Scaling behavior of impurities in mesoscopic Luttinger liquids

V. Meden,[1] W. Metzner,[2] U. Schollwöck,[3] and K. Schönhammer[1]
[1]*Institut für Theoretische Physik, Universität Göttingen, Bunsenstr. 9, D-37073 Göttingen, Germany*
[2]*Institut für Theoretische Physik C, RWTH Aachen, D-52056 Aachen, Germany*
[3]*Sektion Physik, Universität München, Theresienstr. 37, D-80333 München, Germany*
(Received 3 October 2001; published 4 January 2002)

Using a functional renormalization group, we compute the flow of the renormalized impurity potential for a single impurity in a Luttinger liquid over the entire energy range from the microscopic scale of a lattice-fermion model down to the low-energy limit. The nonperturbative method provides a complete real-space picture of the effective impurity potential. We confirm the universality of the open chain fixed point, but it turns out that very large systems (10^4-10^5 sites) are required to reach the fixed point for realistic choices of the impurity and interaction parameters.

DOI: 10.1103/PhysRevB.65.045318 PACS number(s): 71.10.Pm, 73.22.−f, 73.63.−b

The low-energy physics of one-dimensional interacting electron systems with Luttinger liquid (LL) behavior is dramatically affected by the presence of a single impurity.[1–6] The problem is usually mapped onto an effective-field theory using bosonization, where terms which are expected to be irrelevant in the low-energy limit are neglected.[1–5] Then forward and backward impurity scatterings decouple, and the more important backscattering processes are modeled by a single amplitude V_B. From a perturbative bosonic renormalization-group (RG) calculation[4] and a boundary conformal field theory analysis,[5] the following picture emerged: In a chain of spinless fermions[7] with repulsive interactions (LL parameter $K_\rho<1$) the backscattering amplitude V_B is a relevant perturbation which grows as $\Lambda^{K_\rho-1}$ when the flow parameter Λ is sent to zero, and the perturbative analysis breaks down. This behavior can be traced back to the power-law singularity of the $2k_F$ density response function in a LL.[1,2] On the other hand, a weak hopping t_w between the open ends of two semi-infinite chains is irrelevant and scales to zero as $\Lambda^{K_\rho^{-1}-1}$.[4] *Assuming* that the open chain represents 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 chains with open boundary conditions at the end points.[4] Here we focus mainly 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 a *boundary exponent* $\alpha_B=K_\rho^{-1}-1$ which only depends on the interaction strength and band filling, but *not* on the impurity parameters, was predicted.[4] Within the bosonic field theory the above conjecture was verified by refermionization,[4] quantum Monte Carlo calculations,[8,9] and the thermodynamic Bethe ansatz.[10]

To confirm the field theoretical scenario and the validity of the underlying assumptions for a microscopic fermionic system with LL behavior, numerical methods [exact diagonalization (ED), density-matrix renormalization group (DMRG)] were applied to the lattice model of spinless fermions with nearest-neighbor interaction.[5,11–13] Comparing ED data for up to $N=23$ sites with the field theoretical prediction for the finite-size corrections of energies, the expected scaling was confirmed for both weak impurities and weak hopping.[5] 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 open boundary fixed point (BFP) was successfully demonstrated,[11,12] although this strong statement is not really supported by the numerical data presented. The smallest temperature discussed in Ref. 12 corresponds to a system of around 300 lattice sites; the largest system considered in Ref. 11 was $N=52$, while in Ref. 13 it was shown that $N\approx10^2$ 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.

Recently functional RG methods, originally developed in a field-theoretical context, have been introduced as a powerful tool in the theory of interacting Fermi systems,[14] with applications so far concentrating on translationally invariant two-dimensional systems.[15,16] In this paper we apply such a functional RG scheme to a spinless fermion model with site or hopping impurities. We compute the complete *coupled* flow of the renormalized on-site energies and the renormalized hopping amplitudes from the microscopic energy scale down to the infrared fixed point. The flow equations are *nonperturbative in the impurity strength* and 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 convincingly confirm the universality of the BFP. However, it turns out that very large systems (10^4-10^5 sites) are required to reach the BFP for intermediate impurity and interaction parameters. Our RG scheme is checked against numerical exact DMRG data for systems with up to $N=768$ sites.

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

$$H_0=-\sum_j\,(c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j)+U\sum_j\,n_jn_{j+1} \qquad (1)$$

in standard second-quantized notation. Here we focus on the half-filled band case, repulsive interaction, and the LL phase, i.e., $0<U<2$. To the Hamiltonian H_0, we add either a site impurity $H_s=Vn_{j_0}$ or a hopping impurity $H_h=(1-t_{j_0})\,(c^\dagger_{j_0}c_{j_0+1}+\text{H.c.})$.

In a weakly interacting spinless LL with an open end the local spectral weight $\rho_j(\omega)$ near the boundary can, to a surprisingly good approximation, be obtained from a non-self-consistent Hartree-Fock (HF) approximation.[17] It is instructive also to consider the impurity problem within the HF approximation, before turning to the RG treatment. The impurity leads to Friedel oscillations in the noninteracting density profile $\langle n_j\rangle_0$, which for large $|j-j_0|$ behaves as $R\cos(2k_F|j-j_0|)/|j-j_0|$, where R is the reflection amplitude of the bare impurity. Similar oscillations are found in the matrix element $\langle c^\dagger_j c_{j+1}\rangle_0$. Thus both the Hartree potential $U(\langle n_{j-1}\rangle_0+\langle n_{j+1}\rangle_0)$ and the Fock "hopping correction" are oscillatory and of long range. One then has to solve a (nontrivial) one-particle problem within such a potential and with modulated hopping. Taking into account the Hartree term only, the resulting spectral weight for $|\omega|\to 0$ shows a power-law behavior with an exponent which is proportional to the amplitude UR of the oscillations.[18] We have checked numerically (for systems of up to 10^6 lattice sites[17,19]) that this behavior is not changed when the Fock term is included. Thus, due to the *long-range* nature of the effective potential and the hopping modulation, the HF approximation, already 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.

It is tempting to extend the HF study using the self-consistent HF approximation.[20] However, it turns out that an iterative solution of the self-consistent HF equation leads for all U to a charge-density-wave ground state,[19,20] which is qualitatively incorrect since a single impurity cannot change bulk properties of the system.

We now treat the problem using a fermionic functional RG approach. Cutting off the free propagator on a scale Λ, and differentiating with respect to this flow parameter, an exact infinite hierarchy of coupled differential flow equations for the one-particle irreducible vertex functions can be derived.[21–23] For the impurity problem it is technically advantageous to use a frequency cutoff for the free propagator $G^{0,\Lambda}(i\omega)=\Theta(|\omega|-\Lambda)G^0(i\omega)$, where G^0 is the free propagator without cutoff and ω the Matsubara frequency. Λ flows from ∞ to 0. For spinless fermions the electron-electron interaction is renormalized only by a finite amount of order U^2.[24] Hence we can replace the renormalized two-particle vertex to leading order in U by the antisymmetrized bare interaction. In this way the exact hierarchy of flow equations is truncated, and one obtains a simple one-loop flow equation for the self-energy Σ, where only the (full) propagator G and the bare electron-electron interaction U enter. Using the above approximation we can expect our results to be quantitatively correct for small U. Below, we will show that the RG also provides qualitatively correct results for U of the order of 2. Carrying out a Matsubara sum and choosing a real-space representation of G and Σ, one obtains the flow equations (at temperature $T=0$)

$$\frac{d}{d\Lambda}\Sigma^\Lambda_{j,j}=-\frac{U}{2\pi}\sum_{s=\pm 1}\sum_{\omega=\pm\Lambda}G^\Lambda_{j+s,j+s}(i\omega), \tag{2}$$

$$\frac{d}{d\Lambda}\Sigma^\Lambda_{j,j\pm 1}=\frac{U}{2\pi}\sum_{\omega=\pm\Lambda}G^\Lambda_{j,j\pm 1}(i\omega). \tag{3}$$

The self-energy is frequency independent and tridiagonal, since the bare interaction is instantaneous and restricted to nearest neighbors. The full propagator G^Λ on the right-hand side of the flow equations is obtained by inverting the matrix $[G^0]^{-1}-\Sigma^\Lambda$. The bare site and/or hopping impurity enter as *initial conditions* for Σ^Λ at $\Lambda=\infty$. For a site impurity V at j_0, one sets $\Sigma^{\Lambda=\infty}_{j_0,j_0}=V$, and, for a hopping impurity between j_0 and j_0+1, one has $\Sigma^{\Lambda=\infty}_{j_0,j_0+1}=\Sigma^{\Lambda=\infty}_{j_0+1,j_0}=1-t_{j_0}$, while the other matrix elements are initially zero. The above flow equations are *nonperturbative* in the impurity parameters, in contrast to the perturbative bosonic RG equation. Written in momentum space, the different scattering channels $\Sigma_{k,k'}$ are coupled. The self-energy at $\Lambda=0$ can be given a simple physical meaning: $\Sigma^{\Lambda=0}_{j,j}$ represents an effective one-particle potential and $\Sigma^{\Lambda=0}_{j,j+1}$ is an effective modulation of the hopping. To calculate $\rho_j(\omega)$, one determines the spectral weights of the remaining one-particle problem.

For a small impurity strength V, after transforming to momentum space and taking $N\to\infty$, Eqs. (2) and (3) can be solved *analytically*, as long as Σ^Λ stays small. For the backscattering this gives $\Sigma^\Lambda_{k_F,-k_F}\sim\Lambda^{-\eta}$ with $\eta=U[1-\cos(2k_F)]/(\pi v_F)$ and the Fermi velocity v_F. To leading order in U, the exponent η is just $K_\rho-1$,[17] which shows that the nonperturbative fermionic RG equation captures the power-law increase found in the perturbative bosonic RG equation.

Numerically integrating the RG equations for finite systems, we can go beyond the perturbative regime. In each step of the integration we have to invert an $N\times N$ matrix. If we assume open boundary conditions in H_0, $[G^0]^{-1}-\Sigma^\Lambda$ is tridiagonal in real space and the numerical effort is considerably reduced.[25] This allowed us to treat systems with up to $2^{15}=32\,768$ lattice sites. For finite N the flow is effectively cut off on a scale of the order of $1/N$. For smaller systems we also considered periodic boundary conditions. Figure 1 shows typical results for $\Sigma^{\Lambda=0}_{j,j}$ and $\Sigma^{\Lambda=0}_{j,j+1}$ for a *site impurity* and lattice sites close to j_0. Since Σ is symmetric around j_0, mainly the region $j<j_0$ is shown. Similar to the HF approach the effective potential and hopping are oscillating and slowly decaying. The inset of Fig. 1 shows $\Sigma^\Lambda_{j_0,j_0}$ as a function of Λ for different N. Obviously the renormalized potential at the impurity site remains finite, 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 approach is taken too literally. A singular behavior is only found in $\Sigma^\Lambda_{k,k'}$ for momenta with $k-k'\approx\pm 2k_F$, which is associated with the *long-range oscillations* in real space.

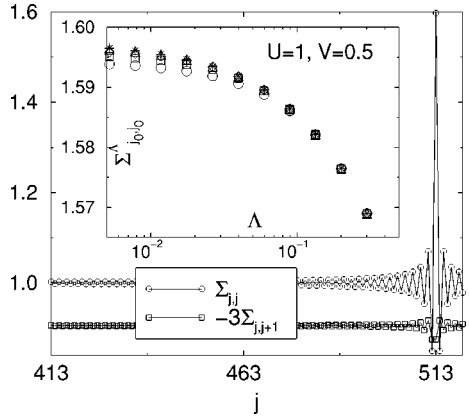

FIG. 1. $\Sigma^{\Lambda=0}_{j,j'}$ for a *site impurity* with $N=1026$ and $j_0=513$. The inset shows $\Sigma^{\Lambda}_{j_0,j_0}$ as a function of Λ for $N=66$ (circles), $N=130$ (squares), $N=258$ (diamonds), $N=514$ (triangles), and $N=1026$ (stars).

In Fig. 2 we present results for a hopping impurity with hopping matrix element $t_{j_0}=0.1$, i.e., in the *weak hopping* limit. It shows the flowing renormalized hopping $\Sigma^{\Lambda}_{j_0,j_0+1}-1$ as a function of Λ for $N=1024$. We have checked that the curve, to a good approximation, already presents the $N\to\infty$ result. In contrast to a simplistic interpretation of the bosonization result, the renormalized hopping $\Sigma^{\Lambda}_{j_0,j_0+1}-1$ does *not* scale to zero. Similar to the case of a site impurity, $\Sigma^{\Lambda=0}_{j,j'}$ shows long-range oscillations. Again this and not the scaling of a single V_j or t_j is the reason for the peculiar behavior of physical observables, as for example $\rho_j(\omega)$, discussed next.

As an inset to Fig. 2 the spectral weight near the impurity, $\rho_{j_0-1}(\omega)$, is presented for a *site impurity*. The data show a suppression of the weight for $|\omega|\to 0$, as expected. Each spike represents a δ peak of the finite system. For the largest system sizes considered $\rho_{j_0-1}(\omega)$ shows a power-law behavior at low energies. At the lowest energies on the other hand, it is cut off due to finite-size effects. To reliably extract the exponent, it is thus advantageous to analyze the finite- size scaling of the spectral weight $W(N)$ at μ, which is the amplitude of the δ peak of $\rho_{j_0-1}(\omega)$ at the chemical potential.[26] The large N dependence of $W(N)$ is given by a power law with the same exponent as the one in $\rho_{j_0-1}(\omega)$ as a function of ω, and the scales on which power-law behavior sets in are comparable.

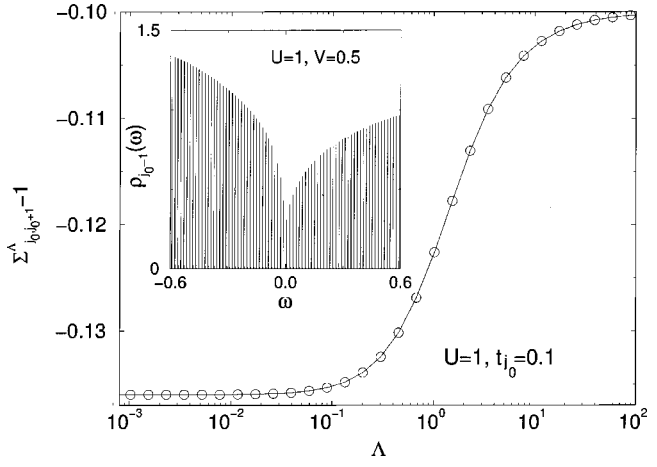

FIG. 2. $\Sigma^{\Lambda}_{j_0,j_0+1}-1$ as a function of Λ for a *hopping impurity* with $t_{j_0}=0.1$, $U=1$, $N=1024$, and $j_0=512$. Inset: $\rho_{j_0-1}(\omega)$ as a function of ω for a *site impurity* with the same parameters as in Fig. 1 ($N=1026$).

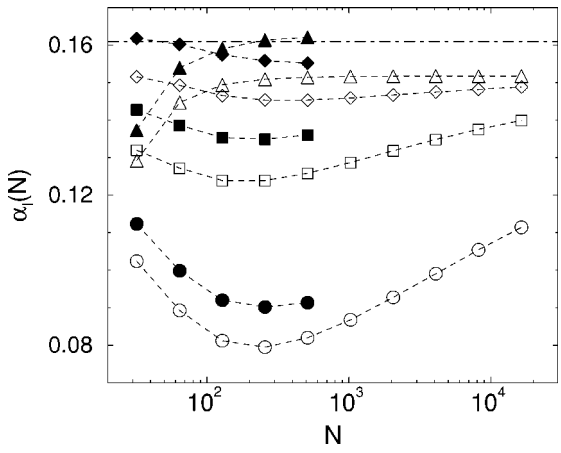

FIG. 3. $\alpha_I(N)$ as a function of N for $U=0.5$ and different V: $V=1$ (circles), $V=2$ (squares), $V=4$ (diamonds), and $V=\infty$ (triangles). The filled symbols are DMRG data, and the open ones obtained from the RG equation. The dash-dotted line gives the exact boundary exponent $\alpha^{\rm ex}_B$.

In Fig. 3 we show the negative of the logarithmic centered differences $\alpha_I(N)$ of $W(N)$ as a function of N for $U=0.5$ and different values of V obtained from RG ($N\leqslant 32\,768$) and DMRG ($N\leqslant 768$) equations. If $W(N)$ decays for $N\to\infty$ as a power law, $\alpha_I(N)$ converges to the respective exponent. For comparison we also calculated $\alpha_B(N)$ for the lattice site next to an open boundary ($V=\infty$). 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 equations capture the essential physics. For $V=\infty$ both methods produce the expected power-law behavior with boundary exponents $\alpha^{\rm DMRG}_B$ and $\alpha^{\rm RG}_B$. $\alpha^{\rm DMRG}_B$ ($N=512$) agrees up to 1% with the exact exponent $\alpha^{\rm ex}_B\approx 0.1609$. $\alpha^{\rm RG}_B$ ($N=16\,384$), which effectively is equal to $\alpha^{\rm RG}_B$ ($N=\infty$), deviates by roughly 6% from $\alpha^{\rm ex}_B$ since the RG equations are only correct to leading order in U. The RG curves for finite V suggest that, for $N\to\infty$, $\alpha^{\rm RG}_I(N)$ converges to the universal (V independent) exponent $\alpha^{\rm RG}_B$. This is in agreement with the field theoretical prediction. It is remarkable that, even for fairly strong impurities ($V=4$), extremely large values of $N=10^4-10^5$ are needed to exclude nonuniversal (V dependent) fixed points with some certainty. Solely relying on DMRG data for a few hundred lattice sites would, in this case, give no definite result.[13] In Fig. 4, RG and DMRG data are presented for intermediate impurity strengths $V=1$ and $V=\infty$ 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 larger U, $\alpha^{\rm RG}_I(N)$ ap-

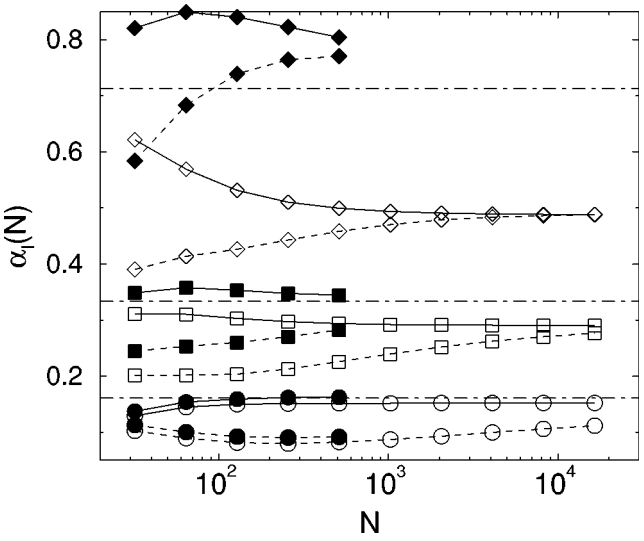

FIG. 4. $\alpha_I(N)$ as a function of N for $V=1$ (dashed lines) and $\alpha_B(N)$ for $V=\infty$ (solid lines) for different U: $U=0.5$ (circles), $U=1$ (squares), and $U=1.8$ (diamonds). Filled symbols are DMRG data, open ones RG results. The dashed-dotted lines give the exact U dependent boundary exponents α_B^{ex}.

proaches α_B^{RG} faster, but even for the largest $U=1.8$ considered here[27] (which corresponds to $K_\rho \approx 0.58$) very large N are needed. This demonstrates that for intermediate V and U, which are experimentally most relevant, very 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.

We finally note that in the fermionic RG scheme used in Ref. 6, flow equations were set up for a single parameter only: the transmission amplitude at the Fermi level. Our functional RG flow, however, indicates that in the nonperturbative regime different momentum channels are strongly coupled. Hence we believe that it is important to take the whole renormalized impurity potential profile into account. The RG equations used in Ref. 6 can also be derived within our formalism, if one makes similar crude approximations.[28] In addition, we did not find signs of an enhanced spectral weight as predicted in Ref. 29.

In summary, by solving a functional flow equation in a fermionic representation, we have shown that, in a one-dimensional lattice electron system with Luttinger-liquid behavior, an impurity makes observables at low-energy scales behave as if the chain is split into two parts with open boundary conditions at the end points. Our fermionic RG equation is nonperturbative in the impurity strength. Long-range oscillations in the effective impurity potential provide a simple real-space picture of the ''splitting'' mechanism. The accuracy of the finite site RG scheme was confirmed by a direct comparison to DMRG data. For realistic parameters very large systems are needed to reach the asymptotic open chain regime. Hence only special mesoscopic systems, such as very long carbon nanotubes, are suitable for experimentally observing the impurity-induced asymptotic open boundary physics. Our method can easily be generalized to the case of several impurities and, e.g., resonance phenomena can be studied.[19]

We would like to thank W. Apel, P. Durganandini, P. Kopietz, N. Shannon, C. Wetterich, and especially M. Salmhofer and H. Schoeller for valuable discussions. U.S. is grateful to the Deutsche Forschungsgemeinschaft for support from the Gerhard-Hess-Preis.

[1] A. Luther and I. Peschel, Phys. Rev. B **9**, 2911 (1974).
[2] D. C. Mattis, J. Math. Phys. **15**, 609 (1974).
[3] W. Apel and T. M. Rice, Phys. Rev. B **26**, 7063 (1982); T. Giamarchi and H. J. Schulz, *ibid.* **37**, 325 (1988).
[4] C. L. Kane and M. P. A. Fisher, Phys. Rev. B **46**, 15 233 (1992); A. Furusaki and N. Nagaosa, *ibid.* **47**, 4631 (1993).
[5] S. Eggert and I. Affleck, Phys. Rev. B **46**, 10 866 (1992).
[6] D. Yue, L. I. Glazman, and K. A. Matveev, Phys. Rev. B **49**, 1966 (1994).
[7] Here we will only discuss spinless fermions.
[8] K. Moon, H. Yi, S. M. Girvin, and M. P. A. Fisher, Phys. Rev. Lett. **71**, 4381 (1993).
[9] R. Egger and H. Grabert, Phys. Rev. Lett. **75**, 3505 (1995).
[10] P. Fendley, A. W. W. Ludwig, and H. Saleur, Phys. Rev. Lett. **74**, 3005 (1995).
[11] S. Qin, M. Fabrizio, and L. Yu, Phys. Rev. B **54**, R9643 (1996).
[12] S. Rommer and S. Eggert, Phys. Rev. B **62**, 4370 (2000).
[13] V. Meden, P. Schmitteckert, and N. Shannon, Phys. Rev. B **57**, 8878 (1998).
[14] M. Salmhofer, *Renormalization* (Springer, Berlin, 1998).
[15] D. Zanchi and H. J. Schulz, Phys. Rev. B **61**, 13 609 (2000); C. J. Halboth and W. Metzner, *ibid.* **61**, 7364 (2000); C. Honerkamp, M. Salmhofer, and N. Furukawa, *ibid.* **63**, 035109 (2001).
[16] Earlier RG studies for the bulk properties of one-dimensional systems are, e.g., reviewed in Ref. 24, and C. Bourbonnais and L. G. Caron, Int. J. Mod. Phys. B **5**, 1033 (1991).
[17] V. Meden, W. Metzner, U. Schollwöck, O. Schneider, T. Stauber, and K. Schönhammer, Eur. Phys. J. B **16**, 631 (2000).
[18] M. Klaus, J. Math. Phys. **32**, 163 (1991).
[19] V. Meden, W. Metzner, U. Schollwöck, and K. Schönhammer (unpublished).
[20] A. Cohen, K. Richter, and R. Berkovits, Phys. Rev. B **57**, 6223 (1998).
[21] C. Wetterich, Phys. Lett. B **301**, 90 (1993).
[22] T. R. Morris, Int. J. Mod. Phys. A **9**, 2411 (1994).
[23] M. Salmhofer and C. Honerkamp, Prog. Theor. Phys. **105**, 1 (2001).
[24] J. Sólyom, Adv. Phys. **28**, 201 (1979).
[25] The open ends are far away from the impurity site j_0 and do not influence the behavior close to j_0.
[26] For a precise definition of $W(N)$, see Ref. 17.
[27] The LL phase is stable only for $U<2$.
[28] We thank H. Schoeller for pointing this out to us.
[29] Y. Oreg and A. M. Finkel'stein, Phys. Rev. Lett. **76**, 4230 (1996).