A Theory of Anisotropic Semiconductor of Heavy Fermions

Hiroaki Ikeda and Kazumasa Miyake

Department of Material Physics, Faculty of Engineering Science, Osaka University, Toyonaka 560

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It is demonstrated that a $k$-dependence of the hybridization matrix element between $f$- and conduction electrons can give rise to an anisotropic hybridization gap of heavy fermions if the filling of electrons corresponds to that of the band insulator. The most interesting case occurs when the hybridization vanishes along some symmetry axis of the crystal reflecting a particular symmetry of the crystal field. The results of a model calculation are consistent with wide range of anomalous properties observed in CeNiSn and its isostructural compounds, the anisotropic semiconductor of heavy fermions. In particular, highly sensitive effect of impurity scattering on the residual density of states for zero energy excitation and the anisotropic temperature dependence of the resistivity are well explained. It is also discussed that a weak semimetallic behavior arises through the weak $k$-dependence of the $f$-electron self-energy $\Sigma_f(k, 0)$.

KEYWORDS: heavy fermion, Kondo insulator, anisotropic hybridization gap, crystal field, CeNiSn, CeRhSb
§1. Introduction

Heavy-fermion systems exhibit a variety of ground states. Among them there is a class, the so-called “Kondo insulator”, which has a narrow energy gap of the order (∼10K) at low temperatures. This class of compounds exhibits the Kondo effect at high temperatures and an insulating behavior at low temperatures. The mechanism of the energy-gap formation at low temperatures has been discussed from a variety of viewpoints. These are classified roughly into two categories, i.e., k-space and real-space approaches. In the former approach, the origin of insulating behaviors is attributed to a hybridization gap which is highly renormalized by the strong correlations among almost localized f-electrons. A circumferential evidence supporting this point of view is that all the compounds called the “Kondo insulator”, except for TmSe, have even number of electrons in the unit cell which is a necessary condition for the band insulator. In the latter approach, on the other hand, it is attributed to the formation of local bound state of one kind of another, such as local singlet due to the strong Kondo effect, the Wigner crystal formation, and so on.

A picture of the renormalized hybridization gap is based on the principle of “adiabatic continuation” which was applied first by Landau in the Fermi liquid theory and then has turned out very useful so far in understanding the low energy properties of wide range of strongly interacting systems as demonstrated by Yamada and Yosida for the impurity Anderson model. While correctness of this picture for the “Kondo insulator” has been suggested by the Gutzwiller approach for the periodic Anderson model for this decade, it was recently shown more vividly on the basis of the numerical renormalization group method, the quantum Monte Carlo calculation, and the exact diagonalization method with the help of the \(d=\infty\) theory. On the other hand, it is reported that a charge gap is different from a spin gap in the \(d=1\) theory on the basis of the exact diagonalization method. This result is against the picture mentioned above. However, we believe that this may come from the particularity of 1-dimensionality.

Among the “Kondo insulators”, CeNiSn and its isostructural compounds have attracted much attention for almost a decade, because they have exhibited, at least for samples of early stage, behaviors of anisotropic semiconductor with highly renormalized energy gap. An anisotropic semiconductor means that the energy gap vanishes in a direction in the \(k\)-space and the density of states (DOS) shows a V-shaped like structure at low energy region. This was first inferred from the measurements of the longitudinal NMR relaxation rate at low temperature and reinforced later by those of the thermodynamic properties (the specific heat, the magnetic susceptibility etc.). In addition, the inelastic neutron scatterings show the existence of anisotropic magnetic excitations in the \(k\)-space. These compounds are also found to be very sensitive to a small amount of impurities such that the residual DOS at zero energy excitations increases drastically in roughly proportional to the square root of impurity concentration.

In this paper we develop a theory of \(k\)-space approach to understand the anomalous properties of
anisotropic semiconductor of heavy fermions, such as CeNiS\\textsubscript{n}. We follow the formalism developed for the Fermi liquid theory of heavy fermions on the basis of the periodic Anderson model while we apply it to the filling corresponding to the band insulator. An essential point of our theory is that the hybridization matrix element can happen to vanish along some symmetry axis (in the $\mathbf{k}$-space) of the crystal for a particular symmetry of the crystal field which is expected to realize in CeNiSn. Then, the hybridization gap also vanishes along the same direction, which can explain wide range of the anomalies observed in CeNiSn.

An idea that the node of the hybridization can possibly give rise to the pseudo-gap structure of quasiparticles has been addressed by Kagan, Kikoin and Prokof’ev, although their theory seems not to have been fully developed and includes some ambiguity. For instance, the condition for the appearance of the node of the hybridization was neither specified, nor the explicit form of the quasiparticle DOS was given. Hereafter we develop the theory on a more solid ground of the formalism.

We develope the formalism of our theory in §2.1 ∼ §2.6 and discuss about DOS in §2.7 and the effect of impurity scattering on DOS in §2.8. §3 is devoted to the discussions of physical properties and those validity: the specific heat (§3.1), the longitudinal NMR relaxation rate (§3.2), the magnetic properties (§3.3 and §3.4), the neutron scattering intensity (§3.5), and the anisotropic temperature dependence of the resistivity (§3.6) are discussed in detail on the model calculations. Furthermore, the effect of pressure (§3.7) and the lifetime of quasiparticles (§3.8) are briefly discussed.

§2. Theory

2.1 Hamiltonian

We start with the periodic Anderson model keeping it in mind that $(4f)^1$ configuration is realized in Ce$^{3+}$ ion in those compounds:

$$H = H_c + H_f + H_{c-f},$$

(2.1)

where $H_c$, $H_f$, and $H_{c-f}$ stands for the Hamiltonian of conduction electrons, $f$-electrons, and the hybridization among them, respectively. The first term in eq. (2.1), $H_c$, is given by

$$H_c = \sum_{k\sigma} \xi_k c_{k\sigma}^{\dagger} c_{k\sigma},$$

(2.2)

where $c_{k\sigma}^{\dagger} (c_{k\sigma})$ creates (annihilates) a conduction electron in a plane wave state labeled by wave vector $\mathbf{k}$ and spin $\sigma(\pm)$. The plane wave state can be expanded around site $i$ ($\mathbf{r}_i$) as follows:

$$|\mathbf{k}\sigma\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}_i} \chi_{\sigma} = \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{i^l j_l(k|r_i|)}{r_i} Y_l^m(\Omega_\mathbf{k}) Y_l^m(\Omega_{\mathbf{r}-\mathbf{r}_i}) \chi_{\sigma},$$

(2.3)
where $\chi_\sigma$ is the spin function, $j_i(kr)$ is the spherical Bessel function, $Y^m_l$ is the spherical harmonics with the argument of solid angle $\Omega_r$ of the position vector $r$ or $\Omega_k$ of the wave vector $k$, and $V$ is the volume of the crystal.

The second term in eq.(2.1), $H_f$, is given by

$$H_f = \sum_{kM} E_M f^\dagger_{kM} f_{kM} + \frac{1}{2} U \sum_{i,M \neq M'} f^\dagger_{iM} f_{iM} f^\dagger_{M'} f_{M'},$$

(2.4)

where $f^\dagger_{iM}(f_{iM})$ is the creation (annihilation) operator of the $f$-electron on the orbital $M$ in the 4f shell at site $i$, and $f^\dagger_{kM}(f_{kM})$ is its Fourier transform, and $E_M$’s denote the energy levels of the 4f-electron which are split into $j=7/2$ and $j=5/2$ multiplets under the spin-orbit interaction and further separated by the crystal-field interaction in general. The angular part of its eigen function is expressed as

$$|M\rangle = \sum_\mu b^M_\mu \sum_m a^\mu_{lma} Y^m_l (\Omega_r - r_i) \chi_\sigma,$$

(2.5)

where $\mu$ is the $z$-component of the total angular momentum, $j$, and $a^\mu_{lma}$ are the Clebsch-Gordan coefficients, and $b^M_\mu$ are coefficients specifying the crystal-field level. The last term in eq.(2.4) represents the Coulomb repulsion $U$ between $f$-electrons in the states $|M\rangle$ and $|M'\rangle$. For simplicity, we neglect $M$- and $M'$- dependence of $U$.

The last term in eq.(2.1), $H_{c-f}$, describes the hybridization between $f$- and conduction electrons:

$$H_{c-f} = \sum_{kM\sigma} (V_{kM\sigma} c^\dagger_{k\sigma} f_{kM} + h.c.),$$

(2.6)

where $V_{kM\sigma}$ is the mixing matrix element which can be calculated with the use of eqs.(2.3) and (2.5) as

$$V_{kM\sigma} = \sqrt{4\pi V_{kl}} \sum_\mu b^M_\mu \sum_m a^\mu_{lma} Y^m_l (\Omega_k).$$

(2.7)

Here, $V_{kl}$ has the energy dependence of the mixing matrix, and is treated as a parameter of our model.

### 2.2 Hybridization and Green Function

Now we consider the case in which the crystal-field splitting is so large that we can neglect the effects of excited crystal-field states in the relevant low-temperature and low-energy phenomena. Then we are left with two conduction bands ($\pm \sigma$) and two $f$-levels($\pm M$). In this case the Green functions of conduction- and $f$-electrons are given by

$$G^c_\sigma(k,\omega) = \frac{1}{\omega - \xi_k - V_f^2(k)},$$

$$G^f_M(k,\omega) = \frac{1}{\omega - E_f - \Sigma_f(k,\omega) - V_f^2(k)},$$

(2.8a)

(2.8b)
where $E_f$ is the lowest crystal-field level and $\Sigma_f(k,\omega)$ is the self-energy of $f$-electrons due to the Coulomb repulsion $U$. The hybridization $V_f^2(k)$ can be regarded as independent of $\sigma$ after an appropriate linear combinations of $|M\rangle$ and $|M\rangle$ have been taken.

$$V_f^2(k) \equiv |V_{kM\sigma}|^2 + |V_{k\bar{M}\sigma}|^2 = |V_{kM\sigma}|^2 + |V_{k\bar{M}\sigma}|^2 \quad (2.9)$$

The $k$-dependence of $V_f(k)$ reflects the symmetry of the lowest crystal-field level in general. For example, in the case of CeNiSn and its isostructural compounds, in which the approximate local symmetry of the crystal field is trigonal $D_3d$, the energy levels split into three doublets: $|5/2, \pm 3/2\rangle, a|5/2, \pm 1/2\rangle + b|5/2, \mp 5/2\rangle$, and $-b|5/2, \pm 1/2\rangle + a|5/2, \mp 5/2\rangle$, with $a$ and $b$ being appropriate constants satisfying $a^2 + b^2 = 1$. Depending on the symmetry of the crystal-field ground state, there occurs various angular dependence of the hybridization $V_f^2(k)$. While the hybridization is finite at any direction of $\hat{k} \equiv k/|k|$ in the state including $|\pm p\rangle \equiv a|5/2, \pm 1/2\rangle + b|5/2, \mp 5/2\rangle$, it vanishes along the quantization axis (z-axis) in $|\pm m\rangle \equiv |5/2, \pm 3/2\rangle$.

$$V_{\pm p}^2(k) = V^2 \left[a^2 (5\hat{k}_z^4 - 2\hat{k}_z^2 + 1) + b^2 5(1 - \hat{k}_z^2)^2 - 4\sqrt{10}ab(\hat{k}_x^2 - 3\hat{k}_y^2)\hat{k}_z \hat{k}_z\right], \quad (2.10a)$$

$$V_{\pm m}^2(k) = V^2(1 - \hat{k}_z^2)(1 + 15\hat{k}_z^2), \quad (2.10b)$$

where $V^2$ gives $|k|$-dependence of $V^2(k)$ and $z$-axis is taken as parallel to the $a$-axis, the symmetry axis of these crystals.

### 2.3 Effective Hamiltonian for Quasiparticles

We are interested in the low temperature region, in which the physical properties can be described by the renormalized quasiparticles near the Fermi level after the many-body effect due to the on-site repulsion $U$ in eq. (2.4) has been taken into account. These quasiparticles are described by the effective Hamiltonian

$$\tilde{H}_{\text{eff}} = \sum_{k\sigma} \xi_k \tilde{c}_k^{\dagger} \tilde{c}_{k\sigma} + \sum_{k} \tilde{E}_f \tilde{f}_k^{\dagger} \tilde{f}_k + \sum_{k} \sum_{M=\pm} (\tilde{V}_{kM\sigma} \tilde{c}_k^{\dagger} \tilde{f}_k + h.c.), \quad (2.11a)$$

where

$$\tilde{E}_f = z_k \left[E_f + \Sigma_f(k,0)\right], \quad (2.11b)$$

$$\tilde{V}_{kM\sigma} = \sqrt{\xi_k} V_{kM\sigma}, \quad (2.11c)$$

where the renormalization amplitude $z_k$ is defined as

$$z_k = \left[1 - \frac{\partial \Sigma_f(k,\omega)}{\partial \omega}\right]_{\omega=0}^{-1} \ll 1 \quad (2.12)$$

Here, the renormalized $f$-level $\tilde{E}_f$ has a $k$-dependence through that of the self-energy $\Sigma_f(k,0)$ in general. However, we first investigate the case where the $k$-dependence can be neglected, because...
the heavy quasiparticles themselves would not be formed if \( \Sigma_f(k,0) \) had appreciable dispersion. The effect of its \( k \)-dependence will be discussed later in relation to the resistivity (§3.6) and the effect of pressure (§3.7).

Then we can rewrite the Green functions, eqs. (2.8), as

\[
G_c^\sigma(k,\omega) = \frac{1}{\omega - \xi_k - \tilde{V}_f^2(k) / (\omega - \tilde{E}_f)} = \frac{A_c^+ (k)}{\omega - E_{k}^+} + \frac{A_c^- (k)}{\omega - E_{k}^-},
\]

(2.13a)

\[
G_f^M(k,\omega) = \frac{z_k}{\omega - \tilde{E}_f - \tilde{V}_f^2(k) / (\omega - \xi_k)} = z_k \left( \frac{A_f^+ (k)}{\omega - E_{k}^+} + \frac{A_f^- (k)}{\omega - E_{k}^-} \right),
\]

(2.13b)

where \( E_{k}^\pm \) are two hybridized-quasiparticle bands given by

\[
E_{k}^\pm = \frac{1}{2} \left[ \xi_k + \tilde{E}_f \pm \sqrt{(\xi_k - \tilde{E}_f)^2 + 4\tilde{V}_f^2(k)} \right],
\]

(2.14)

where

\[
\tilde{V}_f^2(k) = z_k V_f^2(k).
\]

(2.15)

The residues \( A_c^\pm (k) \) and \( A_f^\pm (k) \) in eqs. (2.13) are

\[
A_c^\pm (k) = \left[ 1 + \frac{\tilde{V}_f^2(k)}{E_{k}^\pm - \tilde{E}_f} \right]^{-1},
\]

(2.16a)

\[
A_f^\pm (k) = \left[ 1 + \frac{\tilde{V}_f^2(k)}{E_{k}^\pm - \xi_k} \right]^{-1},
\]

(2.16b)

which give the spectral weight of conduction- and \( f \)-electrons, respectively, in the upper/lower bands.

2.4 Band Insulator of Quasiparticles

In the case of the electron filling corresponding to the band insulator, the renormalized Fermi level is located in between \( E_{k}^+ \) and \( E_{k}^- \) forming the hybridization gap. As we have mentioned above, almost all the compounds called “Kondo insulator” contain even number of electrons in the unit cell and have a right to be a band insulator. A difference from the conventional semiconductor is that the hybridization gap is highly renormalized by strong correlation effect between \( f \)-electrons. Hereafter, we investigate the case where the ground crystal-field level is \(|5/2, \pm 3/2\rangle\), which turn out to be consistent with anomalous properties of CeNiSn as discussed below. Then, due to eqs. (2.10b), (2.14) and (2.15), the hybridization gap \( \Delta (k_B) \) is given by

\[
\Delta (k_B) \simeq 2 \frac{\tilde{V}_f^2(k_B)}{\xi_{k_B}} \simeq 2 z_{k_B} V_f^2(k_B) \equiv T_K (1 - \hat{k}_{Bz}^2) (1 + 15 \hat{k}_{Bz}^2)
\]

(2.17)

where \( k_B \) denotes the wavevector at the zone boundary and \( T_K \equiv 2 z_{k_B} V_f^2 / D \). For simplicity we neglect \(|k|\)-dependence of \( V^2 \) and \( k \)-dependence of \( z_{k_B} \). In deriving eq. (2.17), we have assumed that
the renormalized hybridization $\sqrt{z_{k^2}}V$ is much smaller than the bare band-width of conduction electrons $2D$. Thus the hybridization gap vanishes at points on the zone boundary where $k_Bz = \pm 1$ and becomes a pseudogap. That is, the renormalized DOS have no clear gap threshold. This is to be compared to the “axial-like gap” in anisotropic superconductors, although the resultant DOS is totally different as discussed below.

2.5 Mass Enhancement Factor

The renormalization amplitude $z$ for the particle-hole symmetric case has been calculated by Rice-Ueda,\textsuperscript{10} on the basis of the Gutzwiller approximation, and by Shiba,\textsuperscript{11} on the basis of variational Monte Carlo calculations for the Gutzwiller ansatz, with the use of a model hybridization $V^2(k) = V^2$. A similar but more extended result has recently been obtained by numerical renormalization group method\textsuperscript{12}, quantum Monte Carlo calculation\textsuperscript{13} and the exact diagonalization method\textsuperscript{14} in $d = \infty$ system. We have performed the calculation similar to Rice-Ueda’s with anisotropic hybridization $V^2(k) = V^2(1 - \hat{k}_z^2)$, a simplified version of (2.10b). The result for the filling corresponding to band insulator is

$$z = \frac{e^{19/12}D^2}{4V^2} \exp\left(-\frac{3UD}{32V^2}\right)$$

(2.18a)

which is compared with that of Rice-Ueda

$$z = \frac{D^2}{V^2} \exp\left(-\frac{UD}{8V^2}\right)$$

(2.18b)

where the hybridization gap is constant and fully opened.

In those model calculations, the particle-hole symmetry is assumed, so that the occupation number of $f$-electron $n_f$ per site is exactly unity, i.e. $n_f = 1$. However, this constraint is easily relaxed by introducing the asymmetry of conduction band on the position of the $f$-level. Therefore, it is possible to calculate the mass enhancement factor in the way similar to above not only in the Kondo regime, where $n_f \approx 1$, but also in the valence-fluctuation regime.

2.6 Effect of Impurity Scattering

It can be shown, on the basis of the Ward identity arguments, that the $s$-wave impurity potential $u$ is renormalized by many-body vertex correction as\textsuperscript{15}

$$u \rightarrow \tilde{u} = u \cdot \left[1 - \frac{\partial \Sigma_f(k, \omega)}{\partial \omega}\right]_{\omega=0} = \frac{1}{z}u$$

(2.19)

This renormalization is shown in Fig. 1 in terms of the Feynman diagram. Then, for strongly correlated systems where $z^{-1} = m^* / m \gg 1$, the impurity scattering always becomes that of unitarity limit, i.e., $\tilde{u}N_F \gg 1$, even if the bare potential $u$ is moderate one, i.e., $uN_F \lesssim 1$. Then
the Green functions of the conduction- and $f$-electrons are given by

\[
G^c_{\sigma}(k, \omega) = \frac{1}{\omega - \xi_k - \tilde{V}_f^2(k) + i\tilde{E}_f - \tilde{V}_f \Im \Sigma_{\text{imp}}(\omega)}, \tag{2.20a}
\]

\[
G^f_M(k, \omega) = \frac{z_k}{\omega - \tilde{E}_f - i\tilde{V}_f \Im \Sigma_{\text{imp}}(\omega) - \tilde{V}_f^2(k)}, \tag{2.20b}
\]

where the self-energy $\Sigma_{\text{imp}}(\omega)$ due to impurity scattering is given in the t-matrix approximation by

\[
\Sigma_{\text{imp}}(\omega) = n_{\text{imp}} \frac{\tilde{u}}{1 - \sum_k G^f_M(k, \omega)}, \tag{2.21}
\]

where $n_{\text{imp}}$ denotes the impurity concentration. In deriving eqs.(2.20), the self-energy of conduction electrons due to impurity scattering has been neglected because the renormalization, such as eq.(2.19), does not occur. Equations (2.20) and (2.21) need to be solved self-consistently as in the case of heavy fermion superconductors, where the impurity scattering in the unitarity limit is known to give rise to appreciable residual DOS in the V-shaped gap even for a very small impurity concentration.\(^{37,38}\)

### 2.7 Density of States of Quasiparticles

The quasiparticle DOS are calculated as follows:

\[
\tilde{N}(\omega) = \sum_{k\sigma} \left[ \delta(\omega - E^+_k) + \delta(\omega - E^-_k) \right], \tag{2.22a}
\]

\[
= N_F \int_0^1 d\hat{k}_z \int_{-D}^{D} dE \left( 1 + \frac{\tilde{V}_f^2(\hat{k}_z)}{E^2} \right) \delta(\omega - E) \theta(|E| - \Delta(\hat{k}_z)), \tag{2.22b}
\]

where

\[
\Delta(\hat{k}_z) \equiv T_K(1 - \hat{k}_z^2)(1 + 15\hat{k}_z^2). \tag{2.23}
\]

In deriving eq.(2.22b) from eq.(2.22a), we have assumed for simplicity that the conduction band has a linear dispersion with constant DOS, $N_F$, and extending from $-D$ to $D$, and $\tilde{E}_f = 0$. A result of numerical calculation of $\tilde{N}(\omega)$, eq.(2.22b), is shown in Fig. 2. Here, the relation between the hybridization $V$ and renormalization factor $z$ is determined as $zV^2/D = 0.01D$. The shape of DOS shown in Fig. 2 has two characteristics: (1) $\tilde{N}(\omega = 0)$ is finite, and (2) it exhibits four-peak structure, i.e., there exist two energy scales ($\Delta_1 = T_K = 0.02D, \Delta_2 \approx 0.08D$). The former (1) results from the fact that the hybridization gap vanishes at points ($\hat{k}_z = \pm 1$). The shape of DOS around the Fermi level $\omega = 0$ can be calculated analytically as

\[
\tilde{N}(\omega) \simeq N_F \frac{D^2}{64zV^2} \left[ 1 + 2 \left( 1 + \frac{19D^2}{12 \cdot 32zV^2} \right) \frac{\omega}{D} + \cdots \right]. \tag{2.24}
\]
This is in marked contrast with the case of heavy-fermion superconductors, where the point node leads to DOS proportional to $\omega^2$. The reason for the characteristic (1) to hold is that there exists a singularity $\propto E^{-2}$, in the first factor of the integrand of (2.22b), which arises from the Jacobian $|d\xi/dE| = 1 + \bar{V}_f^2(\hat{k}_z)/E^2$.

The latter characteristic (2) is related to the existence of two extremum values of $\Delta(\hat{k}_z)$, eq.(2.23): $\Delta_1$ corresponds to the minimum of eq.(2.23) at $\hat{k}_z = 0$, at which the hybridization gap is given by $T_K$, and $\Delta_2$ corresponds to the maximum of eq.(2.23) at $\hat{k}_z = \sqrt{7}/15$, in which the hybridization gap becomes maximum. The ratio of $\Delta_2$ and $\Delta_1$ is given as $\Delta_2/\Delta_1 = 64/15$.

2.8 Effect of Impurity Scattering on Density of States

Next let us consider the effects of impurity scattering on quasiparticle DOS. From eqs.(2.20b) and (2.21), DOS is calculated self-consistently as follows:

$$\tilde{N}(\omega) \approx \frac{1}{\pi} \sum_k \frac{-\tilde{z}_k \text{Im}\Sigma_{\text{imp}}(\omega)}{(\omega - \tilde{E}_f - \frac{\tilde{z}_k V_f(k)}{\omega - \xi_k})^2 + [\tilde{z}_k \text{Im}\Sigma_{\text{imp}}(\omega)]^2},$$

$$\text{Im}\Sigma_{\text{imp}}(\omega) = -n_{\text{imp}} \left( \frac{\tilde{u}^2}{\pi \tilde{z}_k \tilde{N}(\omega)} \right)^2.$$

Results of numerical solution of eqs.(2.25) are shown in Fig. 3. One can see that the residual DOS at the Fermi level, $\tilde{N}(\omega = 0)$, is very sensitive to the impurity concentration and drastically increases with the impurity concentration $n_{\text{imp}}$. In Fig. 4 one finds that $\tilde{N}(\omega = 0)$ is roughly proportional to $\sqrt{n_{\text{imp}}}$. Precisely speaking, the residual DOS exists, even if $n_{\text{imp}} = 0$. So, in the limit, $n_{\text{imp}} \to 0$, its $n_{\text{imp}}$-dependence is given by $N_0 \sqrt{1 + c_0 n_{\text{imp}}}$, where $N_0$ is the residual DOS without impurities, and $c_0$ is a proper constant of order unity. This is to be compared with the impurity effects in heavy fermion superconductors.$^{37,38}$ The square-root dependence of the residual DOS has also been derived on the basis of a different picture, where it is understood as an impurity band similar to the doped semiconductor; namely the doping accompanied by variation of carrier number is necessary to obtain finite DOS in the true gap.$^{35,36}$ Our theory has been developed to discuss the case where carrier number does not change, while it is easily extended to the case where carriers are doped.

§3. Physical Properties

In this section, we study the qualitative aspects of several physical quantities and compare them with experiments.
3.1 Specific Heat

The specific heat is calculated on the basis of the quasiparticle picture, and the electronic specific heat coefficient, \( \gamma \equiv C(T)/T \), is given as follows:

\[
\gamma = 2 \int_0^\infty dx \tilde{N}(E)x^2 \text{sech}^2(x),
\]

(3.1)

where \( x = E/2T \). The temperature dependence of \( \gamma \) is calculated with the use of eqs. (2.22) and (2.25) and is shown in Fig. 5. A peak structure is found at \( T \sim \Delta_1/2 \). It is noted that \( \gamma \) is finite at \( T = 0 \), which results from the existence of the residual DOS at \( n_{\text{imp}} = 0 \). If \( \Delta_1 \) is fixed as \( \Delta_1/2 = 7K \), these results are in good agreement with the experimental data at \( T < \Delta_1 \), where the maximum of theoretical curve for \( \gamma \) is adjusted so as to agree with the experiment of ref. 22. We have also verified that the same quality of agreement with the data of ref. 24 is obtained while its absolute value of \( C_m/T \) is about 10% larger than that of ref. 23. However at \( T > \Delta_1 \) the agreement become poor. It is partly improved by considering temperature dependence of the quasiparticle DOS.

Furthermore, assuming that the effect of the magnetic field is only inducing the Zeeman splitting, the magnetic-field dependence of \( \gamma \) is obtained as

\[
\gamma = \int_0^\infty dx \tilde{N}(E) \left[ x_+^2 \text{sech}^2(x_+^2) + x_-^2 \text{sech}^2(x_-^2) \right],
\]

(3.2)

where \( x_{\pm} = (E \pm h)/2T \), \( h = g_J \mu_B |J_z|H \), \( g_J \) being a g-factor. The results for various temperatures are shown in Fig. 6. The coefficient \( \gamma \) at low temperature exhibits two-peak structure, which reflects the peak structure of DOS. This prediction has not yet been observed, partly because the strength of the magnetic field is not enough.

3.2 Longitudinal Relaxation Rate of NMR

The longitudinal NMR relaxation rate, \( 1/T_1 \), is obtained as follows

\[
\frac{1}{T_1 T} \propto \lim_{\omega \to 0} \sum_{\mathbf{q}} \frac{\text{Im} \chi^{-+}(\mathbf{q}, \omega)}{\omega},
\]

(3.3a)

\[
\propto \int_0^\infty dE \tilde{N}(E)^2 \text{sech}^2\left( \frac{E}{2T} \right) \frac{1}{T}.
\]

(3.3b)

Here we have assumed that the quasiparticle DOS directly affects \( 1/T_1 \) at Sn site via the \( c-f \) exchange as done in the analysis of experimental data. The results of numerical calculations of (3.3b), together with experimental data [23] are shown in Fig. 7 for the same parameters as in Fig. 5. For the temperature region, \( 0.1 \Delta_1 \lesssim T \lesssim \Delta_1 \approx 0.02D \), \( 1/T_1 \) shows the \( T^3 \)-like behavior reflecting the formation of the pseudogap at \( \omega \approx \Delta_1/2 \) of DOS as shown in Fig. 2, and for \( T \lesssim 0.1 \Delta_1 \), it shows \( T \)-linear behavior reflecting the residual DOS at the Fermi level. These behaviors well reproduce the \( T \)-dependence of \( 1/T_1 \) observed in the experiments. If \( \Delta_1 \) is fixed as \( \Delta_1 = 14K \). In addition, as increasing impurity concentration \( n_{\text{imp}} \), the residual DOS rises up drastically and the \( T \)-linear
behavior masks the $T^3$-like behavior. These are also in agreement with the experiments\textsuperscript{19} where the residual DOS shows the $n_{\text{imp}}$-dependence quite similar to the theoretical curve shown in Fig. 4.

The above results have been derived on the basis of the quasiparticle picture, so that, strictly speaking, its validity is assured only in the low temperature region $T < T_K$. However, it may be extended to much higher temperature region as far as the qualitative aspects are concerned. Indeed, $1/T_1$ in Fig. 7 exhibits the localized character of $f$-electrons for $T > T_K = 0.02D$, $1/T_1 \propto T^0$, and approaches asymptotically to the Korringa-like behavior at much higher temperatures, $1/T_1 \propto T$, as can be inferred from the DOS of quasiparticles shown in Fig. 2. In the latter region, the NMR relaxation is expected to occur mainly through the coupling with the conduction electrons as in LaNiSn\textsuperscript{18}. Recently such a behavior has been recognized by an analysis of the data of $1/T_1$ up to the room temperature.\textsuperscript{20}

3.3 Magnetization

The quasiparticle contribution to the magnetization is calculated as

$$M = \int_{-\infty}^{\infty} dE \left[ f(E-h) - f(E+h) \right] \tilde{N}(E) \quad (3.4)$$

The results are shown in Fig. 8 where one can see that the magnetization, in the unit $g_J \mu_B |J_z|$, is proportional to $h$, in the unit $D$, at low magnetic field and the slope is given by the residual DOS. However, as increasing $h$ the magnetization drastically increases at $h > 0.01D$ owing to the two large humps of DOS at $\omega = \pm \Delta_1/2$. These tendencies are found in the experimental data\textsuperscript{11}. The slope of the magnetization at low field is enhanced by small amount of impurity and the whole structures of $M-h$ curve shade off.

3.4 Uniform Spin Susceptibility

The uniform spin susceptibility along the easily axis ($a$-axis), in the unit $(g_J \mu_B |J_z|)^2 / D$, is given by the derivative of the magnetization as

$$\text{Re} \chi(0,0) = \left. \frac{\partial M}{\partial h} \right|_{h \rightarrow 0} = \int_{-\infty}^{\infty} dE \left[ -\frac{\partial f(E)}{\partial E} \right] \tilde{N}(E). \quad (3.5)$$

Its temperature dependence shown in Fig. 9 exhibits the peak structure like $\gamma$ as discussed in §3.1. However, the temperature at which $\text{Re} \chi(0,0)$ has the maximum ($T \simeq \Delta_1$) is different from that for $\gamma$. Increasing impurity concentration, the sharp dip at low temperature is filled up rapidly. Since the susceptibility (3.5) is given only by the contribution of the quasiparticles, the Van Vleck term is not included. If the latter is simply a constant, the observed Knight shift\textsuperscript{11} for $H||a$ represents the behavior of the uniform spin susceptibility $\chi^a$, which is in agreement with the curves of Fig. 9.
3.5 Neutron Scattering

The imaginary part of the dynamical susceptibility, the spectral weight of spin fluctuations, is calculated at \( T = 0 \) without a vertex correction as

\[
\text{Im} \chi(Q, \omega) \simeq \pi \sum_k \left[ f(E^-_k) - f(E^+_k) \right] \delta(\omega - E^+_k + Q + E^-_k)
\]

where \( f(E) \) is the Fermi distribution function and \( f(E^-_k) = 1 \) and \( f(E^+_k) = 0 \) at \( T \to 0 \). The spectral weight \( \text{eq.}(3.6) \) has been calculated numerically with the use of the quasiparticle dispersion, eq.(2.14), for specified \( Q \)'s. The spectral weight at \( Q = (1/2, 0, 0) \) is shown in Fig. 10 (a), which shows that there exists a broad hump at around \( \omega = 0.08D \). (It is noted that \( x-, y-, \) and \( z\)-axis here corresponds to the \( b-, c-, \) and \( a\)-axis, respectively of CeNiSn; so that \( Q = (1/2, 0, 0) \) implies \( Q = [0, 1/2, 0] \) in the notation of experiments of CeNiSn for instance.) This structure corresponds to the transition from one peak of DOS at \( \omega = -0.04D \) to another at \( \omega = 0.04D \) in DOS. For example, the former peak corresponds to the quasiparticle at \( k_1 = (-1/4, 1/2, 1/2) \), while the latter at \( k_2 = (1/4, 1/2, 1/2) \), because \( \hat{k}_{1z} = \hat{k}_{2z} \sim \sqrt{7/15} \). Thus, \( Q = k_2 - k_1 = (1/2, 0, 0) \).

The spectrum at \( Q = (0, 0, 1/2) \) shown in Fig. 10 (b) has a peak at around \( \omega = 0.06D \), which corresponds to the energy from an edge of the gap at \( \omega = -0.02D \) to one peak at \( \omega = 0.04D \) in DOS. For example, the former peak corresponds to the quasiparticle at \( k_3 = (1/2, 0, 0) \), while the latter at \( k_4 = (1/2, 0, 1/2) \), because \( \hat{k}_{3z} = 0 \) and \( \hat{k}_{4z} \sim \sqrt{7/15} \). Thus, \( Q = k_4 - k_3 = (0, 0, 1/2) \).

It is seen that a difference between the two spectra arises from that of the possibility of the zero energy transition. Since the hybridization gap vanishes along the \( z(a)\)-axis, there exist zero energy excitations for the transition between the points on the \( z(a)\)-axis. This is because we make choice of non-dispersive \( f\)-level. However, generally speaking, \( \text{Im} \chi(Q, 0) \) have to vanish in the normal Fermi liquid theory by the symmetry reason. This anomaly is removed by taking into account the small dispersion of \( f\)-electrons due to a possible weak \( k\)-dependence of the \( f\)-electron self energy, \( \Sigma_f(k, 0) \).

The spectral intensity at \( \omega = 0.08D \simeq \Delta_2 \) and \( Q = (Q_x, 0, 0) = [0, Q_b, 0] \) is computed as a function of \( Q_x(Q_b) \) and shown in Fig. 11. One can see the peak at \( Q_x(Q_b) = 1/2 \). The reason is that the peak shifts to higher energy as deviating from \( Q_x(Q_b) = 1/2 \). These features are consistent with \( Q_b\)-dependence of the intensity at 4.25meV in the inelastic neutron scattering. [3]

The details of these spectra are modified according to choices of the dispersions of conduction electrons, though characteristic structures do not change. However, when the conduction band do not cross the \( f\)-level in some direction in the \( k\)-space, the excitation energy is rather higher and the spectrum can not be observed at low energy region in general. This case may be realized in the low-energy spectrum at \( Q \parallel c\)-axis in the experiment. [3]
3.6 Anisotropy of Resistivity

It is the resistivity that is one of the measures to classify the heavy-fermion materials into “Kondo insulator” or not. The resistivity in heavy fermions exhibits the Kondo effect at high temperature region and metallic or activation-type behavior at low temperature region. We are interested in the behavior at temperatures lower than the coherent temperature $T_{coh}$, in which the current is carried by the quasiparticles. In this case the conductivity can be evaluated by

$$\sigma_{\mu\nu}(T) \propto \sum_{k} J_{k\mu} J_{k\nu} \tau_k \left(-\frac{\partial f(E_k)}{\partial E_k}\right), \quad (3.7)$$

where $J_{k\mu}$ is the velocity of the quasiparticle and $\tau_k$ is its lifetime. Assuming that the microscopic expression of the current is given only by the conduction electrons (neglecting the dispersion of $f$-electrons), the anisotropy of the conductivity is given as follows:

$$\sigma_{||} \propto \sum_{k} A_\pm^c(k)^2 v_z(k)^2 \tau_k \left(-\frac{\partial f(E_k^\pm)}{\partial E_k^\pm}\right), \quad (3.8a)$$

$$\propto \int dE_k \int d\Omega_k \left(\frac{E_k^2}{-z_k \text{Im} \Sigma_f(k, E_k)} \hat{V}_f^2(k) + \left(-\text{Im} \Sigma_c(k, E_k) E_k^2\right) \left(-\frac{\partial f(E_k)}{\partial E_k}\right)\right), \quad (3.8b)$$

$$\sigma_{\perp} \propto \sum_{k} A_\pm^c(k)^2 v_x(k)^2 \tau_k \left(-\frac{\partial f(E_k^\pm)}{\partial E_k^\pm}\right), \quad (3.8c)$$

$$\propto \int dE_k \int d\Omega_k \frac{\sin^2 \theta_k E_k^2}{-z_k \text{Im} \Sigma_f(k, E_k)} \hat{V}_f^2(k) + \left(-\text{Im} \Sigma_c(k, E_k) E_k^2\right) \left(-\frac{\partial f(E_k)}{\partial E_k}\right), \quad (3.8d)$$

where $\sigma_{||}$ and $\sigma_{\perp}$ are the conductivity along the $a$-axis and in the $bc$-plane, respectively, and

$$\frac{1}{\tau_k} = \frac{1}{E_k^2 + \hat{V}_f^2(k)} \left[(-z_k \text{Im} \Sigma_f(k, E_k)) \hat{V}_f^2(k) + \left(-\text{Im} \Sigma_c(k, E_k) E_k^2\right)\right], \quad (3.9a)$$

$$v_z(k) = \frac{\partial \xi_k}{\partial k_z} \quad \text{and} \quad v_x(k) = \frac{\partial \xi_k}{\partial k_x}. \quad (3.9b)$$

Here we have introduced $\Sigma_c(k, E_k)$, the self-energy of the conduction electrons, because $\sigma_{||}$ in pure system diverges logarithmically otherwise, reflecting the fact that the conduction electrons are decoupled from $f$-electrons in the $z$-direction ($a$-axis) where the hybridization vanishes. We regard the renormalization factor of conduction electrons from $\Sigma_c(k, E_k)$ as 1. In this model the conductivity in the $bc$-plane is isotropic unless the anisotropy of the conduction band is taken into account. In deriving (3.8d) from (3.8c), we have taken into account only the low energy excitations around $\hat{k}_z = \pm 1$ so that the obtained result should be regarded as that for asymptotic behavior in the limit $T \to 0$.

In order to discuss the temperature dependence of the conductivity at low temperature region, we must calculate the energy dependence of the imaginary part of the self-energies. For simplicity we calculate these along a standard treatment of the Fermi liquid theory neglecting the momentum...
dependence of the full vertex:

\[ \text{Im}\Sigma_\mu(k, E_k^+) \propto \int dp dq A_{\mu}^+(k - q) A_{\mu}^-(p + q) \delta(E_k^+ + E_p^- - E_{k-q}^+ - E_{p+q}^+), \]

where \( \mu = c \) or \( f \). These integrations are computed by the Monte Carlo calculation. The numerical results are shown in Fig. 12. From this one can see that the energy dependence of \( \text{Im}\Sigma_c(k, E_k) \) and \( \text{Im}\Sigma_f(k, E_k) \) near the Fermi level at zero temperature can be approximated by \( E_k^5 \) and \( E_k^3 \), respectively. Futhermore, we assume that the temperature dependence of \( \text{Im}\Sigma_\mu(k, E_k) \) is given with replacing \( E_k^2 \) by \( \max(E_k^2, (\pi T)^2) \), as can be seen from the structure of the Green functions.

By using these results we can estimate the temperature dependence of the resistivity. Substituting these energy dependence into eqs.(3.8), we obtain up to the logarithmic accuracy

\[ \sigma_\parallel \propto T^{-1}, \quad \text{and} \quad \sigma_\perp \propto T^0, \]

i.e,

\[ \rho_\parallel \propto T, \quad \text{and} \quad \rho_\perp \propto T^0. \]

Next we discuss the effect of impurity scattering on \( \sigma_\parallel \). For simplicity we first assume that the self-energy \( \text{Im}\Sigma_c(k, E_k) \) and \( \text{Im}\Sigma_f(k, E_k) \) are independent of \( E_k \) and proportional to the impurity concentration \( n_{\text{imp}} \). In this case, by using eq.(3.8b), we obtain

\[ \sigma_{\parallel}^{\text{imp}} \propto T^2/n_{\text{imp}}, \quad \text{i.e.} \quad \rho_{\parallel}^{\text{imp}} \propto n_{\text{imp}} T^{-2}. \]

However, if the small dispersion of \( f \)-electrons due to a possible weak \( k \)-dependence of the \( f \)-electron self energy, \( \Sigma_f(k, 0) \), the current can be carried also by \( f \)-electrons, so that

\[ \sigma_\parallel \propto \int dE_k \int d\Omega_k \frac{1}{E_k^2} \frac{\tilde{V}_f^4(k)}{(-z_k \text{Im}\Sigma_f(k, E_k)) \tilde{V}_f^2(k) + (\text{Im}\Sigma_c(k, E_k) E_k^2)} \left( -\frac{\partial f(E_k)}{\partial E_k} \right), \]

\[ \propto \frac{1}{n_{\text{imp}}}. \]

Thus the singularity of the resistivity (3.13) at \( T = 0 \) is suppressed. Nevertheless, the residual resistivity in the limit \( T \to 0 \) increases drastically as increasing the impurity concentration \( n_{\text{imp}} \). If we take all the contributions of the quasiparticles into consideration, including the logarithmic corrections, the resistivity is given by

\[ \rho_\parallel = \rho_0 \left( n_{\text{imp}} + (T/T_K)^3 \right)^{-1} c_1 + \frac{T/T_K}{\log(c_2 T_K/T) + (T/T_K)^2 \log(c_3 T_K/T)} n_{\text{imp}}^{-1}, \]

where \( c_1(\sim 0.1), c_2(\sim 10) \) and \( c_3(\sim 5) \) are fitting parameters, which are connected with the small dispersion of \( f \)-electrons, the interaction between conduction electrons and impurity scattering of conduction electrons with the Born approximation, respectively. \( n_{\text{imp}} \rho_0/c_1 \) is the resistivity at
The resistivity for proper parameters are shown in Fig. 13. These results are in qualitative agreement with the experimental data. In particular, the temperature dependence of $\rho_{\parallel}(\rho_a)$ observed in the best sample to date is well reproduced as seen in Fig. 13. It is also found that the resistivity is sensitive to the concentration of impurities at low temperature in consistent with the experiments.

It should be remarked here that the weak $\mathbf{k}$-dependence of $\Sigma_f(\mathbf{k},0)$ inevitably gives rise to a small semimetallic Fermi surface around X-point (intersection of $a$-axis and the zone boundary) in general, so long as the hybridization vanishes along the $a$-axis as eq.(2.10b). However, such a small Fermi surface is expected to give only little effect on the qualitative behavior of DOS of quasiparticles discussed in previous sections, while it sensitively affects the low temperature behavior of the resistivity especially in the case where the impurity scattering greatly enhances the resistivity as in eq. (3.12) when there exists no $\mathbf{k}$-dependence of $\Sigma_f(\mathbf{k},0)$. In deriving (3.14), we have taken into account the dispersion of $f$-electron through the $\mathbf{k}$-dependence of $\Sigma_f(\mathbf{k},0)$, nevertheless we have used the same DOS as eq.(2.22). In this sense, the calculation is not self-consistent and the resistivity (3.14) should be regarded as a provisional one. However, the expression (3.14) gives a good description for $T \sim \Delta_1/2$, or a good starting point at least.

We should have a few words about $\rho_{\perp}$. The resistivity $\rho_b$ and $\rho_c$ of the same sample as shown in Fig. 13 exhibits a dip at $T \sim 3K$ and saturate at $T \to 0$. This may be understood as follows. Since quasiparticles around $\hat{k}_z = 0$ with excitation energy ($\sim \Delta_1/2$) have large dispersion along $x$- or $y$-direction, those are expected to contribute considerably to the conduction perpendicular to $z(a)$-axis at $T \sim \Delta_1/2$, leading to the suppression of $\rho_{\perp}$ ($\rho_b$ and $\rho_c$). If we use $\Delta_1/2 \approx 7K$ estimated above by means of $1/T_1$’s result, such suppression or dip is expected to occur at $T \leq 7K$ in consistent with the above observation.

Now we briefly discuss about the longitudinal magnetoresistance (MR). The change from the positive MR to the negative MR is observed with increasing magnetic field. The negative MR at higher field region may be caused by the suppression of spin fluctuations by magnetic field such as in the impurity Kondo effect. However, the case of the positive MR at low field is more complicated. We have calculated magnetic-field dependence of the lifetime $\tau_k$ of quasiparticles and verified that $\tau_k$ is a decreasing function of the magnetic field in the low-field region. Although DOS at low energies increases with the magnetic field due to the Zeeman splitting of DOS, shown in Fig. 2, the weight of conduction electrons of those states decreases in general leading to the enhancement of the resistivity. Therefore, MR is determined on such a delicate balance between the effects on the lifetime of the quasiparticles and the details of DOS at the Fermi level. The experimental data can be understood as follows: MR at lower fields is positive by shortening of the lifetime and at higher fields becomes negative due to the drastic increment of quasiparticles which can carry the current.
3.7 Pressure Dependence

Next we discuss the pressure dependence on the property of quasiparticles. As the lattice constant becomes short under the pressure, both the band-width $D$ of conduction electrons and the hybridization $V$ are enlarged. However, the fundamental energy scale $V^2/D$ is expected to be an increasing function of the pressure because $V$ is much more sensitive than $D$ for heavy fermions where $V$ arises through rather small overlap between $f$- and conduction electrons. Much more pronounced effect of pressure on the hybridization gap (2.17) arises through enlargement of the renormalization amplitude $z_k$. This is because $z_k$ is an exponentially small quantity as (2.18) for heavy fermions so that its relative change under pressure is far larger than that for $V$ and $D$ themselves. Therefore, the energy scale of the gap is expected to increase by applying the pressure, and so is the resistivity in eq.(3.14), which is scaled by $T_K$.

This tendency is consistent with the behavior of CeNiSn and CeRhSb where the peak of the resistivity shifts to the high temperature by the pressure\cite{33,41}. And also the suppression of those resistivity with the pressure in the limit $T \to 0$ can be understood as follows. As discussed in §3.6, there exists a very tiny semimetallic Fermi surface at around $k = (0,0,\pm 1)$ in general, so long as $\Sigma_f(k,0)$ has the dispersion along the $a$-axis no matter how small it is. After the Fermi surface grows further under the pressure due to the growth of the dispersion of $\Sigma_f(k,0)$, an apparent semimetallic behavior is expected to prevail leading to the suppression of the resistivity. That is to say, a parameter $c_1$, which corresponds to $\partial \Sigma_f(k,0)/\partial k$, increases with the pressure in the formula (3.14), so that the resistivity in the limit $T \to 0$, $n_{\text{imp}}\rho_0/c_1$, is suppressed.

3.8 Lifetime of Quasiparticles

We have neglected an effect of quasiparticle damping due to inelastic scattering so far. Here we briefly discuss its effect on DOS of quasiparticles and temperature dependence of physical quantities.

According to eq. (3.9a), the lifetime of quasiparticles around $k_z = \pm 1$ is nearly proportional to $(E_k^2 + \tilde{V}_f^2(k))/\tilde{V}_f^2(k)E_k^3$ at low energy region $E_k < \Delta_1$. This lifetime is longer than in the case of the normal Fermi liquid theory for $E_k < \Delta_1$. This is because the scattering between quasiparticles is suppressed at low energy, owing to the restriction of phase space satisfying the energy-momentum conservation law. Namely, the quasiparticles with low energy are located around $(0,0,\pm 1)$, so that such phase space is restricted within narrow region around $(0,0,\pm 1)$. These quasiparticles make the flat part near the Fermi level at DOS of Fig. 2.

The quasiparticle, corresponding to the peak structure at $\omega = \Delta_1/2$ in DOS of Fig. 2, are located along $k_z = 0$. These quasiparticles also suffers little inelastic scatterings, again because of the restriction due to the energy-momentum conservation law. Thus these lifetime is very long, leading to $\text{Im}\Sigma_f(k_z \sim 0, E_k) \sim 0$. So it is expected that the peak structure at $\omega = \Delta_1/2$ in DOS remains even if the effect of inelastic scattering is taken into account.

On the contrary, we have no reason to keep the sharp peak structure at $\omega = \Delta_2/2$ in DOS,
because the restriction due to the energy-momentum conservation does not suppress the inelastic scattering of quasiparticles forming this peak. So the structure at $\omega = \Delta_2/2$ probably becomes a broad hump.

However, we believe that the two peak structure in DOS of Fig. 2 remains even though the effect of inelastic scattering is taken into account. Indeed, the DOS calculated by the second order perturbation theory exhibits two peak structure similar to those of Fig. 2, although the peak at $\omega = \Delta_2/2$ is somewhat broadened. This result will be discussed elsewhere.

Furthermore, $T > \Delta_1$ is the temperature region where the damping effect of the quasiparticles affects temperature dependence of physical quantities. For $T > \Delta_1$, these peak structures of DOS fade out, while the physical quantities are averaged by temperature dependence of the Fermi distribution. Therefore, the neglect of the damping effect may give rise to no serious errors as far as the qualitative temperature dependence is concerned.

§4. Summary and Discussions

On the basis of the idea of “adiabatic continuity”, a theory of the anisotropic semiconductor of heavy fermions has been developed to explain the anomalous properties of CeNiSn and its isostructural compounds. A difference from the conventional semiconductors is that the band gap is formed by the highly renormalized quasiparticles near the Fermi level. So the gap has meaning only at low temperature region $T < \Delta_1$ (corresponding to the hybridization gap), while the coherent peak of quasiparticles fades out exhibiting the behaviors of the Kondo lattice metals.

Wide range of anomalies of CeNiSn can be understood by a model of the anisotropic hybridization gap which vanishes along the a-axis. The anisotropy of the gap reflects a $k$-dependence of hybridization matrix elements between the conduction electrons and the $f$-electron with particular symmetry of the crystal field state. The desirable $k$-dependence occurs if the lowest crystal field state consists mainly of $|5/2, \pm 3/2\rangle$ due to its approximately trigonal symmetry and the conduction electrons near the Fermi level are described by the plane waves, as discussed in §2.1 and §2.2.

Since there is no band calculation of LaNiSn available to date, it is difficult to assess whether the latter condition is fulfilled in CeNiSn. However, it may be not unrealistic to assume that the state of conduction electrons hybridizing with the $f$-electron localized at Ce site can be approximated by the plane waves with the wave vector $|k+G| < several \times (2\pi/a)$, $G$ being some reciprocal lattice vector and $a$ being the lattice constant. This is because the only way for the $f$-electron to mix with electrons on different sites is through the mixing with the plane wave states outside the muffin-tin spheres so long as the conventional LAPW calculation is performed.

Band calculations of CeNiSn shows that the bands around the Fermi level have mainly Ce 4$f$ character with mixture of Ni 3$d$ component. So, in the tight-binding picture, the hybridization is expected to arise through the overlap of Ce 4$f$ wavefunction and tails of Ni 3$d$ wavefunction. It is seen by a simple calculation of the tight-binding model that the hybridization between $f$-electron
in the state $|5/2, \pm 3/2 \rangle$ and $d$-electrons on the surrounding ions with trigonal symmetry vanishes on the $k_z$ axis, i.e., $V(0, 0, k_z) = 0$.

In order to obtain more solid picture of the $k$-dependence of the hybridization, we need more information of the band structure of LaNiSn. It is also interesting to discuss a difference between CeNiSn and the so-called “Kondo insulator”, such as Ce$_3$Bi$_4$Pt$_3$\cite{1} and YbB$_{12}$\cite{12}, with non-vanishing gap in any directions of the Brillouin zone. From the present point of view, its difference is attributed to that of the $k$-dependence reflecting the symmetry of the lowest crystal-field level. We leave such discussions for future studies.

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[1] See, for example, *Valence Fluctuations in Solids*, ed. L. M. Falicov, W. Hanke and B. P. Maple (Nroth - Holland, Amsterdam, 1981)
[2] See also, *Transport and Thermal Properties of f-Electron Systems*, ed. G. Oomi, H. Fujii and T. Fujita (Plenum, New York, 1993)
[3] R. M. Martin and J. W. Allen: p. 85 in ref. \[1\] and references therein; P. S. Riseborough: Phys. Rev. B 45 (1992) 13984.
[4] T. Kasuya: J. Phys. Soc. Jpn. 61 (1992) 1863; J. Phys. Soc. Jpn. 63 (1994) 2037; J. Phys. C, to be published.
[5] K. Tsutsui, Y. Ohta, R. Eder, S. Maekawa, E. Dagotto and J. Riera: preprint cond-mat /9511055.
[6] P. W. Anderson: *Basic Notions of Condensed Matter Physics*, (Benjamin, New York, 1984) Chap. 4.
[7] L. D. Landau: Sov. Phys. JETP 3 (1957) 920; Sov. Phys. JETP 5 (1957) 101; Sov. Phys. JETP 8 (1959) 70.
[8] K. Yamada: Prog. Theor. Phys. 53 (1975) 970; K. Yosida and K. Yamada: Prog. Theor. Phys. 53 (1975) 1286.
[9] T. M. Rice and K. Ueda: Phys. Rev. Lett. 55 (1985) 995.
[10] H. Shiba: J. Phys. Soc. Jpn. 55 (1986) 2765.
[11] O. Sakai: private communications.
[12] T. Mutou and D. S. Hirashima: J. Phys. Soc. Jpn. 63 (1994) 4475.
[13] T. Saso and M. Itoh: preprint.
[14] T. Nishino and K. Ueda: Phys. Rev. B 47 (1993) 12451.
[15] T. Takabatake et al.: Jpn. J. Appl. Phys. 26 Suppl. 26-3 (1987) 547; Phys. Rev. B 41 (1990) 9607; Phys. Rev. B 45 (1992) 5740.
[16] S. K. Malik and D. T. Adroja: Phys. Rev. B 43 (1991) 6277.
[17] Recently, CeRhAs and CeRhBi have been synthesized by S. Yoshii, M. Kasaya, H. Takahashi and N. Mori, Proc. SCES '95, to be published in Physica B.
[18] M. Kyogaku, Y. Kitaoka, H. Nakamura, K. Asayama, T. Takabatake, F. Teshima and H. Fujii: J. Phys. Soc. Jpn. 59 (1990) 1728, Physica B 171 (1991) 235.
[19] K. Nakamura, Y. Kitaoka, K. Asayama, T. Takabatake, G. Nakamoto, H. Tanaka and H. Fujii: Physica B 206-207 (1995) 829; Phys. Rev. B, to be published.
[20] T. Ohama, H. Yasuoka and Y. Isikawa: J. Phys. Soc. Jpn. 64 (1995) No.12.
[21] T. Takabatake, G. Nakamoto, T. Yoshino, H. Fujii, K. Izawa, S. Nishigori, H. Goshima, T. Suzuki, T. Fujita, K. Maezawa, T. Hiraoka, Y. Okayama, I. Oguro, A. A. Menovsky, K. Neumaier, A. Brückl and K. Andres: Physica B, to be published.
[22] G. Nakamoto, T. Takabatake, H. Fujii, A. Minami, K. Maezawa, I. Oguro and A. A. Menovsky: J. Phys. Soc. Jpn., to be published.
[23] S. Nishigori, T. Suzuki, T. Fujita, H. Tanaka, T. Takabatake and H. Fujii: Physica B 199-200 (1994) 473; S. Nishigori: private communications.
[24] H. Suderow and J. Flouquet: private communications.
[25] T. E. Mason, G. Aeppli, A. P. Ramirez, K. N. Clausen, C. Broholm, N. Stücheli, E. Bucher and T. T. M. Palstra: Phys. Rev. Lett. 69 (1992) 490.
[26] H. Kadowaki, T. Sato, H. Yoshizawa, T. Ekino, T. Takabatake, H. Fujii, L. P. Regnault and Y. Isikawa: J. Phys. Soc. Jpn. 63 (1994) 2074; T. J. Sato, H. Kadowaki, H. Yoshizawa, T. Ekino, T. Takabatake, H. Fujii, L. P. Regnault and Y. Isikawa: J. Phys. C 7 (1995) 8009.
[27] S. Kambe, S. Raymond, H. Suderow, J. McDonough, B. Fak, L. P. Regnault, J. Flouquet: preprint.
[28] K. Yamada and K. Yosida: Prog. Theor. Phys. 76 (1986) 621.
[29] Y. Kagan, K. A. Kikoin and N. V. Prokof'ev: JETP Lett. 57 (1993) 600.
[30] K. Yamada, K. Yosida and K. Hanzawa: Prog. Theor. Phys. 108 (1992) 141.
[31] K. Hanzawa, K. Yamada and K. Yosida: J. Phys. Soc. Jpn. 56 (1987) 678.
[32] In Nd$_{0.3}$La$_{0.7}$NiSn, which is isostructural to CeNiSn, the local symmetry of Nd$^{3+}$ was identified with $D_{3d}$ from an analysis of the crystal field level by means of neutron scattering. See, P. A. Alekseev, E. S. Klement'ev, V. N. Lazukov, E. V. Nefedova, I. P. Sadikov, M. N. Khlopkina, A. Yu. Muzychka, I. L. Sashin, N. N. Efremova and W. Bührer: Sov. Phys. JETP 79 (1994) 665.
[33] It is suggested that the crystal-field ground state is $|5/2, \pm 3/2\rangle$ from some experimental data: The analysis of the magnetic anisotropy measured by the polarized neutron scattering shows that the ground state is $|5/2, \pm 3/2\rangle$ or mostly $|5/2, \pm 5/2\rangle$ with negligibly small admixture of $|5/2, \pm 1/2\rangle$ (ref. 26); and the ultrasonic measurement in CePtSn, which has the same crystal structure as CeNiSn, by T. Suzuki, H. Fujisaki, T. Fujita, G. Nakamoto, T. Takabatake, H. Fujii and A. Tamaki: J. Magn. Magn. Mater. 140-144 (1995) 1215, shows that the ground state is predominantly $|5/2, \pm 3/2\rangle$.
[34] This relation was reported without derivation by G. Kotliar, E. Abrahams, A. E. Ruckenstein, C. M. Varma, P. B. Littlewood and S. Schmitt-Rink: Europhys. Lett. 15 (1991) 655.
[35] P. Schlottmann: J. Appl. Phys. 75 (1994) 7044.
[36] R. Shiina: J. Phys. Soc. Jpn. 64 (1995) 702.
[37] S. Schmitt-Rink, K. Miyake and C. M. Varma: Phys. Rev. Lett. 57 (1986) 2575.
[38] P. Hirschfeld, D. Vollhardt and P. Wölfle: Solid State Commun. 59 (1986) 111.
[39] T. Takabatake, M. Nagasawa, H. Fujii, G. Kido, K. Sugiyama, K. Senda, K. Kindo and M. Date: Physica B 177 (1992) 177; K. Sugiyama, T. Inoue, K. Oda, T. Takabatake, H. Tanaka, H. Fujii, K. Kindo and M. Date: Physica B 211 (1995) 223; K. Sugiyama: private communications.
[40] M. Kurisu, T. Takabatake and H. Fujiwara: J. Phys. Soc. Jpn. 59 (1990) 595.
[41] Y. Uwatoko, G. Oomi, S. K. Malik, T. Takabatake and H. Fujii: Physica B 199-200 (1994) 572.
[42] T. Ekino, T. Takabatake, H. Tanaka and H. Fujii: Physica B 206-207 (1995) 837.
[43] A. Yanase and H. Harima: Prog. Theor. Phys. Suppl. 108 (1992) 19.
[44] T. J. Hammond, G. A. Gehring, and M. B. Suvatsini: Phys. Rev. B 51 (1995) 2994.
[45] J. D. Thompson, W. P. Beyermann, P. C. Canfield, Z. Fisk, M. F. Hundley, G. H. Kwei, R. S. Kwok, A. Lacerda, J. M. Lawrence, and A. Severing: p. 35 in ref. 2.
[46] M. Kasaya: p. 27 in ref. 2.
Fig. 1  The diagram for the many-body vertex correction of impurity scattering. The broken line represents the impurity potential $u$ of $s$-wave, the external solid line the Green function of the $f$-electrons, and internal solid line stands both $f$-electrons and conduction electrons. $\Gamma$ is the full vertex due to the Coulomb repulsion between $f$-electrons. $\tilde{u}$ is a renormalized potential of impurity scattering.

Fig. 2  The density of states, $\tilde{N}(\omega)$, of the quasiparticles as a function of $\omega$ in the unit $D$, half the band-width of conduction band. The Fermi level is located at $\omega = 0$.

Fig. 3  The effect of the impurity scattering on the density of states.

Fig. 4  The density of states at the Fermi level as a function of the impurity concentration.

Fig. 5  The temperature dependence of the specific heat coefficient $\gamma$. The unit of the temperature is $D$, half the band-width of conduction electrons. Circles are experimental data ($C_m/T$) of ref. 23. $\Delta_1/2 = 0.01D$ corresponds to 7K.

Fig. 6  The specific heat coefficient, $\gamma$, as a function of the magnetic field, $h$. The unit of $h$ is $D$, half the band-width of conduction electrons.

Fig. 7  The longitudinal NMR relaxation rate, $1/T_1$ (in arbitrary unit), as a function of the temperature $T$ in the unit $D$, half the band-width of conduction electrons. Triangles and crosses are experimental data of ref. 3. $\Delta_1 = 0.02D$ corresponds to 14K.

Fig. 8  The magnetization, $M$ (in the unit $g\mu_B|J_z|$), as a function of the magnetic field $h$ (in the unit $D$) at $T = 0$.

Fig. 9  $T$-dependence of the uniform susceptibility, $\text{Re}\chi(0, 0)$ in the unit $(g\mu_B|J_z|)^2/D$. The unit of $T$ is $D$, half the band-width of conduction electrons.

Fig. 10  The spectral weight of spin fluctuations, $\text{Im}\chi(Q, \omega)$ (in arbitrary unit), as a function of $\omega$ at $T = 0$ for (a) $Q = (1/2, 0, 0) = [0, 1/2, 0]$ and (b) $Q = (0, 0, 1/2) = [1/2, 0, 0]$. $\text{Im}\chi(Q, 0)$ is finite in (b) due to a choice of non-dispersive $f$-level.

Fig. 11  The intensity of $\text{Im}\chi(Q, \omega = \Delta_2)$ in arbitrary unit as a function of $Q_x$ ($Q_y$) of $Q = (Q_x, 0, 0) = [0, Q_y, 0]$ at $T = 0$.

Fig. 12  The energy dependence of the self-energies, (a) $\text{Im}\Sigma_c(k, E_k)$ and (b) $\text{Im}\Sigma_f(k, E_k)$ at zero temperature. The straight line in (a) and (b) shows $E_k^5$ and $E_k^3$ dependence, respectively. The unit of $E_k$ is $D$, half the band-width of conduction electrons.

Fig. 13  The resistivity $\rho_{\parallel}$ as a function of the temperature $T$, in the unit $D$, half the band-width of conduction electrons. The parameters in eq.(3.14) are chosen as $\rho_0 = 400$, $c_1 = 0.1$, $c_2 = 10$ and $c_3 = 5$. Closed circles show the temperature dependence of $\rho_{\alpha}$ of the best sample of CeNiSn$^{21, 22}$.
\[ \sum \omega = u + (1 - \frac{\partial \Sigma}{\partial \omega}) \cdot u = \tilde{u} \]
\[ \tilde{N}(\omega) \]

\[ \frac{\Delta_2}{\Delta_1} \approx \frac{64}{15} \approx 4.2 \]
$\gamma$ (J/K^2 mol)

$T$

- $n_{\text{imp}} = 0.00$
- $n_{\text{imp}} = 0.01$
- $n_{\text{imp}} = 0.10$

CeNiSn (Exp.)
\gamma (\text{J/K}^2\text{mol})

- \(T=0.001\)
- \(T=0.003\)
- \(T=0.005\)
- \(T=0.007\)

\(h\)
\[ \frac{1}{T_1} \propto T^3 \]

CeNiSn (Exp.)

CeNi\textsubscript{1.01}Sn (Exp.)

- \( n_{\text{imp}} = 0.00 \)
- \( n_{\text{imp}} = 0.01 \)
- \( n_{\text{imp}} = 0.10 \)
$\Re \chi(0,0)$ vs $T$ for different values of $n_{\text{imp}}$: $n_{\text{imp}} = 0.00$, $n_{\text{imp}} = 0.01$, $n_{\text{imp}} = 0.10$. The graphs show the real part of the susceptibility $\chi(0,0)$ as a function of temperature $T$. The curves illustrate how the susceptibility changes with increasing temperature for different impurity concentrations.
\( \chi(\mathbf{Q}, \omega) \)
\[ \text{Im} \chi(Q, \omega) \]

\[ Q_x (Q_b) \]
\[ \text{Im} \Sigma_c(k, E_k) \sim E_k^5 \]

\[ \text{Im} \Sigma_f(k, E_k) \sim E_k^3 \]

(a) \[ \text{Log-log plot showing } \text{Im} \Sigma_c(k, E_k) \text{ vs. } E_k \]

(b) \[ \text{Log-log plot showing } \text{Im} \Sigma_f(k, E_k) \text{ vs. } E_k \]
