v}^{\dagger}_{k\sigma}}{\omega-\varepsilon_{k\sigma}}\,, \tag{65}$$

the Green's functions of f- and c-electrons are given by

$$G^{f}_{kMM'}(\omega)=(\hat{F}_k{}^{-1})_{MM'}\,, \tag{66}$$

$$G^{c}_{k\sigma\sigma}(\omega)=\left[\omega-\varepsilon_{k\sigma}-\sum_{MM'}V^{*}_{kM\sigma}\left(\left[\omega\hat{1}-\hat{E}-\hat{\Sigma}_k-\frac{\hat{v}_{k\bar{\sigma}}\hat{v}^{\dagger}_{k\bar{\sigma}}}{\omega-\varepsilon_{k\bar{\sigma}}}\right]^{-1}\right)_{MM'}V_{kM'\sigma}\right]^{-1}$$

$$=\frac{1}{\omega-\varepsilon_{k\sigma}}+\frac{1}{\omega-\varepsilon_{k\sigma}}\sum_{MM'}V^{*}_{kM\sigma}G^{f}_{kMM'}(\omega)V_{kM'\sigma}\frac{1}{\omega-\varepsilon_{k\sigma}}\,. \tag{67}$$

By introducing the unitary matrix $\hat{U}_k$, $\hat{P}_k$ is diagonalized as $\hat{U}_k\hat{P}_k\hat{U}_k{}^{-1}=\hat{Q}_k$ to give eigenvalues E^{*}_{kn} where $n=1, 2, \cdots, N_f+2$. If we follow Luttinger's derivation,[6] the coefficient of the T-linear term in specific heat is obtained as

$$\gamma=\frac{\pi^2}{3}{k_B}^2\sum_{n=1}^{N_f+2}\delta(\mu-E^{*}_{kn})\,. \tag{68}$$

Now we calculate

$$\sum_{n=1}^{N_f+2}\delta(\omega-E^{*}_{kn})=-\frac{1}{\pi}\mathrm{Im}\frac{\partial}{\partial\omega}\log\prod_{n=1}^{N_f+2}(\omega+i\delta-E^{*}_{kn})=-\frac{1}{\pi}\mathrm{Im}\frac{\partial}{\partial\omega}\log|\hat{Q}_k|$$

$$=-\frac{1}{\pi}\mathrm{Im}\frac{\partial}{\partial\omega}\log|\hat{P}_k|=-\frac{1}{\pi}\mathrm{Im}\frac{\partial}{\partial\omega}\{\log|\hat{F}_k|+\sum_{\sigma}\log(\omega+i\delta-\varepsilon_{k\sigma})\}$$

$$=-\frac{1}{\pi}\mathrm{Im}\left\{\sum_{MM'}\left(\delta_{MM'}-\frac{\partial\Sigma_{kMM'}}{\partial\omega}-\sum_{\sigma}\frac{V_{kM\sigma}V^{*}_{kM'\sigma}}{(\omega-\varepsilon_{k\sigma})^2}\right)G^{f}_{kM'M}(\omega+i\delta)\right.$$

$$\left.+\sum_{\sigma}\frac{1}{\omega+i\delta-\varepsilon_{k\sigma}}\right\}$$

$$=-\frac{1}{\pi}\mathrm{Im}\left\{\sum_{MM'}\left(\delta_{MM'}-\frac{\partial\Sigma_{kMM'}}{\partial\omega}\right)G^{f}_{kM'M}(\omega+i\delta)+\sum_{\sigma}G^{c}_{k\sigma\sigma}(\omega+i\delta)\right\}. \tag{69}$$

Generally, the imaginary part of the self-energy vanishes at the Fermi surface, so that the T-linear coefficient of the specific heat is obtained as

$$\gamma=\frac{\pi^2}{3}k_B^2\sum_k\{\mathrm{Tr}(\hat{\gamma}_k(\mu)\hat{n}_k^f(\mu))+\sum_\sigma n_{k\sigma}^c(\mu)\}\,, \tag{70}$$

where $\hat{\gamma}_k(\omega)$ is the $N_f\times N_f$ matrix representing the mass enhancement

$$\hat{\gamma}_k(\omega)=\hat{1}-\frac{\partial\hat{\Sigma}_k}{\partial\omega}\,, \tag{71}$$

and $\hat{n}_k^f(\omega)$ and $n_{k\sigma}^c(\omega)$ are defined by

$$\hat{n}_k^f(\omega)=-\frac{1}{\pi}\mathrm{Im}\hat{G}_k^f(\omega+i\delta)\,, \tag{72}$$

$$n_{k\sigma}^c(\omega)=-\frac{1}{\pi}\mathrm{Im}G_{k\sigma\sigma}^c(\omega+i\delta)\,. \tag{73}$$

The T-linear term in specific heat is proportional to the density of states of quasiparticles at the Fermi energy, in which the f-electron contribution is enhanced by $\hat{\gamma}_k(\mu)$ while the c-electron one is not.

In order to calculate the susceptibility, first we need to know the magnetization. As Luttinger has derived,[6] the magnetization is obtained by differentiating the thermodynamic potential with respect to the magnetic field and making use of its stationary property with respect to variations in the self-energies, as

$$M=\mu_B\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\Big\{\sum_{MM'}\langle M|(l_z+2s_z)|M'\rangle\Big(-\frac{1}{\pi}\mathrm{Im}\Big)G_{kM'M}^f(\omega+i\delta)$$
$$+\sum_\sigma\sigma\Big(-\frac{1}{\pi}\mathrm{Im}\Big)G_{k\sigma\sigma}^c(\omega+i\delta)\Big\}\,, \tag{74}$$

where $f(\omega)$ is the Fermi distribution function. Introducing the $N_f\times N_f$ matrix $\hat{M}$ whose MM' component is given by $\langle M|(l_z+2s_z)|M'\rangle$ and making use of Eqs. (66) and (67) with ω replaced by $\omega+i\delta$, one may rewrite Eq. (74) as

$$M=\mu_B\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\Big(-\frac{1}{\pi}\mathrm{Im}\Big)$$
$$\times\Big\{\mathrm{Tr}(\hat{M}\hat{F}_k^{-1})+\sum_\sigma\frac{\sigma}{\omega+i\delta-\varepsilon_{k\sigma}}+\sum_\sigma\frac{\sigma}{(\omega+i\delta-\varepsilon_{k\sigma})^2}\mathrm{Tr}(\hat{v}_{k\sigma}\hat{v}_{k\sigma}^\dagger\hat{F}_k^{-1}\Big\}\,. \tag{75}$$

If we follow Luttinger's procedure, the next step will be to rewrite Eq. (75) as

$$M=\mu_B\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\Big(-\frac{1}{\pi}\mathrm{Im}\Big)\frac{\partial}{\partial\omega}\mathcal{F}_k(\omega+i\delta)+J\,, \tag{76}$$

where $\mathcal{F}_k(\omega+i\delta)$ is some function, hopefully logarithmic, and to prove $J=0$. If we can obtain such an expression, M is expressed only by the quantities of quasiparticles on the Fermi surface after integrating by parts with respect to ω, because $(\partial/\partial\omega)f(\omega)=-\delta(\mu-\omega)$ at $T=0$K. It may be, however, impossible to obtain such an expression in the cases including the trace of product of matrices in Eq. (75), since commutators of $\hat{F}_k$ with $\hat{M}$, $\hat{v}_{k\sigma}\hat{v}_{k\sigma}^\dagger$ and $(\partial/\partial\omega)\hat{F}_k$ are not proportional to the unit matrix in general, much less vanish. In Ref. 3) in which an orbital degeneracy has been taken

into consideration for localized f electrons, non-commutability between these operators was not correctly treated, and therefore the expression given there for the susceptibility is not correct.

This difficulty comes from the existence of the off-diagonal parts of self-energies in the present case in contrast to the cases of the homogeneous Fermi liquid,[6] the orbitally-nondegenerate periodic Anderson model[2] and the orbitally-degenerate impurity Anderson model.[7),8] The reason why the off-diagonal self-energy parts appear is that the hybridization connects different f states, that is, the off-diagonal elements of the last term in Eq. (65) remain. However, one can find a simple relation that such elements vanish between an f state and its time-reversal state in the absence of the applied magnetic field as shown below. Thus, if we are allowed to consider only a Kramers doublet of f states, we can proceed following Eq. (75) to get an expression for the magnetic susceptibility.

Here we assume the strong limit of spin-orbit coupling and crystal field to consider only a Kramers doublet labeled by M and $\bar{M}$. The matrix $\hat{F}_k$ of Eq. (65) is now 2×2 matrix:

$$\hat{F}_k=(\omega-E)\hat{1}+\hat{M}\mu_B H-\hat{\Sigma}_k{}^{(H=0)}-\left.\frac{\partial\hat{\Sigma}_k}{\partial(\mu_B H)}\right|_{H=0}\mu_B H-\cdots$$

$$-\frac{1}{\omega-\varepsilon_k}\sum_\sigma \hat{v}_{k\sigma}\hat{v}^\dagger_{k\sigma}+\frac{\mu_B H}{(\omega-\varepsilon_k)^2}\sum_\sigma \sigma\hat{v}_{k\sigma}\hat{v}^\dagger_{k\sigma}+\cdots, \tag{77}$$

where we expand it with respect to magnetic field, H, and drop the suffix M of E_M. We take a representation diagonalizing the magnetic moment: $(\hat{M})_{MM}\equiv\mu$, $(\hat{M})_{\bar{M}\bar{M}}=-\mu$, $(\hat{M})_{M\bar{M}}=0$. In the same way that we have shown $B_{k\sigma}(\omega)=0$ and derived Eq. (18) in § 2, it can be shown that the off-diagonal elements of $\sum_\sigma \hat{v}_{k\sigma}\hat{v}^\dagger_{k\sigma}$ vanish and the diagonal elements are equal, namely, $(\sum_\sigma \hat{v}_{k\sigma}\hat{v}^\dagger_{k\sigma})_{MM'}\equiv 2I_k\delta_{MM'}$. Here we have used the expression of the mixing matrix elements, Eq. (6), and the relation between the Clebsch-Gordan coefficients, Eq. (15). The reason why the off-diagonal elements vanish lies in the cancellation of two processes: One is the process that the f electron in M-state transfers to the *spin-up* conduction electron state then back to M-state; the other is that the f electron transfers from M-state to the *spin-down* conduction electron state then back to M-state. Considering the general structure of the diagrams contributing to the self-energies, we can conclude that the cancellation between these two processes results in the diagonal form of the self-energy matrix for $H=0$: $(\hat{\Sigma}^{(H=0)})_{MM'}\equiv\Sigma_k{}^{(0)}(\omega)\delta_{MM'}$. Equation (77), therefore, may be written as

$$\hat{F}_k=f_{0k}(\omega)\hat{1}+f_{1k}(\omega)\hat{M}\mu_B H+\hat{F}'_{1k}\mu_B H+O(H^2), \tag{78a}$$

where

$$f_{0k}(\omega)=\omega-E-\Sigma_k{}^{(0)}(\omega)-\frac{2I_k}{\omega-\varepsilon_k}, \tag{78b}$$

$$f_{1k}(\omega)=1-\left.\frac{\partial\Sigma_{kMM}(\omega)}{\partial(\mu\mu_B H)}\right|_{H=0}+\frac{\sum_\sigma \sigma|V_{kM\sigma}|^2}{\mu(\omega-\varepsilon_k)^2}, \tag{78c}$$

$$(\hat{F}'_{1k})_{MM}=(\hat{F}'_{1k})_{\bar{M}\bar{M}}=0\,, \tag{78d}$$

$$(\hat{F}'_{1k})_{M\bar{M}}=-\frac{\partial\Sigma_{kM\bar{M}}(\omega)}{\partial(\mu_{\mathrm{B}}H)}\bigg|_{H=0}+\frac{\sum_{\sigma}\sigma V_{kM\sigma}V^{*}_{k\bar{M}\sigma}}{(\omega-\varepsilon_k)^2}\,. \tag{78e}$$

It should be noted that $f_{0k}(\omega)$ and $f_{1k}(\omega)$ consist of only diagonal elements, and $\hat{F}'_{1k}$ consists of off-diagonal elements. The inverse of $\hat{F}_k$ is obtained as

$$\hat{F}_k{}^{-1}=\frac{1}{f_{0k}(\omega)}\hat{1}-\frac{f_{1k}(\omega)}{f_{0k}(\omega)^2}\hat{M}\mu_{\mathrm{B}}H-\frac{1}{f_{0k}(\omega)^2}\hat{F}'_{1k}\mu_{\mathrm{B}}H+O(H^2)\,. \tag{79}$$

Noting $\mathrm{Tr}(\hat{M})=0$, $\mathrm{Tr}(\hat{M}^2)=2\mu^2$ and $\mathrm{Tr}(\hat{M}\hat{F}'_{1k})=0$, we have

$$\mathrm{Tr}(\hat{M}\hat{F}_k{}^{-1})=-2\mu^2\mu_{\mathrm{B}}\frac{f_{1k}(\omega)}{f_{0k}(\omega)^2}H+O(H^2)\,. \tag{80}$$

It has been shown that only the diagonal elements of $\hat{F}_k$ contribute to the f-electron part of the magnetic moment up to the order of H^1. To calculate the susceptibility, therefore, it may be sufficient to make use of fictitious f-electron Green's functions constructed from the diagonal elements of $\hat{F}_k$:

$$[g^f_{kmm}(\omega)]^{-1}=\omega-E+\mu_m\mu_{\mathrm{B}}H-\Sigma^{(g)}_{kmm}(\omega)-\sum_{\sigma}\frac{|V_{km\sigma}|^2}{\omega-\varepsilon_{k\sigma}}\,,\quad m=M,\bar{M}\,, \tag{81}$$

where $\mu_M=\mu$, $\mu_{\bar{M}}=-\mu$ and $\Sigma^{(g)}_{kmm}(\omega)$ is the self-energy consisting of $g^f_{kMM}(\omega)$ and $g^f_{k\bar{M}\bar{M}}(\omega)$ as the f-electron propagators. It is shown that $\Sigma^{(g)}_{kmm}(\omega)$ coincides with $\Sigma_{kmm}(\omega)$ up to the order of H^1 as follows. If a diagram contributing to $\Sigma_{kmm}(\omega)$ contains an f-electron line corresponding to the off-diagonal Green's function, the diagram should contain at least another line corresponding to the off-diagonal Green's function for the interaction U of Eq. (8) which conserves the indices M and M'. Noting the fact that the off-diagonal Green's function vanishes if H tends to zero, we obtain immediately the desired result

$$\frac{\partial\Sigma_{kmm}(\omega)}{\partial(\mu\mu_{\mathrm{B}}H)}\bigg|_{H=0}=\frac{\partial\Sigma^{(g)}_{kmm}(\omega)}{\partial(\mu\mu_{\mathrm{B}}H)}\bigg|_{H=0}\,,\qquad \text{thereby}$$

$$g^f_{kmm}(\omega)=\frac{1}{f_{0k}(\omega)}-\frac{f_{1k}(\omega)}{f_{0k}(\omega)^2}\mu_m\mu_{\mathrm{B}}H+O(H^2)\,. \tag{82}$$

Thus we can calculate the f-electron part of the magnetic moment in the accuracy up to the order of H^1 as

$$\mu_{\mathrm{B}}\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\Big(-\frac{1}{\pi}\mathrm{Im}\Big)\mathrm{Tr}(\hat{M}\hat{F}_k{}^{-1})$$

$$=\mu_{\mathrm{B}}\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\Big(-\frac{1}{\pi}\mathrm{Im}\Big)\sum_m\mu_m g^f_{kmm}(\omega+i\delta)=M_0+J+M_1\,, \tag{83a}$$

where

$$M_0=\mu_B\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\left(-\frac{1}{\pi}\mathrm{Im}\right)\sum_m\mu_m\frac{\partial}{\partial\omega}\log[g^f_{kmm}(\omega+i\delta)]^{-1}\,, \tag{83b}$$

$$J=\mu_B\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\left(-\frac{1}{\pi}\mathrm{Im}\right)\sum_m\mu_m g^f_{kmm}(\omega+i\delta)\frac{\partial}{\partial\omega}\Sigma^{(g)}_{kmm}(\omega+i\delta)\,, \tag{83c}$$

$$M_1=-\mu_B\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\left(-\frac{1}{\pi}\mathrm{Im}\right)\sum_{m\sigma}\mu_m\frac{|V_{km\sigma}|^2}{(\omega+i\delta-\varepsilon_{k\sigma})^2}g^f_{kmm}(\omega+i\delta)\,. \tag{83d}$$

We now discuss the zero-temperature limit, where we can put $f(\omega)=\theta(\varepsilon_F-\omega)$, ε_F being the Fermi energy. For M_0, we can integrate by parts, then obtain only the contribution from the Fermi surface. We can show that $J=0$ for the M-independent force U in Eq. (1), using the energy conservation condition at each vertex. Similar relations have been obtained by Luttinger[6] for the homogeneous Fermi liquid and by Shiba[7] for the single-impurity Anderson model with orbital degeneracy. M_1 is a correction term which will be combined with the last term of Eq. (75). Noting Eqs. (78), (79) and (82), we have

$$\begin{aligned}
&\sum_{\sigma mm'}\frac{\sigma V_{km\sigma}V^*_{km'\sigma}G^f_{km'm}(\omega)}{(\omega-\varepsilon_{k\sigma})^2}-\sum_{\sigma m}\frac{\mu_m|V_{km\sigma}|^2g^f_{kmm}(\omega)}{(\omega-\varepsilon_{k\sigma})^2}\\
&\quad=\frac{1}{(\omega-\varepsilon_k)^2f_{0k}(\omega)}\sum_{\sigma m}(\sigma-\mu_m)|V_{km\sigma}|^2\\
&\qquad-\frac{2}{(\omega-\varepsilon_k)^3f_{0k}(\omega)}\sum_{\sigma m}(\sigma^2-\mu_m\sigma)|V_{km\sigma}|^2\mu_BH\\
&\qquad+\frac{f_{1k}(\omega)}{(\omega-\varepsilon_k)^2f_{0k}(\omega)^2}\sum_{\sigma m}(\mu^2-\mu_m\sigma)|V_{km\sigma}|^2\mu_BH\\
&\qquad-\frac{1}{(\omega-\varepsilon_k)^2f_{0k}(\omega)^2}\sum_{\sigma mm'}\sigma V_{km\sigma}V^*_{km'\sigma}(\hat{F}'_{1k})_{m'm}\mu_BH+O(H^2)\\
&\quad=\frac{\partial}{\partial\omega}\left\{\frac{1}{(\omega-\varepsilon_k)^2f_{0k}(\omega)}\right\}\sum_{\sigma m}(\sigma^2-\mu_m\sigma)|V_{km\sigma}|^2\mu_BH+K_k(\omega)\mu_BH+O(H^2)\,,
\end{aligned} \tag{84a}$$

where

$$\begin{aligned}
K_k(\omega)=&\frac{f'_{0k}(\omega)}{(\omega-\varepsilon_k)^2f_{0k}(\omega)^2}4(I_k-J_k)+\frac{f_{1k}(\omega)}{(\omega-\varepsilon_k)^2f_{0k}(\omega)^2}4(\mu^2I_k-J_k)\\
&-\frac{1}{(\omega-\varepsilon_k)^2f_{0k}(\omega)^2}\sum_{\sigma mm'}\sigma V_{km\sigma}V^*_{km'\sigma}(\hat{F}'_{1k})_{m'm}\,,
\end{aligned} \tag{84b}$$

$$2I_k=\sum_\sigma|V_{km\sigma}|^2=\sum_m|V_{km\sigma}|^2\,, \tag{84c}$$

$$4J_k=\sum_{m\sigma}\mu_m\sigma|V_{km\sigma}|^2=2\mu\sum_\sigma\sigma|V_{kM\sigma}|^2\,, \tag{84d}$$

$$f'_{0k}(\omega)=\frac{\partial f_{0k}(\omega)}{\partial\omega}=1-\frac{\partial\Sigma_k{}^{(0)}(\omega)}{\partial\omega}+\frac{2I_k}{(\omega-\varepsilon_k)^2}\,. \tag{84e}$$

Then we obtain the magnetization

$$M=\mu_B\sum_k\left(-\frac{1}{\pi}\mathrm{Im}\right)\sum_m\mu_m\log\Big[\varepsilon_F+i\delta-E+\mu_m\mu_BH-\Sigma^{(g)}_{kmm}(\varepsilon_F+i\delta)$$
$$-\sum_\sigma\frac{|V_{km\sigma}|^2}{\varepsilon_F+i\delta-\varepsilon_{k\sigma}}\Big]$$
$$+\mu_B\sum_k\left(-\frac{1}{\pi}\mathrm{Im}\right)\sum_\sigma\sigma\log(\varepsilon_F+i\delta-\varepsilon_k+\sigma\mu_BH)$$
$$+\mu_B^2\sum_k\left(-\frac{1}{\pi}\mathrm{Im}\right)\frac{\sum_{\sigma m}(\sigma^2-\mu_m\sigma)|V_{km\sigma}|^2}{(\varepsilon_F+i\delta-\varepsilon_k)^2f_{0k}(\varepsilon_F+i\delta)}H$$
$$+\mu_B^2\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\left(-\frac{1}{\pi}\mathrm{Im}\right)K_k(\omega+i\delta)H+O(H^2)\,. \tag{85}$$

The susceptibility is calculated by the formula $\chi=\partial M/\partial H|_{H=0}$ as

$$\chi=2\mu^2\mu_B^2\sum_k\left[1-\frac{\partial\Sigma_{kMM}(\varepsilon_F)}{\partial(\mu\mu_BH)}\Big|_{H=0}\right]n^f_{kMM}(\varepsilon_F)+2\mu_B^2\sum_k n^c_{k\sigma}(\varepsilon_F)$$
$$+\mu_B^2\sum_k\int_{-\infty}^{\infty}d\omega f(\omega)\left(-\frac{1}{\pi}\mathrm{Im}\right)K_k(\omega+i\delta)\,. \tag{86}$$

The first term corresponds to the Pauli susceptibility of f electrons enhanced by the magnetic-field derivative of the self-energy, and the second that of conduction electrons unenhanced. The third term is the correction originating from the orbital moment of f electrons, which should be estimated by numerical calculations.

§ 5. Concluding remarks

On the basis of the periodic Anderson model, we have developed the Fermi liquid theory for a real case in which orbital degeneracy, spin-orbit coupling and crystalline field are taken into account for f electrons.

In the absence of Coulomb repulsion U between f electrons, the formalism can be done quite straightforwardly in spite of the existence of the crystalline field splittings, and usual standard results can be derived characteristic to the Fermi liquid theory for the specific heat and the susceptibility. This is a simple extension of Ref. 4).

In the presence of on-site Coulomb repulsion U between f electrons, the expression for the T-linear coefficient γ of the specific heat can also be derived to lead to the result with a usual form for the present case. However, for the susceptibility situations are somewhat different from simpler cases of the periodic Anderson model in which f orbital has no degeneracy, and the susceptibility contains a part which cannot be expressed by the quantities at the Fermi energy besides the term with a usual Fermi liquid form. The appearance of such correction terms is entirely due to the off-diagonal elements of the f-electron self-energy. However, it seems very difficult to derive each part of the susceptibility separately.

Therefore, we have demonstrated, in this paper, such calculations for a simple

special case in which L-S couplng and crystalline field splittings are large enough to be able to confine our consideration to the lowest Kramers doublet. In this case, the self-energy of f electrons has no off-diagonal elements between two Kramers components when an external field is absent, whereas derivation of the susceptibility for this case is still somewhat complicated.

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References

1) G. R. Stewart, Rev. Mod. Phys. **56** (1984), 775.
2) K. Yamada and K. Yosida, Prog. Theor. Phys. **76** (1986), 621.
3) K. Yamada, K. Okada, K. Yosida and K. Hanzawa, Prog. Theor. Phys. **77** (1987), 1097.
4) K. Hanzawa, K. Yosida and K. Yamada, Prog. Theor. Phys. **77** (1987), 1116.
5) K. Hanzawa, K. Yamada and K. Yosida, J. Phys. Soc. Jpn. **55** (1986), 641.
6) J. M. Luttinger, Phys. Rev. **119** (1960), 1153.
7) H. Shiba, Prog. Theor. Phys. **54** (1975), 967.
8) A. Yoshimori, Prog. Theor. Phys. **55** (1976), 67.