

## Fermi Liquid Theory on the Basis of the Periodic Anderson Hamiltonian

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$T$ -linear term of specific heat and magnetic susceptibility at zero temperature are derived for the heavy electron systems, and relations among these quantities are discussed on the basis of the Fermi liquid theory. Further, a rigorous expression of the  $T^2$ -term of resistivity at low temperatures is also obtained on the basis of Kubo formula. It is shown that the coefficient of the  $T^2$ -term arising from the electron interaction is strongly enhanced though it vanishes because of the momentum conservation for a free electron system possessing no crystal lattice.

### § 1. Introduction

Behaviors shown by heavy fermion systems often realized in Ce-compounds at low temperatures have been investigated theoretically by many authors with several approaches.<sup>1)</sup> Among them, the Fermi liquid approach on the basis of the periodic Anderson model seems to be most appropriate in order to grasp the essential nature of the heavy electron system.

In this paper, we discuss the low temperature behavior of the heavy electron systems by using this approach. For simplicity we neglect the orbital degeneracy. Then, our Hamiltonian is given by

$$H = H_0 + H', \quad (1.1)$$

$$H_0 = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} E_k a_{k\sigma}^\dagger a_{k\sigma} + \sum_{k\sigma} V_k (a_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger a_{k\sigma}) + \frac{U}{4} N \langle n_{0f} \rangle^2, \quad (1.2)$$

$$H' = \sum_{k_1 k_2 q (+0)} \frac{U}{N} a_{k_1 + q}^\dagger a_{k_2 - q}^\dagger a_{k_2} a_{k_1}. \quad (1.3)$$

Creation operator  $c_{k\sigma}^\dagger$  is that for a conduction electron with momentum  $k$ , spin  $\sigma$  and energy  $\varepsilon_k$ ;  $a_{k\sigma}^\dagger$  is for  $f$ -electron with  $k$ ,  $\sigma$  and  $E_k$ . Heavy  $f$ -electrons in the same atom interact with each other via Coulomb repulsion  $U$ . These two kinds of electrons hybridize through matrix element  $V_k$ . In this paper we include the dispersion of  $f$ -electrons. Therefore, in principle, our results can also be applied to transition metal and actinide systems.

### § 2. Specific heat and magnetic susceptibility

The Green's functions of  $f$ -electrons and conduction electrons are given by

$$G_{k\sigma}^f(z) = \left[ z - E_{k\sigma} - \Sigma_{k\sigma}(z) - \frac{V_k^2}{z - \varepsilon_{k\sigma}} \right]^{-1}, \quad (2.1)$$

$$G_{k\sigma}^f(z) = \left[ z - \varepsilon_{k\sigma} - \frac{V_k^2}{z - E_{k\sigma} - \Sigma_{k\sigma}(z)} \right]^{-1}, \quad (2.2)$$

where  $\Sigma_{k\sigma}(z)$  is the true selfenergy part of  $f$ -electrons.

First, we consider the ground state properties.<sup>2)~4)</sup> The eigenvalues of quasi-particles,  $E_{k\sigma}^*$ , are given by the poles of (2.1) or (2.2) and satisfy the equation, ( $z = E_{k\sigma}^*$ ),

$$[z - E_{k\sigma} - \Sigma_{k\sigma}(z)](z - \varepsilon_{k\sigma}) - V_k^2 = 0. \quad (2.3)$$

The density of states of  $f$ -electrons are given by

$$\rho_{\sigma^f}(\omega) = \sum_k \rho_{k\sigma}^f(\omega), \quad (2.4)$$

$$\rho_{k\sigma}^f(\omega) = -\frac{1}{\pi} \text{Im} G_{k\sigma}^f(\omega + i\delta) = a_{k\sigma}^f(E_{k\sigma}^*) \delta(\omega - E_{k\sigma}^*). \quad (2.5)$$

Here we have put as  $a_{k\sigma}^f(E_{k\sigma}^*)$  the residue

$$a_{k\sigma}^f(E_{k\sigma}^*) = \left[ 1 - \frac{\partial \Sigma_{k\sigma}(\omega)}{\partial \omega} + \frac{V_k^2}{(\omega - \varepsilon_{k\sigma})^2} \right]^{-1} \Big|_{\omega = E_{k\sigma}^*}. \quad (2.6)$$

The density of states of conduction electrons is also given by

$$\rho_{\sigma^c}(\omega) = \sum_k \rho_{k\sigma}^c(\omega), \quad (2.7)$$

$$\rho_{k\sigma}^c(\omega) = -\frac{1}{\pi} \text{Im} G_{k\sigma}^c(\omega + i\delta) = a_{k\sigma}^c(E_{k\sigma}^*) \delta(\omega - E_{k\sigma}^*), \quad (2.8)$$

where

$$\begin{aligned} a_{k\sigma}^c(\omega) &= \left[ 1 + \frac{V_k^2}{(\omega - E_{k\sigma} - \Sigma_{k\sigma}(\omega))^2} \left( 1 - \frac{\partial \Sigma_{k\sigma}(\omega)}{\partial \omega} \right) \right]^{-1} \\ &= \left( \frac{V_k}{\omega - \varepsilon_{k\sigma}} \right)^2 a_{k\sigma}^f(\omega). \end{aligned} \quad (2.9)$$

Combining (2.4) and (2.7), we obtain<sup>2)</sup>

$$\rho_{\sigma^c}(\omega) + \sum_k \left( 1 - \frac{\partial \Sigma_{k\sigma}(\omega)}{\partial \omega} \Big|_{\omega = E_{k\sigma}^*} \right) \rho_{k\sigma}^f(\omega) = \sum_k \delta(\omega - E_{k\sigma}^*). \quad (2.10)$$

Thus, we obtain the coefficient of  $T$ -linear term of the specific heat as

$$\gamma = \sum_{k\sigma} \delta(\mu - E_{k\sigma}^*) = \sum_{\sigma} \rho_{\sigma^c}(0) + \sum_{k\sigma} \left( 1 - \frac{\partial \Sigma_{k\sigma}(\omega)}{\partial \omega} \Big|_{\omega=0} \right) \rho_{k\sigma}^f(0), \quad (2.11)$$

where  $\mu$  denotes the Fermi energy which is put as zero. This result means that  $\gamma$  is given by the sum of  $\rho_{\sigma^c}$  and  $\rho_{k\sigma}^f$  enhanced by the factor of  $(1 - \partial \Sigma / \partial \omega|_{\omega=0})$ . The large enhancement of  $\gamma$  in heavy electron systems originates from the second term of (2.11), because this term is enhanced by the strong interaction between  $f$ -electrons.

Now we discuss the magnetic susceptibility. For simplicity, we assume that  $f$ - and conduction electrons have the same  $g$ -value,  $g=2$ . In this case  $E_{k\sigma}$  and  $\varepsilon_{k\sigma}$  are given

under a magnetic field  $H$  by

$$E_{k\sigma} = E_k - H\sigma, \tag{2.12}$$

$$\varepsilon_{k\sigma} = \varepsilon_k - H\sigma, \tag{2.13}$$

where  $H\sigma = g\mu_B H\sigma/2$ ,  $\mu_B$  being the Bohr magneton. Total electron number  $N_e$  and magnetization  $M$  are given by

$$N_e = \sum_{k\sigma} \theta(\mu - E_{k\sigma}^*), \tag{2.14}$$

$$M = \mu_B \sum_{k\sigma} \sigma \theta(\mu - E_{k\sigma}^*), \tag{2.15}$$

where  $E_{k\sigma}^*$  is an eigenvalue of the quasi-particle under the magnetic field. From (2.15), the spin susceptibility is obtained as

$$\begin{aligned} \chi_s &= \lim_{H \rightarrow 0} \mu_B \sum_{k\sigma} \sigma \delta(\mu - E_{k\sigma}^*) (-\partial E_{k\sigma}^* / \partial H) \\ &= 2\mu_B \sum_k \sigma \delta(\mu - E_k^*) (-\partial E_{k\sigma}^* / \partial H|_{H=0}). \end{aligned} \tag{2.16}$$

By using the eigenvalue equation (2.3), we obtain

$$\frac{\partial E_{k\sigma}^*}{\partial H} = \left[ 1 - \frac{\partial \Sigma_k(\omega)}{\partial \omega} + \frac{V_k^2}{(E_k^* - \varepsilon_k)^2} \right]^{-1} (-\mu_B \sigma) \left[ \tilde{\chi}_s(\mathbf{k}) + \frac{V_k^2}{(E_k^* - \varepsilon_k)^2} \right], \tag{2.17}$$

where

$$\tilde{\chi}_s(\mathbf{k}) = \tilde{\chi}_{\uparrow\uparrow}(\mathbf{k}) + \tilde{\chi}_{\uparrow\downarrow}(\mathbf{k}). \tag{2.18}$$

Here we have put

$$\tilde{\chi}_{\uparrow\uparrow}(\mathbf{k}) = 1 - \frac{\partial \Sigma_{k\sigma}(0)}{\partial H_\sigma} \Big|_{H_\sigma=0}, \tag{2.19}$$

$$\tilde{\chi}_{\uparrow\downarrow}(\mathbf{k}) = \frac{\partial \Sigma_{k\sigma}(0)}{\partial H_{-\sigma}} \Big|_{H_{-\sigma}=0}. \tag{2.20}$$

Thus, the spin susceptibility is written as

$$\chi_s = 2\mu_B^2 \left\{ \sum_k \rho_k^f(0) \tilde{\chi}_s(\mathbf{k}) + \rho^c(0) \right\}, \tag{2.21}$$

where  $\rho_k^f(0)$  and  $\rho^c(0)$  are given by (2.5) and (2.7), respectively.

### § 3. Wilson ratio

$T$ -linear coefficient of specific heat given by (2.11) is rewritten as,

$$\gamma = \sum_\sigma \rho_\sigma^c(0) + 2\gamma^f, \tag{3.1}$$

$$\gamma^f = \sum_{\mathbf{k}} \rho_{\mathbf{k}\sigma}^f(0) \tilde{\gamma}_{\mathbf{k}}, \tag{3.2}$$

$$\tilde{\gamma}_{\mathbf{k}} = 1 - \left. \frac{\partial \Sigma_{\mathbf{k}\sigma}(\omega)}{\partial i\omega} \right|_{\omega=0} = \tilde{\gamma}(\mathbf{k}). \tag{3.3}$$

In this section we use the thermal Green's function with imaginary frequency  $i\omega$  as its argument. By differentiating the unperturbed Green's function  $G_{\mathbf{k}}^{0f}(i\omega)$  by  $i\omega$ , we obtain

$$\frac{\partial}{\partial i\omega} G_{\mathbf{k}}^{0f}(i\omega) = -[G_{\mathbf{k}}^{0f}(i\omega)]^2 \left[ 1 + \frac{V_{\mathbf{k}}^2}{(i\omega + \mu - \epsilon_{\mathbf{k}})^2} \right] + \frac{\delta(\omega)}{i} \delta G_{\mathbf{k}}^{0f}, \tag{3.4}$$

where  $\delta G_{\mathbf{k}}^{0f}$  is given by putting  $\Sigma_{\mathbf{k}}(0) = 0$  in  $\delta G_{\mathbf{k}}^f$ .  $\delta G_{\mathbf{k}}^f$  is given by

$$\delta G_{\mathbf{k}}^f = G_{\mathbf{k}}^f(0_+) - G_{\mathbf{k}}^f(0_-) = -2\pi i \rho_{\mathbf{k}}^f(0). \tag{3.5}$$

On the other hand,  $\partial G_{\mathbf{k}}^{0f}(\omega)/\partial \mu$  is given by

$$\frac{\partial G_{\mathbf{k}}^{0f}(\omega)}{\partial \mu} = -[G_{\mathbf{k}}^{0f}(i\omega)]^2 \left[ 1 + \frac{V_{\mathbf{k}}^2}{(i\omega + \mu - \epsilon_{\mathbf{k}})^2} \right]. \tag{3.6}$$

By shifting the frequencies of every closed loop by external frequency  $\omega$  and using (3.4), (3.5) and (3.6), we obtain

$$\frac{\partial \Sigma_{\mathbf{k}\sigma}(\omega)}{\partial i\omega} = \frac{\partial \Sigma_{\mathbf{k}\sigma}(\omega)}{\partial \mu} + \sum_{\mathbf{k}'\sigma'} \frac{\delta G_{\mathbf{k}'\sigma'}}{2\pi i} \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}), \tag{3.7}$$

where the vertex part  $\Gamma_{\sigma\sigma'}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_3, \mathbf{k}_4)$  is shown by the diagram in Fig. 1 and all frequencies in  $\Gamma_{\sigma\sigma'}$  are put as zero. By shifting the frequencies of only closed loops with  $\sigma$  spin by external frequency  $\omega$ , we obtain

$$\frac{\partial \Sigma_{\mathbf{k}\sigma}(\omega)}{\partial i\omega} = \frac{\partial \Sigma_{\mathbf{k}\sigma}(\omega)}{\partial H_{\sigma}} + \sum_{\mathbf{k}'\sigma'} \frac{\delta G_{\mathbf{k}'\sigma'}}{2\pi i} \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}). \tag{3.8}$$

Thus, we obtain the following relation from (2.18), (3.3), (3.5) and (3.8),

$$\tilde{\gamma}(\mathbf{k}) = \tilde{\chi}_{\uparrow\uparrow}(\mathbf{k}) + \sum_{\mathbf{k}'} \rho_{\mathbf{k}'}^f(0) \Gamma_{\sigma\sigma}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}). \tag{3.9}$$

From (3.2) and (3.9),  $\gamma^f$  is given by

$$\gamma^f = \chi_{\uparrow\uparrow}^f + \delta_{\uparrow\uparrow}^f \tag{3.10}$$

with

$$\chi_{\uparrow\uparrow}^f = \sum_{\mathbf{k}} \rho_{\mathbf{k}}^f(0) \tilde{\chi}_{\uparrow\uparrow}(\mathbf{k}), \tag{3.11}$$

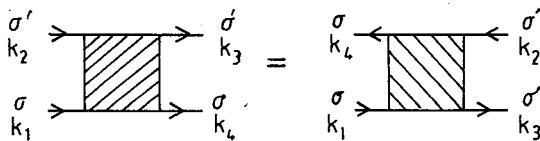


Fig. 1. Four-point vertex  $\Gamma_{\sigma\sigma'}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_3, \mathbf{k}_4)$ .

$$\delta_{\uparrow\uparrow}^f = \sum_{\mathbf{k}\mathbf{k}'} \rho_{\mathbf{k}'}^f(0) \Gamma_{\sigma\sigma}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}) \rho_{\mathbf{k}}^f(0). \tag{3.12}$$

Here  $\Gamma_{\uparrow\uparrow} = \Gamma_{\sigma\sigma}$ , the vertex part between  $f$ -electrons with parallel spins, can be antisymmetrized as

$$\Gamma_{\uparrow\uparrow}^A(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_3, \mathbf{k}_4) = \Gamma_{\uparrow\uparrow}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_3, \mathbf{k}_4) - \Gamma_{\uparrow\uparrow}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_4, \mathbf{k}_3). \quad (3.13)$$

$\Gamma_{\uparrow\uparrow}^A$  vanishes identically for the single impurity case, but does not for the periodic case because of the momentum conservation.<sup>2),5)</sup> Equations (3.7) and (3.8) give the relation

$$\frac{\partial \Sigma_{\mathbf{k}\sigma}(0)}{\partial H_{-\sigma}} = - \sum_{\mathbf{k}'} \frac{\delta G_{\mathbf{k}'}}{2\pi i} \Gamma_{\sigma-\sigma}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}) \quad (3.14)$$

or

$$\tilde{\chi}_{\uparrow\downarrow}(\mathbf{k}) = \sum_{\mathbf{k}'} \rho_{\mathbf{k}'}^f(0) \Gamma_{\sigma-\sigma}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}). \quad (3.15)$$

Thus we obtain

$$\tilde{\chi}_{\uparrow\downarrow}^f \equiv \sum_{\mathbf{k}} \rho_{\mathbf{k}}^f(0) \tilde{\chi}_{\uparrow\downarrow}(\mathbf{k}) = \sum_{\mathbf{k}\mathbf{k}'} \rho_{\mathbf{k}}^f(0) \Gamma_{\uparrow\downarrow}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}) \rho_{\mathbf{k}'}^f(0). \quad (3.16)$$

The charge susceptibility is given by

$$\chi_c = \rho^c(0) + \chi_c^f, \quad (3.17)$$

$$\chi_c^f = \chi_{\uparrow\uparrow}^f - \chi_{\uparrow\downarrow}^f = \sum_{\mathbf{k}} \rho_{\mathbf{k}}^f(0) (\tilde{\chi}_{\uparrow\uparrow}(\mathbf{k}) - \tilde{\chi}_{\uparrow\downarrow}(\mathbf{k})). \quad (3.18)$$

The Wilson ratio is given by

$$R = [\rho^c(0) + \chi_s^f] / [\rho^c(0) + \gamma^f]. \quad (3.19)$$

The ratio due to only  $f$ -electrons is given by

$$\begin{aligned} R^f &= \chi_s^f / \gamma^f = [\chi_{\uparrow\uparrow}^f + \chi_{\uparrow\downarrow}^f] / [\chi_{\uparrow\uparrow}^f + \delta_{\uparrow\uparrow}^f] \\ &= [1 + \chi_{\uparrow\downarrow}^f / \chi_{\uparrow\uparrow}^f] / [1 + \delta_{\uparrow\uparrow}^f / \chi_{\uparrow\uparrow}^f]. \quad (R^f \geq R) \end{aligned} \quad (3.20)$$

Thus,  $R^f$  depends on two parameters,  $\chi_{\uparrow\downarrow}^f / \chi_{\uparrow\uparrow}^f$  and  $\delta_{\uparrow\uparrow}^f / \chi_{\uparrow\uparrow}^f$ . As  $\chi_c^f$  is positive, (3.18) gives

$$\chi_{\uparrow\downarrow}^f / \chi_{\uparrow\uparrow}^f \leq 1, \quad (3.21)$$

and for a large value of  $U$ ,

$$\chi_c^f = 0. \quad (3.22)$$

In this case  $R^f$  is given by

$$R^f = 2 / (1 + \delta_{\uparrow\uparrow}^f / \chi_{\uparrow\uparrow}^f). \quad (\chi_{\uparrow\uparrow}^f = \chi_{\uparrow\downarrow}^f) \quad (3.23)$$

For the case with an attractive interaction between parallel spins ( $\Gamma_{\uparrow\uparrow}^A < 0$ ),  $\delta_{\uparrow\uparrow}^f$  is expected to be negative. In this case  $R^f$  becomes larger than 2. Thus, in principle, if we treat correctly the momentum dependence, the range available for  $R^f$  is extended wider in contrast to the impurity case.<sup>2)</sup> The second-order term of  $\delta_{\uparrow\uparrow}$  is given by

$$\delta_{\uparrow\uparrow}^{(2)} = U^2 \sum_{\mathbf{k}\mathbf{q}} \rho_{\mathbf{k}}^f(0) \rho_{\mathbf{k}+\mathbf{q}}^f(0) [\chi_{\mathbf{q}}^0 - \chi_{\mathbf{q}=0}^0]. \quad (3.24)$$

This result shows that if  $\chi_{\mathbf{q}=0}^0$  is larger than  $\chi_{\mathbf{q}=0}^0$ ,  $\delta_{\uparrow\uparrow}^{(2)}$  is positive and  $\gamma$  increases with

increase of the degree of the coherence. On the other hand, if  $\chi_q^0$  is smaller than  $\chi_{q=0}^0$ ,  $\gamma$  decreases with increasing coherence. According to recent experiments the Wilson ratio of nearly three has been observed in CeCu<sub>2</sub>Si<sub>2</sub>, CeAl<sub>3</sub> and CeCu.<sup>6)</sup>

#### § 4. Resistivity

The resistivity due to the electron interaction has been discussed by several authors.<sup>7-9)</sup> In this paper we pursue the exact coefficient of the  $T^2$ -term in the heavy electron system on the basis of Kubo formula. Current operator  $\tilde{J}$  in our system is given by<sup>\*</sup>

$$\tilde{J} = e \sum_{k\sigma} (v_k^f a_{k\sigma}^\dagger a_{k\sigma} + v_k^c c_{k\sigma}^\dagger c_{k\sigma}), \quad (4.1)$$

where

$$v_k^c = \nabla_k \varepsilon_k, \quad (4.2)$$

$$v_k^f = \nabla_k E_k^0. \quad (4.3)$$

Therefore, conductivity  $\sigma_{\mu\nu}$  is given by the sum of the four parts,

$$\begin{aligned} \sigma_{\mu\nu} &= \sum_{ij} \sigma_{\mu\nu}^{(ij)} \\ &= \sigma_{\mu\nu}^{cc} + \sigma_{\mu\nu}^{cf} + \sigma_{\mu\nu}^{fc} + \sigma_{\mu\nu}^{ff}. \quad (i=c, f; j=c, f) \end{aligned} \quad (4.4)$$

Here  $i$  and  $j$  mean conduction electrons ( $f$ -electron) for  $i=c(f)$  or  $j=c(f)$ .  $\sigma_{\mu\nu}^{(ij)}$  is written by two-particle Green's functions,<sup>7,8)</sup>

$$\sigma_{\mu\nu}^{(ij)} = e^2 \sum_{k\sigma k'\sigma'} v_{k\mu}^{(i)} v_{k'\nu}^{(j)} \lim_{\omega \rightarrow 0} \frac{1}{\omega} \text{Im} K_{k\sigma k'\sigma'}^{(ij)}(\omega + i\delta). \quad (4.5)$$

The retarded two-particle Green's function,  $K_{k\sigma k'\sigma'}^{(ij)}(\omega + i\delta)$ , can be obtained from the thermal two-particle Green's function,  $\tilde{K}_{k\sigma k'\sigma'}^{(ij)}(i\omega)$ , by the analytic continuation,

$$K_{k\sigma k'\sigma'}^{(ij)}(\omega + i\delta) = \tilde{K}_{k\sigma k'\sigma'}^{(ij)}(i\omega). \quad (\omega > 0) \quad (4.6)$$

Thermal two-particle Green's functions are defined by the following,

$$\tilde{K}_{k\sigma k'\sigma'}^{(ij)}(\omega_m) = \int_0^{1/T} d\tau e^{\omega_m \tau} \langle T_\tau \{ A_{k\sigma}^{(i)\dagger}(\tau) A_{k\sigma}^{(i)}(\tau) A_{k'\sigma'}^{(j)\dagger} A_{k'\sigma'}^{(j)} \} \rangle, \quad (4.7)$$

$$A_{k\sigma}^{(i)}(\tau) = e^{(H - \mu N_i)\tau} A_{k\sigma}^{(i)} e^{-(H - \mu N_i)\tau}, \quad (4.8)$$

where  $A_{k\sigma}^{(c)} = c_{k\sigma}$  and  $A_{k\sigma}^{(f)} = a_{k\sigma}$ ,  $\omega_m = 2m\pi i T$ .

As discussed in the preceding section,  $f$ -electrons and conduction electrons hybridize with each other to form quasi-particles. Therefore, conductivity  $\sigma_{\mu\nu}$  can also be written in terms of quasi-particles. We denote by  $\tilde{A}_{k\sigma}$  ( $\tilde{A}_{k\sigma}$ ) creation (annihilation) operator for a quasi-particle with momentum  $k$ , spin  $\sigma$  and energy  $E_k^*$ . In this scheme  $\sigma_{\mu\nu}$  is given by

<sup>\*</sup>) If  $\nabla_k V_k \neq 0$ , we must add a current  $e \sum_{k\sigma} \nabla_k V_k (a_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger a_{k\sigma})$  to (4.1). By this correction,  $\nabla_k V_k^2 / (\mu - \varepsilon_k)$  is added to (4.3).

$$\sigma_{\mu\nu} = e^2 \sum_{k\sigma k'\sigma'} v_{k\mu}^* v_{k'\nu}^* \lim_{\omega \rightarrow 0} \frac{1}{\omega} \text{Im} K_{k\sigma k'\sigma'}^*(\omega + i\delta), \tag{4.9}$$

where  $K_{k\sigma k'\sigma'}^*(\omega + i\delta)$  is obtained from the following thermal Green's function,

$$\tilde{K}_{k\sigma k'\sigma'}^*(\omega_m) = \int_0^{1/T} d\tau e^{\omega_m \tau} \langle T_\tau \{ \tilde{A}_{k\sigma}^+(\tau) \tilde{A}_{k\sigma}(\tau) \tilde{A}_{k'\sigma'}^+(\tau) \tilde{A}_{k'\sigma'}(\tau) \} \rangle. \tag{4.10}$$

Following Éliashberg, we can directly obtain the expression for the conductivity in the quasi-particle scheme mentioned above (see (4.38)), though our system is composed of two kinds of bare electrons.

Now, we discuss the details of our derivation, starting from (4.4). At finite temperatures  $f$ -electrons have a life-time given by the reciprocal of the imaginary part of its selfenergy,

$$\Delta_k(\varepsilon) = -\text{Im}\Sigma_k(\varepsilon), \quad \Delta_k > 0. \tag{4.11}$$

The calculation of this value will be done in the next section. By the life-time of  $f$ -electrons, quasi-particles have also a finite life-time. At finite temperatures the eigenvalue of quasi-particles,  $z = E_k^* - i\Gamma_k^*$  ( $\Gamma_k^* > 0$ ), is determined by

$$(z - \varepsilon_k)(z - E_k^0 - \Sigma_k^R(z)) - V_k^2 = 0. \tag{4.12}$$

As we confine ourselves to low temperatures, we can use the following expansion form of the selfenergy part,

$$\Sigma_k^R(z) = \Sigma_k^R(0) + \frac{\partial \Sigma_k^R(z)}{\partial z} z - i\Delta_k, \tag{4.13}$$

and we put

$$E_k = E_k^0 + \Sigma_k^R(0). \tag{4.14}$$

Then, by using (3.3), we obtain

$$(E_k^* - i\Gamma_k^* - \varepsilon_k) \{ \tilde{\gamma}_k(E_k^* - i\Gamma_k^*) - E_k + i\Delta_k \} - V_k^2 = 0. \tag{4.15}$$

By assuming  $\Gamma_k^* \leq \Delta_k \ll |E_k^*|$  at low temperatures, we can determine the eigenvalue  $E_k^*$  by the equation,

$$E_k^* - \tilde{E}_k - \tilde{V}_k^2 / (E_k^* - \varepsilon_k) = 0, \tag{4.16}$$

$$\tilde{E}_k = E_k / \tilde{\gamma}_k \quad \text{and} \quad \tilde{V}_k^2 = V_k^2 / \tilde{\gamma}_k. \tag{4.17}$$

We can see that a renormalization arising from the selfenergy shift reduces the dispersion of  $f$ -band and  $V_k^2$  by the factor of  $\tilde{\gamma}_k^{-1}$ .<sup>1)</sup> On the other hand, the imaginary part  $\Gamma_k^*$  is given by

$$\Gamma_k^* = \frac{\Delta_k}{\tilde{\gamma}_k + V_k^2 / (E_k^* - \varepsilon_k)^2} = a_k^f \Delta_k, \tag{4.18}$$

where  $a_k^f = a_k^f(E_k^*)$  is given by (2.6). Now, we can represent the Green's functions of  $f$ - and  $c$ -electrons at low temperatures by using that of the quasi-particle,

$$G_k^c(\omega + i\delta) = a_k^c[\omega - E_k^* + i\Gamma_k^*]^{-1}, \tag{4.19}$$

$$G_k^f(\omega + i\delta) = a_k^f[\omega - E_k^* + i\Gamma_k^*]^{-1}, \tag{4.20}$$

$$G_k^{cf}(\omega + i\delta) = G_k^{fc}(\omega + i\delta) = \frac{V_k}{E_k^* - \epsilon_k} G_k^f(\omega) \\ = (a_k^f a_k^c)^{1/2}[\omega - E_k^* + i\Gamma_k^*]^{-1}. \tag{4.21}$$

The velocity of the quasi-particle is derived from the eigenvalue equation (4.12) and is given by<sup>\*)</sup>

$$v_k^* = \nabla_k E_k^* = a_k^f \tilde{v}_k^f + a_k^c v_k^c + a_k^f \frac{1}{\mu - \epsilon_k} \nabla_k V_k^2, \tag{4.22}$$

where

$$\tilde{v}_k^f = \nabla_k E_k = \nabla_k (E_k^0 + \Sigma_k(0)). \tag{4.23}$$

In our system, quasi-particles interact with each other through the Coulomb repulsion between *f*-electrons (see (4.37)).

Now we discuss the two-particle Green's function  $\tilde{K}_{k\sigma k'\sigma'}^{(ij)}$  given by (4.7), which can be written as

$$\tilde{K}_{k\sigma k'\sigma'}^{(ij)}(\omega_m) = -T \sum_n G_{k\sigma}^{(ij)}(\epsilon_n) G_{k'\sigma'}^{(ji)}(\epsilon_n + \omega_m) \delta_{kk'} \delta_{\sigma\sigma'} \\ - T^2 \sum_{nn'} G_{k\sigma}^{(jf)}(\epsilon_n) G_{k'\sigma'}^{(fi)}(\epsilon_n + \omega_m) \Gamma_{k\sigma k'\sigma'}(\epsilon_n, \epsilon_{n'}, \omega_m) \\ \times G_{k'\sigma'}^{(fj)}(\epsilon_{n'}) G_{k\sigma}^{(if)}(\epsilon_n + \omega_m), \tag{4.24}$$

$\epsilon_n = (2n+1)\pi iT$  and  $\epsilon_{n'} = (2n'+1)\pi iT$ . Vertex  $\Gamma_{k\sigma k'\sigma'}(\epsilon_n, \epsilon_{n'}, \omega_m)$  is  $\Gamma_{\sigma\sigma'}(\epsilon_n \mathbf{k}, \epsilon_{n'} + \omega_m \mathbf{k}'; \epsilon_{n'} \mathbf{k}', \epsilon_n + \omega_m \mathbf{k})$  between *f*-electrons defined in Fig. 1 and  $G^{(ij)}$  are given by (4.19) ~ (4.21). Following Eliashberg,<sup>7)</sup>  $K_{k\sigma k'\sigma'}^{(ij)}(\omega + i\delta)$  is given by

$$K^{(ij)}(\omega + i\delta) = -\frac{1}{4\pi i} \int_{-\infty}^{\infty} d\epsilon \left[ \text{th} \frac{\epsilon}{2T} K_1^{(ij)}(\epsilon, \omega) \right. \\ \left. + \left( \text{th} \frac{\epsilon + \omega}{2T} - \text{th} \frac{\epsilon}{2T} \right) K_2^{(ij)}(\epsilon, \omega) - \text{th} \frac{\epsilon + \omega}{2T} K_3^{(ij)}(\epsilon, \omega) \right], \tag{4.25}$$

where

$$K_l^{(ij)}(\epsilon, \omega) = g_l^{(ijji)}(\epsilon, \omega) + g_l^{(ifjf)}(\epsilon, \omega) \\ \times \sum_{m=1}^3 \frac{1}{4\pi i} \int d\epsilon' T_{lm}(\epsilon, \epsilon'; \omega) g_m^{(fjff)}(\epsilon', \omega). \tag{4.26}$$

(see Fig. 2)

$g_l^{(ijji)}$  are defined by

$$g_1^{(ijji)}(\epsilon, \omega) = G^{\text{R}(ij)}(\epsilon) G^{\text{R}(ji)}(\epsilon + \omega), \tag{4.27}$$

( $\omega > 0$ )

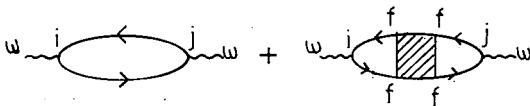


Fig. 2. Two-particle Green's function  $K^{(ij)}(\omega)$ . Vertex  $\Gamma$  is always connected to *f*-electron lines, since the electron interaction exists only between *f*-electrons.

<sup>\*)</sup> Here, we have included a term arising from  $\nabla_k V_k^2$  noted in the footnote of (4.1).



$$g_2^{(ijji)}(\varepsilon, \omega) = G^{A(ij)}(\varepsilon) G^{R(ji)}(\varepsilon + \omega) \tag{4.28}$$

and

$$g_3^{(ijji)}(\varepsilon, \omega) = G^{A(ij)}(\varepsilon) G^{A(ji)}(\varepsilon + \omega). \tag{4.29}$$

Here R and A represent retarded and advanced Green's functions, respectively. The function,  $T_{lm}(\varepsilon, \varepsilon'; \omega)$ , related to vertex function  $\Gamma_{k\sigma k'\sigma'}$  is given by Eq. (12) in Éliashberg's paper.<sup>7)</sup> When  $\omega \ll T$ ,

$$g_1^{(ijji)}(\varepsilon, \omega) \simeq \{G^{R(ij)}(\varepsilon)\}^2 = a_k^i a_k^j (\varepsilon - E_k^* + i\delta)^{-2}, \tag{4.30}$$

$$g_3^{(ijji)}(\varepsilon, \omega) = \{g_1^{(ijji)}(\varepsilon, \omega)\}^*. \tag{4.31}$$

Only the function  $g_2(\varepsilon, \omega)$  depends appreciably on  $\omega$  for small value of  $\omega$ ,

$$g_2^{(ijji)}(\varepsilon, \omega) = 2\pi i a_k^i a_k^j \delta(\varepsilon - E_k^*) / (\omega + 2i\Gamma_k^*). \tag{4.32}$$

Here, we can see from (4.5), (4.25) and (4.30)~(4.32) that a total effective velocity without vertex corrections is given by

$$v_k^t = a_k^f v_k^f + a_k^c v_k^c + a_k^f \frac{1}{\mu - \varepsilon_k} \nabla_k V_k^2, \tag{4.33}$$

and vertex part related to  $T_{lm}$  in (4.26) can be written only by  $f$ -electron Green's functions.

As shown by Éliashberg,  $T_{lm}$  gives the renormalization of the velocity, as given by (4.36), except  $T_{22}$  which has  $g_2$  before and behind it. The velocity renormalized by the interaction between  $f$ -electrons can be derived by using Ward's identities connecting the real part of the selfenergy part of  $f$ -electrons to the vertex corrections. This kind of renormalization can be checked by considering the case  $T=0$  and  $\omega=0$ .

At  $T=0$  and external frequency  $\omega=0$ , vertex correction  $\Lambda_k^0$  is given by

$$\Lambda_{k\sigma}^0(0) = \sum_{k'\sigma'} \int \frac{d\omega'}{2\pi i} \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') [G_{k'}^f(\omega')]^2 \left[ v_{k'}^f + \frac{V_{k'}^2}{(\omega' + \mu - \varepsilon_{k'})^2} v_{k'}^c + \frac{\partial V_{k'}^2 / \partial \mathbf{k}'}{(\omega' + \mu - \varepsilon_{k'})} \right], \tag{4.34}$$

$\Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}')$  being  $\Gamma_{\sigma\sigma'}(\mathbf{k}\mathbf{k}'; \mathbf{k}'\mathbf{k})$ . On the other hand, momentum derivative of the  $f$ -electron selfenergy is given by

$$\begin{aligned} \frac{\partial \Sigma_{k\sigma}(0)}{\partial \mathbf{k}} &= \sum_{k'\sigma'} \int \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') \lim_{q \rightarrow 0} \frac{1}{q} [G_{k'+q}^f(\omega') - G_{k'}^f(\omega')] \frac{d\omega'}{2\pi i} \\ &= \sum_{k'\sigma'} \int \frac{d\omega'}{2\pi i} \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') [G_{k'}^f(\omega')]^2 \left[ v_{k'}^f + \frac{V_{k'}^2}{(\omega' + \mu - \varepsilon_{k'})^2} v_{k'}^c \right. \\ &\quad \left. + \frac{\partial V_{k'}^2 / \partial \mathbf{k}'}{(\omega' + \mu - \varepsilon_{k'})} \right] - \sum_{k'\sigma'} \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') a_{k'}^f \delta(\mu - E_{k'}^*) v_{k'}^*, \end{aligned} \tag{4.35}$$

where  $v_k^*$  is the velocity of the quasi-particle given by (4.22). By adding vertex correction  $a_k^f \Lambda_k^0$  to (4.33), we obtain real velocity  $\mathbf{J}_k$  contributing to the conductivity,

$$\begin{aligned}
 J_k &= a_k^f \left( v_k^f + \Lambda_k^0(0) + \frac{1}{\mu - \epsilon_k} \nabla_k V_k^2 \right) + a_k^c v_k^c \\
 &= a_k^f \left( v_k^f + \nabla_k \Sigma_k(0) + \frac{1}{\mu - \epsilon_k} \nabla_k V_k^2 \right) + a_k^c v_k^c \\
 &\quad + a_k^f \sum_{k'} \Gamma_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') a_{k'}^f \delta(\mu - E_{k'}^*) v_{k'}^* \\
 &= v_k^* + \sum_{k'\sigma'} f_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') \delta(\mu - E_{k'}^*) v_{k'}^* .
 \end{aligned}
 \tag{4.36}$$

The second term of (4.36) represents the backflow<sup>10)</sup> and interaction  $f_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}')$  is given by using  $f$ -electron vertex as

$$f_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') = a_k^f \Gamma_{\sigma\sigma'}(\mathbf{k}\mathbf{k}'; \mathbf{k}'\mathbf{k}) a_{k'}^f .
 \tag{4.37}$$

As the result, we obtain the conductivity in our system as<sup>7)</sup>

$$\begin{aligned}
 \sigma_{\mu\nu}(\omega) &= \frac{i}{2} e^2 \left\{ \sum_k J_{k\mu} \frac{\frac{1}{2T} \text{ch}^{-2}(E_k^*/2T)}{\omega + 2i\Gamma_k^*} J_{k\nu} \right. \\
 &\quad \left. + \frac{1}{2} \sum_{kk'} J_{k\mu} a_{k'}^f \frac{\frac{1}{2T} \text{ch}^{-2}(E_k^*/2T) T_{22}(\mathbf{k}, \mathbf{k}'; \omega)}{(\omega + 2i\Gamma_k^*)(\omega + 2i\Gamma_{k'}^*)} a_{k'}^f J_{k'\nu} \right\} .
 \end{aligned}
 \tag{4.38}$$

The effect of  $T_{22}$  will be discussed in § 6.

### § 5. Imaginary part of the $f$ -electron selfenergy

In this section, we calculate the imaginary part of the selfenergy of  $f$ -electron,  $\Sigma_k^R(\epsilon)$ , up to the order of  $T^2$  or  $\epsilon^2$ . For simplicity we consider the second-order term in  $U^2$  corresponding to the diagram in Fig. 3. Extension to general terms will be discussed later. The second-order selfenergy can be written as follows:

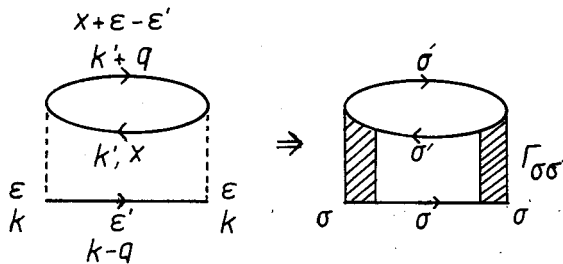


Fig. 3. The second-order selfenergy diagram giving rise to the  $T^2$ -term of its imaginary part. The general diagram giving the  $T^2$ -term is also shown on the right. Dotted line denotes the interaction between  $f$ -electrons and thick solid line  $f$ -electron Green's function.

$$\Sigma_k^{(2)}(\epsilon_n) = U^2 T \sum_{\epsilon_n q} G_{k-q}(\epsilon_n) \chi_q^0(\epsilon_n - \epsilon_n), \tag{5.1}$$

$$\chi_q^0(\epsilon_n - \epsilon_n) = -T \sum_{x_m k'} G_{k'}(x_m) G_{k'+q}(x_m + \epsilon_n - \epsilon_n), \tag{5.2}$$

$$x_m = (2m+1)\pi i T, \quad \epsilon_n = (2n'+1)\pi i T. \tag{5.3}$$

By the analytic continuation of (5.1),  $\Sigma_k^R(\epsilon + i\delta)$  is given by

$$\begin{aligned} \Sigma_k^R(\epsilon + i\delta) = & -U^2 \sum_q \int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \left\{ \text{cth} \frac{\epsilon' - \epsilon}{2T} G_{k-q}^R(\epsilon') \text{Im} \chi_q^{OR}(\epsilon - \epsilon') \right. \\ & \left. - \text{th} \frac{\epsilon'}{2T} \text{Im} G_{k-q}^R(\epsilon') \chi_q^{OR}(\epsilon - \epsilon') \right\}. \end{aligned} \tag{5.4}$$

Then,

$$\text{Im} \Sigma_k^R(\epsilon) = -U^2 \sum_q \int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \left[ \text{cth} \frac{\epsilon' - \epsilon}{2T} - \text{th} \frac{\epsilon'}{2T} \right] \text{Im} G_{k-q}^R(\epsilon') \text{Im} \chi_q^{OR}(\epsilon - \epsilon'), \tag{5.5}$$

$$\begin{aligned} \chi_q^{OR}(\nu) = & -\sum_{k'} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left\{ \text{th} \frac{x}{2T} G_{k'+q}^R(x + \nu) \text{Im} G_{k'}^R(x) \right. \\ & \left. + \text{th} \frac{x + \nu}{2T} G_{k'}^A(x) \text{Im} G_{k'+q}^R(x + \nu) \right\}, \end{aligned} \tag{5.6}$$

$$\text{Im} \chi_q^{OR}(\epsilon - \epsilon') = -\sum_{k'} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \text{th} \frac{x}{2T} - \text{th} \frac{x + \epsilon - \epsilon'}{2T} \right] \text{Im} G_{k'}^R(x) \text{Im} G_{k'+q}^R(x + \epsilon - \epsilon'). \tag{5.7}$$

From (5.5) and (5.7), we obtain

$$\begin{aligned} \text{Im} \Sigma_k^R(\epsilon) = & U^2 \sum_q \int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \left[ \text{cth} \frac{\epsilon - \epsilon'}{2T} - \text{th} \frac{\epsilon'}{2T} \right] \text{Im} G_{k-q}^R(\epsilon') \\ & \times \sum_{k'} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \text{th} \frac{x}{2T} - \text{th} \frac{x + \epsilon - \epsilon'}{2T} \right] \text{Im} G_{k'}^R(x) \text{Im} G_{k'+q}^R(x + \epsilon - \epsilon'). \end{aligned} \tag{5.8}$$

At  $T=0$ ,  $\text{Im} \Sigma_k^R(\epsilon)$  is expanded as follows:

$$\begin{aligned} \frac{\partial}{\partial \epsilon} \text{Im} \Sigma_k^R(\epsilon) = & U^2 \int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \left[ \text{cth} \frac{\epsilon' - \epsilon}{2T} - \text{th} \frac{\epsilon'}{2T} \right] \\ & \times \sum_{k'q} \text{Im} G_{k-q}^R(\epsilon') \int_{-\infty}^{\infty} \frac{dx}{\pi} [-\delta(x + \epsilon - \epsilon')] \text{Im} G_{k'}^R(x) \text{Im} G_{k'+q}^R(x + \epsilon - \epsilon'). \end{aligned} \tag{5.9}$$

By taking the second derivative by  $\epsilon$ , we obtain

$$\begin{aligned} \text{Im} \Sigma_k^R(\epsilon) \simeq & \frac{\epsilon^2 U^2}{2} \int_{-\infty}^{\infty} \frac{d\epsilon'}{\pi} \delta(\epsilon' - \epsilon) \sum_{k'q} \text{Im} G_{k-q}^R(\epsilon') \frac{1}{\pi} \text{Im} G_{k'}^R(\epsilon' - \epsilon) \text{Im} G_{k'+q}^R(0) \\ = & \frac{\epsilon^2 U^2}{2\pi^2} \sum_{k'q} \text{Im} G_{k-q}^R(\epsilon) \text{Im} G_{k'+q}^R(0) \text{Im} G_{k'}^R(0) \\ = & -\frac{\epsilon^2 U^2}{2} \sum_{k'q} \pi \rho_{k-q}(0) \rho_{k'+q}(0) \rho_k(0). \end{aligned} \tag{5.10}$$

At  $\varepsilon=0$ ,  $\text{Im}\Sigma_{\mathbf{k}}^{\text{R}}(0)$  is expanded up to the  $T^2$ -term as follows:

$$\begin{aligned} \text{Im}\Sigma_{\mathbf{k}}^{\text{R}}(0) &= U^2 \sum_q \int_{-\infty}^{\infty} \frac{d\varepsilon'}{2\pi} \left[ \text{cth} \frac{\varepsilon'}{2T} - \text{th} \frac{\varepsilon'}{2T} \right] \text{Im}G_{\mathbf{k}-q}^{\text{R}}(\varepsilon') \\ &\quad \times \sum_{\mathbf{k}'} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \text{th} \frac{x}{2T} - \text{th} \frac{x-\varepsilon'}{2T} \right] \text{Im}G_{\mathbf{k}'}^{\text{R}}(x) \text{Im}G_{\mathbf{k}'+q}^{\text{R}}(x-\varepsilon') \\ &= \frac{U^2}{2\pi} \sum_{\mathbf{k}'q} (\pi T)^2 \frac{\partial}{\partial \varepsilon'} \left[ \text{Im}G_{\mathbf{k}-q}^{\text{R}}(\varepsilon') \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \text{th} \frac{x}{2T} - \text{th} \frac{x-\varepsilon'}{2T} \right] \right. \\ &\quad \left. \times \text{Im}G_{\mathbf{k}'}^{\text{R}}(x) \text{Im}G_{\mathbf{k}'+q}^{\text{R}}(x-\varepsilon') \right]_{\varepsilon'=0} \\ &= -\frac{(\pi T)^2}{2} U^2 \sum_{\mathbf{k}'q} \pi \rho_{\mathbf{k}-q}(0) \rho_{\mathbf{k}'}(0) \rho_{\mathbf{k}'+q}(0). \end{aligned} \tag{5.11}$$

Here we have used the relation,

$$\int_{-\infty}^{\infty} d\varepsilon' \left[ \text{cth} \frac{\varepsilon'}{2T} - \text{th} \frac{\varepsilon'}{2T} \right] F(\varepsilon') \simeq F'(0) (\pi T)^2. \tag{5.12}$$

Combining (5.10) and (5.11), we obtain

$$\text{Im}\Sigma_{\mathbf{k}}^{\text{R}}(\varepsilon) \simeq -\frac{U^2}{2} \sum_{\mathbf{k}'q} \pi \rho_{\mathbf{k}-q}(0) \rho_{\mathbf{k}'}(0) \rho_{\mathbf{k}'+q}(0) [(\pi T)^2 + \varepsilon^2], \tag{5.13}$$

where  $\rho_{\mathbf{k}}(0) = -(1/\pi) \text{Im}G_{\mathbf{k}}^{\text{R}}(0)$ .

We have hitherto considered only the second-order term of selfenergy in  $U$ . If we include the higher order terms, we obtain the following results by using the same derivation as that used for the single impurity case,<sup>11),12)</sup>

$$\begin{aligned} \text{Im}\Sigma_{\mathbf{k}}^{\text{R}}(\varepsilon) &= -(\varepsilon^2 + (\pi T)^2) / 2 \cdot \sum_{\mathbf{k}'q} \pi \rho_{\mathbf{k}-q}^f(0) \rho_{\mathbf{k}'}^f(0) \rho_{\mathbf{k}'+q}^f(0) \\ &\quad \times \left\{ \Gamma_{\uparrow\downarrow}^2(\mathbf{k}, \mathbf{k}'; \mathbf{k}'+\mathbf{q}, \mathbf{k}-\mathbf{q}) + \frac{1}{2} \Gamma_{\uparrow\uparrow}^{\text{A}2}(\mathbf{k}, \mathbf{k}'; \mathbf{k}'+\mathbf{q}, \mathbf{k}-\mathbf{q}) \right\}, \end{aligned} \tag{5.14}$$

where  $\Gamma_{\uparrow\downarrow}$  and  $\Gamma_{\uparrow\uparrow}^{\text{A}}$  are defined as the diagrams in Fig. 1 and (3.13). The result (5.14) is exact as far as  $\varepsilon^2$ - and  $T^2$ -terms are concerned. While  $\rho_{\mathbf{k}}(0)$  in (5.13) is the unperturbed density of states of  $f$ -electrons,  $\rho_{\mathbf{k}}^f(0)$  in (5.14) is the true density of states of  $f$ -electrons with the mutual interaction.

### § 6. Vertex corrections

There are two kinds of vertex corrections. One discussed in § 4 is related to the real part of the selfenergy of  $f$ -electrons by Ward's identities. In the formalism developed by Éliashberg, this correction arises from the vertices connected to  $g_1$  or  $g_3$  at least on one side of it and changes the velocity (4.33) into  $\mathbf{J}_{\mathbf{k}}$  written by (4.36). This correction can be obtained by putting external frequency  $\omega=0$  in the three-point vertex. Another correction arising from  $T_{22}$  in (4.38) is related to the imaginary part of the selfenergy. This correction is essential to obtain the correct result in the thermodynamic limit,  $\omega \rightarrow 0$ . By treating this correction in a consistent way, we can show that the resistivity due to electron interaction vanishes in a free electron system without any crystal potential, as the

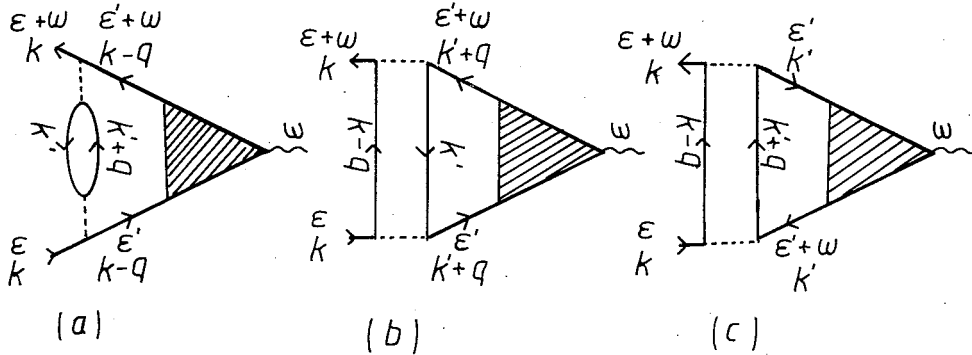


Fig. 4. Three-point vertex corrections indispensable to recover the momentum conservation. These three diagrams are obtained from the second-order selfenergy diagram shown in Fig. 3 by putting the vertex corrections to one of three electron lines in it, respectively. Thick solid line represents electron line and dotted line electron interaction.

result of recovering the momentum conservation. In this section we consider the latter correction.

For simplicity, we explain it by calculating the second-order terms with respect to Coulomb repulsion  $U$ . In order to make vertex corrections consistent with the selfenergy correction, we should take into account of the three diagrams in Fig. 4. We neglect the wave-function renormalization for the moment and take it into account at the last stage.

First we consider diagram (a) in Fig. 4. By using (4.32) and neglecting renormalization factors,

$$\Lambda_k^{(a)}(\varepsilon) = -\frac{U^2}{2\pi} \sum_q \int_{-\infty}^{\infty} d\varepsilon' \left[ \text{cth} \frac{\varepsilon' - \varepsilon}{2T} - \text{th} \frac{\varepsilon'}{2T} \right] \times \text{Im} \chi_q^{\text{OR}}(\varepsilon - \varepsilon') \frac{2\pi i \delta(\varepsilon' + \mu - E_{k-q})}{2i\Delta_{k-q}} \Lambda_{k-q}(\varepsilon'), \quad (6.1)$$

where  $\text{Im} \chi_q^{\text{OR}}(\varepsilon - \varepsilon')$  is given by (5.7),

$$\text{Im} \chi_q^{\text{OR}}(\varepsilon - \varepsilon') = -\sum_{k'} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \text{th} \frac{x}{2T} - \text{th} \left( \frac{x + \varepsilon - \varepsilon'}{2T} \right) \right] \text{Im} G_{k'}^{\text{R}}(x) \text{Im} G_{k'+q}^{\text{R}}(x + \varepsilon - \varepsilon'). \quad (6.2)$$

By a similar way to that used for the imaginary part of the selfenergy in the previous section, we expand  $\Lambda_k^{(a)}(\varepsilon)$  up to  $\varepsilon^2 + (\pi T)^2$  and obtain

$$\Lambda_k^{(a)}(\varepsilon) \simeq U^2 \sum_{k'} \pi \rho_{k-q}(0) \rho_{k'+q}(0) \rho_{k'}(0) \frac{\varepsilon^2 + (\pi T)^2}{2\Delta_{k-q}(\varepsilon)} \Lambda_{k-q}(\varepsilon). \quad (6.3)$$

Figure 4(b) gives the same contribution as  $\Lambda_k^{(a)}(\varepsilon)$ , as seen easily.

$$\Lambda_k^{(b)}(\varepsilon) \simeq U^2 \sum_{k'} \pi \rho_{k-q}(0) \rho_{k'+q}(0) \rho_{k'}(0) \frac{\varepsilon^2 + (\pi T)^2}{2\Delta_{k'+q}(\varepsilon)} \Lambda_{k'+q}(\varepsilon). \quad (6.4)$$

Figure 4(c) gives the following term,

$$\Lambda_k^{(c)}(\varepsilon) = U^2 \sum_{k'} \int_{-\infty}^{\infty} \frac{d\varepsilon'}{2\pi} \left[ \text{cth} \frac{\varepsilon' + \varepsilon}{2T} - \text{th} \frac{\varepsilon'}{2T} \right] \text{Im} \psi_{k+k'}^{\text{R}}(\varepsilon + \varepsilon') \frac{2\pi i \delta(\varepsilon' + \mu - E_{k'})}{2i\Delta_{k'}} \Lambda_{k'}(\varepsilon'), \quad (6.5)$$

where

$$\text{Im}\phi_{k+k^R}(\varepsilon+\varepsilon') = \sum_q \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[ \text{th} \frac{x}{2T} - \text{th} \frac{x+\varepsilon+\varepsilon'}{2T} \right] \text{Im}G_{k-q}^R(x+\varepsilon+\varepsilon') \text{Im}G_{k'+q}^R(-x). \tag{6.6}$$

At  $\varepsilon=0$ ,  $\Lambda_k^{(c)}(0)$  can be expanded with respect to  $T^2$  as follows:

$$\Lambda_k^{(c)}(0) = U^2 \sum_{k'} (\pi T)^2 \frac{\rho_{k'}(0)}{2\Delta_{k'}(0)} \Lambda_{k'}(0) \left[ \frac{\partial}{\partial \varepsilon'} \text{Im}\phi_{k+k^R}(\varepsilon') \right]_{\varepsilon'=0}, \tag{6.7}$$

$$\begin{aligned} \frac{\partial}{\partial \varepsilon'} \text{Im}\phi_{k+k^R}(\varepsilon')|_{\varepsilon'=0} &= - \sum_q \int_{-\infty}^{\infty} \frac{dx}{\pi} \delta(x+\varepsilon') \text{Im}G_{k-q}^R(x+\varepsilon') \text{Im}G_{k'+q}^R(-x)|_{\varepsilon'=0} \\ &= - \sum_q \pi \rho_{k-q}(0) \rho_{k'+q}(0). \end{aligned} \tag{6.8}$$

Thus,  $\Lambda_k^{(c)}(0)$  is given by

$$\Lambda_k^{(c)}(0) = - U^2 \sum_{k'q} \pi \rho_{k-q}(0) \rho_{k'+q}(0) \rho_{k'}(0) (\pi T)^2 \frac{\Lambda_{k'}(0)}{2\Delta_{k'}(0)}. \tag{6.9}$$

At  $T=0$ ,  $\Lambda_k^{(c)}(\varepsilon)$  is expanded with respect to  $\varepsilon$  as follows:

$$\begin{aligned} \frac{\partial}{\partial \varepsilon} \Lambda_k^{(c)}(\varepsilon) &= U^2 \sum_{k'} \int_{-\infty}^{\infty} \frac{d\varepsilon'}{2\pi} \left[ \text{cth} \frac{\varepsilon+\varepsilon'}{2T} - \text{th} \frac{\varepsilon'}{2T} \right] \frac{2\pi \rho_{k'}(\varepsilon')}{2\Delta_{k'}(\varepsilon')} \\ &\quad \times \sum_q \left( -\frac{1}{\pi} \right) \int_{-\infty}^{\infty} dx \delta(x+\varepsilon+\varepsilon') \text{Im}G_{k-q}^R(x+\varepsilon+\varepsilon') \text{Im}G_{k'+q}^R(-x) \Lambda_{k'}(\varepsilon') \\ &= U^2 \sum_{k'q} \int_{-\infty}^{\infty} d\varepsilon' \left[ \text{cth} \frac{\varepsilon+\varepsilon'}{2T} - \text{th} \frac{\varepsilon'}{2T} \right] \rho_{k'}(\varepsilon') \frac{\Lambda_{k'}(\varepsilon')}{2\Delta_{k'}(\varepsilon')} \\ &\quad \times \rho_{k-q}(0) (-\pi) \rho_{k'+q}(\varepsilon+\varepsilon'). \end{aligned} \tag{6.10}$$

Then,

$$\left. \frac{\partial^2}{\partial \varepsilon^2} \Lambda_k^{(c)}(\varepsilon) \right|_{\varepsilon=0} = - \sum_{k'q} 2\pi U^2 \rho_{k'}(0) \rho_{k-q}(0) \rho_{k'+q}(0) \frac{\Lambda_{k'}(-\varepsilon)}{2\Delta_{k'}(-\varepsilon)}. \tag{6.11}$$

Combining (6.9) and (6.11), we obtain

$$\Lambda_k^{(c)}(\varepsilon) = - U^2 \sum_{k'q} \pi \rho_{k-q}(0) \rho_{k'}(0) \rho_{k'+q}(0) [(\pi T)^2 + \varepsilon^2] \frac{\Lambda_{k'}(-\varepsilon)}{2\Delta_{k'}(-\varepsilon)}. \tag{6.12}$$

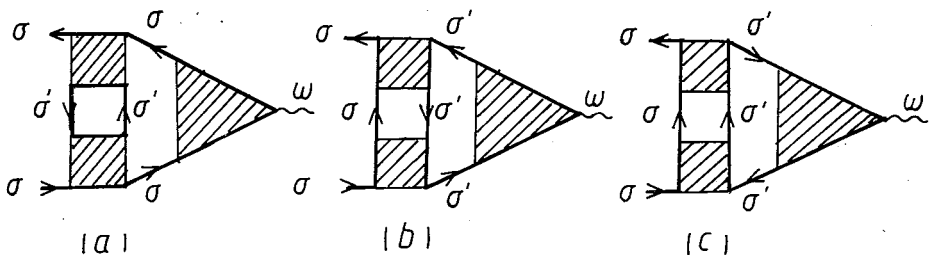


Fig. 5. General vertex corrections giving rise to the  $T^2$ -term. In the irreducible four-point vertices of these diagrams, two four-point vertices are connected only by two electron lines.

Hitherto, we have discussed the second-order term with respect to  $U$ . As far as  $T^2$ -terms are concerned, we have only to consider the diagrams with two electron lines at the same time in irreducible vertex  $\Gamma_{kk'}(\varepsilon_n, \varepsilon_{n'})$  as shown in Fig. 5. In this case four-point vertices contributing to the  $T^2$ -term depend on  $(\varepsilon + \varepsilon')$  or  $(\varepsilon' - \varepsilon)$ , in the same way as the second-order terms in  $U$ . Therefore, the general term can be obtained from the second-order terms by replacing  $U^2$  by

$$\Gamma_{\uparrow\downarrow}^2(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) + \frac{1}{2}\Gamma_{\uparrow\uparrow}^2(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}).$$

This replacement is similar to the imaginary part of selfenergy given by (5.14). Simultaneously with this replacement,  $\rho_k(0)$  is replaced by the true density of states,  $\rho_k^f(0)$ , at the Fermi energy by including the selfenergy corrections.

Now we discuss the renormalization of  $g_2$  in the three-point vertex. By (4.18),

$$\Gamma_k^* = a_k^f(-\text{Im}\Sigma_k(\varepsilon)) = a_k^f\Delta_k, \tag{4.18'}$$

and by (4.32),

$$g_2(\varepsilon) = 2\pi i(a_k^f)^2\delta(\varepsilon - E_k^*) / 2i\Gamma_k^* = \frac{2\pi a_k^f}{2\Gamma_k^*}\rho_k^f(\varepsilon) = \frac{2\pi}{2\Delta_k}\rho_k^f(\varepsilon), \tag{4.32'}$$

where  $\rho_k^f(\varepsilon)$  is the true density of states of  $f$ -electrons, which appeared in (2.5) and (5.14).

Now we show that vertex corrections discussed above are consistent with momentum conservation. The three-point vertex part  $\Lambda_k(\varepsilon)$  can be determined by the equation,

$$\begin{aligned} \Lambda_k(\varepsilon) &= \mathbf{J}_k + \Lambda_k^{(a)}(\varepsilon) + \Lambda_k^{(b)}(\varepsilon) + \Lambda_k^{(c)}(\varepsilon) \\ &= \mathbf{J}_k + \sum_{\mathbf{k}'\mathbf{q}} \Delta_0(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) \left\{ \frac{\Lambda_{\mathbf{k}-\mathbf{q}}(\varepsilon)}{2\Delta_{\mathbf{k}-\mathbf{q}}(\varepsilon)} + \frac{\Lambda_{\mathbf{k}'+\mathbf{q}}(\varepsilon)}{2\Delta_{\mathbf{k}'+\mathbf{q}}(\varepsilon)} - \frac{\Lambda_{\mathbf{k}'(-\varepsilon)}}{2\Delta_{\mathbf{k}'(-\varepsilon)}} \right\}, \end{aligned} \tag{6.13}$$

where

$$\begin{aligned} \Delta_0(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) &= \pi\rho_{\mathbf{k}-\mathbf{q}}^f(0)\rho_{\mathbf{k}'+\mathbf{q}}^f(0)\rho_{\mathbf{k}}^f(0) \\ &\times [\Gamma_{\uparrow\downarrow}^2(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) + \frac{1}{2}\Gamma_{\uparrow\uparrow}^2(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q})] [(\pi T)^2 + \varepsilon^2] \end{aligned} \tag{6.14}$$

and by (4.11) and (5.14)

$$\Delta_k = \frac{1}{2}\sum_{\mathbf{k}'\mathbf{q}} \Delta_0(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}). \tag{6.15}$$

Here it is noted that renormalization factor  $a_k^f$  in the numerator is cancelled out by that in the denominator,  $\Gamma_k^*$ , and  $\Lambda_k(\varepsilon)$  can also be written by unrenormalized quantities even if we include the renormalization.

We put here

$$\Phi_k(\varepsilon) = \Lambda_k(\varepsilon) / 2\Delta_k(\varepsilon) = \Phi_k(-\varepsilon). \tag{6.16}$$

Then, we obtain

$$0 = \mathbf{J}_k + \sum_{\mathbf{k}'\mathbf{q}} \Delta_0(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) [\Phi_{\mathbf{k}-\mathbf{q}} + \Phi_{\mathbf{k}'+\mathbf{q}} - \Phi_{\mathbf{k}'} - \Phi_{\mathbf{k}}]. \quad (6 \cdot 17)$$

Here if we put

$$\Phi_{\mathbf{k}} = \mathbf{k}F, \quad (6 \cdot 18)$$

the second term in (6·17) vanishes because of the momentum conservation.

On the other hand, in the periodic case we have Umklapp processes in  $f$ -electron scattering and (6·17) can be written by

$$\mathbf{J}_k - \sum_{\mathbf{k}'\mathbf{q}} \Delta_0(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) \sum_i \mathbf{K}_i F = 0. \quad (6 \cdot 19)$$

Here we have put

$$\Phi_{\mathbf{k}-\mathbf{q}} + \Phi_{\mathbf{k}'+\mathbf{q}} - \Phi_{\mathbf{k}'} - \Phi_{\mathbf{k}} = - \sum_i \mathbf{K}_i F, \quad (6 \cdot 20)$$

where  $\mathbf{K}_i$  is a reciprocal lattice vector and we have assumed that  $\Delta_0$  with reciprocal lattice vector in its arguments can be replaced by the corresponding value in the reduced zone, for simplicity. From (6·15), (6·18) and (6·19),

$$\Phi_{\mathbf{k}} = \frac{\mathbf{k}}{2\Delta_{\mathbf{k}}} \cdot \frac{\mathbf{J}_k \cdot \mathbf{k}}{\sum_i \mathbf{K}_i \cdot \mathbf{k}} \quad \text{and} \quad \mathbf{J}_k \propto \mathbf{k}. \quad (6 \cdot 21)$$

The conductivity given by (4·38) is written as

$$\sigma_{\mu\nu}(0) = e^2 \sum_{\mathbf{k}} J_{\mathbf{k}\mu} \left( - \frac{\partial f(x)}{\partial x} \right)_{x=E_{\mathbf{k}}^*} \frac{\Lambda_{\mathbf{k}\nu}}{2\Gamma_{\mathbf{k}}^*}. \quad (6 \cdot 22)$$

Inserting (6·21) into (6·22), we obtain

$$\sigma_{\mu\nu}(0) = e^2 \sum_{\mathbf{k}} \delta(\mu - E_{\mathbf{k}}^*) J_{\mathbf{k}\mu} \frac{1}{2\Gamma_{\mathbf{k}}^*} \frac{k^2}{\sum_i (\mathbf{K}_i \cdot \mathbf{k})} J_{\mathbf{k}\nu}. \quad (6 \cdot 23)$$

In this expression,  $\mathbf{J}_k$  and  $\Gamma_{\mathbf{k}}^*$  are renormalized by  $a_k^f$  and density of states of quasi-particles  $\rho_{\mathbf{k}}^*(0) = \delta(\mu - E_{\mathbf{k}}^*)$  is enhanced by  $[a_k^f]^{-1}$ . Therefore, all renormalizations cancel out with each other and the resistivity is proportional to  $\Delta_{\mathbf{k}}$ , which is given by the  $T^2$ -term with a strongly enhanced coefficient. This is one of important results obtained by the present theory.

The factor  $2\Delta_{\mathbf{k}}$  is given by

$$2\Delta_{\mathbf{k}} \simeq \frac{4}{3} (\pi T)^2 \sum_{\mathbf{k}'\mathbf{q}} \pi \rho_{\mathbf{k}-\mathbf{q}}^f(0) \rho_{\mathbf{k}'}^f(0) \rho_{\mathbf{k}'+\mathbf{q}}^f(0) \left[ \Gamma_{\uparrow\downarrow}^2(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) + \frac{1}{2} \Gamma_{\uparrow\uparrow}^{A2}(\mathbf{k}, \mathbf{k}'; \mathbf{k}' + \mathbf{q}, \mathbf{k} - \mathbf{q}) \right]. \quad (6 \cdot 24)$$

Here, if we neglect the momentum dependence in  $\Gamma_{\uparrow\uparrow}^A, \Gamma_{\uparrow\downarrow}^A = 0$ . Further, if we assume a large Coulomb repulsion giving rise to  $\chi_c^f = 0$ , from (3·9) and (3·18) we have

$$\tilde{\chi}_{\uparrow\downarrow}(\mathbf{k}) = \tilde{\chi}_{\uparrow\uparrow}(\mathbf{k}) = \tilde{\gamma}(\mathbf{k}), \quad (6 \cdot 25)$$



and from (3·15)

$$\tilde{\chi}_{\uparrow\downarrow}(\mathbf{k}) = \sum_{\mathbf{k}'} \rho_{\mathbf{k}'}^f(0) \Gamma_{\uparrow\downarrow}(\mathbf{k}, \mathbf{k}'; \mathbf{k}', \mathbf{k}). \quad (6\cdot26)$$

It can be understood from (6·24) ~ (6·26) that the coefficient of  $T^2$ -term of the resistivity,  $A$ , is proportional to  $\gamma^2$ , if we can neglect the momentum dependence (especially on  $\mathbf{q}$  in (6·24)) in  $\Gamma_{\uparrow\downarrow}$ . Thus  $A$  can be strongly enhanced as observed in experiments in Ce and U systems.

## § 7. Conclusions

In this paper we have studied low temperature properties of the heavy fermion system on the basis of the periodic Anderson Hamiltonian. The treated properties are electronic specific heat, susceptibility and electrical resistivity. The coefficient of  $T$ -linear specific heat,  $\gamma$ , is given by the density of states of quasi-particles at Fermi energy and consists of two parts; one is a part arising from conduction  $c$ -electrons and the other a part from  $f$ -electrons which is given by the sum over the density of states of wave vector  $\mathbf{k}$ ,  $\rho_{\mathbf{k}}^f(0)$ , multiplied by enhancement factor  $\tilde{\gamma}_{\mathbf{k}}$ . This enhancement factor gives a main origin of heavy electrons.

The susceptibility is also given by two contributions from  $c$ -electrons and  $f$ -electrons. The latter contribution is given by the sum of two susceptibilities  $\chi_{\uparrow\uparrow}^f$  and  $\chi_{\uparrow\downarrow}^f$ . The contribution to  $\gamma$  from  $f$ -electrons,  $\gamma^f$ , is connected to the sum of  $\chi_{\uparrow\uparrow}^f$  and vertex functions of two  $f$ -electrons with parallel spins, (3·10) ~ (3·12). This relation is derived by Ward's identities. The parallel spin vertex function vanishes in the case of single impurity, while this does not vanish in the periodic case because of the momentum conservation. This point is an important difference between single impurity and periodic cases. As a result of it, Wilson ratio in the limit of large  $U$  can be larger or smaller than the corresponding value of the single impurity case, 2, depending on the sign of their parallel spin vertex function.

At low temperatures, the repulsive interaction between  $f$ -electrons gives rise to the  $T^2$ -resistivity for quasi-particles in the crystal. However, if there is no crystal lattice, this resistivity automatically vanishes, because of the momentum conservation. Therefore, the  $T^2$ -resistivity arises from mainly Umklapp processes.

Resistivity can be calculated mainly along the line layed by Éliashberg. The obtained expression for the conductivity (6·23) includes quasi-particle density of states, two current components in the numerator and the reciprocal life-time of quasi-particles in the denominator. Renormalization factors in these quantities are cancelled out and resistivity becomes finally proportional to the reciprocal life-time of  $f$ -electrons,  $\Delta_{\mathbf{k}}$ . This  $\Delta_{\mathbf{k}}$  is proportional to the square of the enhancement factor  $\tilde{\gamma}_{\mathbf{k}}$  and gives large  $T^2$ -resistivity to the heavy fermion system.

All these properties derived in this paper can explain at least qualitatively the low temperature behaviors of the heavy electron systems in many Ce-compounds represented by CeAl<sub>3</sub>, CeCu<sub>2</sub>Si<sub>2</sub>, CeCu<sub>6</sub>, etc. The present theory, however, includes several quantities characteristic of the Fermi liquid, the selfenergy of  $f$ -electrons as a function of  $\mathbf{k}$  and  $\omega$  and two kinds of vertex functions between two  $f$ -electrons with parallel and antiparallel spins. These quantities were left as unknown functions in this paper.

The appearance of the quasi-fermion system in Ce compounds at low temperatures is caused by large Kondo temperature  $T_K$  compared with RKKY interaction. It is now recognized that such a large value of  $T_K$  is originated from the degeneracy of  $4f$ -orbitals. In this sense, the present Anderson model is not sufficient, and present calculations should be extended to the periodic Anderson model in which are taken into account the orbital degeneracy and also crystalline field splittings for  $4f$ -orbitals. Nevertheless, the results obtained in this paper would remain with only minor modifications for such a real system.

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