Duality in the Kondo model and perturbative approach to strong coupling theory

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We investigate the duality in the Kondo model. Starting from the s-d model with the coupling constant \( J \), the strong coupling model with the constant of \( 1/J \) is identified. The model shows the unitary limit of the conductance, \( G = 2e^2/h \) at zero temperature. The perturbation theory of the model gives qualitative agreement with the results of numerical renormalization group and Bethe ansatz near \( T = T_K \).

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Ever since Kondo elucidated the origin of logarithmic divergence of the resistivity in dilute alloy systems, various aspects of the Kondo effect have been investigated, including recent experimental realizations in quantum dot systems. When the temperature or a characteristic energy scale is larger than the Kondo temperature \( T_K \), the system is in the weak coupling regime while it is smaller, the system is in the strong coupling regime. In these regimes, the Kondo model exhibits duality. It was pointed out from the exact solution in Refs. \[12, 13\]. In particular, the resistivity has calculated beyond the Fermi liquid regime, from the point of view of the duality. The duality also plays an important role in quantum dissipative systems, which are closely related with quantum impurity problems. It is possible to approach perturbatively for a strong coupling regime using a similar way in a corresponding weak coupling regime.

We are presenting yet another duality for \( S = 1/2 \) Kondo model with the coupling constant \( J \). The motivation of this work comes from the following two points. The first one is a recent active interest on the Kondo screening cloud. At low temperatures, conduction electrons and the impurity form the Kondo singlet state, accompanying a screening cloud. The nature of the cloud is still under debate, and accordingly many works have been investigated to detect the cloud in nano structures. The second one is the notion of the strong coupling theory itself. The Fermi liquid theories of the Kondo effect have been developed and they successfully explain low temperature behavior of the Kondo effect. Although it is stated that strong coupling theories describe the low temperature regime, simple questions have not yet answered clearly: What is the action (Hamiltonian) with the coupling constant of \( 1/J \) if it exists?, and how does the perturbation with respect to \( 1/J \) work in the theory?

We will explain that the concept of the screening cloud naturally leads to a duality in the Kondo problem. We will identify the model which has a very large cloud starting from the conventional weak coupling s-d model and show it has the coupling constant of \( 1/J \). Electron transport of this model will be investigated, which shows the unitary limit of the conductance at zero temperature. A perturbative calculation with respect to \( 1/J \) with the poorman’s scaling is performed, giving good qualitative agreement with the results of numerical renormalization group (NRG) and Bethe ansatz around \( T = T_K \).

Weak coupling model.— We start from the s-d model. The action \( S = S_0 + S_1 \) is

\[
S_0 = \int d\omega \sum_{k,\sigma} \bar{\psi}_{\sigma}(\omega) (\omega - \epsilon_k) \psi_{\sigma}(\omega),
\]

\[
S_1 = J \int dt \left[ \bar{\psi}_1(t) \bar{\psi}_2(t) \right] M \left[ \psi_1(t) \psi_2(t) \right],
\]

where the action can be written only by the surface field operator \( \psi_{\sigma} = \sum_k \psi_{k\sigma} \), which is the conduction electron field at the impurity site \( (z = 0) \). For simplicity, we have disregarded the potential scattering term.

The two conduction electron fields, \( \psi_{\sigma} \) and \( \psi_{k\sigma} \) can be treated independently if we introduce a Lagrange multiplier \( \lambda_{\sigma} \) and add a constraint term to the action:

\[
\int dt \sum_{\sigma} \bar{\lambda}_{\sigma}(t) \left( \psi_{\sigma}(t) - \sum_k \psi_{k\sigma} \right) + \text{H.c.}
\]

The action can be written only by the surface field \( \psi_{\sigma} \) after integrating over \( \psi_{k\sigma} \) and \( \lambda_{\sigma} \):

\[
S = \sum_{\sigma} \int d\omega \bar{\psi}_{\sigma}(\omega) G^{-1}(\omega) \psi_{\sigma}(\omega) + S_1,
\]

where \( G(\omega) \) is the Green function of conduction electrons. At zero temperature, \( G(\omega) = i/2 (2\pi\nu \text{ sgn}(\omega)) \) with the density of states \( \nu \) in the lead and the sign function \( \text{sgn}(x) \). For finite temperature, it is convenient to introduce the Keldysh Green function (matrix)

\[
G(\omega) = \begin{pmatrix}
2\pi i \nu \left[ \frac{1}{2} + f(\omega) \right] & 2\pi i \nu f(\omega) \\
2\pi i \nu \left[ f(\omega) - 1 \right] & 2\pi i \nu \left[ \frac{1}{2} + f(\omega) \right]
\end{pmatrix}
\]
where the matrix is defined on the Keldysh space [(1,1) component of the matrix gives the time-ordered Green function, for example.]

**Strong coupling model.** — Now we show the duality of the Kondo model. Instead of integrating over \( \lambda_\sigma \), we integrate over \( \psi_\sigma \) and \( \psi_{i\sigma} \), and then the action is represented by \( \lambda_\sigma \) in the form:

\[
S = \int d\omega \lambda_\sigma(\omega) g^{-1}(\omega) \lambda_\sigma(\omega) + \frac{16}{3J} \int dt \left( \lambda_+ \cdot \lambda_- \right) M^{-1} \left( \lambda_+ \right)
\]

with

\[
M^{-1} = \left( \begin{array}{cc}
\frac{1}{2}S_+ + \frac{1}{4} & \frac{1}{2}S_- + \frac{1}{4} \\
\frac{1}{2}S_- - \frac{1}{4} & \frac{1}{2}S_+ - \frac{1}{4}
\end{array} \right)
\]

where we have used the identity of \((\hat{\sigma} \cdot \hat{S})(\hat{\sigma} \cdot \hat{S}) = S^2 + i\hat{\sigma} \cdot \hat{S} \times \hat{S}\), and \( \hat{S} \cdot \hat{S} = i\hat{S} \). The Green function \( g(\omega) \) is the inverse of \( G(\omega) \). For example, \( g(\omega) = -2i/(2\pi\nu) \operatorname{sgn}(\omega) \) for zero temperature, and the Keldysh Green function is

\[
g(\omega) = \left( \begin{array}{cc}
\frac{\nu}{2\pi} f(\omega) & \frac{\nu}{2\pi} f(\omega) \\
-\frac{\nu}{2\pi} f(\omega) & \frac{\nu}{2\pi} f(\omega)
\end{array} \right).
\]

Equation 7 looks quite similar to the weak coupling model; it includes the s-d interaction as in Eq. 2, with the coupling constant proportional to \( 1/J \) instead of \( J \). It also contains an additional “potential scattering” term which comes from the commutation relation among spin operators. We call this model as the strong coupling Kondo model, and define \( j = 16/(3J) \).

Now we discuss the procedure has been made. The role of the Lagrange multiplier is to enforce the surface field \( \psi_\sigma \) to locate at the impurity site; the interaction with the impurity is allowed only at the origin. As the temperature decreases, conduction electrons start to screen the impurity, accompanying the screening cloud, which is the sign of the Kondo effect. The size of the cloud is \( \sim \nu_F/T_K \) with the Fermi velocity \( \nu_F \) of conduction electrons. It is estimated to be the order of \( 1\mu m \) in a recent experiment [1]; it is much larger than the size of the quantum dot. The large cloud means that conduction electrons away from the origin can interact with the impurity strongly. Thus the surface field, which interacts with the localized spin, is no longer unnecessary to locate at the origin. As a result, \( \psi_\sigma - \sum_k \psi_{i\sigma} \) fluctuates when the cloud is formed, and accordingly should be integrated out from the action. This means that the conjugate field, \( \lambda_\sigma \) now describes the low energy physics instead. In this sense, the strong coupling model 4 will describe the low temperature regime of the Kondo effect. In particular, this point is examined.

**Poorman’s scaling.** — Next we discuss the scaling of \( j \) of the strong coupling model using the poorman’s scaling as in the weak coupling theory 5, 4. To begin with this, we includes the “potential scattering” term as the zeroth order action. Then the time-ordered Green function is

\[
g(\omega) = \frac{-4i\nu(-1/2 + f(\omega))}{2\pi(1 + (j/2\pi\nu)^2)} \left( \frac{1}{1 + (j/2\pi\nu)^2} + \frac{(j/2\pi\nu)^2}{1 + (j/2\pi\nu)^2} \right)
\]

We perform the second order perturbation expansion with respect to \( j \) and then the RG equation reads

\[
\frac{dj}{d\log D} = \left( \begin{array}{c}
\frac{1}{1 + (j/2\pi\nu)^2} \\
\frac{j^2}{1 + (j/2\pi\nu)^2}
\end{array} \right)
\]

with an energy cut-off \( D \). The second term in the time-ordered Green function does not induce the logarithmic contribution.

There is an important difference in this RG; the sign of the right hand side is the opposite to the one in the weak coupling model. It comes from the difference in the sign of the time-ordered Green function. This result means that \( j \) becomes smaller as \( D \rightarrow 0 \); the s-d interaction is less prominent at low temperatures, and eventually vanishes at \( T = 0 \). In terms of the weak coupling model, \( j = 0 \) corresponds to \( J \rightarrow \infty \), a strong coupling fixed point. Note that the scaling flow is formally the same as in the ferromagnetic Kondo model. The scaling flow allows to disregard \( j \) in the denominator in Eq. 11, which comes from the potential scattering term. Thus we disregard this term in the following. Then the solution is

\[
j(D) = \frac{j_0}{1 + j/j_0 \log d_0/D},
\]

where \( j_0 = j(d_0) \) with the initial cut-off \( d_0 \).

To make a connection between the weak and strong coupling theories, \( j_0 \) and \( d_0 \) should be represented by \( J_0 \) and \( D_0 \). The first condition is \( j(D_0)/\nu = 16/3(1/\nu J(d_0)) \) with \( \nu J(d_0) = 1/\log(d_0/T_K) \). \( d_0 \) should be larger than \( T_K \). This results in

\[
\frac{j_0(D)/\nu}{\nu} = \frac{1}{16 \log(d_0/T_K) + 1/\pi \log(d_0/D)}.
\]

The value of \( d_0 \) is still arbitrary, and the second condition is required. Equation 13 diverges at \( D = d_1 \), which is a function of \( d_0 \). We impose the condition \( d_1/d_0 = 0 \) because the divergence should not depend on the artificial parameter \( d_0 \). This gives \( d_0 = \exp(\sqrt{3/16\pi})T_K \sim 1.36T_K \). The two conditions eventually yield

\[
j(D)/\nu = \frac{\pi^2}{\log(T_K/D)} \quad (D < d_0),
\]

with \( T_K = \exp(2\pi\sqrt{3/16})T_K \sim 15.1T_K \). Since \( T_K \) is larger than \( T_K \), \( j \) is a smooth function of \( D \) near \( T = T_K \), while \( J \) diverges at \( T_K \). This provides a contrast between two perturbation theories as will be shown below.

**The expression of the current.** — We shift our discussion to electron transport, and consider the model with the impurity attached to two leads \( \alpha = L, R \) with a chemical potential difference \( \mu \). The Hamiltonian is \( H_0 + H_1 \) with

\[
H_0 = \sum_{\alpha,k,\sigma} \psi_{\alpha k\sigma}(\omega - \mu/2 - \epsilon_k)\psi_{\alpha k\sigma}, \quad \text{the sign}
\]
of $+(-)$ is for $L(R)$, and $H_1 = J \sum_{\alpha, \alpha'} \bar{\psi}_\alpha \bar{S} \cdot \sigma \psi_{\alpha'}$. We have assumed fully symmetric constants between $\alpha = L, R$ for simplicity. The model is simplified, when we apply a unitary transformation between the conduction electron fields, $\varphi^{(k)\sigma} = 1/\sqrt{2}(\psi_{L(k)\sigma} + \psi_{R(k)\sigma})$ and $\psi^{(k)\sigma} = 1/\sqrt{2}(\psi_{L(k)\sigma} - \psi_{R(k)\sigma})$. The $\psi^{(k)\sigma}$ field is decoupled from the impurity, and it simply represents free electron gas. A similar transformation is used in the Anderson model [35]. We discuss the conductance through the impurity. The current operator $I(t) = \frac{ie}{\hbar} [\bar{\psi}_L(t) \bar{S} \cdot \sigma \psi_R(t) - \bar{\psi}_R(t) \bar{S} \cdot \sigma \psi_L(t)]$ is also rewritten by

$$I = \frac{ie}{\hbar} \int dt \eta(t) [\bar{\phi} \bar{S} \cdot \sigma \phi - \bar{\psi} \bar{S} \cdot \sigma \psi]. \quad (15)$$

This term is added to the action in the form of $\int dt \eta(t) I(t)$.

We repeat a similar procedure as above, rewriting the action using the Lagrange multiplier $\lambda_{\phi}$. Applying the unitary transformation for $\lambda_{\phi}$, $\lambda_{\psi} = 1/\sqrt{2}(\lambda_L + \lambda_R)$ and $\lambda_{\psi} = 1/\sqrt{2}(\lambda_L - \lambda_R)$, the two lead $s$-$d$ model including the current generating term is given by

$$S = \int d\omega (\lambda_{\phi} \bar{\phi}) \left( \begin{array}{cc} A & B \\ C & D \end{array} \right) \left( \begin{array}{c} \lambda_{\phi} \\ \lambda_{\psi} \end{array} \right)$$

$$+ \int d\omega \left[ \bar{\psi}_\lambda \lambda_{\psi} + \lambda_{\phi} \phi \right] + \int dt \left[ \bar{\phi} = \lambda_{\phi} \phi + \lambda_{\psi} \psi \right]$$

$$+ 2J \int dt \bar{\phi} M \phi + eJ \int dt \eta(t) \bar{\phi} M \psi - \bar{\psi} M \phi$$

$$+ \left( \begin{array}{c} A \\ C \end{array} \right) \left( \begin{array}{c} \psi_L \\ \psi_R \end{array} \right)$$

$$+ \left( \begin{array}{c} A \\ C \end{array} \right) \left( \begin{array}{c} \lambda_{\psi} \\ \lambda_{\phi} \end{array} \right)$$

$$+ \frac{16}{3}(2J) \int dt \lambda_{\phi} M^{-1} \lambda_{\phi} + \bar{\psi} M \phi - \bar{\phi} M \psi$$

$$= \left( \begin{array}{c} A \\ C \end{array} \right) \left( \begin{array}{c} \psi_L \\ \psi_R \end{array} \right)$$

$$+ \left( \begin{array}{c} A \\ C \end{array} \right) \left( \begin{array}{c} \lambda_{\psi} \\ \lambda_{\phi} \end{array} \right)$$

$$+ \frac{16}{3}(2J) \int dt \lambda_{\phi} M^{-1} \lambda_{\phi} + \frac{e}{2} \int dt \eta(t) \left[ \bar{\lambda}_{\phi} \phi - \bar{\psi} M \phi \right]$$

$$+ \frac{16}{3}(2J) \int dt \lambda_{\phi} M^{-1} \lambda_{\phi} + \frac{e}{2} \int dt \eta(t) \left[ \bar{\lambda}_{\phi} \phi - \bar{\psi} M \phi \right]$$

with $A = \left( \begin{array}{cc} \frac{1}{2}(f_K + g_K) \\ 0 \end{array} \right)$, $B = \left( \begin{array}{cc} 0 \\ \frac{1}{2}(f_K - g_K) \end{array} \right)$, and $f_K = -i(2\pi\nu) \tan(\omega - \mu/2)/2$ and $g_K = -i(2\pi\nu) \tan(\omega + \mu/2)/2$. In these matrices, we have represented them in the Keldysh rotation representation.

The low energy action should be represented by $\lambda_{\phi}$ and $\lambda_{\psi}$ because the $\phi$ field participates in the screening while the $\psi$ field does not. Accordingly integrating over $\varphi$ and $\lambda_{\psi}$, we obtain

$$S = \int d\omega (\lambda_{\phi} \bar{\phi}) \left( \begin{array}{c} a \\ -b \end{array} \right) \left( \begin{array}{c} \lambda_{\phi} \\ \lambda_{\psi} \end{array} \right)$$

$$+ \frac{16}{3}(2J) \int dt \lambda_{\phi} M^{-1} \lambda_{\phi} + \frac{e}{2} \int dt \eta(t) \left[ \bar{\lambda}_{\phi} \phi - \bar{\psi} M \phi \right]$$

$$+ \frac{16}{3}(2J) \int dt \lambda_{\phi} M^{-1} \lambda_{\phi} + \frac{e}{2} \int dt \eta(t) \left[ \bar{\lambda}_{\phi} \phi - \bar{\psi} M \phi \right]$$

with $a = e^{-1}$, $b = \left( \begin{array}{cc} 0 \\ \frac{-(f_K - g_K)}{2\pi\nu} \end{array} \right)$. The important result of this action is that the current generating term represented by $\lambda_{\phi}$ and $\lambda_{\phi}$ is independent on $J$ and has no spin dependence although initially it depends on $J$ and the spin. The lowest order of the conductance together with the result of the RG gives the unitary limit of $G = 2e^2/h$.

FIG. 1: The conductance as a function of log$_{10}(T/T_K)$ calculated by various methods. The dots and thin solid line are for NRG [32] and Bethe ansatz [33], respectively. The data is taken from Ref. [32]. The thick solid line is for the strong coupling perturbation theory. The broken line for the weak coupling perturbation theory [32].

**Strong coupling perturbation theory.**—We apply the perturbation theory with respect to $1/J$. The leading and next to leading order contributions give

$$G = \frac{2e^2}{h} \left[ 1 - \frac{3j^2}{8(2\pi\nu)^2} \right]$$

while $G = \frac{2e^2}{h} (2\pi\nu J)^2$ for the weak coupling model [32]. We have disregarded the potential scattering term. To include the Kondo effect, the coupling constants should be replaced by the renormalized ones; $J \rightarrow J(D)$ and $j \rightarrow j(D)$.

In Fig. 1, the conductance is plotted as a function of log$_{10}(T/T_K)$, calculated by various methods: the weak coupling perturbation theory [32], NRG [32], Bethe ansatz [33], and the strong coupling perturbation theory. The data of NRG and Bethe ansatz is taken from Ref. [32]. The perturbative strong coupling theory (the thick solid line) qualitatively coincides with the results of NRG and Bethe ansatz (the dots and thin solid line) near $T < T_K$. As $T$ increases above $T_K$, the deviation from the results becomes larger. It is in contrast to the result of the weak coupling theory, where $G$ deviates from the results when $T < 10T_K$. This difference describes the character of the Kondo screening cloud. When $T > 10T_K$, it is less prominent, and grows during $T_K < T < 10T_K$. When $T < T_K$, it is fully developed.

Although the perturbation theory shows the unitary limit of the conductance, it does not reproduce the Fermi liquid picture at low temperatures; log$(T)$ behavior still appears. This point is in contrast to the conventional notion of the strong coupling fixed point. The discrepancy comes from the limit of the perturbative RG approach. In the weak coupling theory, the perturbation with respect to $J$ goes wrong as $D$ decreases because it starts...
Nevertheless, the strong coupling perturbation theory provides a simple approach to the crossover regime between the Fermi liquid and the weak coupling theories, where has been treated only by more sophisticated or numerical methods. Furthermore, it elucidates that there is no transition around $T = T_K$, as has been shown.

In conclusion, we have investigated the duality in the Kondo model to identify the strong coupling Kondo model with the coupling constant of $1/J$ in a simple manner. The conductance calculated by the perturbation theory with the poorman’s scaling qualitatively agrees with the exact results near $T = T_K$.

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