Impurity Effects in Strongly Correlated Metals: Large Pressure Dependence of Residual Resistivity of Heavy Fermions

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It is shown on the basis of the Fermi liquid theory that the s-wave scattering potential due to nonmagnetic impurity is strongly enhanced by the mass enhancement factor \(1/z\). As a result the impurity potential with moderate strength, of the order of the bandwidth of conduction electrons, gives scattering in the unitarity limit in strongly correlated metals as heavy fermions. This effect is embodied by large pressure dependence of residual resistivities in heavy fermion systems, since the pressure decreases the degree of correlations, which makes the Kondo temperature increase rapidly. This accounts for the large pressure dependence of the residual resistivity observed in heavy fermion metals, such as CeInCu\(_2\), CeCu\(_6\), CeAl\(_3\).

KEYWORDS: Impurity scattering in Fermi liquid, Ward identity, Periodic Anderson model, unitarity limit, strongly correlated system, pressure dependence of residual resistivity

A bunch of careful experiments under pressure for heavy fermion metals have been carried out recently. Especially, the systematic variations of resistivity in the normal state have been investigated in detail. It is reported for instance that the temperature \(T_{\text{max}}\), which corresponds to the maximum of resistivity and is regarded as being proportional to the Kondo temperature \(T_K\), tends to increase rapidly with increasing pressure. This fact can be understood, on the basis of a periodic Anderson model, in such a way that the increase of hybridization under pressure causes rapid increase of the renormalization factor \(z\) which is proportional to \(T_K\).

Futhermore, the residual resistivity in many heavy fermion metals is reported to decrease drastically under pressure. This decrease is too large to be explained by only an effect of variation of the density of states due to that of hybridization. On the other hand, it has been believed that the renormalization effect associated with large mass enhancement cancels out leaving the residual resistivity unchanged. So, such large pressure dependence may be attributed to the effect that the impurity potential itself is drastically renormalized due to the many-body effect. The purpose of this paper is to show, on the basis of the Fermi liquid theory, that this is the case.

The results are summarized as follows: 1) It is derived on the basis of the Ward identity argument that the s-wave scattering potential due to nonmagnetic impurity is strongly enhanced by the mass enhancement factor \(1/z\). This is one of the characteristic phenomena specific to strongly correlated systems. 2) The impurity potential with moderate strength gives scattering in the unitarity limit in strongly correlated metals as heavy fermions. 3) This can account for the large pressure dependence of the residual resistivity observed in heavy fermion metals, such as CeCuIn, CeCu\(_6\), CeAl\(_3\), since the degree of correlations is decreased by applying the pressure making the Kondo temperature increase rapidly.

Hereafter we discuss, on the basis of the Fermi liquid theory, the interplay between many-body effect and s-wave impurity scattering without the so-called quantum corrections. Namely, for the vertex correction, we take into account all the orders of perturbation in short-ranged repulsive interaction but only the non-crossing terms in the s-wave impurity scattering. Such a treatment may be valid for the Fermi liquid which is suffered from scattering of impurities with dilute enough concentration. In other words, we assume that these impurities do not break down the framework of Fermi liquid itself but give a quasiparticle near the Fermi level a finite life time. At first, we discuss the system consisting of single component of fermion, and then the periodic Anderson model later.

To begin with, we discuss how the structure of vertex correction of particle-hole channel is modified by the presence of impurity scattering. The coherent part of the Green function, which governs physical properties at low temperatures, is given as

\[
G(p, \varepsilon) = z / [\omega - v(|p| - p_F) - i \gamma_p \text{sign}(|p| - p_F) - i \frac{\text{sign}(|\varepsilon|)}{2\tau}],
\]

where \(z\) is the renormalization amplitude, and \(\gamma_p\) and \(1/\tau\) are the damping rate of quasiparticle due to the inelastic scattering by the repulsive interaction and the elastic one by the impurity potential. It should be understood that (0.1) is obtained after the average over configurations of impurities have been taken. The expression (0.1) smoothly connects with that of the Fermi liquid theory in the limit \(1/\tau \propto n_{\text{imp}} \rightarrow 0\), \(n_{\text{imp}}\) being the impurity concentration. The damping rate of quasiparticle with low energy is determined predominantly by \(1/\tau\) which is finite even in the low-energy limit.

Then, we consider the asymptotic properties of the vertex function in the particle-hole channel, \(\Gamma(p_1, p_2; p_1 + p_2)\):
$k, p_2 - k \equiv \Gamma(p_1, p_2; k)$, in the limit $k = (\mathbf{k}, \omega) \to 0$, which plays an important role in the Fermi liquid theory. As in the pure limit, $\Gamma$ satisfies the following equation:

$$\Gamma(p_1, p_2; k) = \Gamma^{(1)}(p_1, p_2) - i \int \Gamma^{(1)}(p_1, p) \varphi(p) \Gamma(p, p_2; k) \frac{d^4 p}{(2\pi)^4}, \quad (0.2)$$

where $\Gamma^{(1)}$ denotes the irreducible vertex part with respect to particle-hole lines. We have set $k = 0$ in $\Gamma^{(1)}$, since it has no singularities at $k = 0$. In the pure limit, the singular contribution arises from the “anomalous” part of particle-hole pair, $G^R G^A$, in the integral in (0.2). Other combinations, $G^R G^R$ and $G^A G^A$, gives regular contributions. Thus, if $\tau$ is long enough, an explicit form of the pair $G(p) G(p + k)$ in the neighborhood of $|p| = p_F, \varepsilon = 0$ can be written as

$$G(p) G(p + k) = A \delta(\varepsilon) \delta(|p| - p_F) + \varphi(p), \quad (0.3)$$

where $\varphi(p)$ represents the regular part in which we have set $k = 0$ in $\varphi(p)$.

The coefficient $A$ can be determined by integrating $G(p) G(p + k)$ with respect to $\varepsilon$ and $|p|$, and is found to be

$$A = \frac{2\pi i z^2}{v} \frac{\omega}{\omega - v \cdot k + i \text{sign}(\omega)/\tau}, \quad (0.4)$$

where $v$ is the velocity of quasiparticle with momentum $p$. Important differences from the Fermi liquid in the pure limit are that there exists the finite life time $\tau$ due to impurity scattering and the numerator is proportional to $\omega$. Namely, the coefficient $A$, (0.4), vanishes for both limits, $k$-limit and $\omega$-limit, in contrast with the case of the Fermi liquid where $A = (2\pi i z^2 v) \times v \cdot k / (\omega - v \cdot k)$ remains finite in the $k$-limit while it vanishes in the $\omega$-limit.

Thus, under the existence of impurities, the vertex $\Gamma \equiv \Gamma^{\omega} = \Gamma^{k}$ in the neighborhood of $|p| = p_F, \varepsilon_i = 0$ satisfies the following integral equation

$$\Gamma(p_1, p_2) = \Gamma^{(1)}(p_1, p_2) - i \int \Gamma^{(1)}(p_1, p) \varphi(p) \Gamma(p, p_2; k) \frac{d^4 p}{(2\pi)^4}, \quad (0.5)$$

which is the same as that for $\Gamma^{\omega}$ in the pure limit. Among the diagrams of $\Gamma^{(1)}$, those representing the pure impurity scattering may be neglected, because they give small quantum corrections, of $O(p_F \ell)$, without order diagrams. As we discussed above, diagrams of Fig. 1(a), (d), (e) and (f) give negligible contributions of $O(p_F \ell)$. Diagrams of Fig. 1(g) and (h) give also a small correction to $\Gamma^{(1)}$ of $O(p_F \ell)$. Thus, the vertex correction arises predominantly from the diagram of the type Fig. 1(b) and (c), and its higher order terms. It is seen easily in these diagrams that the scattering component with the higher angular momentum, such as $p_-$, $d$-wave etc., emerge from the many-body effect due to the repulsive interaction among electrons, even if the bare impurity potential $u$ has only the s-wave component. Nevertheless, the most important scattering process is expected to arise through the s-wave channel, because the partial-wave phase shifts satisfy the Friedel sum rule and the phase shift with higher partial wave gives less contribution in gerneral for local perturbation. Since the scattering probability of s-wave does not depend on the momentum transfer, it is estimated by that of the forward scattering process.

Then, we can estimate the vertex correction for s-wave impurity scattering with the use of the Ward-Takahashi identity

$$\Sigma(p + k) - \Sigma(p - k) = \int \{ G(q + k) - G(q - k) \} \times \Gamma^{(1)}(q - k, p; k, q + k) d^4 q / (2\pi)^4, \quad (0.6)$$

and the relation (0.5): The renormalized s-wave scattering potential $\tilde{u}$ is given by

$$\tilde{u} = \left[ 1 + \Gamma(p, p) \right] u = \left( 1 - \frac{\partial \Sigma(p)}{\partial \omega} \right) u \quad (0.7)$$

This renormalization is represented by the Feynman diagrams as in Fig. 2. The self-energy $\Sigma(p)$ in (0.7) includes the effect of impurity scattering. However, its effect may be small for the case with small impurity concentrations where the quantum corrections, of $O(p_F \ell)$, can be neglected. Thus eq. (0.7) is approximated by

$$\tilde{u} = \frac{1}{\varepsilon} u, \quad (0.8)$$

where $\varepsilon$ is the renormalization factor for the Fermi liquid. The relation (0.8) has been given by Kotliar et al without detailed derivation, and its derivation has been given very briefly by the present authors in the theory of anisotropic semiconductors or semimetals of heavy fermions. The relation (0.8) can be interpreted in such a way that the quasi-particles feel the bare potential $u$, because the potential which the quasiparticle fell is multiplied by $\varepsilon$, the weight of quasiparticle in the bare single-electron state.

In strongly correlated system, such as heavy fermions, $\varepsilon$ is far less than 1 and inversely proportional to the mass enhancement. Therefore, the renormalized impurity potential $\tilde{u}$ can become very strong leading to the scattering in the unitarity limit, even if the bare potential $u$ is moderate one.
Next, we proceed to calculate the life time $\tau$. The self-energy $\Sigma_{\text{imp}}(p)$ due to the renormalized $s$-wave scattering potential above is given in the $t$-matrix approximation by

$$\Sigma_{\text{imp}}(\omega) = n_{\text{imp}} \frac{\tilde{u}}{1 - \tilde{u} \sum_k G(k; \omega)}. \quad (0.9)$$

The life time $\tau$ is related with $\text{Im} \Sigma_{\text{imp}}(\omega)$ as $1/2\tau = -z \times \text{Im} \Sigma_{\text{imp}}(\omega)$. So, in order to determine $\tau$, eqs. (0.1) and (0.9) need to be solved self-consistently, in general, as in the case of heavy fermion superconductors and anisotropic Kondo insulators. However, in the case where $N(\omega)$, the density of states of quasiparticles in the pure limit, does not vanish for $\omega = 0$, the summation over $k$ in (0.9) is approximately given as

$$\sum_k G(k; \omega) \simeq -i\pi z N(\omega), \quad (0.10)$$

where the particle-hole symmetry is assumed for quasiparticle dispersion. Thus, the life time $\tau$ is given by

$$\frac{1}{\tau} = \frac{2\pi \tilde{u}^2 z N(\omega)n_{\text{imp}}}{1 + (\pi \tilde{u} z N(\omega))^2}. \quad (0.11)$$

Here, we should note that in the unitarity limit, $\tilde{u} z N(\omega) \gg 1$, $1/\tau \simeq 2/\pi N(\omega)$ does not depend on the impurity potential at all.

Now, to discuss the residual resistivity of Ce-based heavy fermions, let us consider the periodic Anderson model with a small amount of impurities. Here the bare impurity potential for conduction electron is different from that for $f$-electron in general. However, we neglect the difference for a moment. Repeating the above discussions, it is shown that the impurity potential for the $f$-electrons is enhanced by a factor $1/z_f \simeq 1 - \partial \Sigma_f(p)/\partial \omega$, while the one for conduction electron is not. Since the impurity potential for conduction electron is not renormalized and the quasiparticles near the Fermi level is composed almost from $f$-electrons, the effect of impurity scattering comes predominantly from impurity potential acting on the $f$-electron provided that the bare impurity potential is not very strong. This may justify to neglect the difference between impurity potential for conduction electron and $f$-electron.

Then the life time of the quasiparticle near the Fermi level is given by the expression similar to (0.11):

$$\frac{1}{\tau} = \frac{2z_f \pi \tilde{u}^2 z_f \langle A_f \rangle N(\omega)n_{\text{imp}}}{1 + (\pi \tilde{u} z_f \langle A_f \rangle N(\omega))^2}, \quad (0.12)$$

where $\langle A_f \rangle$, the average weight of $f$-electron contained in the quasiparticle state on the Fermi surface, is given as

$$A_f = \frac{1}{2} \left[ 1 - \frac{\xi_f - \xi_k}{\sqrt{(\xi_f - \xi_k)^2 + 4z_f |V_k|^2}} \right], \quad (0.13)$$

where the notations are standard ones.

In the strongly correlated limit, $\langle A_f \rangle \simeq 1$ as mentioned above.

The residual resistivity $\rho_0$ is given by the Drude formula as

$$\rho_0 = \frac{m^*}{ne^2} \langle A_f \rangle, \quad (0.14)$$

where $m^*$ is the effective mass of hybridization band enhanced by $1/z_f$. Substituting (0.13) into (0.14), the $z_f$-dependence of $\rho_0$ is given as follows:

$$\rho_0 \propto \frac{u^2 \langle A_f \rangle N(\omega)}{z_f^2 + (\pi u \langle A_f \rangle N(\omega))^2}. \quad (0.15)$$

where $N(\omega) = z_f N(\omega)$ is the density of states of hybridization band without the repulsive interaction. It is to be noted that $\rho_0$, (0.13), does not depend on the renormalization factor $z_f$ in the strongly correlation limit, $z_f \ll 1$. However, the $z_f$-dependence in eq. (0.15) can be observed if the value of $u z_f \langle A_f \rangle N(\omega)$ is varied from $\sim 1$ to $\gg 1$. Indeed, such variations can be realized by applying hydrostatic pressure, because the mass enhancement (∝ $1/z_f$) sensitively depends on the hybridization between $f$-electron and conduction electron in heavy fermions.

Applying the pressure to heavy fermion metals, such as CeInCu$_2$, CeCu$_6$, CeAl$_3$, the temperature $T_{\text{max}}$ at which the resistivity exhibits maximum increases rapidly. This is considered to be due to the rapid increase of $z_f$. Correlating with this, $\rho_0$ shows the rapid decrease which is too rapid to be explained by the change of band structure under pressure as observed in ordinary metals. For example, $\rho_0$ of CeInCu$_2$ decreases from 85 $\mu\Omega$cm at ambient pressure to 20 $\mu\Omega$cm at $P = 8$ GPa, while its $T_{\text{max}}$ increases from 27 K to 1000 K correspondingly.

This behavior is consistent with the one expected from eq. (0.15). Thus, the large pressure dependence of $\rho_0$ observed in heavy fermions reveals explicitly the way of mass enhancement in which the large frequency dependence of the self-energy plays a crucial role.

However, as $z \to 1$, the specific properties of compound, such as anisotropy of the density of states at the Fermi level and impurity potential with higher partial wave component beyond $s$-wave, should be taken into account.

In summary, we have discussed the effect of impurity scattering in strongly correlated metals on the basis of the Fermi liquid theory. We have found that the difference between $k$-limit and $\omega$-limit of the vertex in the particle-hole channel disappears due to the damping by the impurity scattering. In this case the $s$-wave scattering process is enhanced by a factor $1/z$ so that this renormalization process is very important in the strongly correlated systems where $z \ll 1$. And then, we have taken into account the effect of this renormalized impurity scattering through the $t$-matrix approximation. As a result, the residual resistivity $\rho_0$ shows a large dependence on $z$ as $z \to 1$. This is consistent with the large pressure dependence of $\rho_0$ observed in many heavy fermions.

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**Fig. 1** Diagrams for vertex corrections. The broken line represents the impurity potential \( u \) of \( s \)-wave component and the wavy line the Coulomb interaction. The solid line represents the bare Green function. \( \Gamma \) is the full vertex due to the Coulomb repulsion and impurity potential.

**Fig. 2** Vertex correction of impurity potential of \( s \)-wave channel.
\[ \Sigma = \mathbf{u} \mathbf{u} \mathbf{u} /c_1 \]