Scaling of the conductance in a quantum wire

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The conductance $G$ of an interacting nano-wire containing an impurity and coupled to non-interacting semi-infinite leads is studied using a functional renormalization group method. We obtain results for microscopic lattice models without any further idealizations. For an interaction which is turned on smoothly at the contacts we show that one-parameter scaling of $G$ holds. If abrupt contacts are included we find power-law suppression of $G$ with an exponent which is twice as large as the one obtained for smooth contacts and no one-parameter scaling. Our results show excellent agreement with the analytically known scaling function at Luttinger liquid parameter $K = 1/2$ and numerical density-matrix renormalization group data.

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The interplay of electron correlations and a single impurity in one-dimensional electron systems leads to striking effects in the low-energy physics. Using bosonization and including a single impurity in an idealized manner the application of a perturbative (in the strength of the impurity) renormalization group (RG) method to the resulting local sine-Gordon model (LSGM) led to a simple picture: at low energy scales physical observables behave as if the system is split in two chains with open boundary conditions at the end points. The bulk part of the model studied is known to capture the universal bulk Luttinger liquid (LL) parameter, which is characterized by the interaction dependent LL parameter $K < 1$ (repulsive interaction). Considering the conductance $G$ as a function of the temperature $T$ and the strength of the impurity $v$ it was argued that for fixed $K$ the RG flow from weak to strong impurity strength determines a scaling function $\tilde{G}_K(x)$ on which the data for different $T$ and $v$ can be collapsed (one-parameter scaling). Going beyond the perturbative RG it was shown that scaling indeed holds for the LSGM. Applying the thermodynamic Bethe ansatz (BA) $\tilde{G}_K$ was determined explicitly for $K = 1/2$ and $K = 1/3$. In Refs. 5, 7, 8 the transport in fractional quantum Hall effect systems was studied and thus an infinite LL without leads was considered. Then in the impurity free case the conductance is renormalized by the interaction, $G^* = K e^2/h$. If the connection of a finite LL quantum wire to non-interacting leads is modeled by a position dependent LL parameter $K(x)$ which takes the value one in the leads (local LL description), the conductance is given by $G^* = e^2/h$ in the impurity free case. The question how the one-parameter scaling of the conductance of the system with an impurity is modified in the presence of leads was not addressed before.

Using numerical methods it was shown that the LSGM captures the behavior observed in a microscopic lattice model in the limits of weak and strong impurities. Based on these results it is generally believed that (i) one-parameter scaling holds for a large class of models of correlated electrons with a single impurity and (ii) the data always scale on the universal scaling function $\tilde{G}_K$ found within the LSGM. The issue of universality is of special importance since transport experiments have been interpreted in terms of scaling.

Here we study the transport through an interacting nano-wire with an impurity connected to non-interacting semi-infinite leads. The wire is modeled by the lattice model of spinless fermions with nearest-neighbor interaction and a hopping impurity. Using a fermionic functional RG method we are able to calculate $G$. We show that for a single impurity, if the interaction is turned on very smoothly starting at the contacts and no one-particle scattering terms (see Eq. (1)) at the contacts are considered (smooth contacts) one-parameter scaling holds also in the presence of leads. For $K = 1/2$ the data perfectly match the LSGM curve $\tilde{G}_{K=1/2}$ provided the impurity free conductance $G^*$ is taken to be $e^2/h$ instead of $Ke^2/h$ as appropriate for systems with leads. The latter gives us confidence that, despite the approximate treatment of the interaction our approach captures the relevant physics. This is further supported by a comparison to numerical data for the conductance obtained by the density-matrix renormalization group (DMRG) method. In the more generic case with abrupt contacts, i.e. if the interaction is turned on more rapidly or one-particle scattering terms at the contacts are included, we find a low-energy power-law suppression of $G$ with an exponent which is twice as large as the one obtained for smooth contacts and no one-parameter scaling. Evidently in most experiments with quantum wires the contacts are abrupt.

The model we study is given by the Hamiltonian

$$H = -\sum_{j=-\infty}^{\infty} \left( c_j^\dagger c_{j+1} + h.c. \right)$$

$$-t_1 \left( c_0^\dagger c_1 + h.c. \right) - t_r \left( c_{Nw}^\dagger c_{Nw+1} + h.c. \right)$$

$$-\rho \left( c_{Nw/2}^\dagger c_{Nw/2+1} + h.c. \right)$$

$\rho$, $t_1$, and $t_r$ are coupling constants, $\rho = 1/2\times10^{-7}$.
\[ + \sum_{j=1}^{N_W-1} U_j \left( n_j - \frac{1}{2} \right) \left( n_{j+1} - \frac{1}{2} \right), \] (1)

in standard second-quantized notation. The sum in the first line runs over all lattice sites \( j \) excluding \( j = 0, N_W/2, \) and \( N_W \), which is indicated by the prime. The hopping matrix element and the lattice constant are set to 1. We consider an even number \( N_W \) of lattice sites in the interacting region (the wire). A single hopping impurity of strength \( \rho \leq 1 \) and modified hopping matrix elements \( t_{l/r} \leq 1 \) in and out of the wire are included. Here we focus on the half-filled system. The nearest-neighbor interaction \( U \) close to the contacts at sites 1 and \( N_W \) is assumed to be spatially varying. The constant bulk value of the interaction is denoted by \( U \). The bulk LL parameter is given by \( K = \left[ \frac{2}{\pi} \arccos \left( -\frac{U}{2} \right) \right]^{-1} \), for \( U \leq 2 \), as follows from the BA solution.\(^{14,15}\)

In linear response and at \( T = 0 \) the conductance can be determined from the one-particle Green function of the interacting wire taken at the chemical potential and calculated in the presence of the non-interacting semi-infinite leads.\(^{16}\) For the half-filled case we obtain \( G = 4e^2t^2_{l/r} \left| G_{N_W,1}(0) \right|^2 / h \), with the Green function \( G_{N_W,1} \).

In our earlier applications of the RG method\(^{13,17}\) we neglected the flow of the two-particle vertex and considered the flow of the self-energy only. Within this approximation the LL exponents relevant for the impurity problem turned out to be correct to leading order in the interaction. We here go beyond this and include the flow of the vertex in an approximate way. We replace the three-particle vertex by its initial value 0. The flow equation for the two-particle vertex then reads

\[
\partial_\Lambda \Gamma^A(\alpha, \beta; \gamma, \delta) =
- \text{Tr} \left\{ P^A \Gamma^A(\ldots; \gamma, \delta) \left[ \Gamma^A \right]^{-1} \Gamma^A(\alpha, \beta; \ldots) \right\}
- \text{Tr} \left\{ P^A \Gamma^A(\alpha, \ldots; \gamma, \delta) \Gamma^A(\beta, \ldots; \delta \ldots) \right\}
- \left[ \alpha \leftrightarrow \beta \right] \left[ \gamma \leftrightarrow \delta \right] + \left[ \alpha \leftrightarrow \beta, \gamma \leftrightarrow \delta \right].
\]

The Greek letters stand for the quantum numbers of the basis in which the problem is considered and the Matsubara frequencies. On the right hand side \( \Gamma^A \) is understood as a matrix in the variables which are not written. \( P^A = G^A \left( \partial_\Lambda \left[ \left[ G^{0A} \right]^{-1} \right] \right) \), with \( G^A = \left[ \left[ G^{0A} \right]^{-1} - \Sigma^A \right]^{-1} \)

and the cut-off dependent self-energy \( \Sigma^A \). \( G^{0A} \) is the non-interacting impurity free propagator supplemented by an infrared cut-off. As before we use a frequency cut-off \( G^{0A} = \Theta(\omega - \Lambda)G^0 \), with \( \Lambda \in [\infty, 0] \). In the flow of the vertex we replace \( \Gamma^A \) by \( G^{0A} \). We neglect the frequency dependence of the vertex which leads to a frequency independent self-energy. Due to this the bulk LL properties of the model are only partially captured by our approximation. In particular we miss the bulk anomalous dimension which is small compared to the impurity contribution included in our approach. We parameterize \( \Gamma^A \) by an effective nearest-neighbor interaction with a renormalized amplitude \( U^A \), whose flow is determined by projecting onto the Fermi points. In this way the fixed point coupling is guaranteed to be correct to order \( U^2 \). The coupling to the leads is neglected. Within these approximations the flow equation for \( U^A \) closes. In the thermodynamic limit it can be integrated analytically leading to

\[
\frac{U^A}{U} = \left( 1 + \frac{\Lambda U}{2\pi} - \frac{U}{2\pi} \frac{2 + \Lambda^2}{\sqrt{4 + \Lambda^2}} \right)^{-1}.
\]

Details of this approximation scheme are presented elsewhere.\(^{18}\) The one-particle Green function of the interacting wire in the presence of the semi-infinite leads and thus the conductance can then be determined numerically by integrating Eqs. (14) and (15) of Ref. 13 using \( U^A \) instead of \( U \). On the right hand side of Eq. (14) the self-energy on sites 1 and \( N_W \) has to be modified: due to the coupling to the leads terms which can be expressed by \( t_{l/r} \) and the \( t_{l/r} = 0 \) Green function of the leads at sites 0 and \( N_W + 1 \) have to be added. The initial condition for \( \Sigma^A \) is given by the impurity potential. Below we show that the above approximation scheme leads to exceptionally good results.

![Fig. 1. Conductance as a function of \( U \) for \( N_W = 12 \), \( \rho = 0.5 \), \( t_{l/r} = 1 \). The interaction is turned on sharply.](image-url)
numerically integrated the finite size flow equation for 
the vertex, but even for $N_W = 12$ the difference between 
using this and the $N_W \to \infty$ result of Eq. (2) is only 
marginal.

For the results presented below we choose 
$\rho = 1$, $t_{i/r} = 1$ (impurity free; circles), $\rho = 0.5$, $t_{i/r} = 1$ 
(squares), and $\rho = 0.5$, $t_{i/r} = 0.7$ (diamonds). The interaction 
is turned on sharply.

Assuming an interaction which is turned on (and off) 
sharply (in space), i.e. $U_j = U$ for $j = 1, 2, \ldots, N_W - 1$, 
leads already in the absence of single particle scattering 
terms (i.e. $t_{i/r} = \rho = 1$) to a conductance which depends 
on $U$ and $N_W$.\cite{23, 20, 17} For large $N_W$, i.e. at low energy 
scales, $G$ goes to zero with a power-law as shown in Fig. 2 
(circles). This strong influence of an abrupt contact has 
not been discussed before. To unambiguously determine 
the exponent exceptionally large wires of up to $10^6$ lattice 
sites have to be considered.\cite{24} For smaller $U$ even larger 
$N_W$ are required. We find that $G \sim N_W^{2(1/1-K)}$. Since 
our approach involves an approximate treatment of the 
interaction we only obtain an approximation $K_{RG}$ for $K$.

For $U = 1.5$ we find $K_{RG} = 0.643$, in excellent agreement 
with the BA result $K = 0.649$. The above exponent is 
equivalently the one found in the LSGM including one impurity\cite{5} 
if $T$ is replaced by $1/N_W$ (see below). The other curves 
of Fig. 2 will be discussed later. To avoid the suppression 
of $G$ due to the contacts and to investigate the role of a 
single impurity in the wire we now turn on the interaction 
smoothly: $U_j = U \pi/2 + \arctan (s(j - j_s/2))/\pi$ for $j = 1, 2, \ldots, j_s - 1$, $U_j = U$ for $j = j_s, \ldots, N_W/2$, and $U_{N_W-j} = U_j$ for $j = N_W/2 + 1, \ldots, N_W - 1$. The larger 
$N_W$ and $U$ the smoother $U_j$ has to be varied to obtain the 
incomplete free conductance for $t_{i/r} = \rho = 1$. This procedure 
enables us to quantify the terms “perfectly” and 
“adiabatically” connected used in the field theoretical 
modeling of transport through an impurity free LL.\cite{9, 10}

In the absence of an impurity we find $G^* = e^2/h$ in agreement 
with the local LL description mentioned earlier.\cite{9, 10}

For the results presented below we choose $s$ and $j_s$ such 
that for $t_{i/r} = \rho = 1$ the relative deviation of the con-
ductance from $e^2/h$ is less than $2 \times 10^{-4}$. For the system 
sizes considered in the following ($N_W \geq 256$) we do not 
expect the local change of the interaction strength over 
a few lattice sites to have a relevant effect on the flow of 
the bulk two-particle vertex and thus neglect this local 
change in the flow of the vertex. It turned out that 
as long as the switching on of the interaction is smooth 
and the bulk part of the wire is large compared to 
the switching region, $G$ is independent of the details of 
the switching procedure as expected. To determine $U^A$ 
we use Eq. (2) obtained for $N_W \to \infty$.

In the LSGM the conductance is studied as a function of temperature.\cite{5, 7, 8} Here we limit ourselves to $T = 0$ 
but treat wires of finite length. We expect that the tem-
perature scaling can directly be translated into a scal-
ing in $1/N_W$ and thus study $G$ as a function of $1/N_W$. 
For a certain value of $U$ we later confirm this by a di-
rect comparison of the scaling function calculated by us 
with $G_{K=1/2}$ obtained within the LSGM. The variable in 
which scaling is expected is $N_W/N_0$, where $N_0$ denotes 
a non-universal length scale, i.e. $N_0$ depends on the details 
of the model and its parameters [here $N_0 = N_0(U, \rho)]$.

FIG. 2. Conductance as a function of $N_W$ for $U = 1.5$, 
$\rho = 1$, $t_{i/r} = 1$ (impurity free; circles), $\rho = 0.5$, $t_{i/r} = 1$ 
(squares), and $\rho = 0.5$, $t_{i/r} = 0.7$ (diamonds). The interaction 
is turned on sharply.

FIG. 3. Scaled conductance for an interaction which is 
turned on smoothly with the bulk strength $U = 1$ and 
$t_{i/r} = 1$. Different symbols stand for different $\rho$ and 
$N_W = 256, 512, \ldots, 4096$ in each case.

For the universality of scaling to hold it is necessary 
that $G$ for small impurity strength, i.e. $1 - \rho \ll 1$, and 
small $N_W$ scales as $1 - G/(e^2/h) \sim N_W^{2(1-K)}$ and 
for large impurity strength, i.e. $\rho \ll 1$, and large $N_W$ as 
$G/(e^2/h) \sim N_W^{2(1-K)}$.\cite{5} Using the functional RG we find 
power-law behavior in both these limits with exponents 
which according to the above two relations can be ex-
pressed consistently in terms of a single approximate LL 
parameter $K_{RG}$. For example we find $K_{RG}(U = 0.5) = 
0.858$ and $K_{RG}(U = 1) = 0.741$ both in excellent agreement 
with the exact values $K = 0.861$ and $K = 0.75$ obtained 
from the BA. To demonstrate one-parameter 
scaling we calculated $G$ for $\rho = 0.99, 0.98, \ldots, 0.95,$
\( \rho = 0.9, 0.85 \ldots, 0.05, N_W = 256, 512, \ldots, 4096, j_x = 22, s = 2, \) and various \( U. \) As an example Fig. 3 shows that for \( U = 1 \) the data can be collapsed on a single curve \( G_{\text{RG}}/(e^2/h) \) with \( x = [N_W/N_0(U, \rho)]^{1-K_{\text{RG}}} \) as a scaling variable. The limiting behavior discussed above leads to the asymptotic \( x \) dependence (solid lines) indicated in the figure.

**FIG. 4.** The same as in Fig. 3 but for \( U = 2.23. \) The solid line is the \( K = 1/2 \) scaling function of the LSGM.

After showing that we find one-parameter scaling for the lattice model considered also in the presence of leads (provided the contacts are assumed to be smooth) we now compare the resulting scaling function to the one determined analytically within the LSGM for \( K = 1/2.^{5} \) We find that \( U = 2.23 \) leads to \( K_{\text{RG}} \approx 1/2. \) This is fairly close to \( U = 2 \) which in the BA solution gives \( K = 1/2. \) Within our approximation the RG method does not capture the charge density wave ordering transition at \( U = 2 \) occurring in the exact treatment of the impurity free model.\(^{15} \) A comparison of the RG data (\( \rho, N_W, j_x, \) and \( s \) as above) with the LSGM function (solid line) is presented in Fig. 4. The excellent agreement shows that in both physical situations the same scaling function is found if the conductance is divided by \( e^2/h \) instead of \( K e^2/h, \) which is appropriate when no leads are present. The assumed equivalence of \( T \) and \( 1/N \) scaling holds and our method captures the relevant physics quantitatively despite our approximate treatment of the interaction. Obviously (see Figs. 3 and 4) the scaling function depends on the interaction, i.e. the LL parameter, as expected from the LSGM. This has to be contrasted to the fermionic RG procedure of Ref. 25, where the scaling function for arbitrary interaction turns out to be the non-interacting one, if the scaling variable \( x \) is defined as above.

For \( U = 0.5, 1, \) and 2.23 the length scale \( N_0 \) is shown in Fig. 5 as a function of the non-interacting reflection amplitude \( |R| = (1-\rho^2)/(1+\rho^2). \) For \( N_0 \gg 1 \) this scale provides a measure for how large \( N_W \) has to be for a given \( \rho \) and \( U \) before the strong impurity limit is reached. Using a site impurity, a combination of site and hopping impurities, and different positions of the local impurity we have verified that scaling holds for generic types of impurities and that independently of the type of impurity for fixed \( U \) the same scaling function is found.

We next study the more generic case of a single impurity in an interacting wire taking abrupt contacts into account. They are modeled considering either \( t_{l/r} < 1 \) or an interaction which is turned on sharply, i.e. \( U_j = U \) for \( j = 1, 2, \ldots, N_W - 1. \) For the latter case \( G \) as a function of \( N_W \) is shown in Fig. 2 (squares) for \( \rho = 0.5, t_{l/r} = 1, \) and \( U = 1.5. \) We find that the suppression of \( G \) in the low energy limit again follows a power-law but with the exponent \( 4(1 - 1/K) \) which is twice as large as the one obtained for smooth contacts. The same holds if the contacts are modeled by additional reduced \( t_{l/r} \) independent of whether the interaction is turned on smoothly or sharply. In this case the asymptotic regime is reached for much smaller systems as can be seen in Fig. 2 for \( \rho = 0.5, t_{l/r} = 0.7 \) (diamonds). In both the above cases the data for different \( \rho \) and \( N_W \) cannot be collapsed on a single curve by a one-parameter scaling ansatz. Considering other types of impurities, asymmetric coupling to the leads, and different positions of the local impurity we have verified that the exponent \( 4(1 - 1/K) \) is found generically. We thus believe that the low-energy and resonant tunneling properties in most transport experiments on interacting quantum wires including a single impurity and coupled to non-interacting leads via contacts are governed by the exponent \( 4(1 - 1/K) \) instead of \( 2(1 - 1/K). \) One-parameter scaling cannot be expected to hold. This observation might be relevant for the attempts to interpret recent resonant tunneling experiments on carbon nanotubes.\(^{26} \)

In summary, using a functional RG method we have shown that in a lattice model of interacting one-dimensional electrons with a single impurity one-parameter scaling of the conductance holds even in
the presence of non-interacting leads if smooth contacts are considered, that is if the interaction is turned on smoothly and no additional one-particle scattering terms at the contacts are included. By comparison to numerical DMRG data and the $K = 1/2$ scaling function of the LSGM we have verified that the approximate treatment of the interaction is valid up to fairly large interactions. We have shown that in the impurity free case a sharp onset of the interaction leads to a power-law suppression of $G$ with an exponent $2(1 − 1/K)$ which is the same as the one found for a single impurity within the LSGM. In the generic case of abrupt contacts and a single impurity in the wire we do not find one-parameter scaling and the low-energy properties are governed by the exponent $4(1 − 1/K)$. The functional RG approach has the important advantage that it is very flexible and allows to determine the conductance for microscopic lattice models of correlated electrons without any further idealizations. The spin degree of freedom can be included. For further studies the combination of the fermionic lattice description and the functional RG approach allows for a more realistic microscopic modeling of contacts and leads.

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