Renormalization group flows in one-dimensional lattice models: impurity scaling, umklapp scattering and the orthogonality catastrophe

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We show that to understand the orthogonality catastrophe in the half-filled lattice model of spinless fermions with repulsive nearest neighbor interaction and a local impurity in its Luttinger liquid phase one has to take into account (i) the impurity scaling, (ii) unusual finite size L corrections of the form \( \ln(L)/L \), as well as (iii) the renormalization group flow of the umklapp scattering. The latter defines a length scale \( L_u \) which becomes exceedingly large the closer the system is to its transition into the charge-density wave phase. Beyond this transition umklapp scattering is relevant in the renormalization group sense. Field theory can only be employed for length scales larger than \( L_u \). For small to intermediate two-particle interactions, for which the regime \( L > L_u \) can be accessed, and taking into account the finite size corrections resulting from (i) and (ii) we provide strong evidence that the impurity backscattering contribution to the orthogonality exponent is asymptotically given by 1/16. While further increasing the two-particle interaction leads to a faster renormalization group flow of the impurity towards the cut chain fixed point, the increased bare amplitude of the umklapp scattering renders it virtually impossible to confirm the expected asymptotic value of 1/16 given the accessible system sizes. We employ the density matrix renormalization group.

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I. INTRODUCTION

Early indications that a single local impurity has dramatic effects on the low-energy physics of a one-dimensional (1D) Luttinger liquid (LL) were phrased in the modern language of renormalization group (RG) relevance and RG flows in the seminal work of Ref. 3. Considering the field theoretical Tomonaga-Luttinger model (TLM)\(^{4,5}\) and using perturbative RG in the impurity strength as well as the amplitude of a weak hopping between two open chains it was shown that for repulsive two-particle interactions a weak impurity with a finite backscattering contribution is a relevant perturbation, while a weak hopping is RG irrelevant.\(^{2}\) The RG flow from the perfect to the cut chain fixed points within the continuum TLM was later confirmed by nonperturbative approaches.\(^{6,7}\) These works were mainly concerned with transport and spectral properties of inhomogeneous LLs but, soon after, other quantities indicative of the impurity RG flow were investigated as well.

A rather fundamental one is the overlap \( O \) between the ground state of the homogeneous system and the one of the same system supplemented by a single local impurity. As shown by Anderson\(^{8}\) for noninteracting fermions this overlap vanishes as a function of the system size \( L \) following a power law \( O \sim L^{-\alpha} \). The orthogonality exponent (OE) \( \alpha > 0 \) of this orthogonality catastrophe is fixed by the scattering phase shifts of the impurity.\(^{9,10}\) It enters the exponents of edge singularities in x-ray spectra of metals\(^{11–13}\) as well as the low-energy properties of prototypical quantum dot models such as the interacting resonant level model in and out of equilibrium.\(^{14–16}\)

If the potential of the bare impurity varies weakly on the scale of \( k_F^{-1} \), such that the backscattering vanishes, the changes of the OE due to two-particle interactions can be computed exactly within the 1D continuum TLM by bosonization.\(^{15–17}\) Here \( k_F \) denotes the Fermi wave vector. The amplitude of the forward impurity scattering does not flow and thus the forward scattering contribution to the OE is only weakly affected by interactions.\(^{16,17}\) Furthermore, due to the linearization of the single-particle dispersion inherent to the construction of the TLM\(^{4,5}\) this contribution reduces to the Born approximation for the forward scattering phase shift at vanishing two-particle interaction. Bosonization thus only makes a prediction for the forward scattering contribution of the OE for very weak impurities.\(^{12}\) In the present work we do not consider impurity forward scattering. Instead, we study a particle-hole symmetric lattice model which is tailored such that forward scattering vanishes.\(^{12}\)

In the presence of even a small impurity backscattering, however, the consequences of the impurity RG flow towards the cut chain fixed point are striking: on low energy scales, that is for large system sizes \( L \), even a weak impurity effectively acts as an open boundary leading to a value \( \alpha = 1/16 \) of the OE—related to a phase shift of \( \pm \pi/2 \)—which is independent of the bare impurity strength and the two-particle interaction of the TLM.\(^{20–22}\)

Early attempts to confirm the impurity RG scaling close to the perfect and cut chain fixed points in microscopic lattice models using exact diagonalization\(^{23}\) were latter complemented by functional RG\(^{24}\) results which reveal the full crossover flow for spectral and transport properties.\(^{25–27}\) The expectation that the impurity RG flow of the TLM supplemented by a local impurity should...
also be observable in lattice models is based on the observation that the translational invariant TLM forms the low-energy fixed point model of a large class of homogeneous 1D metallic Fermi systems. This lies at the heart of LL universality. To show this type of universal behavior one has to understand the RG flow of different two-particle scattering processes (gology model). In lattice models of spinless fermions, which we consider here, particular attention has to be paid to umklapp scattering. More specifically, we study the lattice model of spinless fermions with nearest neighbor hopping $t$ and nearest neighbor interaction $U$ at half filling. This model falls into the LL universality class for $-2 < U/t < 2$. Within this parameter regime umklapp scattering is RG irrelevant. It becomes relevant for $U/t > 2$ leading to the transition into a charge-density wave state.

For lattice models with repulsive two-particle interaction the value $1/16$ for $\alpha$ was so far not convincingly demonstrated. Early attempts using density matrix renormalization group (DMRG) pointed towards this value. However, closer inspection within a comprehensive DMRG study using larger systems with up to 100 lattice sites showed that the results were inconclusive; see Fig. 5 of Ref. 10. We here revisit this problem. Our study is based on (a) recent field theoretical insights on the overlap of a 1D system (b) the finding that umklapp scattering cannot be ignored for $U/t \lesssim 1$, as well as (c) the progress in computer speed and the DMRG algorithm.

DMRG combines two advantages vital for our investigation: it provides highly accurate ground state wave functions and allows to study larger systems than obtainable by any other numerically exact approach to 1D quantum many-body systems.

In a series of papers it was argued that the logarithm of the ground state overlap of an open chain and an open chain additionally cut in the middle (infinite impurity strength) can be viewed as the free energy of a 1+1-dimensional classical boundary problem as long as the chain can be described by a field theory. Based on this it was shown that this specific overlap is characterized by unusual finite size corrections of the form $\ln(L)/L$. We here show that these corrections are also crucial to understand the system size dependence of the overlap in our interacting lattice model including the case of a finite impurity and thus the OE in general. We first study the overlap of the ground states of an open chain and an open chain with a bond impurity in the middle and second the one of a periodic chain and a periodic chain with a bond impurity. Considering the logarithm of the overlap as a free energy provides the justification to add a typical impurity scaling term $\sim L^{1-1/K}$ to the finite size scaling of $\ln |O|$ with $1/K$ being the scaling dimension of the residual hopping close to the cut chain fixed point and $K \leq 1$ the LL parameter of the lattice model which depends on $U/t$. By taking these finite size corrections as well as a standard term $\sim 1/L$ into account our results of the OE turn out to be consistent with the asymptotic $\alpha = 1/16$ for $U/t \lesssim 1$. Interestingly, the interplay of the impurity scaling $\sim L^{1-1/K}$ and the $\ln(L)/L$ correction leads to highly unusual finite size scaling of the backscattering component of the OE. It should however be noted that, although we provide evidence that the asymptotic OE is $1/16$ for $U > 0$, the system sizes corresponding to the asymptotic regime cannot be reached for small $U/t$, neither in numerical simulations nor in actual experiments.

As $K$ decreases with increasing interaction strength $U$ one is tempted to consider two-particle interactions close to the transition into the charge-density wave phase at $U/t = 2$ for which $K = 1/2$. In this limit the finite size corrections by the impurity flow vanish faster. However, for $U/t \rightarrow 2$ the amplitude of the flowing umklapp scattering at the largest accessible system sizes (up to a few thousand lattice sites) is still too large to be negligible and field theory cannot be employed. This renders it virtually impossible to conclusively demonstrate the asymptotic value $\alpha = 1/16$ for $U/t \gg 1$. The umklapp scattering defines a length scale $L_u$ which strongly increases the closer the system comes to its phase transition. In short, to understand the orthogonality catastrophe in our lattice model for the accessible system sizes of up to a few thousand lattice sites one has to consider both the single-particle impurity RG flow as well as the flow of components of the two-particle interaction. The appearance of a scale which restricts field theoretical behavior, e.g. typical LL power laws, to exceedingly large systems the larger $U$ was earlier shown—but not fully analyzed—for the momentum $k$ distribution function $n(k)$ of our translational invariant lattice model. To complement our results for $L_u$ extracted from the overlap we repeat this study and provide evidence that also this scale stems from umklapp scattering.

The remainder of this paper is organized as follows. In Sect. III we introduce our lattice model and briefly discuss the weak coupling RG flow of umklapp scattering (gology) as well as prior results on the impurity scaling obtained for the microscopic model. We discuss basics on wave function overlaps, their finite size dependence, and our way of analyzing the numerical data for $O$ in Sect. IV. In Sect. V we relate the umklapp scales $L_u$ extracted from the $L$-dependence of the overlap, the $k - k_F$-dependence of the momentum distribution of the translational invariant lattice model as well as the weak coupling RG of the continuum gology model. Section VI contains our DMRG results of the OE for systems with open (OBC) and periodic boundary conditions (PBC). Our results are summarized in Sect. VII. The appendices A and B contain details of our fitting procedures and the DMRG implementation, respectively.

II. MODEL

In the following we consider interacting spinless fermions on a lattice (lattice constant $a = 1$) described...
Thus need not be introduced. The Hamiltonian containing these two-particle scattering processes is given by a free bosonic field theory, the TLM,

\[ H_0 = \frac{1}{2\pi} \int dx \left\{ vK[\partial\theta(x)]^2 + \frac{v}{K}[\partial\phi(x)]^2 \right\}. \tag{3} \]

Here \( \theta(x) \) and \( \phi(x) \) are bosonic fields and the model parameters are the charge velocity \( v \) and the dimensionless LL parameter \( K \). Using the above described 'constructive' bosonization of the lattice model it is only possible to extract the \( U \) and \( t \) dependence of \( v \) and \( K \) for \( U/t \ll 1 \).

For the lattice model Eq. (11) at half filling one additionally encounters an umklapp scattering term \( g_3 \), for which momentum is conserved only up to a vector of the reciprocal lattice. This gives rise to an interacting contribution (\( y \sim g_3 \))

\[ H_u \sim y \int dx \cos[4\phi(x)] \tag{4} \]

to the bosonized Hamiltonian \( H = H_0 + H_u \) leading to the sine-Gordon model.\(^{16}\) Umklapp scattering breaks scale invariance and the large amount of results for the TLM associated to the latter are not applicable for \( y \neq 0 \). Fortunately, using a weak coupling RG treatment of the umklapp scattering term, with \( y \sim U \) assumed to be small, one can show, that it is RG irrelevant. As the details of the RG flow do not matter in the present section the corresponding flow equations\(^{4,31}\) are given in Eq. (12) below. Under the RG flow, that is for decreasing energy scales (increasing length scales), the umklapp scattering is renormalized to zero and scale invariance is restored. At the end of the flow, where the flow parameter \( \ell \rightarrow \infty \), an approximation to the renormalized value of \( K \) is obtained by \( K(\infty) \). However, it is a priori not clear how small the energy scales of a given microscopic model, e.g. our lattice model Eq. (11), has to be, such that the umklapp scattering contribution can be safely neglected. Furthermore, the perturbative nature of the RG treatment restricts its range of validity to small interaction strength \( (U/t \ll 1) \).

Fortunately, for the model of Eq. (11) one can find an exact solution via Bethe ansatz. The exact values of \( v \) and \( K \) at half-filling and \( |U| < 2t \) can be extracted from the Bethe ansatz expression for the ground state energy and read\(^{19}\)

\[ K_B = \frac{\pi}{4\eta}, \]
\[ v_B = t \frac{\pi \sin(2\eta)}{\pi - 2\eta}, \tag{5} \]
\[ 2\eta = \arccos \left( \frac{-U}{2t} \right). \]

For interactions \( 0 \leq U/t < 2 \), \( K_B \) assumes values \( 1/2 < K_B \leq 1 \). By a series expansion of \( K_B \) in \( U/t \) one recovers to leading order the results obtained for \( K(\infty) \)

| symbolic representation | OBC | PBC |
|-------------------------|-----|-----|
| perfect chain \( b = 1 \) | ☑  | ☑  |
| impurity \( b < 1 \) | ☑  | ☑  |

TABLE I. Symbols used for the different setups featuring OBC and PBC each with \( b = 1 \) (perfect chain) or \( b < 1 \) (hopping impurity at center of chain).

The linearization of the dispersion leads to the linear part of the dispersion around the Fermi points in compliance with energy and momentum conservation is kept. The low-energy physics (\( L \rightarrow \infty \)) of the impurity free model defined in Eq. (11) is known to be characterized by the g-ology model.\(^{20}\) In this continuum model only the linear part of the dispersion around the Fermi points as well as the dominant low-energy interaction processes in compliance with energy and momentum conservation are kept. The linearization of the dispersion leads to branches of left (\( k \approx -k_F \)) and right (\( k \approx k_F \)) moving fermions. After performing the continuum limit and linearizing the dispersion relation for the model given in Eq. (11) one can classify different interaction processes. One involves two fermions on the same branch denoted as \( g_4 \) and one two particles on different branches denoted as \( g_2 \). Note that in the present spinless case \( g_2 \) processes with small momentum transfer and \( g_1 \) processes with momentum transfer \( 2k_F \) are indistinguishable. The latter thus need not be introduced. The \( g_4 \) and \( g_2 \) processes conserve momentum. Using standard bosonization\(^{15}\) the

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at the end of the flow of the perturbative RG. Furthermore, \( y_B = 0 \) is found in accordance with \( y(\infty) = 0 \) of the weak coupling RG. For \( U/t > 2 \) umklapp scattering turns RG relevant, signaling the phase transition to a charge-density wave state. This transition (at \( K = 1/2 \)) is also captured by the perturbatively motivated RG equations, although they cannot be used to determine \( K(\infty) \) and \( y(\infty) \) any longer as \( y \) flows to strong coupling. To summarize, for \( U/t \leq 2 \) the g-ology RG equations\(^\_12\) describe qualitatively (and for small \( y \) even quantitatively) the fate of the umklapp scattering and its effect on the LL parameter \( K \) of the impurity free lattice model.

A comprehensive picture of the spectral and transport properties of our lattice model Eq. \((8)\) supplemented by a local impurity, such as e.g. \( H_\text{imp} \) Eq. \((9)\), at small to intermediate interactions was obtained using functional RG\(^\_27–\_29\). The effect of the perfect and cut chain fixed points, the corresponding scaling dimensions, as well as the full crossover flow on the corresponding observables (local single-particle spectral function, linear conductance) found within the functional-RG approach are in accordance with the results derived from the TLM Eq. \((10)\) supplemented by an impurity\(^\_34–\_36\). The latter corresponds to the local sine-Gordon Hamiltonian\(^\_1\). In particular, the effect of a hopping between two decoupled chains vanishes as \( \Lambda^{1/K-1} \), where \( \Lambda \) denotes an infrared cutoff, such as e.g. temperature or inverse system size \( L^{-1} \). In the applied approximation, which is controlled for \( U/t \lesssim 1 \), the functional RG has the distinct advantage that very large systems of up to \( 10^7 \) lattice sites and thus very low energy scales are accessible. However, it cannot directly be employed to compute the overlap \( O \) as it does not aim at wave functions but rather \( n \)-particle Green functions. We note in passing that the approximate functional RG method does not capture the phase transition at \( U/t = 2 \) and thus the divergence of the scale \( L_d \). We here resort to a different approach and use DMRG. For details of our DMRG implementation, see Appendix\(^\_\_B\).

### III. WAVE FUNCTION OVERLAPS

The central quantity to study in the context of the OC is the overlap \( O \) of two ground state wave functions—one of a system with an impurity \( (b < 1) \) and one of a perfect system \( (b = 1) \). In this work we study two types of overlaps which differ by the boundary conditions of the models. In the case of open boundary conditions, we consider the overlap \( O = \langle \ldots | \ldots | \ldots \rangle \) between ground states of a perfect chain and a chain with a bond impurity \( b < 1 \) in the center. For periodic boundary conditions, we study the overlap \( O = \langle \ldots | \ldots | \ldots \rangle \). These overlaps depend on the system size \( L \) in a characteristic way. The OC owes its name to the limiting behavior \( \lim_{L \to \infty} O = 0 \), i.e., the fact that the ground states of two infinitely large systems are zero even though they differ only by the presence of a local impurity\(^\_\_2,\_10\).

We are particularly interested in the approach of this limit when the systems under consideration are still finite. For a noninteracting system one can show\(^\_\_19\) that

\[
O \sim L^{-\alpha}, \quad \alpha > 0.
\]

At \( U = 0 \) the OE \( \alpha \) of our model given by \( H + H_\text{imp} \) Eqs. \((11)\) and \((12)\) at half filling can be computed using scattering theory\(^\_19\).

\[
\alpha_{U=0} = \frac{1}{4\pi^2} \arcsin^2 \left( \frac{1 - b^2}{1 + b^2} \right).
\]

Combining this result with the expectation that in the interacting model \( b \) effectively approaches 0 (cut chain fixed point) for large systems one can conjecture that

\[
\alpha_{U>0} = \frac{1}{16}.
\]

However, it remains to be shown that this is indeed the case. Earlier attempts to do so using DMRG and systems of up to 100 sites indicated a tendency towards this value but turned out to be inconclusive under closer inspection\(^\_19,\_32,\_33\).

In order to thoroughly investigate the finite-size behavior of \( O \) and to establish the OE from numerical calculations of wave function overlaps in finite size systems, it is customary to study the logarithmic derivative of \( |O| \). From the DMRG calculations of \( O(L) \) we derive the logarithmic derivative

\[
D(L + \Delta L/2) = -\frac{\ln |O(L + \Delta L)| - \ln |O(L)|}{\ln(L + \Delta L) - \ln(L)}.
\]

For \( L \to \infty \), \( D(L) \) should thus converge to the correct OE \( \alpha \). It turns out, however, that supporting this statement with numerical data is exceedingly difficult without further knowledge about the finite-\( L \) functional form of \( D(L) \). In the following we discuss two unusual terms in the finite-size scaling, which are of utmost importance for a conclusive analysis of the numerical data.

A series of recent conformal field theory (CFT) studies\(^\_\_34–\_36\) provided surprising insights on the finite-\( L \) scaling of \( \ln |O(L)| \) and thus \( D(L) \) for 1D interacting field theories. More specifically the authors studied the overlap of an open chain and an open chain cut in the middle, that is \( O = \langle \ldots | \phantom{=} \quad | \phantom{=} \ldots \rangle \) in our short hand notation. The impurity scaling does not play a role for this setup as one already starts at the cut chain fixed point with \( b = 0 \). The authors of Refs.\(^\_\_33,\_36\) argued that \( \ln |O| \) can be viewed as the free energy of a 1+1-dimensional classical boundary problem. From this they extracted the leading behavior \( \ln |O(L)| \sim -\frac{1}{16} \ln(L) \) and showed that the stress tensor at the boundary leads to the unusual leading finite size correction \( \ln(L)/L \) which must be supplemented by a regular \( 1/L \) term. For \( D(L) \) we thus expect to find

\[
D(L) \approx \alpha + \frac{1}{16} \ln \frac{L}{\lambda} + \frac{1}{L}.
\]
we show that this form indeed allows for convince fits of our DMRG data from which $\alpha = 1/16$ can eventually be concluded even for $b > 0$ and small to intermediate interactions $U/t \lesssim 1$. 

IV. THE UMKLAPP SCALE $L_u$

The finite size corrections to the OE of the form of Eqs. (10) and (11) can be applied if the relevant physics is described by a CFT. In the bosonic representation of the lattice model, however, there is an umklapp term which breaks scale invariance. The coupling constant of this term renormalizes to zero as the system is studied on increasingly large length scales. In other words, field theory results generally do not relate to all observables of the corresponding microscopic theory, but only to those measuring the system on certain length scales. The lower bound of this range of length scales is not sharply defined. Instead, understanding the umklapp scale $L_u$ as the typical length above which the umklapp term is ‘too small to be noticed’ turns out to be convenient. Of course, there is no unique way to determine $L_u$. Different ‘measurements’ and the corresponding definitions of what means ‘too small to be noticed’ will give rise to different representations of $L_u$ (we indicate this by superscripts RG, O, and n in the following). However, they agree in their qualitative behavior, namely that $L_u$ is atomically small for $U/t \ll 1$ and diverges for $U/t \rightarrow 2$.

We shall first analyze the g-ology RG of the translational invariant model and identify the above-described effect in the RG flow. The umklapp term Eq. (11) in the bosonized theory with a coupling constant $y$ breaks the scale invariance, but is irrelevant in the RG sense for $U/t < 2$. In general, the RG produces a sequence of effective low-energy theories which are capable of describing the physics on increasingly large length scales. In this sequence $y$ decreases to zero and $K$ approaches $K_B$ as determined from the Bethe ansatz. However, an ‘exact RG’, which is valid for all $y$, is not known. Instead one usually resorts to perturbative RG equations, valid for small umklapp amplitudes

$$\frac{dy(l)}{dl} = -y(l)[4K(l) - 2], \quad \frac{dK(l)}{dl} = -y(l)^2K(l)^2$$

(12)

where $L = e^l$ is the length scale above which the renormalized theory is valid. Clearly, for $1/2 < K < 1$ (corresponding to $2 > U/t > 0$), $y = 0$ is a stable fixed point of the flow equations. The initial conditions for $K$ and $y$ can be obtained perturbatively from the lattice model.
that is for $U/t \ll 1$. However, since we are more interested in the end of the RG flow than in its beginning, it is convenient to fix the end point $[K(\infty), y(\infty)] = [K_B, 0]$ with the help of the Bethe ansatz solution of our translational invariant lattice model. Thus, the question is: ‘For which length scale $L_u = e^y$ is $y < y_0$ for a certain small $y_0$, which we are free to choose.’

Figure 2 shows the solution of the approximate flow equations \(^2\) for various $0 < U/t \leq 2$. The RG flow always seems to reach its fixed point $[K_B, 0]$, but Fig. 2(b) makes clear that the flow equations must be integrated over increasingly large scales $l$ as $U/t$ gets close to its critical value 2. We may now define the weak coupling RG-based umklapp scale $L_u^{\text{RG}}$ implicitly by

$$y(\ln[L_u^{\text{RG}}]) = y_0.$$  \hspace{1cm} (13)

We choose $y_0 = 0.002$ and plot $L_u^{\text{RG}}$ as a function of $U/t$ in Fig. 3 as a solid line. It is apparent that this representative of the umklapp length scale becomes exceedingly large as $U/t \to 2$.

A second way of determining $L_u$ is based on the power-law behavior of the momentum distribution function $n(k) = \langle c_k^\dagger c_k \rangle$ for $k \approx k_F$. From bosonization it is known

![FIG. 2. (Color online) Perturbative RG flow for different $U$. Part (a) shows the flow in the $K\gamma$-plane for $U = 0.2, 0.4, \ldots, 2$. Part (b) shows $y(l)$ for $U = 0.2, 0.5, 1, 1.5, 1.9, 1.99, 1.999, 2$ on a log-log scale. The dashed (green) line represents the $y_0$ we have chosen for determining $L_u^{\text{RG}}$.](image)

![FIG. 3. (Color online) $U$-dependence of different representatives of the umklapp length scale $L_u$: The RG-based $L_u^{\text{RG}}$, the $n(k)$-based $L_u^n$, and the overlap-based $L_u^O$.](image)

![FIG. 4. (Color online) Exponents $\gamma$ of the momentum distribution function $n(k)$ for $U = 0.2, 0.25, \ldots, 1.95$ (from bottom to top). The dashed (blue) lines represent the expectations $\gamma_B = (K_B + 1/K_B - 2)/2$ from the Bethe ansatz. The solid red lines are the logarithmic derivatives $\gamma(k)$ (see Eq. (15)).](image)
A third way to determine $L_u$ is based on fitting the CFT form Eq. (11) to overlaps between ground states of the lattice model of size $L$ with (infinite) bond impurity $b = 0$ and without the latter (OBC; see Fig. 4). If one restricts the $L$-range of the data to be fitted to $[L_r - \Delta L, L_r + \Delta L]$, one observes convergence of the extrapolated exponent $\alpha$ as the range is shifted towards larger $L_r$. From the systematic investigation of how large systems are needed in order to predict the correct asymptotic exponent $\alpha = 1/16$, one may extract the overlap-based umklapp scale $L_u^{\text{RG}}$. Details about this procedure can be found in Appendix A.

In Fig. 5 we compare the three length scales $L_u^{\text{RG}/a/O}$, which are all representatives of the same physical effect, namely that the lattice model’s correspondence with a CFT requires exceedingly large length scales as $U/t$ is increased towards its critical value $2$. It is not surprising that the representatives differ significantly from each other in their detailed form, since the criterion “too small to be noticed” is not directly comparable for the different aspects discussed above. In fact, the excellent agreement of $L_u^{\text{RG}}$ and $L_u^{O}$ should be viewed as a coincidence. The essential feature shared by all the related length scales is that they are atomically small for $U \approx 0$ and grow exponentially for $U/t \gtrsim 1$. As exemplified considering $n(k)$ typical LL power laws can only be expected on momentum scales smaller than $L_u^{-1}$ (see also Ref. 39). While the appearance of such an interaction dependent scale associated to RG irrelevant two-particle scattering terms is routinely considered in spinful lattice models such as the 1D Hubbard model (flow of $g_{1,L}$-term in the g-ology classification) its role was so far not fully appreciated in studies of the spinless lattice model with nearest-neighbor interaction.

For our further analysis this means that one should always keep in mind that a minimum system size is required if CFT arguments are to be used, and that this minimum system size grows very strongly for $U/t \gtrsim 1$.

V. BOND IMPURITIES

We are now prepared to investigate the OC in our lattice model with finite bond impurity $0 < b < 1$ considering OBC (overlap $\langle \cdots | t = 0 \rangle$) as well as PBC (overlap $\langle \cdots | t > 0 \rangle$). As before, we study the length dependence of the discrete logarithmic derivatives of ground state overlaps $D(L)$ Eq. (11) and now fit the form Eq. (11) to those. It is the combination of three ‘subleading effects’ that governs the approach to the large-$L$ limit: (i) the systems must be longer than the umklapp scale $L_u$, which we ensure by considering $U/t \lesssim 1$ only. (ii) The stress-tensor-based subleading correction $\sim \ln(L)/L$ must be respected. (iii) The impurity scaling term $\sim L^{-1/\kappa}$ must be included, as well. In our fits for finite $b$ and $U > 0$, we fix $\alpha = 1/16$ and $K = K_B$, which leaves us with the three fit parameters $\beta$, $\lambda$, and $\kappa$. For $U = 0$, the exponent of the impurity scaling term is zero and we may absorb $\kappa$ into $\alpha$, thus leaving the OE exponent as a fit parameter in this non-interacting limit as well.

We start out with OBC as those were also considered in the $b = 0$ field theory studies Refs. 34–36 and analyze the overlap $\langle \cdots | t > 0 \rangle$. Figure 5 shows the DMRG-based logarithmic derivatives of the overlaps $D(L)$ for $U/t = 0$, $U/t = 0.2$, and $U/t = 1$. The fits for $U/t = 0$ are shown as a function of $1/L$ for systems with up to $L = 2000$ lattice sites. For $U = 0$ the curves extrapolate to the non-interacting exponents Eq. (8). For $U > 0$ all curves extrapolate to 1/16 for $L \rightarrow \infty$. The dotted (green) horizontal line indicates the limiting exponent 1/16. The dashed lines show fits with an additional $L^{-2}$ term. Note the different $y$-axis scales of (a)-(c).
and show the fits for the overlap to the form with the limiting exponent $1/16$.

For $L=0$ all curves extrapolate to $1/16$ for $L \to \infty$. Note the nonmonotonic behavior. The dotted (green) horizontal line indicates the limiting exponent $1/16$.

$D(L)$ as a function of $1/L$ (circles) together with fits of form Eq. (11) (solid lines) for systems of up to $L = 256$ lattice sites. For $U=0$ the curves extrapolate to the noninteracting exponents Eq. (7). For $U > 0$ all curves extrapolate to $1/16$ for $L \to \infty$. The dotted (green) horizontal line indicates the limiting exponent $1/16$.

The situation improves for $U/t \approx 1$ [Fig. 6(c)] and the data are closer to the asymptotic value. Note the different $y$-axis scales of Fig. 6(a)-(c). The finite-size fits for open boundary conditions in Fig. 6(c) to the form with $L^{-1}$ as the most quickly decaying term show slight deviations from the numerical data for small $L$ (solid lines in Fig. 6). Including a further term $\sim L^{-2}$ in the functional form improves the fit quality considerably (dashed lines in Fig. 6).

Even though for $U > 0$ we fixed $\alpha$ to $1/16$ we judge the excellent agreement between the DMRG data and the fits to provide strong evidence for the asymptotic value $1/16$ of the backscattering component of the OE in our lattice model. Furthermore, the quality of the fits gives us confidence that the scaling form Eq. (11) which was based on field theoretical arguments indeed presents the leading finite size corrections of $D$ of the microscopic model.

Figures 6 and 7 show the fits for the overlap $O = \langle \langle D(b) \rangle \rangle$ and system sizes of up to $L = 264$. It is inherent to the DMRG algorithm that for PBC the numerical resources are exhausted faster than for OBC which explains the difference in reachable system sizes. For $U=0$ the numerical data again extrapolates to the known noninteracting OE Eq. (7). For $U > 0$ our conclusions are identical to the case of OBC. We note, however,
that the quality of the fits to Eq. (11) without an additional $L^{-2}$ term is as good as the one of the fits for OBC including this term. Since finite size effects are expected to be more severe for OBC than for PBC, this is not surprising. The excellent quality of the fits provides evidence that the CFT arguments, employed for OBC, which led us to consider the form Eq. (11) of the finite size corrections are applicable to both, OBC as well as PBC. Note, that for $U = 0$ and $b = 0$ this was already hinted at in Ref. [36].

The excellent agreement between the DMRG data for $D(L)$ and the fits by the form Eq. (11) for OBC and PBC is naturally linked to our conclusion that the backscattering contribution to the OE in the microscopic model is indeed given by $1/L$.

It is worth noting that the prefactors of the $\ln(L)/L$ terms have opposite signs for different boundary conditions, while the impurity scaling term has equal signs. Since these are the most slowly decaying finite size contributions, this sign difference leads to counterintuitive behavior of the logarithmic derivatives for PBC: as shown in Fig. 6 and in particular Fig. 7 for certain parameter combinations $U/t$ and $b$, $D(L)$ seems to decrease monotonously and even appears to converge, until for system sizes beyond the reach of numerical techniques it turns up and finally approaches the asymptotic regime with $\alpha = 1/16$. This explains why the results of the earlier DMRG studies performed for PBC turned out to be inconclusive.19,32,33

VI. SUMMARY

Using state of the art DMRG we have studied the orthogonality catastrophe in the lattice model of spinless fermions with repulsive nearest-neighbor interaction at half band filling. We were able to provide convincing evidence for the expected backscattering contribution $1/16$ to the asymptotic orthogonality exponent for weak to intermediate interactions. This was only possible by carefully considering finite size corrections stemming from the field theoretical insight that the logarithm of the overlap can be viewed as a free energy. For chains with periodic boundary conditions the interplay of these terms results in nonmonotonic scaling behavior for system sizes $L \rightarrow \infty$ (compare also Fig. 5 of Ref. [19]). For interactions approaching the one at which umklapp scattering becomes RG relevant and the system enters a charge-density wave phase we were not able to confirm $\alpha \rightarrow 1/16$. For such results from scale invariant field theory cannot be employed on the reachable length scales of up to a few thousand lattice sites due to residual umklapp scattering.

For the overlap between ground states of a homogeneous and a not perfectly cut system ($b > 0$) the true asymptotic regime for the orthogonality exponent, where all subleading terms are negligibly small, is virtually unreachable for small interactions $U$. It is important to note that the system sizes needed for reaching the asymptotic regime not only exceed the computational resources, but are also beyond experimental reach. For instance, at $U/t = 0.1$ and $b = 0.05$ (compare also Fig. 7), at $L = 10^6$ lattice sites, corresponding to system sizes in the meter range, the observed exponent $0.058$ is still closer to $\alpha_{U=0} \approx 0.055$ than to the asymptotic $1/16 = 0.0625$. Moreover, for reasonable system sizes the exponent seems to converge to a value less than $1/16$.

We expect to find similar behavior in other half-filled lattice models. Our study highlights the importance of scaling of single-particle inhomogeneities as well as two-particle scattering in 1D correlated electron systems in their Luttinger liquid phase.

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Appendix A: Variable window fits of overlaps

For investigating the asymptotic behavior of a quantity and especially for extracting this behavior from numerical data, it is not always useful to use the full range of data points at hand for one single fit. Instead, one may restrict the range of fit data to a certain window of all available data and shift this window up and down. From such a procedure, one can learn something about the stability of such a fit. Moreover, effects which are not accounted for in the fit function, but are only present in a certain regime, can be identified. It is the latter aspect we are interested in, in the present context.

In this procedure, which we call variable window fitting, we restrict the numerical data for a particular fit to the window $[L_w - \Delta L/2, L_w + \Delta L/2]$. The size of the window $\Delta L$ is fixed and must be sufficiently large for the individual fits to be numerically stable. The best fit parameters can then be studied as functions of the center of the data window $L_w$. Here we are especially interested in the $L_w$-dependence of the extrapolated exponent $\alpha(L_w)$.

For overlaps with $b = 0$ impurities the impurity scaling is irrelevant and thus the form Eq. (10) should be used for fitting the discrete logarithmic derivatives of the numerically calculated overlaps [see Eq. (9)]. However, since Eq. (10) originates from a CFT analysis, the umklapp process [described by Eq. (3)] present in the interacting lattice model Eq. (1) with $U > 0$, which is the basis of the numerical simulation, is not accounted for in this fit.
form. As the length scales on which the system is studied is increased, the coupling constant $y$ of this umklapp process scales to zero. Thus, if such an umklapp term is present, one expects that the fit is only stable for sufficiently large $L_w$.

Figures 8 and 9 show the variable window fits for $U = 0$ and 1 in systems with OBC and PBC, respectively. The different curves in the main plot correspond to different window centers $L_w$. We have chosen $\Delta L = 40$ for the OBC and $\Delta L = 14$ for the PBC data. Two effects leading to different curves for different $L_w$ should be distinguished. One is due to the quickly decaying contribution of the standard higher order finite-size corrections, such as $L^{-n}$ terms with $n \in \mathbb{N}$ and $n \geq 2$, which in the present case might be supplemented by terms $\ln(L)/L^{n}$ [15,34-36].

In the $U = 0$ plots [parts (a) of Figs. 8 and 9], due to the absence of the umklapp term in the noninteracting limit, this is the only effect that can be observed. In this case, the convergence to $\alpha(L_w) \approx 1/16$ is reached already for small $L_w$, as can be seen in the corresponding insets. The second reason for deviating fits is the presence of terms in the Hamiltonian which are not captured by the scaling form Eq. (10). This effect can be observed in parts (b) of Figs. 8 and 9 showing the $U/t = 1$ data with their corresponding variable window fits. As can be seen in the corresponding insets, the typical system sizes needed to achieve convergence to $\alpha = 1/16$ are much larger than in the $U = 0$ case. We attribute this to the umklapp length scale $L_u$ which diverges as $U/t$ approaches its critical value 2.

From the variable window fits we may extract a further representative of $L_u$, namely the overlap-based umklapp scale $L_u^O$. For this we fix an acceptance interval of a certain width $\Delta \alpha$ around $\alpha = 1/16$. If the extrapolation $\alpha(L_w)$ from a certain data window $L_w$ is in this interval, then the $L_w > L_u^O$. Thus, $L_u^O$ is defined as the $L_w$ for which the curve $\alpha(L_w)$ enters the acceptance interval. We have chosen $\Delta \alpha = 0.0002$ as the interval width from which the $L_u^O$ in Fig. 8 has been extracted.

**Appendix B: Details about the DMRG calculations**

All numerical results discussed in this work have been acquired by the DMRG method. We have employed two versions of the general DMRG concept [37]. For the ground states of the lattice models with finite size $L$ we have used the standard iterative ground
state finder with a two site update, formulated in matrix product state (MPS) language. In order to increase
the efficiency of our code, we have explicitly used the conservation of the total particle number. The method
is limited by the discarded terms in the wave function. After each two site optimization, the wave function is
Schmidt-decomposed into the form

$$|\psi\rangle = \sum_a s_a |a\rangle_L |a\rangle_R, \quad (B1)$$

where $0 < s_a < 1$ are the Schmidt-weights and $|a\rangle_L$ ($|a\rangle_R$) is the left (right) part of the corresponding term in
the wave function. If $s_a$ is below a certain threshold, the term is discarded. Typically, this threshold is between
$10^{-6}$ and $10^{-8}$. For all calculations we have checked that the result does not change as the threshold is further
decreased. In the calculations with the lowest thresholds and the largest system sizes, the resulting bond dimen-
sions are on the order of $10^4$.

For both, PBC and OBC, our MPS ansatz for the ground state of the finite systems is of the form

$$|\psi\rangle = \sum_{\mu_1 \mu_2 \ldots \mu_L} M_{\mu_1}^L \cdots M_{\mu_L}^{L} |\mu_1\rangle |\mu_2\rangle \cdots |\mu_L\rangle, \quad (B2)$$

with $|\mu_j\rangle$ the state of the $j$th site and $\mu_j$ running over the
basis states of the local Hilbert space at this site. The first and last matrices $M_{\mu_1}^{L_1} \in \mathbb{C}^{L \times d}$ and $M_{\mu_L}^{L} \in \mathbb{C}^{L \times 1}$
with $d, d' \geq 1$, which means that the periodic boundary conditions are not built into the MPS. Instead, we explic-
ically add one long-range term connecting the first and the last site of the chain to the matrix product operator
which represents the Hamiltonian with respect to which the ansatz Eq. (B2) is optimized. For small systems it has
been checked with exact diagonalization that the ground states of the periodic systems are correct. However, the
bond dimension needed to reach a similar ground state accuracy is considerably higher for the periodic boundary
conditions.

Once the optimal ground states have been found, which usually is the case after 5-10 sweeps, the desired wave
function overlaps can be calculated straightforwardly.

For the calculation of the momentum distribution function $n(k)$ we have employed the iDMRG algorithm de-
scribed in Ref. 40. Here we have fixed the bond dimension to 1600. Convergence of the ground state requires
typically between 50.000 and 100.000 iterations. The particle number conservation law has been employed as well.
For calculating $n(k)$ we follow closely Ref. 33, i.e., we measure the single-particle Green function $G_j = \langle c_j | c_0 \rangle$
and compute the Fourier transform $n(k) = \sum_j e^{-ik} G_j$.

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