Impurity in a Luttinger liquid: a numerical study of the finite size energy spectrum and of the orthogonality catastrophe exponent

Shaojin Qin†, Michele Fabrizio* and Lu Yu†‡

† International Center for Theoretical Physics, P.O. Box 586, 34100 Trieste, Italy.
* International School for Advanced Studies, Via Beirut 2-4, I-34014 Trieste, Italy, and Istituto Nazionale di Fisica della Materia, INFN.
‡ Institute of Theoretical Physics, Academia Sinica, Beijing 100080, China.

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Abstract

The behavior of a single impurity in a one-dimensional Luttinger liquid is numerically investigated by means of the density matrix renormalization group. By analyzing the finite size scaling behavior of the low energy spectrum, we confirm the theoretical prediction of Kane and Fisher [Phys. Rev. Lett. 68, 1220 (1992)] both for attractive and repulsive interactions. Moreover, we calculate the exponent of the orthogonality catastrophe, which gives a further support to the above theoretical prediction.
The problem of an impurity in a one-dimensional (1D) interacting Fermi system (Luttinger liquid) has become quite popular in recent years for its implications to a variety of physical problems as for instance the behavior of quantum wires (see e.g. Refs. [1,2]) or the tunneling through a constriction in the fractional quantum Hall regime [3].

The interesting feature of this problem lies in the fact that the competition between the impurity potential and the electron-electron interaction leads to quite surprising effects. If the interaction is repulsive, the electrons at low energy see the potential barrier as if it were effectively infinite. On the contrary, for an attractive interaction the effective scattering close to the Fermi energy is vanishingly small (see e.g. Ref. [4]). The two different behaviors have a quite simple physical interpretation: in 1D the electron gas is quasi-ordered, i.e. it shows power law decaying correlation functions of the order parameter. Specifically, for repulsive interaction it has a charge density wave, while for attractive interaction a superconductive quasi-long-range order. It is then clear that the two different orderings lead to opposite behavior in the presence of a local potential, which tends to pin the charge density wave but has minor effects for a superconductor.

From the theoretical point of view, the problem has many similarities with the Kondo effect. In fact the problem of a magnetic impurity in a metal can also be transformed into a one-dimensional model of electrons in the presence of a local potential. Moreover, in both cases a perturbation expansion in powers of the impurity potential breaks down at low energy due to the appearance of logarithmic singularities. A standard approach based on renormalization group leads in both cases to the conclusion that the impurity potential flows either to infinity or to zero, depending on the the sign of the exchange in the Kondo model or of the interaction in the Luttinger liquid. Therefore, analogously to the Kondo effect, a low energy description of an impurity in a Luttinger liquid needs a correct identification of the low energy fixed point. In particular, Kane and Fisher [4] (KF) argued that the fixed point corresponds to a chain disconnected at the impurity site for repulsive interaction.

This interpretation has been recently questioned by Oreg and Finkel'stein [7] (OF), specifically in the context of the X-ray edge singularity. These authors find in fact an expo-
ponent of the absorption spectra at the threshold which is not equal to the value compatible with a disconnected chain fixed point [8]. It is however unclear whether they would extend their criticism to all the results which have been obtained on the basis of the disconnected chain fixed point, or if they only doubt about the X-ray edge singularity results. In fact, for other properties, like for instance the finite size spectrum [9] or the conductance through the barrier [9], there exist exact numerical calculations which support KF’s hypothesis, while for the X-ray edge singularity only approximate analytical results are till now available [8].

In this paper we investigate this problem by numerical methods, closely following the kind of analysis in Ref. [9]. In particular we study the low energy spectrum for 1D periodic chains of spinless fermions interacting either with attractive or repulsive interaction in the presence of a local potential. Our numerical results show that this spectrum is compatible with a disconnected chain fixed point for repulsive interaction and with a periodic chain if the interaction is attractive. We also calculate the exponent of the orthogonality catastrophe from the overlap between the ground states in the presence and in the absence of the local potential. This exponent is related to the X-ray edge singularity exponent, and therefore our results can solve the above mentioned controversy. We find that the orthogonality catastrophe exponent again points in favor of the KF hypothesis.

The development of the density matrix renormalization group (DMRG) method [9] has made possible the study of the ground state and low excited states of one-dimensional systems with large number of sites. Previous DMRG studies on $S = 1/2$ chains has proved also quite successful in determining the finite size behavior of the low excitation energies, correlations and Friedel’s oscillation due to boundary effects [10]. In this paper, we use DMRG to study the low energy spectrum for anisotropic $S = 1/2$ Heisenberg chains with a local perturbation. This model can be mapped through a Jordan-Wigner transformation onto a model of interacting spinless fermions with a local impurity potential.

An $S = 1/2$ spin-anisotropic Heisenberg chain with open boundary conditions (OBC) is described by the Hamiltonian

$$H = \sum_{i} (J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) + \sum_{i} V_i S_i^z$$
\[ H = \sum_{i=1}^{L-1} \left[ \frac{J_{xy}}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + J_z S_i^z S_{i+1}^z \right], \]  

where \( S_i^+ \) and \( S_i^- \) are spin raising and lowering operators at site \( i \), \( S_i^z \) being its z-component.

For periodic boundary conditions (PBC) the \( L^{th} \) and 1st site are also coupled by the same exchange couplings \( J_{xy} \) and \( J_z \). An impurity site potential is introduced by adding a nonzero local magnetic field at the 1st site in the periodic chain. An impurity bond is instead introduced by coupling the \( L^{th} \) and 1st site with exchanges \( J'_{xy} \) and \( J'_z \) different from the bulk values \( J_{xy} \) and \( J_z \).

Eggert and Affleck [5] have shown that the systems flow to the OBC fixed point whenever the impurity bond strengths between the 1st and \( L^{th} \) sites differs from the bulk values. They have studied odd length chains under global SU(2) symmetry (\( J_{xy} = J_z \) and \( J'_{xy} = J'_z \)) by comparing the parity, multiplicity, and magnitude of energies of the ground state and the lowest excited states. We have extended their analysis by considering both even and odd length chains, either for site impurity or bond impurity, and also in the case when SU(2) symmetry is explicitly broken.

Particularly, in the presence of spin anisotropy, we find numerically that the low energy spectrum in the presence of a local potential flows to the OBC spectrum if \( 0 < J_z/J_{xy} < 1 \), and to the PBC spectrum if \( -1 < J_z/J_{xy} < 0 \), thus in agreement with the theoretical prediction of Ref. [4]. For the sake of clarity, we are going to present our numerical data for the specific case of even length chains with bulk anisotropies \( J_z/J_{xy} = 0.5 \) and \(-0.5\), which correspond, respectively, to repulsive and attractive interactions in the equivalent spinless fermion model.

We introduce the impurity potential by bond couplings \( J'_z = bJ_z \) and \( J'_{xy} = bJ_{xy} \), and denote the anisotropy by \( a = J_z/J_{xy} \). We calculate the ground state energy \( E_0 \) and the first excited energy \( E_1 \) for even length chains by DMRG. The ground state and the first excited state are the lowest energy states in the sectors with z-component of the total spin \( S_z^{\text{tot}} = 0 \) and 1, respectively. We use the parity of the ground state as a reference, and we consider as quantum numbers of the lowest energy states their z-component of the total spin and their
parity. Each state is therefore represented by a fixed value of $S_z^{+(-)}$, where $+$ is the parity of the ground state and $-$ denotes the opposite parity. The ground state is then represented by $0^+$ and the first excited state $E_1$ by $1^-$. The two energy levels of the low energy spectrum we choose to study are $0^-$ and $1^+$, and we denote their energies by $E_2$ and $E_3$, respectively.

For different impurity bond strength $b$, $L[E_1(a,b) - E_0(a,b)] = \pi v_F$ is a bulk property and therefore remains the same for fixed anisotropy $a$. This is shown in Fig.1 for $a = \pm 0.5$ and $b = 0, 0.1$ and 1, ($b = 0$ and 1 are the values for OBC and PBC, respectively). The behavior of the low energy spectrum in the presence of the local potential is instead made evident by the flow of the two energy levels $E_2$ and $E_3$. We use the energy unit $\pi v_F/L$, i.e. we scale the energy as

$$e_2(a,b) = \frac{E_2(a,b) - E_0(a,b)}{E_1(a,b) - E_0(a,b)},$$
$$e_3(a,b) = \frac{E_3(a,b) - E_0(a,b)}{E_1(a,b) - E_0(a,b)}.$$ (2)

For attractive electron-electron interaction ($a = -0.5$), we plot in Fig.2 $e_2(-0.5,b)$ and $e_3(-0.5,b)$ for different $b$-values: $b = 0$, corresponding to OBC; $b = 1$ for PBC, and $b = 0.1$ for an intermediate case. It is clear from Fig.2 that $e_2(-0.5,0.1)$ and $e_3(-0.5,0.1)$ flow to $e_2(-0.5,1)$ and $e_3(-0.5,1)$, respectively, i.e. they flow to PBC. We just mention that other energy levels of the spectrum for attractive interaction $-1 < a < 0$ also flow to those with PBC. For repulsive electron-electron interaction ($a = 0.5$), we plot in Fig.3 $e_2(0.5,b)$ and $e_3(0.5,b)$ for different $b$-values. The energy levels of the spectrum for repulsive interaction flow to those with OBC.

The same conclusions can be drawn for other values of the spin-anisotropy $a$ and other impurity bond strength $b$, or by substituting the bond potential with a site potential provided by a local magnetic field, or else for the odd length chain case (which however has already been extensively discussed in Ref. [5]).

Therefore our numerical results show that PBC is the fixed point towards which the system in the presence of a local potential flows when the interaction is attractive, while OBC is the fixed point for systems with repulsive interaction.
An interesting quantity which can also be evaluated numerically and which further supports the interpretation of the strong coupling fixed point in terms of a perfectly reflecting barrier is the exponent $\alpha$ of the orthogonality catastrophe [11]. This exponent is defined through the overlap between the ground state wave functions for a system of size $L$ in the presence, $|\phi\rangle$, and in the absence, $|\phi_0\rangle$, of the impurity potential. In particular,

$$\langle \phi|\phi_0 \rangle \sim \left(\frac{1}{L}\right)^\alpha.$$  \hspace{1cm}(3)

The orthogonality exponent is intimately related to the exponent of the X-ray edge singularity. Let us assume that the scattering potential is present if some localized level is empty and is absent otherwise. The localized state Green function can be shown to decay at long times like:

$$G(t) = \langle \phi_0|d(t)d(0)|\phi_0 \rangle = \langle \phi_0|e^{i\hat{H}_0 t}e^{-i\hat{H}t}|\phi_0 \rangle \sim e^{-iE_{\text{edge}}t} \left(\frac{1}{t}\right)^{2\alpha},$$  \hspace{1cm}(4)

where $d$ is the operator which empties the localized level, $\hat{H}_0$ and $\hat{H}$ the Hamiltonians in the absence and in the presence of the scattering potential, respectively. In the absence of electron-electron interaction, the exponent $\alpha$ can be exactly determined [11] and is given by:

$$2\alpha = \left(\frac{\delta_{e\pi}}{\pi}\right)^2 + \left(\frac{\delta_{o\pi}}{\pi}\right)^2.$$  \hspace{1cm}(5)

The phase shifts of the even ($\delta_e$) and odd ($\delta_o$) scattering channels can in turn be related to the properties of the barrier, since

$$\delta_{e(o)} = \frac{1}{2} \left(\delta_\mp \tan^{-1} \frac{|r|}{|t|}\right),$$  \hspace{1cm}(6)

where the transmission amplitude $t = |t|e^{i\delta_t}$, and $r$ is the reflection coefficient.

In order to simplify the interpretation of the numerical results, we consider an anisotropic Heisenberg chain of length $L$. The ground state is in the subspace with total spin $z$-component $S_z = 0$. The impurity potential is provided by modifying the exchange of a single bond in the chain. This model maps onto a chain of interacting spinless fermions at half filling. The impurity potential is such as to preserve the particle-hole symmetry of the
Hamiltonian. As a consequence, the forward scattering phase shift $\delta_+ = 0$, since a finite $\delta_+$ would imply a breaking of the particle-hole symmetry. Before presenting the numerical results, it is worthwhile to discuss what the theory would predict for the exponent $\alpha$. As we already mentioned, according to Kane and Fisher the strong coupling fixed point towards which the model flows in the long wavelength limit consists of an Heisenberg open chain: the impurity has simply changed the boundary conditions from periodic to open. In this case the exponent is predicted to be $\alpha = 1/16$ \[8\], which corresponds simply to take $\delta_+ = 0$ and $|r/t| \to \infty$ in Eq.(6). As we previously said, the KF interpretation has been questioned by OF in the context of the X-ray edge singularity \[7\]. Following them, we expand the Green function (4) in powers of the impurity potential. Each term in the perturbation expansion can be evaluated exactly in the long-time limit and finally we find, in accordance with OF, that the imaginary time Green function $G(\tau)$ coincides with the partition function of a two-dimensional classical Coulomb gas confined on a line of length $\tau$. The relevance of the impurity potential translates in the language of the Coulomb gas into an increasing fugacity: the gas is therefore in the plasma phase. If $\tau$ is much bigger than the screening length of the plasma $\tau_{scr}$, then OF have predicted that

$$\lim_{\tau \gg \tau_{scr}} G(\tau) = e^{-E_{edge}\tau} \text{const.},$$

which would imply an exponent $\alpha = 0$. As we see the two theoretical approaches lead to two completely different results; therefore the exact numerical approach we are going to describe turns out to be quite decisive.

We denote the overlap integrals to be evaluated numerically and their exponents as:

$$O_P(L) = \langle \phi_{PBC}|\phi \rangle \propto \left(\frac{1}{L}\right)^\alpha,$$

$$O_O(L) = \langle \phi_{OBC}|\phi \rangle \propto \left(\frac{1}{L}\right)^\beta,$$

where the ground states are $|\phi_{PBC}\rangle$ for PBC, $|\phi_{OBC}\rangle$ for OBC, and $|\phi\rangle$ for chains with PBC but in the presence of a modified bond $0 < b < 1$. The exponents $\alpha$ and $\beta$ are given by

$$\alpha(a, b) = \frac{\ln O_P(L+2) - \ln O_P(L)}{\ln L - \ln(L+2)},$$

$$\beta(a, b) = \frac{\ln O_O(L+2) - \ln O_O(L)}{\ln L - \ln(L+2)}.$$
For anisotropy $a = \pm 0.5$ and impurity bond strength $b = 0.1, 0.9$, we calculate the ground states by DMRG method, and then calculate the exponents $\alpha(a, b)$ and $\beta(a, b)$. We plot in Fig.4 the exponents as a function of $-2/[\ln L + \ln(L + 2)]$ for different sizes $L$. The figure shows that $\alpha(a, b)$ flows to $1/16$ and $\beta(a, b)$ to $0$ for repulsive interaction ($a = 0.5$), and vice versa for attractive interaction ($a = -0.5$).

The values $\alpha = 0$ and $\beta = 1/16$ which we find for attractive interaction are in agreement with the flowing of the system to the PBC fixed point. On the other hand, $\alpha = 1/16$ and $\beta = 0$ for repulsive interaction show that the system flows indeed to the OBC fixed point, thus in agreement with Kane and Fisher’s interpretation of the strong coupling fixed point and with the analytical results of Refs. [8].

In conclusion, we have investigated by numerical DMRG method the impurity problem in a Luttinger liquid. All our results, which include a detailed analysis of the finite size scaling behavior of the low energy spectrum and the evaluation of the orthogonality catastrophe exponent, suggest that at low energy the barrier acts as it were perfectly reflecting. The orthogonality catastrophe exponent result may help to clarify the controversy recently raised by the authors of Ref. [7] about the X-ray edge singularity [12].

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FIGURES

FIG. 1. The first excitation energy $E_1(a, b) - E_0(a, b)$ multiplied by chain length $L$ is plotted v.s. $1/\ln L$, $L = 4, 6, \cdots, 60$, for different values of the anisotropy $a = \pm 0.5$ and impurity bond strength $b = 0, 1, 0.1$.

FIG. 2. The scaled low energy levels $e_2(a, b)$ and $e_3(a, b)$ of Eq.(2) for attractive interaction ($a = -0.5$) are plotted v.s. $1/\ln L$, $L = 4, 6, \cdots, 50$. $e_2(-0.5, 0)$, $e_3(-0.5, 0)$ is for OBC ($b = 0$), $e_2(-0.5, 1)$, $e_3(-0.5, 1)$ for PBC ($b = 1$), and $e_2(-0.5, 0.1)$, $e_3(-0.5, 0.1)$ for impurity chains.

FIG. 3. The scaled low energy levels $e_2(a, b)$ and $e_3(a, b)$ of Eq.(2) for repulsive interaction ($a = 0.5$) is plotted v.s. $1/\ln L$, $L = 4, 6, \cdots, 40$. $e_2(0.5, 0)$, $e_3(0.5, 0)$ is for OBC ($b = 0$), $e_2(0.5, 1)$, $e_3(0.5, 1)$ for PBC ($b = 1$), and $e_2(0.5, 0.1)$, $e_3(0.5, 0.1)$ for impurity chains.

FIG. 4. The exponents $\alpha(a, b)$ and $\beta(a, b)$ of Eq.(10) are plotted for both repulsive and attractive interactions $a = \pm 0.5$ and impurity bond strength $b = 0.1, 0.9$ as a function of $-2/[\ln L + \ln(L + 2)]$ with $L = 4, 6, \cdots, 48$. The fitting lines indicate that $\alpha(-0.5, 0.1)$ and the $\beta(0.5, 0.1)$ flow to zero, while $\alpha(0.5, 0.1)$ and $\beta(-0.5, 0.1)$ flow to $1/16$. 
Fig. 1 Qin, Michele, and Yu

\[ L(E_1 - E_0) \]

- \( a = 0.5, b = 0.0 \)
- \( a = -0.5, b = 0.0 \)
- \( b = 0.1 \)
- \( b = 1.0 \)

fitting lines
Fig. 2 Qin, Michele, and Yu

$e_2$ and $e_3$

$1/\ln(L)$

fitting lines
Fig. 3 Qin, Michele, and Yu

$\text{fitting lines}$

- $e_2(0.5, 1.0)$
- $e_3(0.5, 1.0)$
- $e_2(0.5, 0.1)$
- $e_3(0.5, 0.1)$
- $e_2(0.5, 0.0)$
- $e_3(0.5, 0.0)$

$e_2$ and $e_3$
Fig. 4 Qin, Michele, and Yu

$\alpha(0.5,0.1)$
$\alpha(-0.5,0.1)$
$\beta(0.5,0.9)$
$\beta(-0.5,0.9)$
fitting lines