Effect of conduction electron interactions on Anderson impurities

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Abstract

The effect of conduction electron interactions for an Anderson impurity is investigated in one dimension using a scaling approach. The flow diagrams are obtained by solving the renormalization group equations numerically. It is found that the Anderson impurity case is different from its counterpart – the Kondo impurity case even in the local moment region. The Kondo temperature for an Anderson impurity shows nonmonotonous behavior, increasing for weak interactions but decreasing for strong interactions. The implication of the study to other related impurity models is also discussed.

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Recently there has been much interest in magnetic impurities interacting with a one-dimensional (1D) correlated fermion system [1–3]. On the one hand, the progress in the nanofabrication technology could make the question accessible experimentally. On the other hand, it would shed some light on the impurity as well as lattice systems in \( D > 1 \) in the presence of conduction electron correlations. It has been found that localized electrons interact with strongly correlated conduction electrons in many materials, particularly in high-\( T_c \) superconductors and the heavy-fermion-like compound \( \text{Nd}_{1.8}\text{Ce}_{0.2}\text{CuO}_4 \) [3].

It is known that electrons in 1D systems are in a Luttinger liquid state [8]. A Kondo impurity in a Luttinger liquid was studied recently by Lee and Toner [1], and Furusaki and Nagaosa [2]. They found that the Kondo temperature \( T_K \) has an algebraic dependence on the Kondo coupling rather than the exponential dependence of the usual Kondo impurity, and always rises as the strength of conduction electron interactions increases. In effect, there is no competition between electron correlations and the Kondo effect.

The usual Anderson impurity Hamiltonian with a free conduction bath can be transformed into the Kondo Hamiltonian with an irrelevant potential scattering [4] using the Schrieffer-Wolff transformation in the local moment regime. However, when the Schrieffer-Wolff transformation is applied in the presence of conduction electron interactions, the effective Kondo coupling strongly depends on the interactions. Moreover, the impurity spin will interact not only with conduction electron spins at the impurity site but also with spins at neighboring sites [10]. The potential scattering is also relevant in a Luttinger liquid [11,5]. One would expect that an Anderson impurity behave differently from a Kondo impurity when conduction interactions are included even in the local moment region.

In this paper, we mainly report results for an Anderson impurity in a Luttinger liquid. Using the scaling approach of Anderson-Yuval-Hamanna (AYH) [12] and Cardy [13], we obtain the renormalization group (RG) equations, which are solved exactly by numerical methods. We find that there is a strong interplay between the Kondo effect and the electron interactions for the Anderson impurity, unlike the Kondo impurity case. The Kondo temperature is enhanced for weak electron interactions but reduced for the strong interacting
case. The zeroth-order approximation which is widely used in the literature for solving the RG equations is checked against our numerical results. It suggests that the zeroth-order approximation could be very misleading.

The Anderson impurity in a Luttinger liquid is described by the Hamiltonian

\[ H = H_L + H_f + H_{c-f}, \]

\[ H_L = v_F \sum_{k,\sigma} k (c_{k,1,\sigma}^\dagger c_{k,1,\sigma} - c_{k,2,\sigma}^\dagger c_{k,2,\sigma}), \]

\[ + \frac{g_2}{N} \sum_{k_1,k_2,p,\sigma_1,\sigma_2} c_{k_1,1,\sigma_1}^\dagger c_{k_2,2,\sigma_2}^\dagger c_{k_{2+p,2,\sigma_2}} c_{k_{1-p,1,\sigma_1}}, \]

\[ H_f = E_0^f \sum_{\sigma} n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}, \]  

\[ H_{c-f} = \frac{t}{\sqrt{N}} \sum_{k,i,\sigma} (c_{k,i,\sigma}^\dagger f_\sigma + H.c.), \]

Where \( c_{k,1,\sigma} (c_{k,2,\sigma}) \) is the annihilation operator of right-moving (left-moving) electrons with spin \( \sigma \) and momentum \( k \), \( f_\sigma \) is the annihilation operator for localized electrons, \( n_{f\sigma} = f_\sigma^\dagger f_\sigma \), and \( N \) is the number of lattice sites. \( H_L \) is the so-called Tomonaga-Luttinger Hamiltonian, where the \( g_2 \) term represents forward scattering. \( H_L \) generally describes 1D fermion systems away from half-filling and with repulsive interactions, for which umklapp and backward scattering can be ignored. \( H_f \) and \( H_{c-f} \) are the local and mixing terms, respectively. In the case of \( g_2 = 0 \), the total Hamiltonian \( H \) reduces to the usual Anderson Hamiltonian.

We will derive the partition function using bosonization technique \[7\] and then obtain the renormalization group equations applying the scaling approach of Anderson-Yuval-Hamann \[12\] and Cardy \[13\]. The partition function of the system is \( Z = \int DcDf \exp \left[ -S_0 - \int_0^\beta d\tau H_{c-f}(\tau) \right] \), where \( S_0 \) is the action corresponding to \( H_L + H_f \). Paralleling the previous studies on impurity problems \[14\] \[15\], the strategy for finding \( Z \) is the following. First, \( Z \) is expanded and is written in terms of histories of the impurity. In this paper we will take the on-site Coulomb repulsion \( U \to \infty \). The history for the \( n \)-th term is thus a sequence of transitions, taking place at the imaginary time \( 0 < \tau_1 < ... < \tau_n < \beta \), between the three local \( f \) states \( |\alpha\rangle \) with \( \alpha = 0 \) (i.e., the \( f^0 \) configuration), \( \sigma \) (here \( \sigma = \pm 1 \) stands for the \( f^1 \) configuration with spin-up and spin-down, respectively). The degrees of
freedom of conduction electrons left in $Z$ are then treated using bosonization. This gives

$$Z = Z_0 \sum_{n=0}^{\infty} \sum_{\alpha, \alpha_1, \ldots, \alpha_n} \sum_{l_1 \ldots l_n} \int_0^\beta \frac{d\tau_n}{\xi} \int_0^{\tau_n-\xi} \frac{d\tau_{n-1}}{\xi} \ldots \int_0^{\tau_2-\xi} \frac{d\tau_1}{\xi} \exp[-S_{(\alpha l)}(\tau_1 \ldots \tau_n)].$$  \hspace{1cm} (2)

where $Z_0$ is the partition function for $H_L + H_f$, and the cut-off is $\xi = 1/W$ ($W$ is the conduction electron bandwidth). Furthermore, $l_i$ in the summation takes 1 and 2, labelling the left and right movers, and

$$S_{(\alpha l)}(\tau_1 \ldots \tau_n) = -\sum_{i<j} (-1)^{i+j} K_{ij}^{l_{ij}} \ln \frac{\tau_j - \tau_i}{\xi} - n \ln y_{\alpha_i, \alpha_{i+1}} + \sum_i h_{\alpha_{i+1}} \frac{\tau_{i+1} - \tau_i}{\xi}.$$  \hspace{1cm} (3)

The fugacity $y_{\alpha_i, \alpha_{i+1}}$ in (3) is the amplitude associated with a transition from $|\alpha_i\rangle$ to $|\alpha_{i+1}\rangle$. $y_{\sigma} = y_{\sigma 0} = \sqrt{\Delta \xi/\pi}$, here $\Delta$ is the bare hybridization strength, defined by $\pi \rho t^2$ ($\rho$ is the bare density of states of the bath at Fermi level) as usual. The effective “magnetic field” $h_{\alpha_i}$ reflects the differences of the local state energies: $h_0 = -2E_f/3$, $h_\sigma = E_f/3$. $K_{ij}^{l_{ij}}$ corresponding to the scaling dimension is given by

$$K_{ij}^{l_{ij}} = \frac{1}{2} [(1 + 2 \sinh^2 \phi) \delta_{l_i l_j} + \sinh 2\phi (1 - \delta_{l_i l_j}) + m_i m_j \delta_{l_i l_j}],$$  \hspace{1cm} (4)

where $\phi = (1/2) \tanh^{-1}(-g_2/(\pi v_F))$ and $m_i = \alpha_i + \alpha_{i+1}$. The long-range logarithmic interaction in (2) arises from the reaction of the conduction electron bath towards the transition between the local states. So $K_{ij}^{l_{ij}}$ describes the reaction strength with respect to the local disturbance.

Using the partition function (2) and the scaling approach [12, 13], we obtain the following RG equations

$$\frac{d\Delta}{dln\xi} = -\gamma \Delta,$$  \hspace{1cm} (5)

$$\frac{dE_f}{dln\xi} = \frac{\Delta}{\pi} (2e^{-E_f \xi} - e^{E_f \xi}),$$  \hspace{1cm} (6)

$$\frac{d\gamma}{dln\xi} = -4(\gamma + 1) \frac{\Delta \xi}{\pi} (2e^{-E_f \xi} + e^{E_f \xi}),$$  \hspace{1cm} (7)

where

$$\gamma = \frac{1}{2} \left[ \frac{1}{\sqrt{1 - \left|g_2/(\pi v_F)\right|^2}} - 1 \right].$$  \hspace{1cm} (8)
The parameter $\gamma$ is just the exponent of the distribution function, $n_{\sigma}(k)$, of conduction electrons at the Fermi surface in the absence of the impurity, i.e., $n_{\sigma}(k) \sim |k - k_F|^{2\gamma}$. It is noted that when the above RG equations are derived, only the hybridization term $H_{c-f}$ is treated as perturbation, while the conduction electron interactions and the “external field”, i.e., the energy level of local electrons are dealt with nonperturbatively. Eqs. (5)-(7) are complicated and will be solved numerically.

The above RG equations have been discussed using the zeroth-order approximation in the literature. In the zeroth-order approximation, the parameter $\gamma$ is not renormalized, i.e., $d\gamma/d\ln\xi \approx 0$ since $\Delta \xi \ll 1$. For $E_f\xi \ll 1$, Eq. (6) is reduced to

$$
\frac{dE_f}{dln\xi} \approx \frac{\Delta}{\pi}.
$$

For $g_2 = 0$ (or $\gamma = 0$), Eqs. (3) and (4) reproduce Haldane’s scaling equations for the usual Anderson model \[14\]. For a constant $\gamma$, integrating (4) and (9), we obtain the flowing resonance width and impurity level

$$
\Delta = \Delta_0 \left( \frac{W}{W_0} \right)^{\gamma},
$$

$$
E_f = E_f^0 - \frac{\Delta_0}{\pi \gamma} \left[ \left( \frac{W}{W_0} \right)^{\gamma} - 1 \right],
$$

(10)

where $\Delta_0$, $E_f^0$ and $W_0$ are initial (bare) values. If the Kondo temperature $T_K$ is estimated from $W \approx -E_f \approx \alpha T_K$ (here $\alpha$ is an universal number characteristic of the crossover) \[14\], using (10) one can obtain

$$
T_K \sim W_0(1 - \frac{\gamma}{J\rho})^{1/\gamma},
$$

(11)

where $J = \Delta_0/(\pi |E_f^0| \rho)$. When $\gamma \geq J\rho$, $T_K$ becomes zero.

Now let us look at numerical solutions of the RG equations (5) - (7). The parameter $\gamma$ as a function of the bandwidth is shown in Fig. 1(a) for various initial values $\gamma_0$ (curves labeled a, b and c correspond to $\gamma_0 = 0.1, 0.5, 1.0$, respectively). It is seen that $\gamma$ decreases fast as the bandwidth reduces. The corresponding resonance width $\Delta$ is shown in Fig. 1(b), compared with the result of the zeroth-order approximation (dashed curves). Since the
perturbative scaling approach is valid in the region $\Delta \ll W$, the straight dotted line $\Delta = W$ marks the rough boundary beyond which the renormalization is incorrect quantitatively. It is noted that even in the region of $W >> \Delta$ where the renormalization is valid, there is a significant difference between exact results and those of the zeroth-order approximation. The corresponding impurity level $E_F$ is shown in Fig. 1(c). It is different from the result of the zeroth-order approximation even for a large bandwidth $W \sim W_0$. It is noted that the zeroth-order approximation gives wrong flows of $E_F$ for small $W$ in the case of large $\gamma$.

One important observation on Fig. 1(a) and 1(b) is that at the points where $\gamma$ flows to zero, the corresponding resonance width $\Delta$ is still much less than the bandwidth. This means that our renormalization process is still valid at $\gamma = 0$. One of the advantages of the scaling approach is that the systems with different parameters on the same flow line in the flow diagrams are indicated to have the same universal behavior. Although this approach does not solve the model, one can know information of other systems if one of the systems on the flow line is soluble. The $\gamma = 0$ system is the usual Anderson impurity problem [16], which is the well-known exactly soluble case [9,17]. The Kondo temperature for the usual Anderson impurity is $T_K = W\sqrt{J\rho}\exp(-1/J\rho)$. We will use this expression to estimate the Kondo temperature for our system. It is noted that all the parameters in the expression should be replaced by the values of the corresponding parameters at $\gamma = 0$, not the initial values.

We obtain the Kondo temperature shown in Fig. 2 for two choices of initial values of parameters (solid curves). $T_K$ increases for small $\gamma_0$ but decreases for large $\gamma_0$. This is consistent with small cluster calculations [4]. Basically the conduction electron interactions have two effects on the Kondo temperature. On the one hand, more conduction electrons could participate in the screening on the impurity spin in the interacting case than in the free conduction electron case where only the electrons near the Fermi surface can contribute to this screening process, so that the Kondo temperature is expected to be enhanced by the conduction electron interactions. On the other, the effective Kondo coupling decreases because the second-order hopping processes contributing to the spin-flip exchange, i.e., the
Kondo scattering, in the Schrieffer-Wolff transformation are unfavorable due to the interactions [10]. The competition of these two effects results in the nonmonotonous behavior of the Kondo temperature. For the Kondo impurity model, in contrast, the Kondo coupling is assumed to be constant so that the Kondo temperature is always enhanced by the conduction electron interactions.

The corresponding Kondo temperatures in the zeroth-order approximation are also shown in Fig. 2 for comparison (the dashed curves). It is seen that the zeroth-order approximation gives a sharp decrease for \( T_K \) as \( \gamma_0 \) increases and predicts a transition at \( \gamma_0 = J \rho \). This artificial transition originates from the incorrect flows of \( E_F \), shown in Fig. 1(c), where the dashed curves do not tend to zero for small \( W/W_0 \) in the case of large \( \gamma_0 \).

Incidentally, we would like to give a remark on the usual Anderson model with the screening channels. This is a model which has attracted much attention recently since it could show non-Fermi liquid behavior [18–21]. The RG equations of this model have the same form as those given in (5)-(7). The parameter \( \gamma \) included is given by the phase shifts of the conduction electrons scattering from the impurity. So the above discussions on the RG equations are also applicable to this case. The Kondo temperature should have the same behavior as that shown in Fig. 2. The renormalization of \( \gamma \) has not been taken into account in discussing physical properties of the system in the literature. The present study strongly suggests that it is important to include this renormalization for a complete understanding of this system.

In conclusion, we have found that there is a basic difference between an Anderson and a Kondo impurity in the presence of conduction electron interactions even in the local moment regime. The conduction electron interactions enhance the Kondo temperature for the weak case, but will compete with the Kondo effect for the strong case. Although the present study is confined in one dimension, we expect that this effect exist for dimensions higher than one. We have demonstrated that the renormalization of the parameter related to interactions is essential for a consistent scaling theory. This is also true for other related impurity models.

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REFERENCES

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[1] D. H. Lee and J. Toner, Phys. Rev. Lett. 69, 3378 (1992).

[2] A. Furusaki and N. Nagaosa, Phys. Rev. Lett. 72, 892 (1994).

[3] A. Schiller and K. Ingersent, Phys. Rev. B 51, 4676 (1995); P. Phillips, preprint (1994).

[4] K. A. Hallberg and C. A. Balseiro, preprint (1994).

[5] M. Fabrizio and A. O. Gogolin, cond-mat preprint (1995).

[6] T. Brugger et al., Phys. Rev. Lett, 71, 2481 (1993); P. Fulde, V. Zevin, and G. Zwicknagl, Z. Phys. B 92, 133 (1993).

[7] For reviews, see, e.g., J. Solyom, Adv. Phys. 28, 201 (1979); V. J. Emery, *Highly Conducting One-dimensional Solids* (Plenum, 1979), p247.

[8] F. D. M. Haldane, Phs. Rev. Lett. 45, 1358 (1980); J. Phys. C 14, 2585 (1981).

[9] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B, Phys. Rev. B 21, 1044 (1980).

[10] T. Schork and P. Fulde, Phys. Rev. B 50, 1345 (1994).

[11] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. 68, 1220 (1992).

[12] P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B 1, 4464 (1970).

[13] J. L. Cardy, J. Phys. A 14, 1407 (1981).

[14] F. D. M. Haldane, Phys. Rev. Lett. 40, 416 (1978); J. Phys. C 11, 5015 (1978).

[15] Q. Si and G. Kotliar, Phys. Rev. Lett. 70, 3143 (1993); Phys. Rev. B 48, 13881 (1993).

[16] For $\gamma = 0$, the impurity spin is coupled with free left and right moving electrons, which
is reminiscent of the two-channel Kondo problem. However, the fixed point would be unstable for the asymmetry of the Kondo couplings of the impurity spin with spins at neighboring sites and the backward Kondo scattering [2].

[17] N. Andrei, Phys. Rev. Lett. 45, 379 (1980); P. B. Wiegmann, JETP Lett. 31, 364 (1980).

[18] T. Giamarchi et. al, Phys. Rev. Lett, 70, 3967 (1993); I. Perakis, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett, 70, 3467 (1993); C. Sire et. al., Phys. Rev. Lett, 72, 2478 (1994).

[19] G. M. Zhang and L. Yu, Phys. Rev. Lett, 72, 2474 (1994).

[20] Y. Yu, Y. M. Li, and N. d’Ambrumenil, Phys. Rev. B (in press) (1995).

[21] G. M. Zhang, Z. B. Su, and L. Yu, Phys. Rev. B 49, 7759 (1994); I. Perakis and C. M. Varma, Phys. Rev. B 49, 39041 (1994).

Fig. 1
The flow diagrams: (a) the parameter $\gamma$ related to the interactions; (b) the resonance width $\Delta$ and (c) the impurity level $E_F$, as functions of the bandwidth $W$ for various initial values of $\gamma_0$. Curves labeled $a, b, c$ are for $\gamma_0 = 0.1, 0.5, 1.0$, respectively. The initial values for $E_F^0$ and $\Delta_0$ are chosen to be $-0.15$ and $0.2\pi|E_F^0|$, respectively. The dashed lines in (b) and (c) are the corresponding quantities in the zeroth-order approximation [given in (10)]. The dotted line in (b) is $\Delta = W$. All energies are in unit of $W_0$.

Fig. 2
The Kondo temperature $T_K$ as a function of $\gamma_0$ for two choices of initial parameters. Curve a: $E_F^0 = -0.15$, $\Delta_0 = 0.2\pi|E_F^0|$; Curve b: $E_F^0 = -0.1$, $\Delta_0 = 0.15\pi|E_F^0|$. The dashed curves are the corresponding results of the zeroth-order approximation [given in (11)].
