

A Single Impurity in a Luttinger Liquid: How it “Cuts” the Chain*

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Using a fermionic renormalization group method we present a simple real space picture of the strong influence an impurity has on the electronic properties of a Luttinger liquid. We compute the flow of the renormalized impurity potential for a single impurity over the entire energy range - from the microscopic scale of a lattice-fermion model down to the low-energy limit. We confirm that low energy properties close to the impurity are as if the chain is cut in two pieces with open boundary conditions at the end points, but show that this universal behavior is only reached for extremely large systems. The accuracy of the renormalization group scheme is demonstrated by a direct comparison with data obtained from the density-matrix renormalization group method.

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1. INTRODUCTION

The detailed theoretical understanding of the low-energy electronic properties of one-dimensional interacting electron systems obtained within the last fifty years has mainly been reached by mapping microscopic models onto an effective field theory using the very powerful technique of bosonization.¹ Bosonization, renormalization group (RG) investigations,² and the use of conformal field theory¹ have led to the concept of Luttinger liquid (LL) behavior which unifies the low-energy physics of a wide class of models. In the mapping process terms which are expected to be irrelevant in the low-energy limit are neglected and the energy scales of the microscopic models get lost.

*Dedicated to P. Wölfle on the occasion of his 60th birthday

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Therefore a direct investigation of lattice models is necessary to obtain informations about the *energy scales* at which the typical LL power-laws and thus *universal behavior* can be expected. This is of special importance in connection with the interpretation of experimental data. Such an investigation might furthermore lead to a more intuitive understanding of the mechanisms involved in the physics of low-dimensional correlated electrons. Here we present such a direct fermionic discussion using analytical and numerical techniques focusing on the drastic influence a single impurity has on the low-energy physics of LL's.^{3,4,5,6,7,8}

Within bosonization an impurity with scattering amplitudes $V_{k,k'}$, (k denotes the wave vector) is modeled by forward and backward scattering only, i.e. k and k' are restricted to $\pm k_F$, where k_F is the Fermi wave vector. Both scattering channels are furthermore decoupled. A perturbative bosonic RG calculation⁶ and a boundary conformal field theory analysis⁷ led to the following picture: For a chain of spinless fermions⁹ with repulsive interactions (LL parameter $K_\rho < 1$) the backscattering amplitude V_B presents a relevant perturbation which grows as $\Lambda^{K_\rho-1}$ when the flow parameter Λ is sent to zero. This leads to a breakdown of the perturbative analysis. The scaling behavior can be traced back to the power-law singularity of the $2k_F$ density response function in a LL.^{3,4} On the other hand⁶ a weak hopping t_w between the open ends of two semi-infinite chains is irrelevant and scales to zero as $\Lambda^{K_\rho-1}$. *Assuming* that the open chain presents the only stable fixed point it was argued that at low energy scales and even for a weak impurity physical observables behave as if the system was split in two semi-infinite chains with open boundary conditions at the end points.⁶ Our main interest will be on the local spectral weight $\rho_j(\omega)$ for lattice sites j close to the impurity and energies ω close to the chemical potential μ . For $\rho_j(\omega)$ a power-law suppression $\rho_j(\omega) \sim |\omega|^{\alpha_B}$ with the *boundary exponent* $\alpha_B = K_\rho^{-1} - 1$ which only depends on the interaction strength and shape and filling of the band, but *not* on the impurity parameters, was predicted.⁶ Within the bosonic field theory the above assumption was verified by refermionization,⁶ quantum Monte Carlo calculations,^{10,11} and the thermodynamic Bethe ansatz.¹² Although this gives a consistent picture there are three important questions which have not been answered using field theory:

- In a more elaborate RG procedure the growing backscattering amplitude feeds back into the flow of all the other scattering channels $V_{k,k'}$ neglected in the field theory. Does this lead to other stable fixed points? Does the above scenario hold for microscopic lattice models?
- Provided the scenario holds what is the scale on which the universal open boundary fixed point (BFP) physics can be observed?

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- Is it possible to obtain a simple physical picture of the “splitting” mechanism?

To numerically investigate the first two questions exact diagonalization (ED) and the density-matrix renormalization group (DMRG) method were applied to the lattice model of spinless fermions with nearest neighbor interaction and a single impurity.^{7,13,14,15} The expected scaling was confirmed for both weak impurities and weak hopping using ED data.⁷ However, due to the limited system size it was impossible to go beyond the perturbative (in either V_B or t_w) regime. Later it was claimed that the full flow from a weak impurity to the BFP was successfully demonstrated using DMRG,^{13,14} although this strong statement is not really supported by the numerical data presented. The smallest temperature discussed in Ref. 14 corresponds to a system of around 300 lattice sites and the largest system considered in Ref. 13 was $N = 52$, while in Ref. 15 it was shown that $N \approx 10^2$ lattice sites are clearly not enough to exclude an asymptotic behavior not governed by the BFP, even if one starts out with a fairly strong impurity.

An attempt to answer the above questions requires a method which is non-perturbative in the impurity strength, does give the LL power-law divergence in the density response function, but is not limited to systems of a few hundred lattice sites. We here use a functional RG method which has recently been introduced as a new powerful tool in the theory of interacting Fermi systems.^{16,17,18} Details of the derivation of the flow equations are given and the RG scheme is applied to the spinless fermion model with site or hopping impurities. In the extended numerical analysis of the flow equations (see Sec. 6.) we mainly focus on the hopping impurity. This complements our earlier publication on the impurity problem.¹⁹ In our RG approach the complete flow of the renormalized on-site energies and the renormalized hopping amplitudes from the microscopic energy scale down to the infrared fixed point is calculated. The flow equations are *non-perturbative in the impurity strength* while perturbative in the electron-electron interaction. We treat the *full functional form* of the renormalized impurity potential as generated by the flow, instead of replacing it approximately by the scattering amplitudes at the Fermi level. Computing the local spectral weight near the impurity we can confirm the flow to the BFP only if we start out with already fairly large impurities even for systems of up to 10^4 - 10^5 lattice sites. This shows that for intermediate impurity and interaction parameters extremely large systems are required to reach the universal BFP. The quality of the approximations involved in our RG scheme is demonstrated by a direct comparison with essentially exact DMRG data for systems with up to $N = 512$ sites.

2. THE MODEL

The one-dimensional lattice model of spinless fermions with nearest neighbor hopping amplitude $t = 1$, lattice constant $a = 1$, and nearest neighbor interaction U is given by

$$H = - \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + U \sum_j n_j n_{j+1}, \quad (1)$$

in standard second-quantized notation. The boundary conditions we consider are discussed below. Here we mainly focus on the half filled band case for which the LL parameter

$$K_\rho = \left[\frac{2}{\pi} \arccos \left(-\frac{U}{2} \right) \right]^{-1} \quad (2)$$

is analytically known from the Bethe ansatz.²⁰ As already indicated by this expression the model at half filling shows LL behavior only for $-2 < U < 2$. For $U > 2$ the groundstate displays charge density wave order and for $U < -2$ phase separation sets in. We restrict ourselves to repulsive interactions in the LL regime, i.e. to $0 < U < 2$. To the Hamiltonian H we either add a site impurity $H_s = V n_{j_0}$ or a hopping impurity $H_h = (1-t')(c_{j_0}^\dagger c_{j_0+1} + \text{h.c.})$. $t' = 0$ corresponds to a vanishing hopping between the sites j_0 and $j_0 + 1$. Taking the thermodynamic limit or assuming open boundary conditions in Eq. (1) a small t' thus models the situation of a weak link between two decoupled chains. In the non-interacting limit the reflection coefficient for scattering of such impurities at $k_F = \pi/2$ is given by¹⁵ $|R_s|^2 = V^2/(4 + V^2)$ for H_s and $|R_h|^2 = (1 - t'^2)^2/(1 + t'^2)^2$ for H_h , which provides us with a measure for the strength of the bare impurity.

3. A HARTREE-FOCK STUDY

As a first step it is instructive to consider the impurity problem within the Hartree-Fock approximation, before turning to the RG treatment. The impurity leads to Friedel oscillations in the non-interacting density profile $\langle n_j \rangle_0$ which for large $|j - j_0|$ behaves as $|R| \sin(2k_F|j - j_0|)/|j - j_0|$.²¹ Similar oscillations are found in the matrix element $\langle c_j^\dagger c_{j+1} \rangle_0$. Thus both the Hartree potential $V_j^H = U(\langle n_{j-1} \rangle_0 + \langle n_{j+1} \rangle_0)$ and the Fock ‘‘hopping correction’’ $U(\langle c_j^\dagger c_{j+1} \rangle_0 + \text{c.c.})$ are oscillating and decay as $1/|j - j_0|$. One then has to solve a (non-trivial) one-particle problem within such a non-local potential. This problem is interesting in itself - a special variant of it has been discussed in the mathematical literature.²² Taking into account the Hartree

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term only, the resulting spectral weight for $|\omega| \rightarrow 0$ shows power-law behavior with an exponent which independently of the local part of the effective potential around j_0 is proportional to the amplitude $U|R|$ of the asymptotic oscillations.²² It can be shown analytically that this behavior is not changed when the Fock term is included. A more detailed discussion of this scattering problem will be given elsewhere.²³ Thus solely due to the oscillations and the very slow $1/|j - j_0|$ decay of the non-local effective potential already HF yields a *power-law* for the spectral weight, but with an exponent which not only depends on U , but via R also on the *bare* impurity strength. This contradiction to the bosonization prediction is not surprising as HF does certainly not contain the renormalization of the impurity strength.

The extension of the HF study using self-consistent HF leads to unphysical results and thus cannot be used to gain further insight. The self-consistent iterative solution of the HF equations generates for all $U > 0$ a groundstate which shows charge density wave order²⁴ which is qualitatively incorrect since a single impurity cannot change bulk properties of the system.

4. THE FERMIONIC RENORMALIZATION GROUP

We now treat the problem using a fermionic functional RG approach.^{16,17,18} Various versions were applied recently to problems of strongly correlated two-dimensional electron systems.²⁵ Here we use the method proposed by Wetterich¹⁶ and Morris,¹⁷ where one introduces a cut-off parameter Λ in the free propagator G^0 cutting out degrees of freedom on energy scales less than Λ and derives an exact hierarchy of coupled differential flow equations for the one-particle irreducible vertex functions by differentiating with respect to Λ , where Λ flows from ∞ to 0.

Before turning to the specific lattice model of spinless fermions with nearest neighbor interaction and hopping we will give a brief introduction to the method for a general lattice model of spinless fermions with interaction and impurity free one-particle states $|\alpha\rangle$ (e.g. Wannier states $|j\rangle$ or momentum states $|k\rangle$), two-body interaction $\frac{1}{4} \sum_{\alpha,\beta,\gamma,\delta} \bar{v}_{\alpha,\beta,\gamma,\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$, and an impurity potential $\sum_{\alpha,\beta} V_{\alpha,\beta} c_\alpha^\dagger c_\beta$. The *exact* flow equation for the selfenergy reads

$$\begin{aligned} \frac{d}{d\Lambda} \Sigma_{\alpha,\beta}^\Lambda(i\omega_n) = & -T \sum_{\omega_l} e^{i\omega_l 0^+} \sum_{\gamma,\delta} \left\{ \left[1 - G^{0,\Lambda}(i\omega_l) \Sigma^\Lambda(i\omega_l) \right]^{-1} \frac{dG^{0,\Lambda}(i\omega_l)}{d\Lambda} \right. \\ & \left. \times \left[1 - \Sigma^\Lambda(i\omega_l) G^{0,\Lambda}(i\omega_l) \right]^{-1} \right\} \Gamma_{\alpha,\gamma,\beta,\delta}^\Lambda(i\omega_n, i\omega_l, i\omega_n, i\omega_l), \end{aligned} \quad (3)$$

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where $G^{0,\Lambda}$ and Σ^Λ are matrices with matrix elements $G_{\alpha,\beta}^{0,\Lambda}$ and $\Sigma_{\alpha,\beta}^\Lambda$, respectively, ω_n denotes a fermionic Matsubara frequency, and T is the temperature. The irreducible four point vertex $\Gamma_{\alpha,\gamma,\beta,\delta}^\Lambda$ obeys a flow equation with terms bilinear in Γ^Λ and a term linear in the irreducible six point vertex. The initial condition is given by $\Sigma_{\alpha,\beta}^{\Lambda=\infty} = V_{\alpha,\beta}$. For spinless fermions the electron-electron interaction is renormalized only by a finite amount of order interaction squared.² Hence as our central approximation we replace the renormalized two-particle vertex to leading order in the interaction by the antisymmetrized bare coupling, i.e. $\Gamma_{\alpha,\gamma,\beta,\delta}^\Lambda \rightarrow \bar{v}_{\alpha,\gamma,\beta,\delta}$. With this approximation Σ^Λ becomes *frequency independent*. For the case of a model including a spin degree of freedom the flow of the two-particle vertex has to be taken into account.² In order to simplify the remaining Matsubara sum in Eq. (3) we take the zero temperature limit and perform the RG flow with a *frequency cut-off*

$$G^{0,\Lambda}(i\omega) = \Theta(|\omega| - \Lambda)G^0(i\omega). \quad (4)$$

The first factor on the right hand side (rhs) of Eq. (3) then involves products of a Dirac delta function and step functions. Using the relation¹⁷

$$\delta_\varepsilon(\omega - \Lambda)f(\Theta_\varepsilon[\omega - \Lambda]) \rightarrow \delta(\omega - \Lambda) \int_0^1 f(t)dt, \quad (5)$$

where ε is a broadening parameter tending to zero and f is a sufficiently smooth function, we obtain

$$\frac{d}{d\Lambda}\Sigma_{\alpha,\beta}^\Lambda = -\frac{1}{2\pi} \sum_{\omega=\pm\Lambda} \sum_{\gamma,\delta} \bar{v}_{\alpha,\gamma,\beta,\delta} G_{\delta,\gamma}^\Lambda(i\omega) e^{i\omega 0^+}, \quad (6)$$

where

$$G^\Lambda(i\omega) = \left\{ \left[G^0(i\omega) \right]^{-1} - \Sigma^\Lambda \right\}^{-1} \quad (7)$$

is the full propagator for the cut-off dependent selfenergy. The convergence factor $e^{i\omega 0^+}$ with $\omega = \pm\Lambda$ is relevant only for determining the flow from $\Lambda = \infty$ down to some arbitrarily large finite Λ_0 . For Λ_0 much larger than the band width this high energy part of the flow can be easily computed analytically and yields the simple contribution $\frac{1}{2} \sum_\gamma \bar{v}_{\alpha,\gamma,\beta,\gamma}$. One can then drop the convergence factor and continue the flow from Λ_0 downwards with the new initial condition

$$\Sigma_{\alpha,\beta}^{\Lambda_0} = V_{\alpha,\beta} + \frac{1}{2} \sum_\gamma \bar{v}_{\alpha,\gamma,\beta,\gamma}. \quad (8)$$

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Within this scheme $\Sigma_{\alpha,\beta}^\Lambda$ is the flowing effective impurity potential. In our RG procedure all the different impurity scattering channels corresponding to transitions from the one-particle states $|\alpha\rangle$ to $|\beta\rangle$ are coupled [see Eq. (6)] and we do not replace them by scattering amplitudes at the Fermi level. This has to be contrasted to the bosonization approach to the problem. The RG is a grand canonical method for which the chemical potential is fixed and the average particle number has to be determined from the Green function. To calculate observables, as e.g. the local spectral weight, we have to determine the selfenergy $\Sigma_{\alpha,\beta}^\Lambda$ at $\Lambda = 0$ and invert the matrix Eq. (7) to obtain the Green function, i.e. solve the one-particle problem of a particle moving in the effective scattering potential $\Sigma_{\alpha,\beta}^{\Lambda=0}$. This gives us a simple picture - in momentum or real space depending on the choice of one-particle states $|\alpha\rangle$ - of the influence an impurity has on the electronic properties of a LL (see below).

Because of the matrix inversion involved in calculating the rhs of Eq. (6) we were not able to analytically solve the flow equation for general parameters. But it is easy to show analytically that in the weak impurity limit Eq. (6) exhibits the scaling predicted from bosonization. For that purpose we work in momentum space and consider $\Sigma_{k,k'}^\Lambda$ for $k - k'$ different from a reciprocal lattice vector K . Then the term linear in Σ^Λ presents the leading approximation in the expansion of G^Λ on the rhs of Eq. (6) and we obtain

$$\begin{aligned} \frac{d}{d\Lambda} \Sigma_{k,k'}^\Lambda &= -\frac{1}{2\pi} \frac{1}{N} \sum_{k_1, k_2} \sum_K [\tilde{v}(k - k') - \tilde{v}(k - k_2)] \delta_{k+k_1, k'+k_2+K} \\ &\quad \times \left[\frac{1}{i\Lambda - \xi_{k_2}} \Sigma_{k_2, k_1}^\Lambda \frac{1}{i\Lambda - \xi_{k_1}} + (\Lambda \rightarrow -\Lambda) \right] \end{aligned} \quad (9)$$

where $\xi_k = \varepsilon_k - \mu$ with the one-particle dispersion ε_k , $\tilde{v}(k)$ is the Fourier transform of the two-particle interaction, and N is the number of lattice sites. We treat the Hartree-type and Fock-type terms separately. The Hartree-type term alone would lead to a selfenergy which depends on $k - k'$ only. In the thermodynamic limit one obtains

$$\begin{aligned} \left[\frac{d}{d\Lambda} \Sigma_{k,k'}^\Lambda \right]_H &= -\frac{1}{2\pi} \tilde{v}(k - k') \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} \left[\frac{1}{i\Lambda - \xi_{k-k'+k_1}} \right. \\ &\quad \left. \times \Sigma_{k-k'+k_1, k_1}^\Lambda \frac{1}{i\Lambda - \xi_{k_1}} + (\Lambda \rightarrow -\Lambda) \right]. \end{aligned} \quad (10)$$

For $k = k_F$, $k' = -k_F$ the k_1 -integration contains a singular contribution proportional to $1/\Lambda$ which leads to the power-law behavior with an exponent

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proportional to $\tilde{v}(2k_F)$ as discussed below. The Fock-type term reads

$$\left[\frac{d}{d\Lambda} \Sigma_{k,k'}^\Lambda \right]_F = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} \tilde{v}(k-k_2) \left[\frac{1}{i\Lambda - \xi_{k_2}} \right. \\ \left. \times \Sigma_{k_2, k_2+k'-k}^\Lambda \frac{1}{i\Lambda - \xi_{k_2+k'-k}} + (\Lambda \rightarrow -\Lambda) \right]. \quad (11)$$

Away from half filling the singular contribution $\sim 1/\Lambda$ for $k = k_F$, $k' = -k_F$ comes from $k_2 \approx k_F$ and is therefore proportional to $\tilde{v}(0)$. If only the singular contributions are kept the differential equation for $\Sigma_{k_F, -k_F}^\Lambda$ reads

$$\frac{d}{d\Lambda} \Sigma_{k_F, -k_F}^\Lambda = - \left[\frac{\tilde{v}(0) - \tilde{v}(2k_F)}{2\pi v_F} \right] \frac{1}{\Lambda} \Sigma_{k_F, -k_F}^\Lambda, \quad (12)$$

where v_F denotes the Fermi velocity. This leads to the scaling

$$\Sigma_{k_F, -k_F}^\Lambda \sim \left(\frac{1}{\Lambda} \right)^{[\tilde{v}(0) - \tilde{v}(2k_F)]/[2\pi v_F]}. \quad (13)$$

To leading order in the interaction the exponent $[\tilde{v}(0) - \tilde{v}(2k_F)]/[2\pi v_F]$ is just $1 - K_\rho$ which shows that our non-perturbative fermionic RG captures the power-law increase found in the perturbative bosonic RG. As Eq. (12) was derived by expanding the Green function G^Λ in powers of the selfenergy, the scaling behavior Eq. (13) can be trusted only as long as Σ^Λ stays small. Eq. (12) also holds in the half filled band case since the two additional terms from the Hartree- and Fock-type contributions cancel each other. The scaling equation (13) can similarly be derived for a continuum model.

5. NUMERICAL SOLUTION OF THE RG EQUATIONS

Numerically integrating the RG equations (6) for finite systems of N lattice sites we can go beyond the perturbative regime. In each step of the integration we have to invert an $N \times N$ matrix. If we now specialize on the lattice model of spinless fermions with nearest neighbor interaction and hopping, treat the problem in real space, and assume open boundary conditions, then $[G^0(i\omega)]^{-1} - \Sigma^\Lambda$ is tridiagonal and Eq. (6) reads

$$\frac{d}{d\Lambda} \Sigma_{j,j}^\Lambda = -\frac{U}{2\pi} \sum_{s=\pm 1} \sum_{\omega=\pm\Lambda} G_{j+s, j+s}^\Lambda(i\omega) \quad (14)$$

$$\frac{d}{d\Lambda} \Sigma_{j, j\pm 1}^\Lambda = \frac{U}{2\pi} \sum_{\omega=\pm\Lambda} G_{j, j\pm 1}^\Lambda(i\omega). \quad (15)$$

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Therefore the numerical effort is considerably reduced which allowed us to treat systems with up to $2^{15} = 32768$ lattice sites. Since the position of the impurity j_0 is chosen to be far away from the open boundaries they do not influence the behavior close to j_0 . We have confirmed this by also investigating systems with periodic boundary conditions, in which case we are limited to smaller systems of the order of 10^3 lattice sites. The initial conditions for the case of a site impurity are $\Sigma_{1,1}^{\Lambda_0} = U/2$, $\Sigma_{N,N}^{\Lambda_0} = U/2$, $\Sigma_{j_0,j_0}^{\Lambda_0} = V + U$, and $\Sigma_{j,j}^{\Lambda_0} = U$ for $j \neq j_0$ and not at the boundaries, while the other matrix elements are initially zero. We started the integration at $\Lambda_0 = 1000$ convincing ourselves that further increasing Λ_0 only leads to negligible changes in the results. For a hopping impurity we start with $\Sigma_{1,1}^{\Lambda_0} = U/2$, $\Sigma_{N,N}^{\Lambda_0} = U/2$, $\Sigma_{j,j}^{\Lambda_0} = U$ and $\Sigma_{j_0,j_0+1}^{\Lambda_0} = \Sigma_{j_0+1,j_0}^{\Lambda_0} = 1 - t'$, while the other matrix elements are again zero.

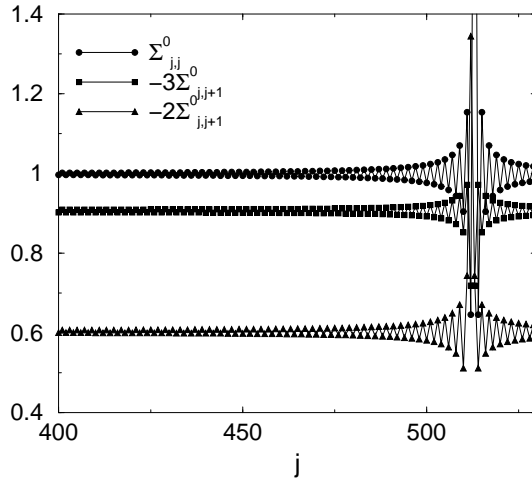


Fig. 1. $\Sigma_{j,j'}^{\Lambda=0}$ for a *site impurity* (circles and squares) with $V = 1$ and a *hopping impurity* (triangles) with $t' = 0.5$, both for $U = 1$. For a clear representation the nearest neighbor parts are multiplied by -3 respectively -2 as indicated in the legend.

Fig. 1 shows typical results for $\Sigma_{j,j}^{\Lambda=0}$ and $\Sigma_{j,j+1}^{\Lambda=0}$ for $U = 1$, with a *site impurity* $V = 1.5$ in one case and a *hopping impurity* $t' = 0.5$ in the other, where both would lead to a transmission probability of $|T|^2 = 0.64$ in a non-interacting system. Since Σ^{Λ} is symmetric around j_0 and the ends of the chain are dominated by the open boundaries mainly the region $1 \ll j < j_0$ is shown. For symmetry reasons in the first case we take $N = 1025$, $j_0 = 513$ and the average number of electrons at $\mu = U$ is $\langle N_F \rangle = 512$

so that we are slightly off half filling. In the latter $N = 1024$, $j_0 = 512$ and $\langle N_F \rangle = 512$. At half filling a hopping impurity leads to the shown long range oscillatory behavior in $\Sigma_{j,j+1}^{\Lambda=0}$ but *not* in $\Sigma_{j,j}^{\Lambda=0}$, similar to the HF approximation. Furthermore both the diagonal and the nearest neighbor part show global shifts. For $\Sigma_{j,j}^{\Lambda=0}$ this shift by U is due to the initial condition and is exactly canceled by the chemical potential which at half filling is given by $\mu = U$. A change in $\Sigma_{j,j+1}^{\Lambda=0}$ is present already in HF and corresponds to an interaction induced broadening of the band.

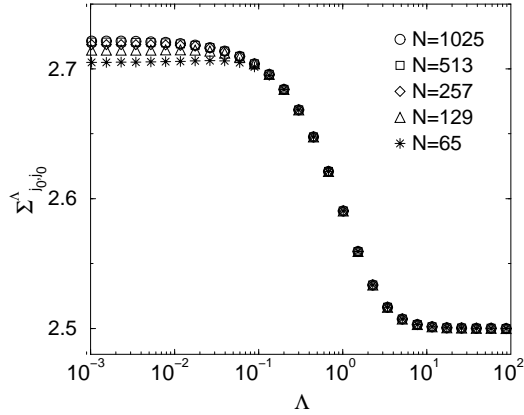


Fig. 2. $\Sigma_{j_0, j_0}^{\Lambda}$ as a function of Λ for a *site impurity* (same parameters as in Fig. 1) and different N .

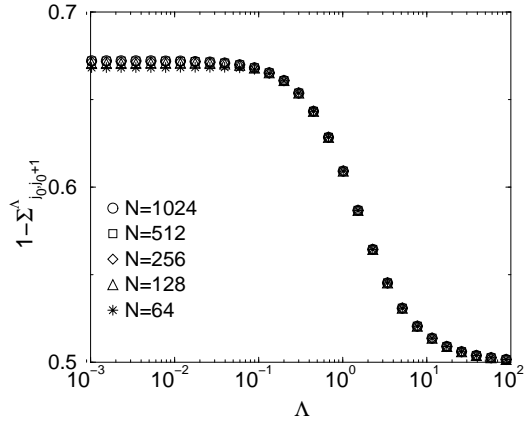


Fig. 3. The effective hopping $1 - \Sigma_{j_0, j_0+1}^{\Lambda}$ between sites j_0 and $j_0 + 1$ as a function of Λ for a *hopping impurity* (same parameters as in Fig. 1) and different N .

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In Fig. 2 we show $\Sigma_{j_0, j_0}^\Lambda$ for the *site impurity* as a function of Λ for different N on a log-linear scale. For finite N the flow is effectively cut off on a scale of the order of $1/N$ and to extrapolate to the thermodynamic limit we have to consider a sequence of N values. Obviously the renormalized potential at the impurity site remains finite in the limit $N \rightarrow \infty$ and the expected “cutting” of the chain does certainly not occur because a single on-site energy diverges, as one might guess if the bosonic RG is taken too literally. Singular behavior is only found in $\Sigma_{k, k'}^\Lambda$ for momenta with $k - k' \approx \pm 2k_F$, which is associated with the *long range oscillations* in real space.

Fig. 3 shows the effective hopping $1 - \Sigma_{j_0, j_0+1}^\Lambda$ for the *hopping impurity* between sites j_0 and $j_0 + 1$ as a function of Λ for different N on a log-linear scale. The effective hopping does *not tend to zero* for $N \rightarrow \infty$ as one could expect from a simplistic interpretation of the bosonization result. As we do not perform a rescaling in our RG analysis the weak hopping has to stay finite because we otherwise would suppress the transmission through the weak link on *all* energy scales. The hopping between j_0 and $j_0 + 1$ even increases upon integrating out degrees of freedom. Again the long range oscillations of the non-local effective impurity potential and not the scaling of a single on-site energy or hopping matrix element is the reason for the peculiar behavior of physical observables, as for example $\rho_j(\omega)$, discussed next.

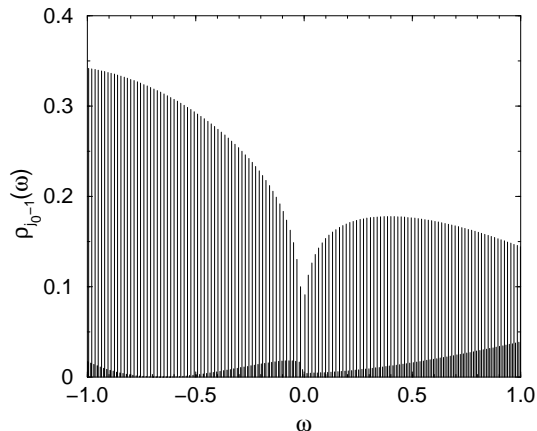


Fig. 4. $\rho_{j_0-1}(\omega)$ as a function of ω for a *site impurity* with the same parameters as in Fig. 1.

The local spectral function at the site $j_0 - 1$, $\rho_{j_0-1}(\omega)$, is presented in Fig. 4 for a *site impurity* with the same parameters as in Fig. 1. The data

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show a suppression of the weight for $|\omega| \rightarrow 0$, i.e. for energies close to the chemical potential, as expected from bosonization. A similar suppression is found in the local spectral weight close to a hopping impurity. Each spike represents a δ -peak of the finite system. For large systems the suppression follows a power-law which similar to the HF description is related to the oscillatory long range nonlocal effective potential. But while the HF exponent depends on the bare impurity strength we expect our RG method to lead to a power law decay described by the boundary exponent $\alpha_B^{\text{RG}}(U)$ independent of the the impurity strength, where $\alpha_B^{\text{RG}}(U)$ can be determined from the same RG analysis for an impurity free system by calculating $\rho_j(\omega)$ for j close to one of the boundaries. The occurrence of $\alpha_B^{\text{RG}}(U)$ can be shown analytically from Eqs. (14) and (15) only for $|V| \gg 1$ or $|t'| \ll 1$. We shortly sketch the argument for the weak hopping case. If one introduces operators \hat{L} and \hat{R} which project on the one-particle states to the left and right of the weak link the resolvents $G^\Lambda(z) \equiv (z - h^\Lambda)^{-1}$ in Eqs. (14) and (15) can be expanded in the effective hopping matrix element $h_{j_0, j_0+1}^\Lambda = -1 + \Sigma_{j_0, j_0+1}^\Lambda \equiv \tilde{\Sigma}_{j_0, j_0+1}^\Lambda$, anticipating that this quantity is small for all values of Λ . One obtains $G_{LL}(z) \equiv \hat{L}G^\Lambda(z)\hat{L} = [z\hat{L} - \hat{L}h^\Lambda\hat{L}]^{-1} + \mathcal{O}\left([\tilde{\Sigma}_{j_0, j_0+1}^\Lambda]^2\right)$ and a corresponding result for $\hat{R}G^\Lambda(z)\hat{R}$. If we denote the leading term as $[G_{LL}^\Lambda(z)]_0$ (and $[G_{RR}^\Lambda(z)]_0$) and also expand $\hat{L}G^\Lambda(z)\hat{R} = [G_{LL}(z)]_0 \hat{L}h^\Lambda\hat{R}G_{RR}(z)$ the equation for $\tilde{\Sigma}_{j_0, j_0+1}^\Lambda$ reads

$$\frac{d}{d\Lambda} \tilde{\Sigma}_{j_0, j_0+1}^\Lambda = \left(\frac{U'}{2\pi} \sum_{\omega=\pm\Lambda} [G_{j_0, j_0}^\Lambda(i\omega)]_0 [G_{j_0+1, j_0+1}^\Lambda(i\omega)]_0 \right) \tilde{\Sigma}_{j_0, j_0+1}^\Lambda. \quad (16)$$

The correction terms to the rhs are of order $(\tilde{\Sigma}_{j_0, j_0+1}^\Lambda)^3$. We also allowed the Coulomb integral U' across the weak link to be different from U . The equations for all other nonvanishing matrix elements of Σ^Λ , apart from higher order corrections, are equations for a chain *split* between the sites j_0 and $j_0 + 1$. Therefore it is obvious that local spectral functions $\rho_j(\omega)$ for j in the neighborhood of j_0 show a power law suppression with the boundary exponent $\alpha_B^{\text{RG}}(U)$. Once the equations for the split chain are solved the result for $\tilde{\Sigma}_{j_0, j_0+1}^{\Lambda=0}$ follows from Eq. (16) by a simple integration. In the special case $U' = 0$ the effective hopping is given by t' for *all* values of Λ . The case of a strong site impurity $|V| \gg 1$ can be mapped to a weak hopping problem with $t' \sim 1/V$ by projecting out the impurity site.

It is advantageous¹⁹ to analyze the finite size scaling of the spectral weight $W(N)$ at μ and $j_0 - 1$ instead of trying to fit a power-law to the fixed N data for $\rho_{j_0-1}(\omega)$ at small ω . If $\rho_{j_0-1}(\omega)$ follows a power-law as a

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function of frequency, we obtain a power-law with the same exponent in the N dependence of $W(N)$. In the next section we investigate the behavior of the exponent as a function of system size and compare the data obtained within the RG scheme with essentially exact data from DMRG focusing on hopping impurities.

6. LARGE N AND COMPARISON WITH DMRG RESULTS

We have calculated the spectral weight $W(N)$ at μ and on the site next to the modulated bond j_0 for different t' , U , and $N = 2^n$. Applying the RG scheme we were able to go up to $n = 15$, while using the DMRG we were limited to $n = 9$. Since we are interested in the exponent of a possible power-law behavior we determine

$$\alpha_I(N = 2^n) = -\frac{\ln [W(2^{n+1})] - \ln [W(2^{n-1})]}{\ln [2^{n+1}] - \ln [2^{n-1}]}.$$
 (17)

If $W(N)$ decays for $N \rightarrow \infty$ as a power-law, $\alpha_I(N)$ converges to the respective exponent.

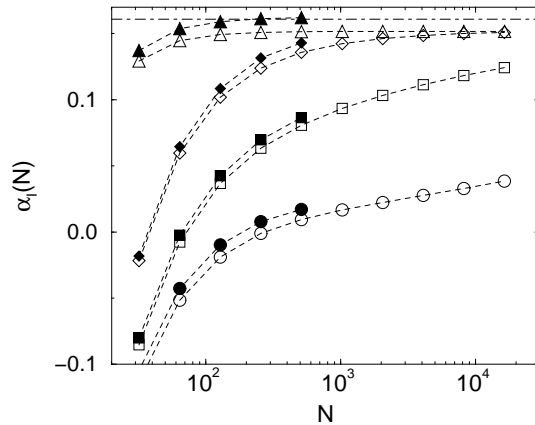


Fig. 5. $\alpha_I(N)$ as a function of N for $U = 0.5$ and different t' : $t' = 0.8$ (circles), $t' = 0.5$ (squares), $t' = 0.2$ (diamonds), and $t' = 0$ (triangles). The filled symbols are DMRG data, while the open ones have been obtained from the RG. The dashed-dotted line gives the exact boundary exponent α_B^{ex} .

Fig. 5 shows $\alpha_I(N)$ for $U = 0.5$ and $t' = 0.8$ (corresponding to $|T|^2 = 0.95$ at $U = 0$, i.e. a very weak impurity), $t' = 0.5$ ($|T|^2 = 0.64$ at $U = 0$,

i.e. an intermediate impurity), and $t' = 0.2$ ($|T|^2 = 0.15$ at $U = 0$, i.e. a weak hopping). For comparison we also calculated $\alpha_B(N)$ for the lattice site next to an open boundary ($t' = 0$). The DMRG and RG data are parallel to each other, which in addition to the analytical arguments is a strong indication that our fermionic RG captures the essential physics. For $t' = 0$ both methods produce the expected power-law behavior with boundary exponents α_B^{DMRG} and α_B^{RG} . $\alpha_B^{\text{DMRG}}(N = 512)$ agrees up to 1% with the exact exponent $\alpha_B^{\text{ex}} \approx 0.1609$ obtained using Eq. (2) and $\alpha_B^{\text{ex}} = K_\rho^{-1} - 1$.²⁶ As our RG is only correct to leading order in U , $\alpha_B^{\text{RG}}(N = 16384)$ which effectively is equal to $\alpha_B^{\text{RG}}(N = \infty)$ deviates by roughly 6% from α_B^{ex} . From the RG curves for small to intermediate bare hopping t' between j_0 and $j_0 + 1$ one can infer that $\alpha_I^{\text{RG}}(N)$ will approach the impurity independent boundary exponent α_B^{RG} for $N \rightarrow \infty$, as predicted by bosonization. We have also determined $\alpha_I^{\text{RG}}(N)$ for a site impurity and three different values of V leading to the same $U = 0$ transmission probabilities $|T|^2$ as for the impurity parameters discussed here (see above). A comparison shows that for the hopping impurity and a fixed $|T|^2$ the convergence to α_B^{RG} is slightly slower. Already for the site impurity extremely large $N = 10^4$ - 10^5 were needed to exclude non-universal (impurity dependent) fixed points with some certainty,¹⁹ and here even longer chains are required.

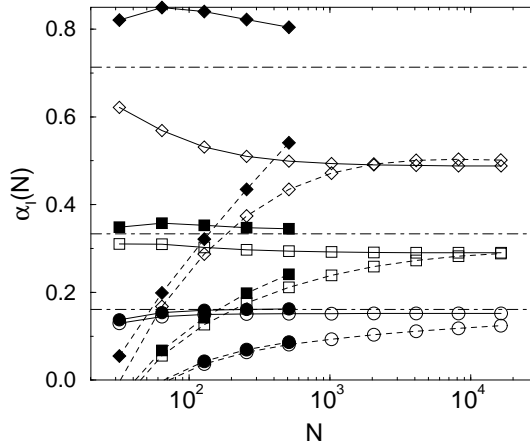


Fig. 6. $\alpha_I(N)$ as a function of N for $t' = 0.5$ (dashed lines) and $\alpha_B(N)$ for $t' = 0$ (solid lines) for different U : $U = 0.5$ (circles), $U = 1$ (squares), and $U = 1.8$ (diamonds). Filled symbols are DMRG data, open ones RG results. The dashed-dotted lines give the exact U dependent boundary exponents α_B^{ex} .

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In Fig. 6 RG and DMRG data are presented for an intermediate impurity strength $t' = 0.5$ and $t' = 0$ for different values of U . Due to higher order corrections in U , the difference between the RG and DMRG data increases with increasing U . For the case of a site impurity the speed of convergence of $\alpha_I^{\text{RG}}(N)$ to α_B^{RG} was increased considerably by increasing U (see Fig. 4 of Ref. 19). In Fig. 6 we also find a tendency towards a faster convergence to α_B^{RG} if U is increased for a fixed t' , but the situation is less clear since the $\alpha_I^{\text{RG}}(N)$ curves at large N cross $\alpha_B^{\text{RG}}(N)$ showing non-monotonic behavior and approach α_B^{RG} from above.

Compared to the case of a site impurity we here find somewhat less clear indications that the boundary exponent and thus the BFP is approached independently of the bare impurity strength. Nonetheless the presented RG data lead us to conclude that the universality of the BFP holds also for a hopping impurity. Our data show that for a hopping impurity and especially for intermediate t' and U , which are experimentally most relevant, exceptionally large systems are needed to observe the universal BFP physics. For chains which are not long enough a strong system size dependence of experimentally extracted exponents must be expected. For both types of impurities it is obvious that a DMRG study alone, which is limited to a few hundred lattice sites, cannot give a definite answer to the question if the BFP is indeed universal.^{15,19} To judge the quality of the approximations made to set up our RG scheme the DMRG data are on the other hand very useful.

7. SUMMARY

In summary, we have applied a functional RG method to a lattice fermion model in order to analyze how and on what scale a single impurity in a Luttinger liquid “cuts” the chain. The method is perturbative in the electron-electron interaction but non-perturbative in the impurity strength. The results have been checked against essentially exact DMRG data for finite systems, with good quantitative agreement for small U . Computing the local spectral weight near a hopping impurity we found a clear indication of the expected BFP physics only for intermediate to strong hopping impurities even for systems of up to $N = 2^{15}$ lattice sites. Having in mind the results of our previous study for site impurities¹⁹ we nevertheless conclude that universal power-law behavior with a boundary exponent depending on the electron-electron interaction and not on the impurity strength also holds for hopping impurities. The functional RG method, where the entire functional form of the impurity potential is renormalized, provides a clear real

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space picture of the cutting mechanism for both site and hopping impurities: while the local impurity strength is not renormalized much, an oscillating, slowly decaying non-local potential develops which at low energies acts as an effective barrier.

It turned out that extremely large systems are required to reach the universal regime, even for intermediate impurity and interaction strengths. Hence only special mesoscopic systems, such as very long carbon nanotubes, under very favorable experimental conditions are suitable for experimentally observing the impurity induced universal boundary physics. A trend *towards* cut chain behavior is certainly easier to observe. In Fig. 4 e.g. a strong suppression of the local spectral weight can be seen already for a chain with $N = 1025$ lattice sites, a system size for which $\alpha_I(N)$ is still far away from the universal boundary exponent α_B . Functional RG methods applied to realistic models should be useful to compute the *non-universal* behavior at intermediate scales, which is more easily accessible to experimentalists.

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