Enhanced Local Moment Formation in a Chiral Luttinger Liquid

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Abstract

We derive here a stability condition for a local moment in the presence of an interacting sea of conduction electrons. The conduction electrons are modeled as a Luttinger liquid in which chirality and spin are coupled. We show that an Anderson-U defect in such an interacting system can be transformed onto a nearly-Fermi liquid problem. We find that correlations among the conduction electrons stabilize the local moment phase. A Schrieffer-Wolff transformation is then performed which results in an anisotropic exchange interaction indicative of the Kondo effect in a Luttinger liquid. The ground-state properties of this model are then equivalent to those of the Kondo model in a Luttinger liquid.

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Hybridization of a magnetic impurity with a band of conduction electrons results in charge fluctuations that ultimately determine the stability of the local moment on the defect. If the defect is modeled with a single orbital that can at most be doubly occupied, the Anderson-U model \[ H_A = \sum_{k,\sigma} \epsilon_k a_{k\sigma}^\dagger a_{k\sigma} + \sum_{\sigma} \epsilon_d a_{d\sigma}^\dagger a_{d\sigma} + \sum_{k,\sigma} V_{kd}(a_{k\sigma}^\dagger a_{d\sigma} + a_{d\sigma}^\dagger a_{k\sigma}) + U_d n_{d\uparrow} n_{d\downarrow} \]

is the simplest description that includes charge fluctuations with the conduction electrons of the host metal. In Eq. (1), \( \epsilon_d \) is the defect energy of the magnetic impurity, \( V_{kd} \) the overlap integral between a band state with momentum \( k \) and the impurity, \( a_{k\sigma}^\dagger \) creates an electron in the band states, \( a_{d\sigma}^\dagger \) creates an electron with spin \( \sigma \) on the impurity, and \( n_{d\sigma} = a_{d\sigma}^\dagger a_{d\sigma} \) is the number operator for an electron of spin \( \sigma \). As a consequence of the on-site repulsion \( (U_d) \), the single particle states on the impurity have energies, \( \epsilon_d \) and \( \epsilon_d + U_d \). At high temperatures, the density of states of this model has two Lorentzian peaks centered at these two energy levels. However, the occupancy of these levels need not be equal. Anderson \[1\] showed that at the Hartree Fock level, \( U_d \rho_d(0) = 1 \) defines the phase boundary demarcating the magnetic (single occupancy) from the non-magnetic (double occupancy) phase. In this relationship, \( \rho_d \) is the defect density of states, \( \epsilon_F = 0 \) and we assumed that \( \epsilon_d < 0 \). At low temperatures, the local moment is quenched by the formation of the Kondo singlet state \[2\]. Although the Kondo resonance is expected to occur for any value of the defect energy within the range \( -U_d < \epsilon_d < 0 \), it is most favourable at the defect energy corresponding to the greatest stability of the local moment at the d-impurity, namely, \( \epsilon_d = -\frac{U_d}{2} \). At this energy \( H_A \) is particle-hole symmetric, and the Kondo resonance is pinned at \( \epsilon_F = 0 \).

If repulsive interactions are now turned on among the conduction electrons, it is unclear at the outset whether they stabilize or destroy the local moment phase of an Anderson-U impurity. Should they destabilize the local moment, then the possibility arises that the Kondo effect might be suppressed. It is precisely the fate of a local moment in a sea of interacting conduction electrons that we address in this paper. Surprisingly, an answer
to this basic question has not been advanced. Magnetic impurities in heavy-Fermion and high-T_c materials are obvious physical realizations of an Anderson-U defect in a strongly correlated system. Hence, formulation of the correlated local moment problem is of extreme physical significance. Recently, Schork and Fulde have considered this problem in the limit that the defect is at most singly-occupied. Consequently, they were not able to obtain the phase diagram demarcating the magnetic from the non-magnetic phase. Others as well have considered the infinite-U limit or Kondo problem in a correlated system. The new physics that has come out of these studies is that the Kondo temperature scales algebraically as $T_k \propto J^{2 \pi v_F / g^2}$, with J the Kondo exchange coupling, $v_F$ the Fermi velocity and $g^2$ the coupling constant for forward electron scattering. This result is valid strictly in the limit of weak Coulomb interactions, $\frac{g^2}{2\pi v_F} << 1$. In addition, the Kondo effect occurs for both ferromagnetic and antiferromagnetic exchange couplings. In a recent paper, Schiller and Ingersent have shown that if the conduction electrons are bosonized and only spin-up right movers and spin-down left movers are retained, all weak coupling features of the Kondo problem in a Luttinger liquid are reproduced, such as the power-law scaling of the Kondo temperature. Below the Kondo temperature, the strong-coupling analysis of Furusaki and Nagaosa results in anomalous exponents for the impurity contribution to the specific heat. The truncation of the full Luttinger liquid made in ref. 6 results in purely Fermi-liquid behaviour. Hence, the truncation introduced by Schiller and Ingersent appears to be valid only in the weak coupling regime.

In this paper, we approach the Anderson-U problem in a Luttinger liquid by coupling chirality to spin as has been done previously in the work of Schiller and Ingersent. We show here that with judiciously-chosen transformations, much of the physics of this problem can be unearthed. Specifically, we show that interactions enhance the local moment. As the local moment phase occurs in the weak coupling limit or equivalently at temperatures high relative to the Kondo temperature, our conclusions that the local moment phase is enhanced is most probably not affected by the truncation of the full Luttinger liquid. We also show that in the Kondo limit, we recover exactly the results of Schiller and Ingersent.
The starting point for our analysis is a Hamiltonian \( H = H_0 + H_L \) that includes the standard Anderson model as well as a 1-dimensional lattice of conduction electrons

\[
H_L = -\frac{t}{2} \sum_{n\sigma} \left[ \Psi_{n\sigma}^\dagger \Psi_{n+1\sigma} + h.c. \right] + U_L \sum_{n\sigma} \rho_{n\sigma} \rho_{n-\sigma}
\]  

interacting via on-site Coulomb repulsions of strength \( U_L \). In equation (3), \( t \) is the hopping matrix element, \( \Psi_{n\sigma} \) annihilates an electron on site \( n \) with spin \( \sigma \) and \( \rho_{n\sigma} = \Psi_{n\sigma}^\dagger \Psi_{n\sigma} \) is the electron density at the \( n \)-th lattice site. To obtain the Luttinger description of our interacting model, we now linearise around the Fermi momentum \( k_F \) and write the electron field as \( \Psi_{n\sigma} = e^{i k_F n} \Psi_{+\sigma} + e^{-i k_F n} \Psi_{-\sigma} \). For each spin there are two electron fields \( \Psi_{\pm\sigma} \) with momentum \( \pm k_F \). We will, for the sake of simplicity, retain only two electron fields. We associate with spin-up the right moving field, \( \Psi_+ \) and spin-down with the left-moving field, \( \Psi_- \). We refer to an interacting system with this constraint as a chiral-spin Luttinger liquid. This coupling of spin to chirality has been shown to have no severe consequences in the Kondo problem in a Luttinger liquid [6] in the weak coupling regime. Hence, it is worth exploring the Kondo limit of the corresponding Anderson model in our chiral-spin liquid.

As there is only a forward interaction term, we can rewrite our electron lattice Hamiltonian in continuum form as

\[
H_L' = -iv_F \sum_{s=\pm} \int_{-L/2}^{L/2} \Psi_s^\dagger(x) \partial_x \Psi_s(x) dx + aU_L \int_{-L/2}^{L/2} \Psi_+^\dagger \Psi_+ :: \Psi_-^\dagger \Psi_- : dx
\]  

where :: indicates normal ordering and \( v_F = a \sin k_F a \) is the Fermi velocity and \( a \) the lattice spacing. We must also recast the impurity Hamiltonian

\[
H_A' = H_d + V_d \left[ \Psi_+^\dagger (x=0) a_d^\dagger + \Psi_-^\dagger (x=0) a_d + h.c. \right].
\]  

with \( H_d \) the second and last terms in Eq. (1). In writing this equation, we have subsumed the \( \sqrt{a} \) continuum factor into the definition of \( V_d \). Because spin and chirality are coupled, hopping of spin-up (spin-down) conduction electrons to the impurity located at \( x=0 \) is mediated by the right (left) moving field \( \Psi_+ (\Psi_-) \).

The lattice degrees of freedom can now be bosonized by writing the left and right moving fields
\[ \Psi_\pm = \frac{1}{\sqrt{2\pi a}} e^{-i\sqrt{\pi} \int_{-\infty}^{\infty} \Pi(x')dx' \mp \Phi(x)} \] (6)

in terms of two real, conjugate Bose fields, \( \Phi(x) \) and \( \Pi(x) \). The Bose fields obey the commutation relation \([\Phi(x), \Pi(y)] = i\delta(x - y)\). If we express the conduction electron degrees of freedom in terms of the Bose fields, we find that the resultant lattice Hamiltonian

\[ H'_L = \frac{\nu_F}{2} \int_{-L/2}^{L/2} \left[ \alpha_- \Pi^2(x) + \alpha_+ (\partial_x \Phi(x))^2 \right] dx \] (7)

can be mapped onto a free Fermion theory

\[ H'_L = \frac{\tilde{\nu}_F}{2} \int_{-L/2}^{L/2} \left[ \tilde{\Pi}^2(x) + (\partial_x \tilde{\Phi}(x))^2 \right] dx \] (8)

once the bare Bose fields are rescaled in the form, \( \tilde{\Pi}(x) = \eta^{1/2} \Pi(x) \) and \( \tilde{\Phi}(x) = \eta^{-1/2} \Phi(x) \). Such a rescaling retains the canonical commutation relations. The constants appearing in the bosonized Hamiltonian are \( \alpha_\pm = [1 \pm g]^{1/2} \), \( \alpha = \sqrt{\alpha_- \alpha_+} \), \( \eta = \sqrt{\alpha_- / \alpha_+} \) and a rescaled Fermi velocity \( \tilde{\nu}_F = \alpha \nu_F \). The strength of the electron correlations is determined by the dimensionless conductance \( g = \frac{aU \pi}{2 \nu_F} \). The range of validity of the approximations used here is the weak-coupling regime, \( g < 1 \). In the rescaled basis, interactions among the conduction electrons simply rescale the original Fermi velocity. It is this rescaling of the Fermi velocity that results in anomalous dimensions and as a consequence Luttinger liquid behaviour of the conduction electrons [7].

While the conduction electron degrees of freedom are now quite simple, the hybridization term in the effective Anderson Hamiltonian

\[ H'_A = H_d + V_d \left[ A_+^\dagger a_d^\uparrow + A_-^\dagger a_d^\downarrow + h.c. \right] \] (9)

depends explicitly on the electron correlations through the operators

\[ A_\pm^\dagger = \frac{1}{\sqrt{2\pi a}} e^{i\sqrt{\pi} \int_{-\infty}^{0} \eta^{-1/2} \Pi(x')dx' \mp \eta^{1/2} \Phi(0)} \] (10)

We will have successfully mapped our impurity problem onto an equivalent non-interacting one if the factors of \( \eta \) in the exponents of \( A_\pm \) can be rescaled to unity. We seek then a transformation that maps the fields \( A_\pm \) to the canonical rescaled fields.
\[ \tilde{\Psi}^\dagger_\pm(x) = \frac{1}{\sqrt{2\pi a}} e^{i\sqrt{\pi} \int_{-\infty}^{x} \tilde{\Pi}(x')dx'} \tilde{\Phi}(x). \] (11)

From the form of the hopping term in \( H_A \), the transformation, should one exist, must amount to a rotation among the states of the impurity. To this end, we investigate a unitary transformation of the form

\[ \hat{T} = e^{i\Phi_{\pm}^\lambda r n_{d\uparrow} + i\Phi_{\pm}^\lambda r n_{d\downarrow}} \] (12)

\[ \Phi_{\pm}^\lambda r = \lambda^{-1} \int_{-\infty}^{0} \tilde{\Pi}(x')dx' \mp \Gamma \tilde{\Phi}(0) \] (13)

where \( \lambda \) and \( \Gamma \) are constants to be determined. We need to evaluate \( \hat{T}(H_L' + H_A')\hat{T}^\dagger = \hat{\tilde{H}} \).

The terms in the Luttinger part of the Hamiltonian transform straightforwardly as

\[ \hat{T}\tilde{\Pi}^2\hat{T}^\dagger = \left(\tilde{\Pi} + \delta(x)\Gamma(n_{d\uparrow} - n_{d\downarrow})\right)^2 \] (14)

\[ \hat{T}(\partial_x \tilde{\Phi}(x))^2\hat{T}^\dagger = \left(\partial_x \tilde{\Phi}(x) + \delta(x)\lambda^{-1}(n_{d\uparrow} + n_{d\downarrow})\right)^2. \] (15)

We will see that it is the \( \delta(x) \) terms that renormalize the site energies as well as the impurity on-site Coulomb repulsion and produce a Kondo exchange interaction.

The hopping term transforms as

\[ \hat{T}A^\dagger_{\pm\sigma}a_{d\pm\sigma}\hat{T}^\dagger = e^{-i\Phi_{\pm}^\lambda r} A^\dagger_{\pm\sigma} a_{d\pm\sigma} + i[\Phi_{\pm}^\lambda r, A^\dagger_{\pm\sigma}]n_{d\pm\sigma}a_{d\mp\sigma} + ... \] (16)

The second term in Eqn. 16 represents a correlated hopping process in which an electron is annihilated from a doubly-occupied impurity state. This term then stabilizes the singly-occupied state of the impurity. The Hermitian conjugate of this term creates a doubly-occupied impurity state from a singly-occupied one. The higher-order terms in Eq. 16 are all of this form. Hence, all higher-order correlated hopping processes produce no net change in the occupancy of the impurity. As a result, we drop these terms and focus solely on the first term in Eqn. 16. The precise form of the transformation can now be found by demanding that \( e^{-i\Phi_{\pm}^\lambda r} A^\dagger_{\pm\sigma} \propto \tilde{\Psi}^\dagger_\pm(x) \). Using the identity for combining products of exponential operators, we find that \( \lambda^{-1} = \sqrt{\pi}(\eta^{-1/2} - 1) \) and \( \Gamma = \sqrt{\pi}(\eta^{1/2} - 1) \). We now combine the results of these calculations to obtain
\( \tilde{H} \approx \tilde{H}_p + \tilde{\epsilon}_d(n_{d\uparrow} + n_{d\downarrow}) + \tilde{U}_d n_{d\uparrow} n_{d\downarrow} + \tilde{V}_d \left[ \tilde{\Psi}_+^\dagger(x = 0)a_{d\uparrow} + \tilde{\Psi}_-^\dagger(x = 0)a_{d\downarrow} + h.c. \right] \\
+ \tilde{v}_F \Gamma \tilde{\Pi}(0)(n_{d\uparrow} - n_{d\downarrow}) + \tilde{v}_F \lambda^{-1} \left( \partial_x \tilde{\Phi}(0) \right) (n_{d\uparrow} + n_{d\downarrow}) \) 

(17)

as our fully-transformed Hamiltonian in the absence of the correlated-hopping processes. As is evident all bare parameters associated with the impurity have now been renormalized by the interactions:

\[
\begin{align*}
\tilde{\epsilon}_d &= \epsilon_d + \frac{\tilde{v}_F \pi}{2a} \left[ (\eta^{-1/2} - 1)^2 + (\eta^{1/2} - 1)^2 \right] > \epsilon_d \\
\tilde{U}_d &= U_d + \frac{\tilde{v}_F \pi}{a} \left[ (\eta^{-1/2} - 1)^2 - (\eta^{1/2} - 1)^2 \right] > U_d \\
\tilde{V}_d &= V_d e^{i\pi/2(\eta^{-1/2} - \eta^{1/2})}
\end{align*}
\]

(18)

Eqs. 17 and 18 represent one of the key results of this paper. Much of the physics of the Anderson model in a Luttinger liquid can be deduced from them.

Insight into the transformed Hamiltonian can be gained initially by ignoring the last two terms in Eq. 17. At this level, \( \tilde{H} \) is identical to the original Anderson Hamiltonian except the matrix elements and site energies now depend on the electron correlations through Eqs. 18. Note first that \( \tilde{U}_d > U_d \). The interactions have effectively increased the on-site Coulomb repulsions on the impurity, thereby increasing the energy cost of doubly occupying the impurity. The hybridization energy is unaffected by the interactions because \( |\tilde{V}_d|^2 = |V_d|^2 \).

As a consequence, the two crucial ratios that determine the stability of the local moment phase \( \frac{\tilde{\epsilon}_d}{\tilde{U}_d} \) and \( \frac{|\tilde{V}_d|^2}{\tilde{U}_d} \) are both smaller than their bare values in the Anderson model. In the Anderson model, local moment formation is expected for \( 0 < \frac{|\epsilon_d|}{U_d} < 1 \) and \( \pi|V_d|^2/U_d < 1 \). At this level of theory, we find that the local moment phase must expand to compensate for the smaller values of \( \frac{\tilde{\epsilon}_d}{\tilde{U}_d} \) and \( \frac{|\tilde{V}_d|^2}{\tilde{U}_d} \). From this analysis, we conclude that correlations stabilise the local moment phase.

What effect do the last two terms have? Recall, \( \tilde{\Pi}(0) = -\sqrt{\pi}j_1(0) \) defines the current and \( \partial_x \tilde{\Phi}(0) = \sqrt{\pi}j_0(0) \) the electron charge density at the defect. In Eq. 17, \( j_1 \) and \( j_0 \) couple respectively to the impurity magnetic moment and charge density. Above the Kondo temperature where local moment formation is favoured, mean-field theory should be
sufficient to describe the effect of these terms. Physically, the charge density term should provide, to leading order, an overall shift in the defect site energy that scales with the filling. The net contribution of these terms to the local moment phase is expected to be small as terms involving a product of two Fermion operators is expected to yield corrections of $O(1/k_B T)$ at high temperatures [8]. To see how this comes about, we calculate the occupancy on the impurity level $\langle n_{d\sigma} \rangle$. This quantity is obtained by integrating the imaginary part of the d-electron Green function, $G_{d\sigma}(\omega) = \langle \langle a_{d\sigma}; a_{d\sigma}^\dagger \rangle \rangle$, weighted with the Fermi-Dirac distribution function. At high temperatures, it is sufficient to use a second level closure of the equations of motion [8] to eliminate the conduction electron Green function $G_{kk'}$ from the expression for $G_{d\sigma}$. If we retain only the leading diagonal term in the equation of motion for $G_{kk'}$, we find that the occupancy on the impurity [9]

$$
\pi \langle n_{d\sigma} \rangle = \cot^{-1} \left[ \frac{\tilde{\varepsilon}_d + \frac{\pi \tilde{v}_F \lambda^{-1} n}{a} - \tilde{\varepsilon}_F + \tilde{U}_e^{\sigma} \langle n_{d-a} \rangle - \frac{\pi^2 \Delta \tilde{v}_F}{2LD} (\lambda^{-1} + sgn(\sigma) \Gamma) \langle n_{d\sigma} \rangle}{\Delta} \right]
$$

(19)

is still of the mean-field Anderson form [1]. In this expression, the energy cutoff is $D \propto k_B T$, $\Delta = \pi |\tilde{V}_d|^2 \rho(\epsilon)/L$, and $n = aN_e/L$ is the filling. We see explicitly now that the charge-density term in Eq. 17 provides a net shift to the defect site energy proportional to the filling in the conduction. Additionally, this term as well as the current term provide corrections to the on-site Coulomb repulsion, $\tilde{U}_e^{\sigma} = \tilde{U}_d - \frac{\pi^2 \Delta \tilde{v}_F}{2LD} (\lambda^{-1} - sgn(\sigma) \Gamma)$ which are $O(1/k_B T)$. The overall effect of this correction is to decrease $\tilde{U}_d$. However, it is straightforward to show that this correction is always smaller than the enhancement in the on-site Coulomb repulsion predicted by Eq.18. Hence, the enhanced stability of the local moment remains intact even if the current and density terms are included. To illustrate the enhancement, we plot the phase boundary in the limit that $D \to \infty$ in Eq. 19. The Anderson mean-field result $g = 0$ corresponds to the solid line in Figure 1. As is evident, the local moment region expands as the strength ($g$) of the interactions among the conduction electrons increases. As expected, the filling correction provides a net shift in the defect site energy. It appears then that the increased stability of the local moment phase can be understood simply from the enhancement of the Coulomb repulsion induced by the electron correlations on the impurity.
To understand the Kondo limit of our effective Hamiltonian, it is expedient to introduce the anti-commuting Fourier components $\tilde{\Psi}_\pm(x) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} c_{k\pm\sigma}$. In terms of the $c_k'$s, the transformed Hamiltonian becomes,

$$\tilde{H} = \sum_k \epsilon(k) \chi_k^\dagger \sigma_k \chi_k + \tilde{\epsilon}_d \chi_d^\dagger \chi_d + \tilde{U}_d n_d^\dagger n_d + \frac{\tilde{V}_d}{\sqrt{L}} [\chi_k^\dagger \chi_d + h.c.] + a J_z^U \sum_{k,k'} (\chi_k^\dagger \sigma_k \chi_{k'}) \cdot (\chi_d^\dagger \sigma_d \chi_d) + \sqrt{\pi} v_F \lambda^{-1} \sum_{k,k'} \chi_k^\dagger \chi_{k'}^\dagger \chi_d^\dagger \chi_d$$

with $\epsilon(k) = k L \tilde{v}_F / 2$, $J_z^U = \tilde{v}_F \pi (1 - \eta^{1/2}) / a$, and $\chi_{k(d)}$ are two-components spinors composed of the up and down components of $c_{k\sigma}(a_{d\sigma})$ scaled by $1/\sqrt{L}$. It is the current density, $j_1(0)$, that gives rise to the new diagonal spin-exchange process. This term is identical to the one derived by Schiller and Ingersent [6] in the context of the Kondo effect in a chiral-spin Luttinger liquid. To see this more clearly, we perform a Schrieffer-Wolff transformation [2]. The hopping term in Eq. 20 produces the standard spin-flip term $4|\tilde{V}_d|^2 / \tilde{U}_d (\chi_k^\dagger \sigma_k \chi_{k'}) \cdot (\chi_d^\dagger \sigma_d \chi_d)$. As a result, the net diagonal spin-exchange matrix element $\tilde{J}_z = 4|\tilde{V}_d|^2 / \tilde{U}_d + \frac{\tilde{v}_F \pi}{a} (1 - \eta^{1/2})$ consists of two contributions: the usual hybridization-mediated exchange and an additional term arising from the interactions among the conduction electrons. The perpendicular component of the exchange $J_\perp = 4|\tilde{V}_d|^2 / \tilde{U}_d$ depends only on the hybridization-mediated interaction. It is this anisotropy that is responsible for the algebraic scaling of the Kondo temperature in a Luttinger liquid [6].

Although an exact solution has not been found, it is reassuring that the chiral model is in agreement with simple physical arguments that electron correlations enhance local moment formation. The success of the chiral-spin model is due in part to the fact that it retains spin-flip backscattering at the impurity. Lee and Toner [4] were first to point out that spin-flip backscattering is the dominant scattering process among the conduction electrons, at least for the Kondo problem. Ultimately it would be preferable to solve the local moment problem in a full Luttinger liquid. It turns out that a transformation that solves the full problem is quite dissimilar from the one constructed here, because the bosonized Hamiltonian for the full Luttinger liquid [7] cannot be mapped onto a non-interacting Fermion problem. However, the charge and spin sectors independently satisfy such a mapping, at least away from the Kondo limit.
from half-filling. Hence, the analogous transformation must involve a rotation among the charge and spin sectors of the Luttinger liquid as well as the states on the impurity.

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Figure Captions

Figure 1: a) Local moment phase diagram calculated using Eq. [9] with $D = \infty$. The curves indicate equal occupancy of the up and down spin states on the impurity as a function of $x = \frac{\epsilon_d - \epsilon_f}{U_d}$, $v = \Delta/U_d$, and the filling $n = aN_c/L$. The solid curve corresponds to $g = 0.0$ whereas $g = 0.7$ in the other two. In all the curves $U_L = 0.5U_d$. The local moment ceases to exist on and to the right of each curve.