Kondo screening cloud in a one dimensional wire: Numerical renormalization group study

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We study the Kondo model – a magnetic impurity coupled to a one dimensional wire via exchange coupling – by using Wilson’s numerical renormalization group (NRG) technique. By applying an approach similar to which was used to compute the two impurity problem we managed to improve the bad spatial resolution of the numerical renormalization group method. In this way we have calculated the impurity spin – conduction electron spin correlation function which is a measure of the Kondo compensation cloud whose existence has been a long standing problem in solid state physics. We also present results on the temperature dependence of the Kondo correlations.

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Introduction— As being one of the most interesting quantum impurity problems, the Kondo effect [1] – when a localized impurity spin interacts with the itinerant electrons via spin exchange coupling – has been studied for decades both theoretically and experimentally [2] and has recently come to its renaissance when it has been predicted to appear [3] and observed [4] in quantum dot systems. Even though the Kondo effect seems to be well-understood now, still, there is a controversial question which has not been clarified yet: Whether there exists an extended “Kondo screening cloud” or not?

In case of the single channel Kondo problem – when the local spin is coupled to one band of conduction electrons – the interaction with the electrons lifts the ground state degeneracy of the isolated spin resulting in an effective “screening” of the impurity spin below a certain energy scale, the so-called Kondo temperature $T_K$. It is adequate to ask the question what is the typical length scale in which the impurity spin gets screened. As a simple estimate, just by comparing the scales of the competing kinetic and binding energies, one easily gets a length scale, the so-called Kondo coherence length, $\xi_K = h v_F / K_B T_K$. By substituting the typical Fermi velocity $v_F$ in metals, and taking a typical Kondo temperature $T_K \sim 1K$, one gets $\xi_K \sim 1\mu m$, which is comparable with, or even larger than the typical dimension of today’s mesoscopic devices. However, to measure that screening cloud is highly non-trivial from experimental point of view.

In order to observe the screening cloud, one has to measure correlations between the impurity spin and the conduction electron spin density. It is very difficult to imagine such kind of a measurement in bulk metallic samples. Recently, it has become possible to perform scanning tunneling microscopy (STM) measurements on metallic surfaces addressing a single magnetic impurity and its close neighborhood [5]. In those experiments the screening cloud was not observed since the STM tip probes the local charge density of states which is affected by the Kondo correlations in the close neighborhood of the impurity only. Even in case of having spin-polarized STM tips, it is very difficult to measure the spin correlations since the Kondo effect manifests itself in continuous, coherent spin flip processes at a time scale $\sim 1/T_K$ meaning that one has to measure at a frequency of tens of gigahertz. The idea of suppressing the impurity spin fluctuations by applying a local magnetic field is doomed to fail since a magnetic field which is large enough to suppress the spin fluctuations is necessarily large enough to destroy Kondo correlations as well.

There were experimental setups proposed in order to measure the Kondo cloud in confined systems [6], e.g. in case of a quantum dot attached to one dimensional lead with length shorter than, or comparable with $\xi_K$. Such kind of a proposal suffers from the facts that it is destructive, i.e. the Kondo effect disappears for one dimensional leads shorter than $\xi_K$ and one can still argue that the suppression of the Kondo effect is a result of having the level spacing in the lead $\delta \epsilon > T_K$ for short enough leads therefore one does not need the theoretical construction of the screening cloud to explain the experimental findings. In case of an impurity embedded into a higher dimensional environment, another length scale $l_K$ emerges [7] by equating $\Delta (l_K) = T_K$ where $\Delta (l_K)$ stands for the mean level spacing in a box with size $l_K$. For the case of $D \geq 2$ that length scale can be substantially smaller than $\xi_K$. In 1D systems, which are in the focus of the present paper, the two length scales are essentially equal.

Despite those challenges, there were proposals published to observe the Kondo screening cloud. These proposals deal with the Knight shift [8], persistent current [9] or conductance of mesoscopic systems [10].

Very recently, Hand and his coworkers established a proportionality between the weight of Kondo resonance and the spatial extension of the Kondo correlations in mesoscopic systems [11]. This fact allows another, spectroscopic way to observe the Kondo screening cloud. Those proposals are very promising even though the ex-
Since we know that the ground state of the Hamiltonian \( T \) by Eq. (1) forms a singlet below the Kondo temperature \( T_K \) As it is mentioned above, the system described stands for the electron spin density at the position of the impurity. \( c_{\mu} \) and \( c_{\mu}^\dagger \), conduction electron spin density at position \( x \), \( \rho \), \( \Lambda \), \( n \), a quantity which measures the spatial extension of the singlet, the equal-time correlator of the impurity spin and conduction electron spin density at position \( x \):

\[
\chi_{t=0}(x) = \langle S\bar{\sigma}(x) \rangle_{t=0}.
\]

Since we know that the ground state of the Hamiltonian Eq. (1) is a singlet, we can easily derive a sum rule for the equal time correlator at zero temperature:

\[
\int_0^\infty \langle S\bar{\sigma}(x) \rangle_{t=0} dx = \frac{3}{4}.
\]

Method — To calculate spatial correlations is a non-trivial task since most of the methods used to investigate the Kondo model are not able to reproduce correlation functions. Comparatively only a very little of the theoretical study has been focused on spatial correlations: Perturbative calculations have been performed as well as Monte Carlo analysis. In the present paper, we extend NRG to compute the Kondo correlations. Wilson’s NRG—the most useful numerically exact method to obtain correlation functions — suffers from the very bad spatial resolution away from the impurity. This fact is a direct consequence of the corner stone of the method, the logarithmic discretization of the conduction band. In Wilson’s NRG technique, one introduces a discretization parameter, \( \Lambda \) and with the help of that discretizes the conduction band logarithmically by dividing it into intervals (i.e. the \( n \)th interval is \( ] - D_0A^{-n}; -D_0A^{-n}^{-1} \) for negative, and \( [D_0A^{-n}; D_0A^{-n}^{-1}] \) for positive energies measured from the Fermi energy and \( D_0 \) stands for the half bandwidth) and keeping one mode per interval only. As a next step, one maps the problem onto a semi-infinite chain with the impurity at the end by means of a Lanczos transformation. As a consequence of the logarithmic discretization, the hopping amplitude falls off exponentially along the chain allowing us to diagonalize the problem iteratively. As is shown in Ref. [12], the states represented as on-site states on the Wilson-chain correspond to extended states in real space with a typical spatial extension

\[
r_N \sim \frac{1}{k_F} \Lambda^{N/2},
\]

where \( N \) is the site index along the chain. It is obvious that the numerical renormalization group method has a good spatial resolution at the position of the impurity. (See Fig. 1a.) Of course, these fields are not orthogonal, i.e., they do not fulfill the canonical anticommutational relations. As a next step, we can introduce the proper linear combinations of these fields,

\[
\psi_{\pm} = 1/\sqrt{2}(\psi_0 \pm \psi_1)
\]

which are now anticommuting but the corresponding density of states is modified i.e., it acquires energy dependence, e.g., for 1D electrons \( g_{1D}^{\pm}(x) = \varepsilon_0/2[1 \pm \cos(\varepsilon x/v_F)] \). (In 2D the density of states reads \( g_{2D}^{\pm}(x) = \varepsilon_0/2[1 \pm J_0(\varepsilon r/v_F)] \) where \( J_0 \) is the zeroth Bessel function, while in 3D \( g_{3D}^{\pm}(x) = \varepsilon_0/2[1 \pm \sin(\varepsilon r/v_F)/(\varepsilon r/v_F)] \).
As we see, the oscillations of the even/odd density of states decay as \( \sim r^{-(D-1)/2} \), where \( D \) is the dimensionality of the problem.) In the new basis the Kondo Hamiltonian reads

\[
H = \frac{1}{2} J\bar{S}(\psi_+^\dagger + \psi_-^\dagger)\bar{\sigma}(\psi_+ + \psi_-) + \sum_{i=\pm,\mu=\uparrow,\downarrow} \int d\varepsilon \bar{g}(\varepsilon) c_{i\varepsilon\mu}^\dagger c_{i\varepsilon\mu}.
\]  

In this representation \( \bar{\sigma}(x) = 1/2[\psi_+^\dagger - \psi_-^\dagger] \sigma[\psi_+ - \psi_-] \) is represented in a high accuracy. In brief, the main idea behind the above transformation is that one can get a very good spatial resolution at the impurity site as well as at another freely chosen position \( x \) if one is willing to pay the price of (a) having two electron channels mixed by the interaction, (b) having energy dependent density of states and (c) having a separate NRG iteration for every different \( x \) values. Those difficulties are possible to be handled: The most serious one amongst them is the extension of NRG to arbitrary density of states which has been solved by Bulla et al.\(^\text{[18]}\).

Results—In this NRG scheme the calculation of the equal time correlation function is rather simple: \( \chi_{t=0}(x) \) appears to be a static thermodynamic quantity which can be evaluated with a high precision. The results for different Kondo couplings are shown in Fig. 2: the correlation function oscillates as \( \sim \cos^2(k_F x) \). As it is shown in the inset of Fig. 2 the envelope of the correlation function for different Kondo couplings nicely collapse into one universal curve (apart from the points \( x \lesssim \pi/k_F \) which show non-universal, coupling-dependent behavior, not plotted in the inset). The envelope curve (i.e.\( \chi_{t=0}(x = n\pi/k_F) \)) for different \( n \)'s, different couplings and different temperatures: Any finite temperature introduces another energy scale, \( \xi_T = \hbar/2k_BT \) at which the envelope function crosses over from an algebraic to an exponential decay.
its integral. This fact enters the numerical calculation through the $\sim r^{-(D-1)/2}$ decay of density of states oscillations and makes the calculation of $\chi_{t=0}(x)$ challenging for dimensions higher than $D = 1$.

Up to this point we have considered the case of zero temperature $T = 0$. However, it is known that the temperature plays an essential role in Kondo physics: Kondo correlations are destroyed when the temperature reaches the Kondo scale $T \sim T_K$. It is adequate to ask the question how does this fact show up in $\chi_{t=0}(x)$?

Since $\chi_{t=0}(x)$ is a static quantity we obtain its complete temperature dependence by numerical renormalization as the iteration proceeds. In Fig.3 we show the results for $T = 0$, $T = T_K/3$, $T = T_K$, and $T = 3T_K$. As it is transparent from the curves, the effect of finite temperature shows up in the appearance of another length scale, the thermal length scale, $\xi_T = h\nu_F/k_BT$. For $x < \xi_T$ the correlation function $\chi_{t=0}(x)$ is not much affected while for $x > \xi_T$ the correlations are cut off exponentially.

Based on those results we can now interpret the role of finite temperature in Kondo screening as follows: The fact that the impurity spin is perfectly screened at $T = 0$ is reflected in the sum rule given by Eq. [3]. At any finite temperature the integral is reduced and can approximately rewritten as $\int_0^{\xi_T} \chi_{t=0}(x)dx$. When the temperature is lower than the Kondo temperature $T < T_K$, the corresponding thermal length scale is larger than $\xi_K$. Since $\chi_{t=0}(x)$ has its most weight in the region $x < \xi_K$, the effect of a small temperature is just a small correction to the perfect screening obtained at $T = 0$. Given that in the $x > \xi_K$ regime $\chi_{t=0}(x) \sim x^{-2}$, the correction appears to be linear in $T$. In contrast, for $T > T_K$ the corresponding $\xi_T$ is shorter than $\xi_K$ and the correction to the integral is not small and consequently, we cannot speak about the screening of the local moment any more.

Conclusions — We have shown that Wilson’s NRG technique is capable to handle spatial correlations if we apply a straightforward extension. To demonstrate that we have computed the $\langle \hat{S}_i \hat{S}_j(x)\rangle_{t=0}$ correlator for a one dimensional Kondo system and shown that the decay of spin correlations crosses over from $\sim x^{-1}$ to $\sim x^{-2}$ at around the Kondo coherence length, $\xi_K = h\nu_F/k_BT_K$. We have shown by calculating the temperature dependence that any finite temperature introduces a new energy scale beyond which the Kondo correlations vanish exponentially. Our method — apart from the numerical challenges — easy to generalize to other impurity models. A very attractive example would be the two channel Kondo model to see how the non-Fermi liquid nature of the ground state shows up in the spatial spin correlations.

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