Entanglement of an impurity and conduction spins in the Kondo model

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Based on Yosida’s ground state of the single-impurity Kondo Hamiltonian, we study three kinds of entanglement between an impurity and conduction electron spins. First, it is shown that the impurity spin is maximally entangled with all the conduction electrons. Second, a two-spin density matrix of the impurity spin and one conduction electron spin is given by a Werner state. We find that the impurity spin is not entangled with one conduction electron spin even within the Kondo screening length $\xi_K$, although there is the spin-spin correlation between them. Third, we show the density matrix of two conduction electron spins is nearly same to that of a free electron gas. The single impurity does not change the entanglement structure of the conduction electrons in contrast to the dramatic change in electrical resistance.

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Entanglement, the quantum correlation between subsystems, is considered to be one of the key concepts in quantum mechanics and quantum information science. A study of entangled structures of quantum many-body systems is of great importance for providing us not only a new view on their physical properties but also the basic knowledge for fabricating quantum information processors. For example, entanglement of the ground states of one-dimensional quantum spin lattice models has been intensively investigated in context of quantum phase transition. In a non-interacting electron gas, entanglement of two electron spins due to the Pauli exclusion principle has been studied in connection with its characteristic length scale, the Fermi wavelength $\lambda_F$. Entanglement of two electron spins of a BCS superconductor has also examined with relation to the coherence length $\xi_0$.

The Kondo model describing the exchange interaction between the impurity spin and the conduction electrons has been one of challenging quantum many-body problems in condensed matter physics. Various theoretical tools such as Anderson’s scaling theory, Wilson’s numerical renormalization group approach, and the Bethe ansatz, etc. have been applied to the Kondo model. Recently, Kondo effects in nanodevices have been revisited with potential applications to spin devices or spin qubits. Although the Kondo model have been very intensively studied, its entanglement structure remains to be explored. In this paper we investigate three kinds of entanglement between the impurity spin and conduction electron spins as shown in Fig. 1. From this study on the entanglement structure of the Kondo model we provide a clear view on the Kondo screening cloud with the size of the Kondo screening length $\xi_K$, which is the holy grail in the Kondo physics. Also we discuss a possibility for the use of an electron gas in coupling spin qubits.

Let us consider the spin-$\frac{1}{2}$ Kondo Hamiltonian

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} - 2JS \cdot s(0),$$

where $S$ is the spin of the magnetic impurity, $s(0)$ the spin of the conduction electrons at $r = 0$, and $c_{k\sigma}^\dagger$ creates a conduction electron with momentum $k$ and spin $\sigma$. The exchange interaction $J$ is assumed to be negative, so the impurity spin is anti-parallel to the conduction spins.

Yosida presented the variational ground state of Eq. (1) given by a singlet state

$$|\Psi_s\rangle = \frac{1}{\sqrt{2}} (|\phi_u\rangle|\chi_t\rangle - |\phi_t\rangle|\chi_u\rangle),$$

where $|\chi_t\rangle$ is the spin-up state of the impurity spin and $|\phi_u\rangle$ denotes the state of conduction electrons with one excess down spin. The simplest form of $|\phi_u\rangle$ is the state...
with one down spin added outside the filled Fermi sphere

\[ |\phi_\downarrow\rangle = \frac{1}{\sqrt{N}} \sum_{k > k_F} \Gamma_k c^\dagger_k |F\rangle, \]

where \( \Gamma_k \) are variational parameters, \( N \) the normalization factor, and \( |F\rangle = \prod_{k \leq k_F} e^{i\phi_k} |0\rangle \) the filled Fermi sphere. The variational parameters \( \Gamma_k \) are given by

\[ \Gamma_k = \frac{1}{\epsilon_k + E_B}, \]

where \( E_B = k_B T_K = D \exp[2/3JN(0)] \). Here \( T_K \) is called the Kondo temperature, \( 2D \) the bandwidth of the conduction electrons, and \( N(0) \) the density of states of the conduction electrons. The characteristic length scale of the Kondo model is the Kondo screening length \( \xi_K \), the size of the Kondo screening cloud

\[ \xi_K = \frac{\hbar v_F}{k_B T_K} = \frac{E_F}{k_B T_K} \frac{2}{k_F}, \]

where \( v_F \) is the Fermi velocity, \( E_F \) the Fermi energy, and \( k_F \) the Fermi momentum. Since \( E_F \gg k_B T_K \), \( \xi_K \) is much larger than the Fermi wavelength \( \lambda_F = 2\pi/k_F \).

(i) Entanglement between the impurity spin and the conduction electrons. As depicted in Fig. 1(a), let us investigate entanglement between the impurity spin and all the conduction electrons. Since the total state, Eq. (2), is a pure state, entanglement between them is quantified by the von Neumann entropy of the reduced density matrix \( \rho_{\text{im}} \) of the impurity spin, \( S(\rho_{\text{im}}) = -\text{Tr}[\rho_{\text{im}} \log \rho_{\text{im}}] \). Here the subscript ‘im’ represents the impurity. By tracing out the degrees of freedom of the conduction electrons in Eq. (2), one easily obtains \( \rho_{\text{im}} = \text{Tr}_{\text{con}}|\Psi_s\rangle\langle\Psi_s| \). It is given by the fully mixed state

\[ \rho_{\text{im}} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \]

which gives the maximum entropy \( S(\rho_{\text{im}}) = 1 \). Thus we find that the impurity spin is maximally entangled with the conduction electrons.

(ii) Entanglement of the impurity spin and one conduction electron. If a magnetic impurity is immersed in a Fermi sea, conduction electrons will align in order to screen the magnetic field by the impurity. To put it simply, this magnetic disturbance is called the Kondo screening cloud of electrons (or an electron) with the size of order \( \xi_K \), forming a singlet with an impurity \([12]\). So one may expect some correlation or entanglement between the impurity spin and a conduction electron in the Kondo screening cloud.

Let us consider the impurity spin and one conduction spin at \( \mathbf{r} \) from the impurity as shown in Fig. 1(b). Entanglement between them can be measured if one obtains the two-spin density matrix by tracing out all the degrees of freedom of Eq. (2) except the impurity spin and one conduction spin at \( \mathbf{r} \). In the second quantization, it is given as follows

\[ \rho^{(2)}_{\alpha\beta,\alpha'\beta'}(\mathbf{r}) = \frac{1}{2} \langle \Psi_s | \hat{\psi}^+_\beta(\mathbf{r}) \hat{\phi}_{\alpha'}(0) \hat{\phi}_{\alpha}(0) \hat{\psi}_{\beta'}(\mathbf{r}) | \Psi_s \rangle, \]

where an operator \( \hat{\psi}_{\beta}(\mathbf{r}) \) creates a conduction electron with spin \( \beta \) at \( \mathbf{r} \) and \( \hat{\phi}_{\alpha}(0) \) is a creation operator of the impurity spin \( \alpha \) at origin. Here \( \alpha, \alpha', \beta, \beta' \) refer to the spin indices, i.e., \( \uparrow \) or \( \downarrow \).

From Eqs. (2) and (7), we obtain

\[ \rho^{(2)}(\mathbf{r}) = \frac{1}{2} \begin{bmatrix} \rho_{\uparrow\uparrow;\uparrow\uparrow} & 0 & 0 & 0 \\ 0 & \rho_{\uparrow\downarrow;\downarrow\uparrow} & \rho_{\uparrow\downarrow;\uparrow\downarrow} & 0 \\ 0 & \rho_{\downarrow\uparrow;\uparrow\downarrow} & \rho_{\downarrow\uparrow;\downarrow\uparrow} & 0 \\ 0 & 0 & 0 & \rho_{\downarrow\downarrow;\downarrow\downarrow} \end{bmatrix}, \]

where the diagonal elements are given by

\[ \rho_{\uparrow\uparrow;\uparrow\uparrow} = \langle \phi_\uparrow | \hat{\psi}_\uparrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) | \phi_\uparrow \rangle, \]

\[ \rho_{\uparrow\downarrow;\downarrow\uparrow} = \langle \phi_\uparrow | \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) | \phi_\downarrow \rangle, \]

\[ \rho_{\downarrow\uparrow;\uparrow\downarrow} = \langle \phi_\downarrow | \hat{\psi}_\uparrow(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) | \phi_\uparrow \rangle, \]

\[ \rho_{\downarrow\downarrow;\downarrow\downarrow} = \langle \phi_\downarrow | \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) | \phi_\downarrow \rangle, \]

and the off-diagonal elements are given by

\[ \rho_{\uparrow\downarrow;\downarrow\uparrow} = -\langle \phi_\uparrow | \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) | \phi_\downarrow \rangle = \rho_{\downarrow\uparrow;\uparrow\downarrow}. \]

Since the state \( |\phi_\downarrow\rangle \) has \( N/2 \) up and \( N/2+1 \) down spins of the conduction electrons, the matrix element \( \rho_{\uparrow\uparrow;\uparrow\uparrow} \) is given by the electron density with up spin

\[ \rho_{\uparrow\uparrow;\uparrow\uparrow} = \frac{N}{2V} = \frac{n}{2}, \]

where \( V \) is the volume of the conduction electrons and \( n \) is the electron density. Similarly we have \( \rho_{\downarrow\downarrow;\downarrow\downarrow} = n/2 \). The matrix element \( \rho_{\uparrow\downarrow;\downarrow\uparrow} \) is given by

\[ \rho_{\uparrow\downarrow;\downarrow\uparrow} = \frac{n}{2} + f(\mathbf{r}), \]

where \( f(\mathbf{r}) \) is defined by

\[ f(\mathbf{r}) \equiv \frac{1}{\sqrt{4N}} \sum_{k k' > k_F} \Gamma_k \Gamma_{k'} e^{-i(k'-k)\mathbf{r}}. \]

The system is isotropic, so \( f(\mathbf{r}) \) depends only on the distance \( r \). We get the off-diagonal element \( \rho_{\downarrow\uparrow;\uparrow\downarrow} = -f(\mathbf{r}) \). Thus \( \rho^{(2)} \) is given by the sum of the fully mixed state and a spin-singlet state

\[ \rho^{(2)} = \frac{1}{2} \begin{bmatrix} \frac{n}{2} & 0 & 0 & 0 \\ 0 & \frac{n}{2} + f(\mathbf{r}) & -f(\mathbf{r}) & 0 \\ 0 & -f(\mathbf{r}) & \frac{n}{2} + f(\mathbf{r}) & 0 \\ 0 & 0 & 0 & \frac{n}{2} \end{bmatrix}, \]

\[ = \frac{1}{4} + f(\mathbf{r}) |\Psi^{-}\rangle \langle \Psi^{-}|, \]
where $|\Psi(-)\rangle = \frac{1}{\sqrt{2}}(|\uparrow \downarrow \rangle - |\downarrow \uparrow \rangle)$ and $I$ is the 4 x 4 unit matrix. The meaning of Eq. (13) is that the first term is the uniform background and the second is the singlet state forming a Kondo screening cloud.

Since $\text{Tr} \rho^{(2)} = n + f(r)$, let us introduce the normalized two-spin density matrix $\rho$ defined by $\rho^{(2)} = (n + f)\rho$. Then we find that $\rho$ is given by the Werner state $\rho$:

$$\rho = (1 - p)\frac{1}{4} + p|\Psi(-)\rangle\langle\Psi(-)|,$$  \hspace{1cm} (14)

where $p = f/n + f$. The impurity spin is entangled with one conduction electron spin at $r$ if $p > 1/3$, that is, $f > n/2$.

Let us examine whether $\rho$ is entangled or not by calculating $f(r)$. Since $\Gamma_k$ is real, we rewrite $f(r) = V\tilde{f}(r)^2/N$ where the function $\tilde{f}(r)$ is defined by

$$\tilde{f}(r) = \frac{1}{V} \sum_{k > k_F} \Gamma_k e^{ikr}.$$  \hspace{1cm} (15)

After some calculations, $\tilde{f}(r)$ becomes the integral form

$$\tilde{f}(r) = \frac{N(0)}{k_F r} \int_0^{D/E_F} \sin \left[ k_F r \sqrt{1 + t E_B/E_F} \right] \frac{dt}{t + 1},$$  \hspace{1cm} (16)

where $N(0)$ is the density of state at Fermi level and becomes $N(0) = mk_F/2\pi^2h^2 = 3n/4E_F$ for a free electron gas. The normalization factor $N$ is given by

$$N = \sum_{k > k_F} \Gamma_k^2 = \frac{V N(0)}{E_B} y(D, E_B, E_F),$$  \hspace{1cm} (17a)

where the definite integral $y(D, E_B, E_F)$ is defined by

$$y(D, E_B, E_F) = \int_0^{D/E_F} \sqrt{1 + t E_B/E_F} \frac{dt}{(1 + t)^2}.$$  \hspace{1cm} (17b)

Thus we obtain

$$f(r) = \frac{3n}{4} \frac{E_B}{E_F} \frac{f_N(r)^2}{y(D, E_B, E_F)},$$  \hspace{1cm} (18)

where $f_N(r) \equiv \tilde{f}(r)/N(0)$. The condition of entanglement of $\rho$, $f > n/2$, becomes

$$\frac{3}{2} \left( \frac{E_B}{E_F} \right) \frac{f_N(r)^2}{y(D, E_B, E_F)} > 1.$$  \hspace{1cm} (19)

For usual Kondo systems, the Kondo temperature $T_K$ ranges from few to hundreds Kelvin, $T_K \approx 1 \sim 300 K$. The Fermi temperature $T_F = E_F/k_B$ is about $T_F \approx 10^4 K$. This implies $E_B/E_F \approx 10^{-2} \sim 10^{-4}$. However, according to Eq. (5), the small ratio of $E_B/E_F = k_B T_K/E_F$ indicates the Kondo screening length $\xi_K$ is much larger than the Fermi wavelength $\lambda_F$. If the bandwidth $D$ is assumed to be $E_B \ll D \ll E_F$, we have $y(D, E_B, E_F) \approx 1$. Also $f_N(r) \approx O(1)$ as shown in Fig. 1 (c). The density matrix $\rho_{\text{con}}$ of all the conduction electrons has been calculated by Chen et al. [16] and by Gubernatis et al for the Anderson model [17]. It is interesting that $\rho^{(2)}$ is given by a pseudo entangled state in liquid-state NMR [11, 18]. The Kondo screening cloud could be detected through the extra Knight shift experiment which measures $f(r)$.

Our result shows that even if there is the spin-spin correlation between the impurity and a conduction electron in the Kondo screening cloud, entanglement between them vanishes. A simple explanation for this is as follows. Since many conduction electrons are coupled to a single impurity, the quantum correlation between the impurity and each conduction electron is very tiny so there is no entanglement between them.

(iii) Entanglement between two conduction electron spins. It has been believed that conduction electrons within the Kondo screening cloud are mutually correlated because they have information on the same impurity [4]. We examine whether the impurity spin induces the non-classical correlation, i.e., entanglement between conduction electrons.

Consider two conduction spins at $\mathbf{r}_1$ and $\mathbf{r}_2$ as shown in Fig. 1 (c). The density matrix $\rho_{\text{con}}$ of all the conduction electrons is noting but the spin-spin correlation function between the impurity spin and the conduction spin at $\mathbf{r}$,

$$\langle \sigma^z_{im} \sigma^z_{im} \rangle = \rho_{\uparrow \uparrow \uparrow \uparrow} + \rho_{\downarrow \downarrow \downarrow \downarrow} - \rho_{\uparrow \downarrow \downarrow \uparrow} - \rho_{\downarrow \uparrow \uparrow \downarrow}$$  \hspace{1cm} (20)

Notice that $f(r)$ is qualitatively similar to the spatial spin-spin correlation function $\langle \mathbf{S} \cdot \mathbf{S}(\mathbf{r}) \rangle = \frac{3}{2} \langle \sigma^z_{im} \sigma^z_{im} \rangle$, which was calculated by Chen et al. [16] and by Gubernatis et al for the Anderson model [17]. It is interesting that $\rho^{(2)}$ is given by a pseudo entangled state in liquid-state NMR [11, 18]. The Kondo screening cloud could be detected through the extra Knight shift experiment which measures $f(r)$.
electrons is given by the mixture of $|\phi_F\rangle$ and $|\phi_L\rangle$
\begin{equation}
\rho_{\text{con}} = \text{Tr}_{\text{im}} |\Psi_s\rangle \langle \Psi_s| = \frac{1}{2} (|\phi_F\rangle \langle \phi_F| + |\phi_L\rangle \langle \phi_L|). \tag{21}
\end{equation}

From Eq. (21), the density matrix $\rho(2)$ of two conduction electron spins is written by
\begin{equation}
\rho_{\sigma_1,\sigma_2}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2} \text{Tr} \left[ \hat{\psi}_{\sigma_1}^{\dagger}(\mathbf{r}_2) \hat{\psi}_{\sigma_1}(\mathbf{r}_1) \hat{\psi}_{\sigma_2}(\mathbf{r}_1) \hat{\psi}_{\sigma_2}(\mathbf{r}_2) \rho_{\text{con}} \right]. \tag{22}
\end{equation}

After a lengthy calculation, we obtain
\begin{equation}
\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \rho^{(2)}_{\text{free}}(\mathbf{r'}) + \Delta \rho(\mathbf{r}_1, \mathbf{r}_2), \tag{23}
\end{equation}
where $\mathbf{r'} = \mathbf{r}_1 - \mathbf{r}_2$ and $\rho^{(2)}_{\text{free}}(\mathbf{r'})$ is the density matrix of two electron spins of a free electron gas $\frac{\hbar^2}{8}$
\begin{equation}
\rho^{(2)}_{\text{free}}(\mathbf{r'}) = \frac{n^2}{8} \begin{bmatrix}
1 - g^2 & 0 & 0 & 0 \\
0 & 1 - g^2 & 0 & 0 \\
0 & 0 & 1 - g^2 & 0 \\
0 & 0 & 0 & 1 - g^2
\end{bmatrix}, \tag{24}
\end{equation}
with $g(\mathbf{r'}) \equiv \sum_{k \leq k_F} e^{i k \mathbf{r'}}$. The small change is
\begin{equation}
\Delta \rho(\mathbf{r}_1, \mathbf{r}_2) = \frac{n^2}{8} \begin{bmatrix}
3 E_B & a + b & 0 & 0 \\
0 & a & b & 0 \\
0 & b & a & 0 \\
0 & 0 & 0 & a + b
\end{bmatrix}, \tag{25}
\end{equation}
where $a \equiv g(0) \left[ f_N(r_1)^2 + f_N(r_2)^2 \right]/2$ and $b \equiv g(\mathbf{r'}) f_N(r_1) f_N(r_2)$. Since $E_B/E_F$ is very small, we have $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \approx \rho^{(2)}_{\text{free}}(\mathbf{r}_1, \mathbf{r}_2)$. Of course, if $r_1, r_2 > \xi_K$, then one gets $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \rho^{(2)}_{\text{free}}(\mathbf{r}_1, \mathbf{r}_2)$.

This result implies that the entanglement structure of the conduction electrons is little affected by the single impurity. In contrast to the traditional belief, the mutual correlation between conduction electrons is mainly due to the Pauli exclusion principle not due to the impurity. So their correlation length is the Fermi wavelength. The reason is that the number of conduction electrons are very large so they act as a reservoir. Although $|\phi_F\rangle$ is orthogonal to $|\phi_i\rangle, |\phi_F\rangle$ differs from $|\phi_L\rangle$ and from $|F\rangle$ by a single spin.

Before conclusion, we would like to mention an interesting experiment which reported the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction of two spin qubits on quantum dots mediated by an electron gas $\frac{\hbar^2}{8}$. The RKKY interaction may be used to couple spin qubits. However, our result implies that a spin qubit could be maximally entangled with the electron gas and become fully mixed if one does not deal with a quantum sate of a spin qubit and the electron gas as a whole. Our another study $\frac{\hbar^2}{8}$ on a two-spin boson model, similar to the two-impurity Kondo model, suggests that the electron gas could be used for an interaction mediator if the electron gas are separable from two spin qubits.

Our analysis is based on Yosida’s ground state which describes the Kondo physics in an simple but effective way. There are another ways to solve the problem: the variational ground state of the Anderson Hamiltonian $\frac{\hbar^2}{8}$, the quantum Monte Carlo method $\frac{\hbar^2}{8}$, the perturbative renormalization $\frac{\hbar^2}{8}$, and the density matrix renormalization group for a tight-binding model $\frac{\hbar^2}{8}$.

In conclusion, we have studied entanglement of the impurity spin and the conduction electron spins in the Kondo model based on Yosida’s ground state. First, it has been shown that the impurity spin is maximally entangled with all the conduction electrons. Second, the two-spin density matrix of the impurity spin and one conduction electron spin at $\mathbf{r}$ is given by a Werner state. It has been found that the impurity spin is not entangled with a conduction electron spin within the Kondo screening cloud even though there exists the spin-spin correlation between them. Third, the entanglement structure of the conduction electrons is little affected by the impurity in contrast to the strong effect on electrical resistance.

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