The interacting Rice-Mele model – bulk and boundaries

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We investigate the interacting, one-dimensional Rice-Mele model, a prototypical fermionic model of topological properties. To set the stage, we firstly compute the single-particle spectral function, the local density, and the boundary charge in the absence of interactions. The boundary charge is fully determined by bulk properties indicating a bulk-boundary correspondence. In a large parameter regime it agrees with the one obtained from an effective low-energy theory (arXiv:2004.00463). Secondly, we investigate the robustness of our results towards two-particle interactions. To resum the series of leading logarithms for small gaps, which dismantle plain perturbation theory in the interaction, we use an essentially analytical renormalization group approach. It is controlled for small interactions and can directly be applied to the microscopic lattice model. We benchmark the results against numerical density matrix renormalization group data. The main interaction effect in the bulk is a power-law renormalization of the gap with an interaction dependent exponent. The important characteristics of the boundary charge are unaltered and can be understood from the renormalized bulk properties, elevating the bulk-boundary correspondence to the interacting regime. This requires a consistent treatment not only of the low-energy gap renormalization but also of the high-energy band width one. In contrast to low-energy field theories our renormalization group approach also provides the latter. We show that the interaction spoils the relation between the bulk properties and the number of edge states, consistent with the observation that the Rice-Mele model with finite potential modulation does not reveal any zero-energy edge states.

I. INTRODUCTION

For noninteracting quantum many-body systems the relation between the topological properties and the behavior of typical observables is well understood [1–7]; see Refs. [8–12] for reviews and textbooks. However, in many respects this understanding relies on ideas which make explicit use of the concept of independent particles. Insights on the relation between topology and the physics of interacting many-body systems are based either on case studies for specific models or on general considerations of how to extend the concept of topological invariants to the realm of correlated systems [13–23].

We here provide a case study for the interacting, one-dimensional (1d), and spinless Rice-Mele (RM) model [24]. For vanishing interaction and up to isolated points in the space of the single-particle parameters the model is an insulator with phases of distinct topological properties. It is one of the most elementary models with a band gap in the spectrum and was set up in the early eighties when investigating the electronic properties of linear polymers [25]. The model consists of two-site unit cells with an intra-cell hopping matrix element $t_1$ and alternating onsite energies $V_1$ and $V_2$. The unit cells are coupled by a nearest-neighbor inter-cell hopping $t_2$. For degenerate onsite energies it becomes the famous Su-Schriefer-Heeger (SSH) model [26]. We add a nearest-neighbor two-particle interaction of amplitude $U$ to the Hamiltonian.

One of the hallmarks of topological systems is the bulk-boundary correspondence (BBC) [27–34]. In the traditional form, denoted as orthodox BBC in the following, it is formulated in terms of a connection between topological bulk invariants and the appearance of edge states. For 1d systems it is known that topological invariants are related to the number or parity of zero-energy edge states. However, one can view the BBC from a more general point of view by raising the question if other properties of a system close to a boundary can solely be understood based on bulk characteristics. This is of particular interest since topological invariants (like Chern and winding numbers) can only be defined for clean and non-interacting systems. Here, we will focus on this aspect and call it generalized BBC in the following to distinguish it from the orthodox one.

To investigate the generalized BBC we first solve the noninteracting infinite and semi-infinite RM model. We focus on three observables to analyze their potential to be candidates for the formulation of a generalized BBC: The local single-particle spectral function, the local density, and the so-called boundary charge accumulated close to the boundary. Edge states show up as in-gap $\delta$-peaks in the local single-particle spectral function and their appearance and energy can be used to investigate the generalized BBC. The boundary charge, which is computed from the local density, is influenced by the number of edge states via an integer number. However, the fractional part of the boundary charge is an alternative and fundamentally different observable for the formulation of a generalized BBC. It is influenced by the whole spectrum of extended states, which carry also important information from the boundary. As shown for noninteracting and clean systems via the polarization in terms of...
the Zak-Berry phase and recently also for disordered and interacting systems the fractional part of the boundary charge shows characteristics which follow directly from bulk properties. Furthermore it is an interesting observable in its own right as it indicates various universal properties, such as the linear phase-dependence against continuous translations of the lattice, the possibility to realize rational quantization in the presence of symmetries, and a universal low-energy behavior for very small gaps. Our first important step is thus to compute the boundary charge for the noninteracting RM model and illustrate the above mentioned characteristics resulting from bulk properties. We show that results obtained from an effective low-energy theory for gaps much smaller than the band width hold in a surprisingly large parameter regime. In addition, we find an interesting quantization of the boundary charge in the limit of large gaps.

In 1d metallic systems two-particle interactions imply correlations which strongly alter the low-energy physics. They lead to Tomonaga-Luttinger liquid behavior which can not be captured by perturbation theory in the limit of large gaps. DMRG was earlier applied to models of topological RG results for the above observables to numerically compute the boundary charge for the noninteracting RM model and illustrate the above mentioned characteristics resulting from bulk properties. We show that results obtained from an effective low-energy theory for gaps much smaller than the band width hold in a surprisingly large parameter regime. In addition, we find an interesting quantization of the boundary charge in the limit of large gaps.

To study the interacting RM model we follow an alternative route and use an essentially analytical but approximate truncated functional renormalization group (RG) approach. This has the distinct advantage that it can directly be applied to the microscopic lattice model and consistently treats interaction effects on all energy scales, from the high-energy band width down to the low-energy gap. The approximations required to derive a finite set of RG flow equations for the components of the static self-energy are controlled for small interactions. Crucially, the solution of these leads to a proper resummation of the leading logarithms to a power law (for related examples, see Ref.). We benchmark our functional RG results for the above observables to numerical density matrix renormalization group data (DMRG). DMRG was earlier applied to models of topological insulators. However, to reach the low-energy regime for systems with boundaries requires the study of exceedingly large systems which provides a computational challenge to this approach.

We show that the interaction can induce in-gap δ-peaks that is “effective edge states”, in the local single-particle spectral function, which are absent for $U = 0$. They originate from the local modulation of the self-energy close to the open boundary and cannot be explained based on renormalized bulk properties. Therefore, the appearance of edge states can not be used as an indicator to formulate a generalized BBC. These modulations also affect the local density close to the boundary. However, the characteristic features of the fractional part of the boundary charge remain unaffected and can be explained from the bulk properties of the interacting model. This provides evidence that the boundary charge might turn out to be the more appropriate indicator of a generalized BBC for interacting systems.

This paper is structured as follows. In Sect. II we present the model and introduce the observables of interest to us. For vanishing interactions, we compute all eigenenergies and wavefunctions for periodic as well as open boundary conditions—including possible (topological) edge states. From these we determine the local single-particle spectral function, the local density, as well as boundary charge accumulated close to the boundary. Details of these calculations are given in the Appendix. In Sect. III we next present the quantum many-body methods we employ to investigate the interacting RM model: Functional RG and DMRG. Our results for the bulk properties of the interacting model are presented in Sect. IV, while Sect. V is devoted to the study of the physics in the presence of an open boundary. In Sect. VI we provide a—taken the length our paper—short summary of our results. As the individual sections end with summaries of the corresponding parts, we this way avoid a doubling. In addition, we present an outlook.

II. THE MODEL AND ITS PHYSICS AT VANISHING INTERACTION

A. The model

The noninteracting RM model is one of the basic models discussed in connection with edge state physics and topological properties. In 1d, for spinless fermions, and in the Wannier state basis (with lattice site index $j$) it is given by the Hamiltonian

$$H_0 = \sum_j \left( V_j n_j - t_j c_{j+1}^\dagger c_j + \text{H.c.} \right)$$

(1)

with the site-density operator $n_j = c_j^\dagger c_j$. Standard second quantized notation is used. The on-site potentials $V_j = V_{j+Z}$ and hoppings $t_j = t_{j+Z}$ are periodic with period $Z = 2$, defining the number of lattice sites of the unit cell. With the average hopping $t = (t_1 + t_2)/2$ and
half the difference $\delta t = (t_1 - t_2)/2$, we parametrize $V_j$ and $t_j$ by

$$V_1 = -V_2 = V, \quad t_{1/2} = t \pm \delta t > 0. \quad (2)$$

We take $t$ as our unit of energy and set $t = 1$. In analytic calculations we still find it advantageous to introduce a symbol for an energy scale associated to this average hopping. We use $W = 2t$, as it reminds us that $2t$ is half the band width of the gapless model with $\delta t = 0 = V$. For compactness we refer to $2W$ as the band width.

As discussed in more detail in Sect. the RM model displays two bands separated by a single particle gap of minimal size $2\Delta$ (taken at wavevector $k = \pm \pi$, with the lattice constant $a = 1$) with

$$\Delta = \sqrt{V^2 + 4\delta t^2}. \quad (3)$$

It is convenient to define a phase $\gamma \in \mathbb{R}$ via the complex gap parameter

$$\Delta e^{i\gamma} = V + i2\delta t. \quad (4)$$

We vary $\gamma$ to modulate the staggered hopping and onsite energies such that the complex gap parameter stays on a circle in the complex plane defined by $(V, 2\delta t)$.

For $V = 0$ the RM model becomes the SSH model [24].

The Hamiltonian $H_0$ is complemented by a homogeneous two-particle interaction of nearest neighbor type

$$H_{\text{int}} = U \sum_j \left( n_j - \frac{1}{2} \right) \left( n_{j+1} - \frac{1}{2} \right), \quad (5)$$

with amplitude $U$. Subtracting $1/2$ from the local density operator $n_j$, the interaction is written in a particle-hole symmetric form.

We take the number of lattice sites $L$ to be even such that all unit cells remain intact. We are interested in the bulk properties as well as the boundary ones. In the former case we consider periodic boundary conditions (PBCs). The site index $j$ in the sum of Eq. (1) and Eq. (5) runs from 1 to $L$ and site indices are considered modulo $L$. For open boundary conditions (OBCs) the sum in the first term of Eq. (1) runs from 1 to $L$ while in the second one of Eq. (1) and in Eq. (5) it only extends up to $L - 1$.

For $\delta t = 0 = V$ the elementary unit cell has a single site and $H = H_0 + H_{\text{int}}$ is the Bethe ansatz solvable (single-band) lattice model of spinless fermions with nearest-neighbor hopping $t = 1$ and nearest-neighbor interaction $U$; see e.g. Ref. [19]. For $|U|$ being smaller than a filling dependent critical interaction it shows metallic behavior. E.g. for half filling the model remains gapless for $-2 < U < 2$. In this regime the system is a Tomonaga-Luttinger liquid with all low-energy excitations being of collective bosonic nature (instead of being fermionic quasi-particles) and correlation functions decay as power laws with interaction dependent exponents [19, 50]. Outside the metallic Tomonaga-Luttinger liquid phase correlations induce a gap. Here we are not interested in the interplay of the single-particle gap $2\Delta$ of the noninteracting RM model and the interaction induced gap and always consider interactions so small that the latter does not open. For results on this interplay, see Ref. [19].

Before discussing our results on the interaction effects of the spinless 1d RM model we investigate its $U = 0$ properties in the next section. For details, see the Appendix. We also use this section to introduce our observables of interest. A particular emphasize is put on the boundary charge accumulated close to an open boundary, as it is an interesting quantity to characterize topological properties and indicates a generalized BBC—its main characteristics can be understood solely based on bulk properties of the Hamiltonian.

### B. Spectra and the density

For PBC the noninteracting Hamiltonian Eq. (1) can easily be diagonalized. For this we rewrite the Wannier states as

$$|j\rangle = |n\rangle \otimes |i\rangle \quad (6)$$

with the unit cell index $n$ and the index $i = 1, 2$ for the two sites within the unit cell. They are related to the lattice site index via

$$j = 2(n - 1) + i, \quad (7)$$

a relation which is used implicitly in the following.

In the single-particle subspace $H_0$ can then be rewritten as

$$H_0 = \sum_{n=-\infty}^{\infty} \langle n | \otimes h(0) + | n + 1 \rangle \otimes h(1) + \text{H.c.},$$

with the $2 \times 2$-matrices

$$h(0) = \begin{pmatrix} V_1 & -t_1 \\ -t_1 & V_2 \end{pmatrix}, \quad h(1) = \begin{pmatrix} 0 & -t_2 \\ -t_2 & 0 \end{pmatrix}, \quad (9)$$

in the $i = 1, 2$ basis. Here we have already taken the thermodynamic limit $L \to \infty$ (infinite system, bulk properties). We next define $k$-states

$$|k\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} e^{ikn} |n\rangle, \quad (10)$$

with $k \in [-\pi, \pi)$. Taking these as our basis the Hamiltonian reads

$$H_0 = \int_{-\pi}^{\pi} dk \langle k | \otimes h_k, \quad (11)$$

with

$$h_k = \sum_{\delta=0,\pm 1} h(\delta)e^{-ik\delta} = \begin{pmatrix} V_1 & -t_1 - t_2e^{-ik} \\ -t_1 - t_2e^{ik} & V_2 \end{pmatrix}. \quad (12)$$
The eigenenergies are given by the eigenvalues of $h_k$ as
\[
\varepsilon_k^{(\alpha)} = \alpha \varepsilon_k = \alpha \sqrt{V^2 + t_1^2 + t_2^2 + 2t_1 t_2 \cos k}, \tag{13}
\]
with the band index $\alpha = \pm$. We used $V_1 = -V_2 = V$. We thus find two bands separated by a single-particle energy gap which takes its minimal value $2\Delta$ at $k = \pm \pi$, with $\Delta$ defined in Eq. (3).

The single-particle wave functions of the infinite (bulk) system are given by the Bloch states
\[
\psi_{k,\text{bulk}}^{(\alpha)}(j) = \frac{1}{\sqrt{2\pi}} \chi_k^{(\alpha)}(i) e^{ikj}, \tag{14}
\]
where
\[
\chi_k^{(\alpha)}(1) = \frac{t_1 + t_2 e^{-ik}}{\sqrt{N_k^{(\alpha)}}}, \quad \chi_k^{(\alpha)}(2) = \frac{V - \alpha \varepsilon_k}{\sqrt{N_k^{(\alpha)}}}, \tag{15}
\]
with the normalization factor
\[
N_k^{(\alpha)} = 2\varepsilon_k(e_k - \alpha V). \tag{16}
\]

We here exclusively consider the case with the chemical potential $\mu$ lying in the gap between the valence and conduction band as well as temperature $T = 0$, such that the lower band is completely filled and the upper one is empty.

Integrating over the absolute values squared of the wave functions in the lower band we obtain the bulk density. It is translationally invariant by two lattice sites and is given by
\[
\rho_{\text{bulk}}(j) = \int_{-\pi}^{\pi} dk \left| \psi_{k,\text{bulk}}^{(-)}(j) \right|^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \left| \chi_k^{(-)}(i) \right|^2 = \frac{1}{2} + (-1)^j \frac{V}{4\pi} \int_{-\pi}^{\pi} dk \frac{1}{\varepsilon_k}, \tag{17}
\]
where we made use of Eqs. (14)-(16) for the Bloch states and used Eq. (7) relating the indices $i$ and $j$. Closing the integration contour in the upper half we show in the Appendix that the bulk density can be calculated very efficiently from the integral
\[
\rho_{\text{bulk}}(j) = \frac{1}{2} + (-1)^j \frac{V}{2\pi} \int_{0}^{\infty} dk \frac{1}{\sqrt{-R(\kappa)}}, \tag{18}
\]
with
\[
R(\kappa) = V^2 + t_1^2 + t_2^2 - 2t_1 t_2 \cosh (\kappa + \kappa_{bc}) \tag{19}
\]
and
\[
\kappa_{bc} = \ln \frac{\Delta^2 + 2t_1 t_2 + \Delta \sqrt{\Delta^2 + 4t_1 t_2}}{2t_1 t_2}. \tag{20}
\]
As we will see below the length scale $\kappa_{bc}^{-1}$ corresponds to the decay length of the exponential localization of the excess density for a semi-infinite system at the boundary.

The fact that this length scale appears also in the calculation of the bulk density provides an interesting link between bulk and boundary quantities.

The eigenstates of a semi-infinite chain with an open boundary (boundary properties), obtained by starting with OBC and taking $L \to \infty$, are given by
\[
\psi_k^{(\alpha)}(j) = \frac{1}{\sqrt{2\pi}} \left[ \chi_k^{(\alpha)}(i) e^{ikj} - \chi_k^{(\alpha)}(j) e^{-ikj} \right], \tag{21}
\]
with $k \in [0, \pi]$. The dispersion remains the same as for the infinite chain; see Eq. (13).

It is well established that for $t_1 - t_2 < 0$ the set of extended eigenstates of a semi-infinite chain Eq. (21) is complemented by an edge state with wavefunction
\[
\psi_e(j) = \delta_{i,1}(-1)^{n+1} \left( \frac{t_2}{t_1} - 1 \right)^{1/2} e^{-\kappa_e n}, \tag{22}
\]
and
\[
\kappa_e = \ln \frac{t_2}{t_1}. \tag{23}
\]
It has weight exclusively on the sites with $i = 1$ within the unit cell and decays (purely) exponentially in the unit cell index $n$ away from the boundary. The characteristic length scale is $\kappa_e^{-1}$. The edge state is located at energy $V$ within the energy gap. Accordingly, at $T = 0$ the edge state is filled for $V < \mu$ and empty for $V > \mu$. For $V = \mu$ it is half-filled. In the SSH model limit with $V = 0$ the edge state is located at vanishing energy and classified as topologically protected within the standard nomenclature of topological insulators. The existence of the edge state follows from a property of the bulk parameters, namely $t_1 - t_2 < 0$. This can be used as an indicator for a generalized BBC.

From the eigenenergies and the eigenstates the local single-particle spectral function $A_j(\omega)$ of the semi-infinite system can be computed as
\[
A_j(\omega) = \sum_{\alpha=\pm} \int_{0}^{\infty} dk \left| \psi_k^{(\alpha)}(j) \right|^2 \delta (\omega - \alpha \varepsilon_k) + \left| \psi_e(j) \right|^2 \delta (\omega - V). \tag{24}
\]
Figure 1 shows results for different $j$. The parameters are $\delta t = -0.04$, and $V = -0.01$, thus from the regime featuring an edge state. Therefore, the spectral function shows an in-gap $\delta$-peak at energy $\omega = \varepsilon_e = V$ on odd sites with a weight which according to Eq. (22) decays exponentially for increasing $j = 2(n - 1) + i$. In the figure it is indicated as a vertical arrow. The height of the arrow is proportional to the weight of the $\delta$-peak. The gap is clearly visible. Close to the boundary the spectral weight generically (for an exception, see Sect. V A) vanishes in a semi-circular way when the energy approaches the band edges. For larger $j$ inverse square-root-like van-Hove singularities typical for the density of states of 1d systems develop. For $\omega \to \pm \Delta$ this is visible only for larger $j$ than shown in Fig. 1.
The local single-particle spectral function $A_j(\omega)$ of the noninteracting RM model as a function of energy $\omega$ for different lattice sites $j$ close to an open boundary. The in-gap edge state is indicated by a vertical arrow of height proportional to its weight. The parameters are $\delta t = -0.04$, and $V = -0.01$.

We note that the results of Fig. 1 were computed for a finite system of $L = 4096$ sites with PBC by numerical diagonalization. To obtain a smooth function out of the sum of $\delta$-peaks (finite system size) we averaged the spectral weight in the bands over several eigenenergies. Increasing the system size the curves do not change on the scale of the plot and the data can be considered to be in the thermodynamic limit.

The local density of the semi-infinite system can be written as

$$\rho(j) = \int_0^\pi dk \left| \psi_k(j) \right|^2 + \rho_e(j) = \rho_{\text{bulk}}(j) + \rho_F(j) + \rho_e(j),$$

(25)

where $\rho_e(j)$ denotes the edge state density which is given by

$$\rho_e(j) = \Theta(t_2 - t_1) \left| \psi_e(j) \right|^2 \frac{1}{2} [1 + \text{sign}(\mu - V)],$$

(26)

with $\text{sign}(0) = 0$. As outlined in the Appendix the Friedel density $\rho_F$ can be split into a pole and branch cut contribution

$$\rho_F(j) = -\frac{1}{2\pi} \int_{-\pi}^\pi dk \left\{ \psi_k(i) \right\}^2 e^{2ikn}$$

(27)

$$= \rho_F^{(\text{pole})}(j) + \rho_F^{(\text{bc})}(j),$$

(28)

given by

$$\rho_F^{(\text{pole})}(j) = -\rho_e(j)|_{\mu=0},$$

(29)

$$\rho_F^{(\text{bc})}(n, 1) = -\frac{V}{2\pi} e^{-2\kappa_{bc}n}$$

$$\times \int_0^\infty d\kappa \left( t_1 - t_2 e^{\kappa + \kappa_{bc}} \right)^2 e^{-2\kappa n},$$

(30)

$$\rho_F^{(\text{bc})}(n, 2) = -\frac{V}{2\pi} e^{-2\kappa_{bc}n} \int_0^\infty d\kappa \frac{1}{\sqrt{R(\kappa)}} e^{-2\kappa n},$$

(31)

with $R(\kappa)$ and $\kappa_{bc}$ defined in Eqs. (19) and (20). The pole contribution coincides with the negative edge state density at $\mu = 0$. Therefore, for $\mu = 0$ it exactly cancels the edge state density $\rho_e(j)$ in Eq. (25). The second term of $\rho_F(j)$ arises from a branch cut contribution and decays exponentially (to zero) for large $n$, i.e. large $j = 2(n - 1) + i$, with the characteristic length scale $\kappa_{bc}^{-1}$. Therefore, for $j \rightarrow \infty$ the total density Eq. (25) for the semi-infinite chain approaches the bulk values Eq. (17) as expected. This holds for any $\mu$ located in the gap. Inserting Eqs. (28) and (29) in Eq. (25) one finds that the only term depending on such a chemical potential is the difference

$$\rho_e(j) - \rho_e(j)|_{\mu=0} = \Theta(t_2 - t_1) |\psi_e(j)|^2$$

$$\times \frac{1}{2} \left[ \text{sign}(\mu - V) - \text{sign}(-V) \right].$$

In the following we mostly consider the case of vanishing chemical potential

$$\mu = 0,$$

(33)

in which the right hand side of Eq. (32) is zero. Therefore, the difference of the densities of the semi-infinite and infinite system is given by the branch cut contribution of the Friedel density

$$\delta \rho(j) = \rho(j) - \rho_{\text{bulk}}(j)$$

(34)

$$= \rho_F(j) + \rho_e(j) = \rho_F^{(\text{bc})}(j),$$

(35)

In the SSH model limit with $V = 0$ we find $\kappa_{bc} = \kappa_e$. In this case and for $\mu = 0$ the total density of the semi-infinite chain is given by $1/2$ independent of the lattice site index $j$. This follows from particle-hole symmetry.

In particular we are interested in the limit that the gap is smaller than the energy scale associated to the band width $2W$ of the gapless model: $\Delta \ll W$. As shown in the Appendix in this case the branch cut contribution of the Friedel density decays asymptotically as

$$\rho_F^{(\text{bc})}(j) \sim -\frac{1}{\sqrt{n}} e^{-2\kappa_{bc}n}, \quad n \gg \frac{W}{\Delta} \gg 1$$

(36)

with the decay length $\kappa_{bc}^{-1}$ and a prefactor which depends on $i$.

The main part of Fig. 2 shows $\delta \rho(j)$ for $\delta t = 0.000125$, and $V = 0.001$, that is, for a very small gap. A very
The difference $\delta\rho(j)$ of the density of the semi-infinite and infinite system constructed from the extended eigenstates of the noninteracting RM model as a function of the unit cell index $n$ for chemical potential $\mu = 0$. Data for the two different lattice sites $i = 1, 2$ within the unit cell are shown. The single-particle parameters are $\delta t = 0.000125$ and $V = 0.001$. Inset: The logarithmic derivative of the pre-exponential inverse square root behavior of Eq. (36) must be accessed. Note that for $\mu = 0$, $\rho_{(bc)} = \delta\rho$ holds. The Friedel density on the second sites of every unit cell ($i = 2$) takes longer to decay to zero as compared to the one on the first sites ($i = 1$). We return to these observations in Sect. V when studying the interacting RM model.

C. The boundary charge

In this section we discuss the boundary charge $Q_B$ of the noninteracting RM model. It is defined as the charge accumulated close to an open boundary. We closely follow the treatment of Ref. [48]. Here we summarize the most important results; see the Appendix for the technical details. The boundary charge $Q_B$ of the semi-infinite large but finite system with OBC and $L = 200000$ sites was considered. On the scale of the plot the data are free of finite size corrections and for all practical purposes can considered to be in the thermodynamic limit. In the inset the “centered logarithmic differences”

$$\alpha(n) = \frac{\ln[f(n+1)] - \ln[f(n-1)]}{\ln(n+1) - \ln(n-1)}$$

(37)

with $f(n) = e^{2\kappa_{bc}n} |\rho_{(bc)}|$ are shown for $i = 1, 2$. If $f(n)$ shows power-law scaling for large $n$, $\alpha(n)$ approaches a constant in this limit with $\lim_{n\to\infty} \alpha(n)$ being the exponent. The inset of Fig. 2 indicates that to identify the pre-exponential function computed according to Eq. (37). The asymptotic inverse square-root decay of the pre-exponential function is only reached for very large $n$.

RM model for $\mu = 0$ can be computed as

$$Q_B = \lim_{M \to \infty} \lim_{N \to \infty} \sum_{j=1}^{\infty} \left[ \rho(j) - \frac{1}{2} \right] f_{N,M}(j),$$

(38)

where $f_{N,M}(j)$ is an envelope function changing smoothly from 1 to zero when going from the boundary towards the bulk. It characterizes a macroscopic charge measurement probe; see Fig. [3] from which the definition of the parameters $M$ and $N$ is apparent. Using Eq. (34), $Q_B$ can be split as

$$Q_B = Q_P + \delta Q_B,$$

(39)

$$Q_P = \lim_{M \to \infty} \lim_{N \to \infty} \sum_{j=1}^{\infty} \left[ \rho_{\text{bulk}}(j) - \frac{1}{2} \right] f_{N,M}(j) = -\frac{1}{2} \sum_{i=1,2} \left[ \rho_{\text{bulk}}(i) - \frac{1}{2} \right],$$

(40)

$$\delta Q_B = \sum_{j=1}^{\infty} \delta\rho(j).$$

(41)

Here, $Q_P$ is the polarization charge determined by the bulk density. Using the translational invariance $\rho_{\text{bulk}}(j = 2[n-1]+i) = \rho_{\text{bulk}}(i)$ and expanding the envelope function in $i$ one proceeds from the first to the second line of Eq. (40), see Ref. [48] for details. The term $\delta Q_B$ involves the exponentially decaying part $\delta\rho(j)$ for which the $f_{N,M}(j)$ function can be set to 1. Inserting Eqs. (17), (30), (31), and (35) for the various parts of the density, together with the explicit solution Eq. (15) for the Bloch states, we show in the Appendix that the total boundary charge can be calculated very efficiently as

$$Q_B = -\frac{1}{4} \text{sign}(V) - \frac{V(t_2^1 - t_1^1)}{4\pi} \int_0^\infty dk \frac{1}{\sqrt{-R(k)}} \frac{1}{|V^2 - R(k)|},$$

(42)

where $R(k)$ is defined in Eq. (19). This holds for the special case $\mu = 0$. For finite $\mu$ one has to add the difference of the edge state charge corresponding to Eq. (42)

$$Q_e(j) - Q_e(j)|_{\mu=0} = \Theta(t_2 - t_1)$$

(43)

$$\times \frac{1}{2} \left[ \text{sign}(\mu - V) - \text{sign}(-V) \right].$$
There are four characteristics of the boundary charge discussed in Refs. [44, 48] which all can be derived from properties of the bulk Hamiltonian. This provides a manifestation of a generalized BBC. (i) Transformation property of $Q_B$ when shifting the lattice by one site towards the boundary (also referred to as the universal linear slope of $Q_B$ as a function of the phase variable $\gamma$). (ii) Transformation property of $Q_B$ under local inversion. (iii) Low-energy behavior of $Q_B$ for small gaps $\Delta \ll W$. (iv) Quantization of $Q_B$ in the presence of local and nonlocal symmetries. These four features are specified in the following for the noninteracting RM model employing the above formulas and further alternatives to write Eq. (42) (see the Appendix).

(i) **Transformation of $Q_B$ under translations.** Using the parametrization of the single-particle parameters Eq. (3) in terms of the phase variable $\gamma$, one can describe a translation of the lattice by one site towards the boundary as a phase change by $\pi$, which corresponds to $V_1 \leftrightarrow V_2 = -V_1$ (or $V \to -V$) and $t_1 \leftrightarrow t_2$. Using Eq. (42) we find

$$\Delta Q_B(\gamma) = Q_B(\gamma + \pi) - Q_B(\gamma) = \frac{1}{2} \text{sign}(V).$$

This agrees with the general result derived in Refs. [47, 48] for all single-channel and nearest neighbor hopping models that $Q_B$ changes either by the average particle charge per site $\bar{\rho}$ or the average hole charge per site $\bar{\rho} - 1/2$. For the RM model at $\mu = 0$ we have $\bar{\rho} = \frac{1}{2}$ leading to $\pm \frac{1}{2}$ for $\Delta Q_B$ consistent with Eq. (44). We note that, for finite $\mu$, we have to add the change of Eq. (43) under translation, which gives

$$\Delta Q_B(\gamma) = \frac{1}{2} \Theta(t_1 - t_2) \text{sign}(\mu + V) - \Theta(t_2 - t_1) \text{sign}(\mu - V).$$

Again we see that the change of $Q_B$ can only take the values $\pm \frac{1}{2}$.

(ii) **Transformation of $Q_B$ under local inversion.** A local inversion for the RM model is defined within a unit cell by the transformation $V_1 \leftrightarrow V_2 = -V_1$ (or $V \leftrightarrow -V$) but leaving the hoppings invariant. In Ref. [44] it was shown that $Q_B$ changes its sign under local inversion $\bmod(1)$ for generic tight-binding models in 1d (for special cases see also Refs. [45, 46, 48]). Using Eq. (42) we find for the particular case of the RM model

$$Q_B(-V) = -Q_B(V).$$

(iii) **Low-energy theory for small gaps.** In the low-energy limit of a very small gap $\Delta \ll W$ and using the definition Eq. (4), we show in the Appendix that the boundary charge can be written approximately in the universal form

$$Q_B \approx \frac{\gamma}{2\pi} - \frac{1}{4} - \Theta_{\frac{1}{2}\pi < \gamma < 2\pi}.$$

for $0 < \gamma < 2\pi$ and periodic continuation to other intervals. Here, $\Theta_{a < x < b} = 1$ for $a < x < b$ and zero otherwise. The universal linear behavior in $\gamma$ has been found in Ref. [44] for any single-channel and nearest-neighbor hopping model in the low-energy limit (note that in this reference $\gamma' = \gamma - \pi$ with $-\pi < \gamma' < \pi$ defines the phase of the gap parameter).

(iv) **Quantization of $Q_B$.** In the presence of special symmetries the boundary charge is quantized to some rational number. For local inversion or local chiral symmetry $Q_B$ is quantized in half-integer units. This was shown via the quantization of the Zak-Berry phase $\gamma_Z$ in units of $\pi$ [73, 74], which is related to the boundary charge by $Q_B = -\frac{\gamma_Z}{2\pi} \bmod(1)$ [45, 48]. In the presence of nonlocal symmetries it was shown recently [44] that any rational quantization of the boundary charge is possible in combinations of multiples of half of the average particle or hole charge per site $\frac{1}{2}\bar{\rho}$ or $\frac{1}{2}(\bar{\rho} - 1)$. Since $\bar{\rho} = \frac{1}{2}$ for the RM model this means that both cases of $\frac{1}{2}$ and $\frac{1}{4}$ quantization can occur for $Q_B$.

For the RM model a local inversion or local chiral symmetry is present for $V_1 = V_2 = V = 0$, which corresponds to the SSH model. Due to particle-hole symmetry at $\mu = 0$ this gives $Q_B = 0$. For $|V| \ll |\delta t|$ we show in the Appendix [note that sign(0) = 0]

$$Q_B = -\frac{1}{2} \Theta(t_2 - t_1) \text{sign}(V) + O\left(\frac{V}{\delta t}\right),$$

This gives half-integer quantization.

A nonlocal chiral symmetry occurs for the RM model for $t_1 = t_2$. In this case one obtains for $Q_B$ the novel quantization value $\frac{1}{4}$, see Ref. [44]. For $|\delta t| \ll |V|$ we show in the Appendix

$$Q_B = -\frac{1}{4} \text{sign}(V) + O\left(\frac{W \delta t}{V_{\text{max}}(|V|, W)}\right),$$

leading to the expected $\frac{1}{2}$-quantization.

The main characteristics (i)-(iv) suggest the boundary charge to be an interesting quantity to characterize topological properties and to use it as an indicator of the generalized BBC. In contrast, the orthodox BBC is discussed in terms of the connection between topological bulk invariants and the appearance of edge states which, for 1d systems, have to be at zero energy [27, 34]. Our results of Sects. V A and V C indicate that the boundary charge might be a more robust signature of a generalized BBC as compared to the number of edge states when the interaction is turned on.

The features (i), (ii), and (iv) can be seen clearly in Fig. 4 where we show the boundary charge as function of the two parameters $V$ and $2\delta t$ defining the real and imaginary part of the quantity $\Delta e^{i\gamma}$ of Eq. (4). Therefore, $\gamma$ corresponds to the polar angle and $\Delta$ to the radial component in Fig. 4. The data were computed for $L = 2000$ but are essentially free of finite size corrections. A translation by one lattice site towards the boundary corresponds to a sign change of $V$ and $\delta t$, i.e., changes of
FIG. 4. The boundary charge $Q_B$ of the noninteracting RM model as a function of $V$ and $2\delta t$ or the polar coordinates $\Delta$ and $\gamma$, see Eq. (4)

FIG. 5. Main panel: The boundary charge as a function of the polar angle $\gamma$ [see Eq. (4)] for different $\Delta$. Inset: Derivative of the data of the main panel with respect to $\gamma$. This highlights the remarkable linearity even for sizable $\Delta$; see Eq. (47) and the discussion in the main text.

the angle $\gamma$ by $\pi$. According to Eq. (44) this leads to a change of $Q_B$ by $\frac{1}{2}\text{sign}(V)$ which is consistent with Fig. 4. The transformation Eq. (46) under local inversion means that $Q_B$ is antisymmetric when changing the sign of the variable $V$ in Fig. 4. The quantization rules Eqs. (48) and (49) can be seen on the axis $V = 0$ and $\delta t = 0$ in Fig. 4, respectively.

Of particular interest is the validity range of the low-energy behavior (iii) of $Q_B$ according to Eq. (47), i.e., the universal linear behavior as a function of the angle $\gamma$ if the gap $2\Delta$ is very small compared to the band width. This is shown in Fig. 5 (again obtained for $L = 2000$). Strikingly, the linear behavior is observed to a high accuracy in the whole parameter regime $\Delta < W$ extensively beyond the low-energy regime $\Delta \ll W$ where it is expected to hold. As shown in the Appendix the stability of the low-energy result up to values $\Delta \sim W$ can be explained by calculating the leading order correction to Eq. (17). According to Eq. (A.40) it is given by $1/(8\pi)\sin(2\gamma)(\Delta/W)^2\ln(\Delta/W)$. This is in full agreement with the inset of Fig. 5 showing the derivative of $Q_B$ with respect to $\gamma$, where the corrections to the linear slope are zero for $\cos(2\gamma) = 0$ and largest for $\cos(2\gamma) = \pm1$. Only for $\Delta \gg W$ visible deviations from linear behavior occur and in the atomic limit $\Delta \gg W$ one obtains the universal result of $\frac{1}{4}$-quantization

$$Q_B \approx -\frac{1}{4}\text{sign}(V)\left[1 - \frac{W\delta t}{V^2}\right], \quad (50)$$

see the Appendix for details.

Therefore, we find two universal regimes of the boundary charge for the noninteracting RM model, given by the linear dependence in the phase $\gamma$ of the gap parameter for $\Delta < W$, and the $\frac{1}{4}$-quantization of $Q_B$ for $\Delta \gg W$. Moreover, in Sect. V C we demonstrate that this interesting behavior is stable against weak two-particle interactions.

III. MANY-BODY METHODS

Already in the early eighties it was suggested to use field theoretical models to study the universal low-energy physics of lattice models for linear polymers (such as the RM and the SSH models) with small single-particle gaps. Continuum models also provide a straightforward way to include two-particle interactions. It was shown that the interaction leads to logarithmic terms of the form $g^n\ln^n(2\Delta)$ in the first ($n = 1$) and second ($n = 2$) order perturbative expressions for the effective renormalized gap $2\Delta^{\text{ren}}$ as a function of the bare one $2\Delta$ [51–53]. Here $g$ denotes the coupling constant of the field theory. As the gap is small this logarithmic dependence severely limits the applicability of perturbation theory to tiny couplings $g$. However, the leading-log series can be resummed by either using field-theoretical RG or by adapting results from the Bethe ansatz solution of the massive Thirring model [51]. In fact, in the field theoretical model the effective gap depends on the bare one in a power-law fashion. Up to linear order in the coupling constant one finds $\Delta^{\text{ren}} \sim \Delta^{1-g/9c}$, with a characteristic interaction scale $g_c$.

We are not aware that this power-law renormalization has so far been verified directly for a microscopic lattice model, i.e. without the intermediate approximate step of mapping it to a continuum field theory. However, expecting to find this and being interested in the entire space of noninteracting parameters, including the small gap limit, we cannot use simple perturbation theory to investigate the interaction effects in the RM model. Instead we employ the functional RG in its lowest order truncation.
In addition, we benchmark our approximate results by comparing to numerical ones obtained by DMRG.

We note that recently the use of field theoretical models and tools (such as bosonization) to investigate the low-energy properties of (topological) insulators experienced a revival. In Ref. [54] they were used to not only study the gap renormalization but in addition the edge state and in Ref. [44] to investigate the boundary charge. In Refs. [44, 51] it has furthermore been established how to express the parameters of a continuum Dirac model in 1 + 1 dimension in terms of microscopic lattice model parameters. However, by neglecting fast oscillating terms in these approaches one has to assume that the gap is much smaller than the band width and it is quite difficult to determine the quality of the low-energy results beyond this regime. The functional RG used here treats the microscopic details of the lattice model on all energy scales and thus can cover the entire parameter range from small to large gaps. Also, high-energy properties such as the renormalization of the band width are treated consistently in functional RG. This will turn out to be crucial to establish a generalized BBC for the boundary charge in the presence of two-particle interactions. Field theories do not capture high-energy features and will thus fail in this respect.

A. The functional RG

1. The basic idea

It was earlier shown that functional RG in its lowest-order truncation [53] can be used to properly resum leading logs in extended 1d models of correlated fermions [67] as well as for quantum dot models with local two-particle interactions [68]. In Sect. IV A it will be shown analytically that this also holds in the (single-particle) gaped RM model with nearest-neighbor interaction.

The functional RG has the distinct advantage over other RG methods that it is directly applicable to microscopic lattice models. It does not require the intermediate (approximate) step of the mapping to a field theory. It thus does not only capture the low-energy physics but the one on all energy scales. Functional RG still inherits the RG idea of a successive treatment of energy scales. A comprehensive account is given in Ref. [53] (see also Ref. [54]). For completeness we here present the basic idea and the important equations.

The fundamental steps of the application of FRG to interacting fermionic systems are the following:

1. Write the partition function as a coherent state functional integral (within the Matsubara formalism).

2. Replace the noninteracting propagator \( G_0(i\omega) \) which inherits all the single-particle physics by one decorated by a cutoff \( \Lambda \). For the initial value \( \Lambda_i \), the free propagation must be restored. One often uses \( G_0^A(i\omega) = \Theta(|\omega| - \Lambda)G_0(i\omega), \Lambda_i = \infty, \) and \( \Lambda_\text{f} = 0 \). When \( \Lambda \) is sent from \( \infty \) to \( 0 \) (see below) this incorporates the RG idea of a successive treatment of energy scales. Here we will also use this cutoff.

3. Differentiate the generating functional of one-particle irreducible vertex functions with respect to \( \Lambda \).

4. Expand both sides of the functional differential equation with respect to the vertex functions. This leads to an infinite hierarchy of coupled differential equations for the vertex functions. The lowest order vertex function is the self-energy \( \Sigma \).

The hierarchy of coupled flow equations presents an exact reformulation of the quantum many-body problem. Integrating it from \( \Lambda_i \) to \( \Lambda_f \) leads to exact expressions for the vertex functions. From those observables, such as the single-particle spectral function can be computed.

In practice, truncations of the hierarchy are required, resulting in a closed finite set of equations. The integration of this leads to approximate expressions for the vertices and, thus, for observables. We here employ the lowest-order truncation in which the flowing two-particle vertex is replaced by the bare interaction. What remains within this scheme is a set of coupled differential equations for the matrix elements of a frequency independent self-energy. This approximation contains all leading order in \( U \) terms [55] but in addition selected higher order ones. As will be seen a posteriori in Sect. IV A this includes all leading log terms of the form \( U^n \ln^n(2\Delta) \). In this context we also show how to reproduce the perturbative results from the functional RG.

The frequency independence of the self-energy has the distinct advantage that it leads to an effective single-particle picture at the end of the RG flow. All single-particle parameters of the model, that is all hoppings and onsite energies get renormalized by the interaction and in the final step of computing the renormalized propagator a single-particle Hamiltonian of the form Eq. (1) needs to be solved. We emphasize that for open boundaries the single-particle parameters acquire a spatial dependence beyond the underlying unit cell structure (see below). We will employ this effective single-particle picture in the interpretation of our results, however, we already now emphasize that it should not be overstressed. E.g. the wave functions obtained from diagonalizing the effective single-particle Hamiltonian do not have a direct physical meaning (similar to their role in Hartree-Fock or density-functional theory). This includes energetically isolated “effective single-particle edge states”.

Within our approximation the local spectral function can be obtained by simply taking

\[
A_j(\omega) = -\frac{1}{\pi} \text{Im} G(i\omega \to \omega + i0),
\]  

(51)
with $G(i\omega)$ computed using Eq. \[52\] and $\Sigma$ taken at the end of the RG flow.

As discussed in the introduction and Sect. \[118\] we are also interested in the spatial dependence of the local density of the interacting RM model with open boundaries. As it is well known the density on site $j$ can be computed by integrating the $(j,j)$-matrix element of the full propagator (Dyson equation)

$$G(i\omega) = \left\{ \left[ G_0(i\omega) \right]^{-1} - \Sigma \right\}^{-1} \tag{52}$$

over the Matsubara frequency. However, truncated functional RG is not a so-called conserving approximation. It is thus not guaranteed that computing the density along this line will lead to the same result as computing it in a more consistent way via its own RG flow equation. In fact, it was earlier shown that the above frequency integration over the full approximate propagator does not capture the typical Tomonaga-Luttinger liquid power-law decay of the Friedel density oscillations away from an open boundary or an impurity for vanishing gap. In contrast, (the leading) interaction dependence of the exponent is properly captured if a flow equation for the self-energy at this value of the cutoff \[55\]. For PBC the self-energy only depends on the site index $i = 1, 2$ within the unit cell only. The translation symmetry by two sites is preserved. In contrast, for open boundaries $\Sigma^\Lambda$ acquires a nontrivial dependence on $n$ in addition to the one on $i$.

To consistently compute the local density $\rho(j)$ we set up according flow equations for this observable

$$\frac{\partial}{\partial \Lambda} \rho^\Lambda(j) = -\frac{1}{2\pi} \sum_{\omega+\pm\Delta} \text{tr} \left[ e^{i\omega 0^+} G^\Lambda(i\omega) R^\Lambda(i\omega) \right]. \tag{55}$$

They involve a density response vertex $R^\Lambda_{j,j}$ which obeys the flow equation

$$\frac{\partial}{\partial \Lambda} R^\Lambda_{j,j,l,l} = -\frac{U}{2\pi} \sum_{\omega=\pm\Delta} \sum_{l'=r\pm1} \sum_{l''=r,0} \sum_{l'=0,\pm1} G^\Lambda_{j+r,l',l''}(i\omega) \times R^\Lambda_{j+r,l',l''} G^\Lambda_{j+r,l'+r,l''}(i\omega), \tag{56}$$

$$\frac{\partial}{\partial \Lambda} R^\Lambda_{j,j,\pm1} = -\frac{U}{2\pi} \sum_{\omega=\pm\Delta} \sum_{l'=r,0} \sum_{l''=0,\pm1} G^\Lambda_{j+r,l',l''}(i\omega) \times R^\Lambda_{j+r+l',l''} G^\Lambda_{j+r+l',l''}(i\omega).$$

Details on this can be found in Ref. \[69\].

The flow is uniquely determined by this set of coupled first order differential equations and the initial conditions at $\Lambda = \infty$. However, the numerical solution of the equation have to start at a large but finite cutoff $\Lambda_0$. One can integrate over the flow equation Eq. \[53\] from $\Lambda = \infty$ to $\Lambda = \Lambda_0$ analytically to obtain the initial condition for the self-energy at this value of the cutoff \[55\]. For PBC it is given by $\Sigma^\Lambda_0 = U$ and $\Sigma^\Lambda_{j,\pm1} = 0$. For OBC the initial condition on the diagonal of the self-energy matrix and the sites $j = 1$ and $j = N$ has to be changed to $\Sigma^\Lambda_{1,1} = \Sigma^\Lambda_{N,N} = U/2$. Moreover, the initial condition for the local density and density response vertex at $\Lambda_0$ are $\rho^\Lambda_0 = \frac{1}{2}$ and $R^\Lambda_{j,j,l'} = \delta_{jj} \delta_{l'}$, respectively. The corrections are of order $1/\Lambda_0$. To obtain the data shown below we set $\Lambda_0 = 10^8$.

Note that $\Sigma^\Lambda$ and $G_0^{-1}$ are both tridiagonal matrices in real space. Using a particular algorithm \[69\], the tridiagonal matrix elements of the the cutoff dependent propagator Eq. \[54a\] needed on the right hand side of the flow equations \[55\] can be computed with an $O(L)$ computational effort. Similarly, the right hand side of the flow equation of the density response vertex which involves the product of inverted tridiagonal matrices and the vertex itself can be computed in $O(L)$. We can therefore easily deal with very large systems with $L \approx 10^8$ sites.

At the end of the flow at $\Lambda = 0$, one can decompose the self-energy into unit cell index $n$ independent and dependent parts, labeled by “bulk” and “F” respectively. For $j = 2(n-1) + i$,

$$\Sigma^\Lambda_{j,j} = \Sigma^\Lambda_{\text{bulk}} + \Sigma^\Lambda_{\text{F}}(n),$$

$$\Sigma^\Lambda_{j,j+1} = \left\{ \begin{array}{ll} \Sigma^\Lambda_{\text{intra}} + \Sigma^\Lambda_{\text{F}}(n) & \text{for } i = 1 \\ \Sigma^\Lambda_{\text{inter}} + \Sigma^\Lambda_{\text{F}}(n) & \text{for } i = 2. \end{array} \right. \tag{57}$$

Finally, the renormalized onsite potentials and hoppings are determined by

$$V^\text{ren}_{j=2(n-1)+i} = V^\text{ren}_i + V^\text{F}_i(n),$$

$$t^\text{ren}_{j=2(n-1)+i} = t^\text{ren}_i + t^\text{F}_i(n). \tag{58}$$
with
\[ V_i^{\text{ren}} = V_i + \Sigma_i^{\text{bulk}}, \]
\[ V_i^F(n) = \Sigma_i^F(n), \]
\[ t_i^{\text{ren}} = \begin{cases} t_1 - V_i^{\text{bulk}} & \text{for } i = 1, \\ t_2 - V_i^{\text{inter}} & \text{for } i = 2, \end{cases} \]
\[ t_i^F(n) = \begin{cases} -\Sigma_i^{\text{intra}}(n) & \text{for } i = 1 \\ -\Sigma_i^{\text{inter}}(n) & \text{for } i = 2. \end{cases} \]

For PBCs the unit cell index dependent interaction induced Friedel parts vanish. For OBC, however, they lead to a modulation of the potential and hopping landscape close to the boundary (and beyond the unit cell structure). The approach of the renormalized bulk values is dominated by an exponential decay in the unit cell index (see Fig. 8 below). We can thus expect that local properties, such as the weight of in-gap \( \delta \)-peaks of the single-particle spectral function, which for \( U = 0 \) are associated to single-particle edge states, are altered by the two-particle interaction. We will even show that peaks can be generated which do not have any analog at \( U = 0 \) and are thus purely interaction induced. The \( \delta \)-peaks are signatures of the edge states of the effective single-particle Hamiltonian to be diagonalized at the end of the RG procedure.

B. The density matrix renormalization group

We use a “numerically exact” DMRG approach set up in the language of matrix product states \(^{[57]}\) to compare to and to benchmark the results obtained within the approximate functional RG method described above. The model defined in Eqs. \((1)\) and \((6)\) can be mapped directly to a spin model by a Jordan-Wigner transform \(^{[70]}\) rendering it amendable to standard DMRG implementations, such as the one outlined in Ref. \(^{[57]}\). We will here use two algorithms.

1. Iterative ground state search

First, an iterative two-site update sweeping procedure to obtain the ground state of a system with OBC is employed. We follow precisely the procedure outlined in section 6 of Ref. \(^{[57]}\). We use 40 sweeps forth and back on the chain and keep the summed discarded weight below \(10^{-7}\) during the update to achieve numerically exact results. After the sweeps are completed we obtain a “numerically exact” approximation to the ground state wavefunction. From this the site-dependent density \( \rho(j) = \langle n_j \rangle \) can be computed.

2. Imaginary time evolution: Finite temperature states

Second, an imaginary time evolution to access the finite temperature properties of an infinite system using purification is used. Here, we follow the procedure described in section 7 of Ref. \(^{[57]}\) for a two site unit cell as outlined in section 10 of the same reference. We use a second order Trotter decomposition with small steps in inverse temperature \( \Delta \beta = 0.001 \) as well as a bond dimension sufficiently high to keep the summed discarded weight below \(10^{-10}\) in all runs. With that we achieve numerically converged results. By calculating the energy \( \langle H \rangle \) in dependence of the temperature we can extract the small temperature behavior of the specific heat. To obtain the excitation gaps we fit this small temperature behavior to an exponential activation, where the fitted rate of the exponential can be identified with the excitation gap.

Alternatively, one could extract the excitation gap by using a sweeping procedure as detailed above, but targeting the first excited state within the same filling sector instead of the ground state. However, for our purposes the simpler imaginary time evolution algorithm, described above, suffices.

For both algorithms we benchmarked the noninteracting case to the exact solution, which provides a nontrivial consistency check for our numerics.

IV. BULK PROPERTIES FOR \( U > 0 \)

We first discuss our results for the bulk properties of the interacting RM model at \( \mu = 0 \) obtained by truncated functional RG as well as by numerical DMRG. In Sect. IV.A we present the analytical solution of the functional RG flow equations \(^{[53]}\) in the limit of small bare gaps \( 2\Delta \). We show that the renormalized gap, displayed in the (interacting) single-particle spectral function, scales as a power law as a function of the bare gap with \( U \) entering in the exponent. In addition, we discuss how the first order in \( U \) perturbative result can be obtained from functional RG. These considerations prove that functional RG in lowest order truncation captures the entire leading log series.

In Sect. IV.B results for the effective gap obtained from a numerical solution of the RG flow equations \(^{[53]}\) are presented and compared to the DMRG results. In the limit of small bare gaps both confirm the analytical insight of Sect. IV.A. In addition, considering bulk properties we provide a first hint that Fig. 4 is only altered quantitatively by small interactions.

A. Analytical insights

We consider periodic boundary conditions. In this case the chain is translational invariant by two lattice sites. For analytic calculations it is advantageous to transform the right hand side of the flow equations \(^{[53]}\) to \( k \)-space. The number of (independent) coupled equations is re-
duced to three: One for the onsite energy

\[ \partial_a \Sigma_{1/2}^{\text{bulk},A} = \frac{2U}{\pi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{ \frac{V_{1A}^A}{a^A + b^A \cos k} \right\}, \quad (63) \]

and one each for the intra and the inter unit cell hopping

\[ \partial_a \Sigma_{\text{intra}}^{\text{bulk},A} = \frac{U}{\pi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{ \frac{t_{1A}^A + t_{2A}^A \cos k}{a^A + b^A \cos k} \right\}, \]

\[ \partial_a \Sigma_{\text{inter}}^{\text{bulk},A} = \frac{U}{\pi} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{ \frac{t_{1A}^A \cos k + t_{2A}^A}{a^A + b^A \cos (k)} \right\}. \quad (64) \]

Here \( a^A = \Lambda^2 + (V_{1A}^A)^2 + (t_{1A}^A)^2 + (t_{2A}^A)^2, \) \( b^A = 2t_{1A}^A t_{2A}^A, \) and \( V_{1A}^A, t_{1/2}^A \) are defined as the effective onsite potential and hopping parameters during the flow, respectively.

Remind that for the bare parameters \( V_1 = -V_2 \) holds. As the consequence, Eq. \((63)\) implies \( -V_2^A = V_1^A = V^A \) during the entire flow including the end \( \Lambda = 0. \)

The \( k \)-integrals in Eqs. \((63)\) and \((64)\) can be performed analytically. Going over from flow equations for the self-energy to the ones for the renormalized single-particle parameters one obtains

\[ \partial_a \frac{V_{1A}^A}{V_{1A}} = \frac{U}{\pi} \frac{1}{b^A} \left\{ 1 - \frac{a^A + b^A}{\sqrt{(a^A)^2 - (b^A)^2}} \right\}, \quad (65) \]

\[ \partial_a \frac{\delta t^A}{t^A} = -\frac{2U}{\pi} \frac{1}{b^A} \left\{ 1 - \frac{a^A - b^A}{\sqrt{(a^A)^2 - (b^A)^2}} \right\}, \quad (66) \]

\[ \partial_a \frac{\delta t^A}{t^A} = -\frac{2U}{\pi} \frac{1}{b^A} \left\{ 1 - \frac{a^A - b^A}{\sqrt{(a^A)^2 - (b^A)^2}} \right\} \]

with \( \delta t^A = (t_{1A}^A - t_{2A}^A)/2 \) and \( t^A = (t_{1A}^A + t_{2A}^A)/2. \) For weak interactions, one can expand the right hand sides of the RG equations in \( U. \) Due to the explicit prefactor \( U, \) the first order correction can be obtained by replacing the renormalized parameters in \( a^A \) and \( b^A \) by the bare ones. We will use this below. Note that this is an additional approximation which comes on top of the truncation of the infinite hierarchy of functional RG flow equations to lowest order. In Sect. \( \text{VIB} \) we avoid this and numerically integrate the full set of truncated flow equations.

The self-energy or the (effective) single-particle parameters within standard first order perturbation theory (for the self-energy, not the Green function) can, as usual, be obtained from the lowest-order truncated RG flow equations by switching off the feedback of the self-energy \([55]\). In Eqs. \((65)\) to \((67)\) we thus do not only have to replace the renormalized parameters by the bare ones in the expressions for \( a^A \) and \( b^A \) on the right hand sides but in addition in the corresponding denominators on the left hand sides. We will return to this.

1. Gap renormalization

For bare gaps \( 2\Delta \) much smaller than the band width \( 2W \) and keeping the leading order in \( U \) only, the right hand sides of the Eqs. \((65)\) and \((66)\) can systematically be expanded leading to

\[ \partial_a \frac{V_{1A}^A}{V_{1A}} = -\frac{U}{\pi A}, \quad \partial_a \frac{\delta t^A}{t^A} = -\frac{U}{\pi A}. \quad (68) \]

Integrating Eq. \((68)\) from the high-energy cutoff \( W \) down to the low-energy scale \( \Delta \) leads to

\[ \frac{V_{\text{ren}}}{V} \sim \left( \frac{\Delta}{W} \right)^{-U/\pi} \sim \frac{\delta t_{\text{ren}}}{\delta t} \quad \text{for} \quad \Delta \ll W. \quad (69) \]

Employing that the renormalized gap, as it shows up in the single-particle spectral function (see Sect. \( \text{V A} \)), can be obtained introducing the renormalized parameters at the end of the flow into Eq. \((3)\) we obtain

\[ \Delta_{\text{ren}}^{\Delta} = \left( \frac{\Delta}{W} \right)^{-U/\pi} \quad \text{for} \quad \Delta \ll W. \quad (70) \]

This result for the ratio of the renormalized and the bare gap as a function of the bare one is fully consistent with the result obtained for a field theoretical model as mentioned in the introduction of Sect. \( \text{III} \) if one identifies \( g/g_c \leftrightarrow U/\pi [51-53]. \) We are not aware that this power-law increase (for repulsive interactions) of the gap was earlier shown directly for a microscopic lattice model, that is without the intermediate approximate step of mapping the lattice model to a continuum field theory.

Evaluating Eqs. \((65)\) and \((66)\) in first order perturbation theory as described above we obtain the perturbative result

\[ \Delta_{\text{ren}} = \Delta \left( 1 - \frac{2U}{\pi W} \ln \Delta \right). \quad (71) \]

It coincides with the leading order in \( U \) expansion of Eq. \((70)\). This logarithmic divergence in the limit of small \( \Delta \) is known from field theory \([31,53]). \) For the present lattice model it can also be obtained directly by employing standard first order perturbation theory.

To summarize this part, we have shown analytically that functional RG in its lowest-order truncation contains all infrared divergent leading log terms and is able to resum this series to a power law.

2. Band width renormalization

After the analysis of the gap renormalization, we next discuss the interaction effect on the band width. Similar to the renormalized gap it will be visible in the local spectral function discussed in Sect. \( \text{V A} \). As for bare gaps \( \Delta \ll W, V_{\text{ren}} \ll \Delta_{\text{ren}}^{\Delta} \leq t_{1\text{ren}}^{\Delta} + t_{2\text{ren}}^{\Delta}, \) it is meaningful to define half the renormalized band width as \( W_{\text{ren}} = t_{1\text{ren}}^{\Delta} + t_{2\text{ren}}^{\Delta} - 2t_{\text{ren}}^{\Delta}. \) Keeping the term to leading order in \( U \) on the right hand side of the RG equation and systematically expanding for \( \Delta \ll \min \{ W, \Lambda \}, \) Eq. \((67)\) becomes

\[ \frac{\partial t^A}{t^A} = -\frac{2U}{\pi W^2} \left( 1 - \frac{\Lambda}{\sqrt{\Delta^2 + W^2}} \right). \quad (72) \]
It can be integrated over $\Lambda$ from $\infty$ (which is possible as the right hand side decays as $1/\Lambda^2$) to $\Delta$ with the solution

$$W^{\text{ren}} = \exp \left\{ \frac{U}{\pi} \left( \frac{\sqrt{\Delta^2 + W^2} - \Delta}{W} \right) \right\}. \quad (73)$$

Expanding this result up to first order in $U$, (half) the renormalized bandwidth is given as

$$W^{\text{ren}} = W \left( 1 + \frac{U}{\pi} \right). \quad (74)$$

This result is again consistent with the one known from first order perturbation theory (for the gapless model).

Note that the “high-energy” band width does not show any divergent behavior. A resummation of (logarithmically) divergent terms inherent to the functional RG procedure is not required. In accordance with the observation that our truncated RG does contain all regular (non-log-divergent) terms to leading order in $U$ only, the higher order terms of Eq. (73) are not systematic in the sense of perturbation theory. Accordingly, we cannot argue that this equation provides a better approximation to the unknown exact renormalization of the band width as compared to the purely perturbative result Eq. (74).

**B. Numerical results**

The effective gap, as it shows up in the spectral function (see Sect. IV A), can be computed using Eq. (3) with the bare $V$ and $\delta t$ replaced by the renormalized values. The main panel of Fig. 6 shows a comparison of the renormalized gap divided by the bare one as a function of the bare gap obtained by the numerical solution of the full truncated functional RG equations to DMRG data for different $U$. In contrast to our analytical considerations of Sect. IV A, we do not employ any additional approximations besides the lowest order truncation. The DMRG data were extracted from the specific heat, as explained in Sect. III B. The single-particle parameters are $V = 0.3\cos \varphi = \delta t$ and $\varphi$ varies between 0 and $\pi/2$. For interactions of up to $U = 0.5$ and not to small bare gaps, the agreement between the functional RG and DMRG data is excellent. The functional RG data show linear behavior on a log-log scale indicating power-law scaling for small bare gaps as discussed in Sect. IV A. The slope and therefore the exponent depends on $U$. As long as the bare gap is not to small the DMRG data confirm this. However, the limited numerical accuracy of the renormalized gap obtained from the specific heat at small bare gaps makes it difficult to confirm the power law with certainty.

The analysis of the approximate functional RG data can, however, be driven to a much higher level. In the inset of Fig. 6 we show the centered logarithmic differences of $2\Delta^{\text{ren}}/(2\Delta)$ as a function of $2\Delta$ computed as in Eq. (37) for different $U$. The single-particle parameters for the inset are $V = (1/2)^l = \delta t$, with $l = 0, 1, \ldots, 15$. For small $U$ these data nicely approach the expected leading order exponent $\beta = -U/\pi$ (indicated as dashed horizontal lines) in the limit of small $\Delta$; see Eq. (70). The deviation at larger $U$ stems from higher-order corrections contained in the numerical solution of the full truncated functional RG equations but not in the analytical solution of Sect. IV A which required additional approximations. Apparently, the prefactor of the $U^2$ term of the exponent is not small compared to the one of the leading term. From the excellent agreement of the DMRG and functional RG data for sizeable $U$ (and not to small bare gaps) as shown in the main part of Fig. 6 we conclude that the higher order functional RG corrections of the exponent show the correct trend as compared to the ones which would show up in a hypothetical exact solution. In other words, the prefactor of, e.g., the $U^2$ term of the exponent obtained within the approximate functional RG is rather close to the unknown exact one. However, the truncations within the functional RG approach do not allow us to argue that both prefactors agree. Overall, this is a rather stringent numerical confirmation that the analytical result Eq. (70) gives the exponent of the power-law renormalization of the gap to leading order.

We can compare this to the result for the exponent from field theory. As discussed in Sect. IV A, the leading order exponents of the lattice model calculation and field theoretical considerations agree if we identify $g/g_c \leftrightarrow U/\pi$. In Ref. [51] an expression for $\beta$, which contains higher order corrections in $g/g_c$, was derived from the Bethe ansatz solution of the massive Thirring
model [71]. However, as discussed there, only the first order term is independent of the ultraviolet regularization of the field theory and thus universal. Furthermore, one cannot expect that the identification $g/g_c \leftrightarrow U/\pi$ between the coupling constant of the field theory and the interaction parameter of the lattice model holds beyond leading order. Accordingly, one cannot expect that the second order correction $(g/g_c)^2$ (with prefactor 1) to the leading term $-g/g_c$ (and, for that matter, any other higher order term) of the Bethe ansatz solution can be found in the lattice model. However, this second order correction shares one feature with our lattice model result for the exponent. It has a prefactor which is not small as compared to the one of the leading linear term.

In addition to the gap, the band width is renormalized by the interaction. As discussed in Sect. IV A 2 this can be computed analytically using functional RG and simple perturbation theory. We note in passing that for sufficiently small $U$ the numerical functional RG data for the renormalized band width given by $2\delta t^{\text{ren}}$ agree well with the perturbative result Eq. (74).

In a first attempt to investigate if the topological properties are altered by the two-particle interaction we study the renormalized $V^{\text{ren}}$ and $\delta t^{\text{ren}}$ at the end of the RG flow as a function of the bare parameters $\delta t$ and $V$. In case $\delta t^{\text{ren}}$ has a sign opposite to $\delta t$ one would naively, that is within an effective single-particle picture, expect that the interaction alters the topological properties as well as Fig. 4 highlighting the characteristic features of the boundary charge. We did not observe this for any parameter set considered. Figure 7(a) shows $\delta t^{\text{ren}}$ (color coded) as a function of $V$ and $\delta t$. Similarly, $V^{\text{ren}}$ stayed positive for all positive $V$ and vice versa; see Fig. 7(b). Still the renormalization leads to nontrivial structures indicated by the bending of the (dashed) equipotential lines.

From the renormalized bulk properties and employing the generalized BBC one would thus conclude that the number of “effective edge states” showing up as in-gap $\delta$-peaks in the single-particle spectral function is not altered by the interaction. We will return to this in Sect. IV A.

\section{V. Systems with Boundary for $U > 0$}

The nontrivial spatial structure of the frequency independent self-energy (or the renormalized single-particle parameters) close to a boundary build up during the RG flow prohibits the analytical solution of the functional RG flow equations [53]. This has to be contrasted to the case with PBC in which this was possible, at least in the limit of small bare gaps; see Sect. IV A. We thus have to rely on a numerical solution of the RG equations. Figure 8 shows the Friedel-part of the renormalized single-particle parameters (or the static self-energy) at the end of the RG flow; see Eqs. (58)-(62). The parameters are $V = -0.25$, $\delta t = 0.001$, $U = 0.25$ and the system size is $L = 10000$. Inset: The absolute value of the data of the main panel on a linear-log sale highlighting the exponential decay. The dashed line shows an exponential function with decay length $1/\kappa_{bc}$ which can be obtained by plugging the renormalized bulk values for $\Delta$, $t_1$, and $t_2$ into Eq. (20).

In the above sections we explained how to obtain the observables of interest from functional RG and DMRG. We focus on $\mu = 0$ and start out with the local spectral function.
FIG. 9. Functional RG data for the local single-particle spectral function of the interacting RM model for the same single-particle parameters as in Fig. 1 and \( U = 0.5 \). The height of the \( \delta \)-peaks (vertical arrows) on the \( i = 2 \) sites is scaled up as compared to the one of the \( i = 1 \) sites.

A. The local spectral function

In Fig. 9 we show functional RG results for the local single-particle spectral function of the interacting RM model with OBC computed using Eq. (51). The single-particle parameters are as in Fig. 1, the interaction is \( U = 0.5 \), and the system size \( L = 4096 \). Similar to the procedure used in the noninteracting case, to obtain a smooth function out of the sum of \( \delta \)-peaks (finite system size) we averaged the spectral weight in the bands over several eigenenergies of the effective single-particle Hamiltonian. Increasing the system size the curves do not change on the scale of the plot.

The interaction effects we expect based on our analysis of the bulk properties can clearly be observed in Fig. 9. In comparison to Fig. 1 the gap size is increased and the bands extend to smaller (valence band) and larger (conduction band) energies (renormalization of the band width). The in-gap \( \delta \)-peak representing the edge state for \( U = 0 \) still appears. We emphasize that strictly speaking the \( \delta \)-peak of the interacting spectral function does not have an interpretation as a single-particle (edge) state.

However, beyond these findings expected from the renormalized bulk properties we observe in Fig. 9 that the \( n \) dependence \( [j = 2(n - 1) + i] \) of the weight of the \( \delta \)-peak on the first site of each unit cell \( (i = 1) \) is modified as compared to the \( U = 0 \) case [see Eq. (22) and Fig. 1]. For generic single-particle parameters and \( U > 0 \) the spectral weight of the peak first increases before it starts to decrease when going from the boundary towards the bulk. This has to be contrasted to the purely exponential spatial decay of the noninteracting case. Furthermore, we observe the appearance of \( \delta \)-peak spectral weight on the second sites of the unit cell \( (i = 2) \). It is much smaller than the one on \( i = 1 \) sites but also shows a nonmonotonic \( n \) dependence. To render the weight on the \( i = 2 \) sites visible they were all scaled up by an (arbitrary) factor as compared to the weights on \( i = 1 \). Both these interaction effects are a consequence of the nontrivial interaction induced spatial dependence of the effective single-particle parameters close to the boundary (and beyond the unit cell structure) acquired during the RG flow.

We observe that also for \( U > 0 \), the energy \( \varepsilon_e \) of the \( \delta \)-peak, indicating the “effective edge state”, turns out to be position independent. Comparing Figs. 1 and 9 one can barely see that \( \varepsilon_e \) is modified by the interaction. To further illustrate this we show the dependence of the peak energy \( \varepsilon_e \) on \( \delta t \) for different \( U \) on a log-log scale in Fig. 10 (symbols). The single-particle parameters are \( V = 0.001 \), and \( \delta t \) varies from \(-0.1\) to \(-0.005\). The system size is \( L = 2048 \). As we are in the limit \( |V| \ll |\delta t| \), according to Eq. (69) \( |\delta t| \) is a measure for the size of the bare gap. The energy of the \( \delta \)-peak thus scales as a power-law (straight line on the log-log scale) as a function of the bare gap with the leading order exponent \(-U/\pi\) known from the scaling of the renormalized gap Eq. (70). Consulting Eq. (69) for the renormalized bulk value of the onsite energy and taking into account that in the noninteracting case \( \varepsilon_e = V \) one might argue that this power-law dependence was to be expected. However, this ignores that the RG flow leads to a nontrivial spatial dependence of the renormalized onsite energies and bond hoppings close to the boundaries. This can be anticipated to affect all properties close to the boundaries. Indeed, for \( U > 0 \) the energy \( \varepsilon_e \) of the in-gap \( \delta \)-peak does not coincide with the renormalized bulk value \( V_{\text{ren}} \) of the onsite energy. The latter is shown as dashed lines in Fig. 10 and shows power-law scaling as a function of \( \delta t \).
(respectively the bare gap) in accordance with Eq. (69).

Although first order perturbation theory for the self-energy misses the power-law renormalization of the gap as well as the power-law dependence of $\varepsilon_e$ it leads to qualitatively the same interaction effects in the single-particle spectral function as discussed above.

We find even more severe interaction effects in the single-particle spectral function associated to “effective edge states”. In the limit $|\delta t| \ll |V|$ the noninteracting gap Eq. (3) is dominated by $|V|$ and the spectral function on site $j = 1$ shows a van-Hove singularity at $V$. This can be seen in the $U = 0$ curve (deep purple) of Fig. 11 which only displays the photoemission part $\omega < 0$ of $A_1(\omega)$. For $\delta t > 0$ no edge state appears. If in this regime of single-particle parameters an interaction is turned on an in-gap $\delta$-peak appears, which can be associated to an “effective edge state”. In fact, it is an edge state of the effective single-particle Hamiltonian to be diagonalized at the end of the RG procedure. The appearance of the in-gap weight can be traced back to the interaction induced spatial modulation of the effective onsite energy and hopping close to the boundary which can obviously alter local properties (such as “effective edge states”). Increasing the interaction the weight of the $\delta$-peak increase as illustrated in Fig. 11. It furthermore shows the characteristics of an edge state as a function lattice site $j$; for large $j$ the weight decays exponentially. This is a property of the eigenstate of the effective single-particle Hamiltonian at the in-gap eigenvalue. However, similar to the peak of Fig. 9 its weight first increases when going towards larger $j$ (not shown).

We emphasize, that the appearance of the interaction induced “effective edge states” is not related to the ability of the lowest-order truncated functional RG to resum the series of leading logarithms. Accordingly, this effect can also be observed in first order perturbation theory for the self-energy.

We conclude that the interaction can alter the number of “effective edge states” (in-gap $\delta$-peaks of the single-particle spectral function). As discussed, this cannot be understood from the bulk properties of the system but follows from the interaction induced spatial modulation of the effective onsite energy and hopping close to the boundary. This insight shows that the number of “effective edge states” (in-gap $\delta$-peaks of the single-particle spectral function) in the interacting case cannot be predicted based on a generalized BBC. As we will discuss in Sect. V C the main features of the boundary charge can be understood from the bulk properties even in the presence of interactions. It might thus be the more appropriate indicator of a generalized BBC in the presence of two-particle interactions.

B. The local density

In the discussion of our functional RG results for the local density modulations induced by an open boundary, we start out with a comparison of functional RG and highly accurate DMRG data. The main panel of Fig. 12 shows results obtained for generic single-particle parameters in the small gap limit $V = 0.0035$, $\delta t = -0.007$, for a weak interaction $U = 0.25$ and system size $L = 1000$. The largest absolute value of the relative difference between the functional RG and DMRG data taken over all lattice sites as a function of $U$. A log-log scale is taken. The dashed line indicates the power-law $U^2$ (line with slope 2 on the log-log scale).
Close to the boundary the density deviates from the bulk values, which, however, are approached for larger $j$. The renormalized (as compared to $U = 0$) bulk value of the density obtained from DMRG is indicated on the right by a triangle. The behavior on the two sites of the unit cell ($i = 1, 2$) differs. Close to the boundary the density is nonmonotonic for the first site ($i = 1$) in each unit cell and monotonic for the second ($i = 2$). This nonmonotonicity is an interaction effect (see below) which vanishes for $U \to 0$. In addition, larger $j$ are required for the $i = 1$ sites (odd $j$) to approach their asymptotic bulk value as compared to the $i = 2$ ones (even $j$). This is opposite to the noninteracting case (see the discussion of Fig. 2) and thus an interaction effect as well. Within the approximate functional RG approach both these interaction effects can be traced back to the nontrivial spatial dependence of the effective single-particle parameters acquired during the RG flow.

Within the approximate functional RG approach the density was computed in two ways: By integrating the $(j,j)$-matrix element of the Green function over Matsubara frequency (label “Green”, diamonds) and by its own flow equation (label “vertex”, squares) in accordance with our discussion in Sect. III A the density computed via the second way agrees better with the highly accurate DMRG data. The inset shows the maximum (over all lattice sites) of the relative difference between the functional RG and DMRG data as a function of $U$. Due to the truncation this difference scales as $U^2$ (dashed line). Deviations from the $U^2$ scaling result from the limited accuracy of the numerical solution of the functional RG flow equations as well as the small errors inherent to the DMRG approach. We emphasize that using the flow equation for the density one does not gain a power in $U$. Rather the difference to the exact prefactor of the $U^2$ term is significantly smaller. From now on we refer to functional RG density data obtained from their own flow equation.

As in the noninteracting case the approach of the bulk value of the density on the two sites of the unit cell is dominated by an exponential factor. The bulk value itself agrees with the one obtained for PBC. The functional RG decay rate $\kappa_{\text{ren}}$ can for small $U$ be obtained by plugging the renormalized bulk values for $\Delta$, $t_1$, and $t_2$ into Eq. (20). In other words, the effective single-particle picture can be used and the leading asymptotic decay is not altered by the spatial modulation of the effective single-particle parameters close to the boundary. This is shown in the main part of Fig. 13 for $\delta t = 0.0001$, $V = 0.002$, $L = 20000$, and different $U$. To avoid overloading the plot we focus on the unit cell index $i = 2$ in the main part (solid lines). After subtracting the bulk value and on a linear-log scale the data for sufficiently large $n$ are linear with the slope given by $-2\kappa_{\text{ren}}$ as computed from the corresponding bulk $\Delta_{\text{ren}}$, $t_{1\text{ren}}$, and $t_{2\text{ren}}$ (see dashed lines).

The advantage of the functional RG approach as compared to DMRG is that it is easily possible to study very large systems (see Sect. III A 2). This is required if one is interested in the spatial dependence of the density beyond the leading exponential behavior. By subtracting the bulk values and factoring out the exponential term discussed in the last paragraph we can extract the large $j = 2(n-1) + i$ behavior of the pre-exponential function.

In the inset of Fig. 13 we show centered logarithmic differences of the pre-exponential function which were computed as in Eq. (37). The same parameters as in the main part are considered. We here show results for both unit cell indices $i = 1$ (solid lines) and $i = 2$ (dashed-dotted lines). In contrast to the noninteracting case the $U > 0$ data do not approach a plateau at $-1/2$ (dotted line). The $1/\sqrt{n}$ decay of the pre-exponential function is thus altered by the interaction. This is a qualitative change of the position dependence of the density due to the interaction. However, this qualitative effect is hidden by an exponential decay and thus difficult to observe. It results from a similar nontrivial pre-exponential function of the spatial dependence of the Friedel part of the renormalized self-energy (the dominant decay being exponential; see Sect. III A 2). The details of the behavior of the pre-exponential functions of the self-energy and the density for $U > 0$ are beyond the scope of the present paper.

We note in passing that we do not observe any remnants of the Tomonaga-Luttinger liquid power-law decay of the Friedel oscillations of the density obtained for a vanishing single-particle gap. As discussed in Sect. III A if present, we should be able to observe this even within our approximate functional RG approach.
This completes our discussion of the spatial dependence of the density close to an open boundary. We now turn to the boundary charge which can be computed from the density.

C. The boundary charge

As our last observable of the interacting RM model with an open boundary we investigate the boundary charge. As in the noninteracting case it can be computed from the density by Eq. (38).

To get an overview of the interaction effects in Fig. 14 we show functional RG data for the boundary charge in the \((V, 2\delta t)\) [or equivalently the \((\Delta, \gamma)\)] plane for \(U = 0.25\). Barely any differences as compared to the noninteracting case Fig. 4 are visible. As discussed in Sect. II C this type of plot nicely illustrates the main characteristics (i), (ii), and (iv) of the boundary charge for noninteracting models. Combined this already indicates that these characteristics are robust towards small two-particle interactions.

For the noninteracting model, the features (i)-(iv) of the boundary charge follow from bulk properties. Thus the apparent robustness of (i), (ii), and (iv) towards interactions [for (iii), see below] in addition provides a first hint that this type of generalized BBC also holds for \(U > 0\). Crucially, the spatial modulations of the renormalized single-particle parameters close to the boundary do not seem to alter the general features of the boundary charge. This has to be contrasted to the number of “effective edge states” (in-gap \(\delta\)-peaks of the single-particle spectral function) which in the interacting case cannot be predicted from bulk properties; see Sect. VA. Next we further substantiate both, the robustness of (i)-(iv) towards two-particle interactions as well as the validity of a generalized BBC for \(U > 0\).

In Fig. 15 we show the difference between the boundary charge with and without interaction as a function of \(U\) for different \(\Delta\) and \(\gamma\) on a log-log scale. First of all, we realize that for small \(U\) the corrections are very small. Still, for generic \(\gamma\) they are of order \(U\). This can be seen from the inset, which shows the logarithmic derivative of the data computed as in Eq. (37). Furthermore, the finite \(U\) corrections depend on (the generic) \(\gamma\) but are only weakly \(\Delta\)-dependent. For \(\gamma\) being a multiple of \(\pi\) (blue symbols in Fig. 15), i.e. \(\delta t = 0\) [see Eq. (4)], the corrections are of order \(U^2\). We note that within our approximate functional RG procedure not all terms of order \(U^2\) are kept. We thus do not control the value of these \(U^2\) corrections. We associate the deviations from the exponent 2 for \(U \lesssim 0.01\) (see the inset of Fig. 15) to small errors of the data for \(Q_B\) obtained by the numerical integration of the RG flow equations. Note that the value of \(\log(Q_B(U) - Q_B(0))\) for \(\gamma = 0\) is already very small and that taking the logarithmic derivative significantly enhances small errors.

In Fig. 16 we show \(Q_B\) as a function of \(\gamma\) for \(U = 0.089\) and different \(\Delta\) (symbols). The linearity in \(\gamma\) for small \(\Delta\) as derived analytically for \(U = 0\) [see Eq. (47)] and illustrated in Fig. 5 is robust against small interactions. However, the interaction enhances the corrections to the linear behavior and for small \(\Delta\) they appear to be independent of the bare gap. This can be seen most clearly by comparing the insets of Fig. 15 and Fig. 5 which show the logarithmic derivatives of the data of the corresponding main panels with respect to \(\gamma\). For \(\Delta \gg W\) the same \(\frac{1}{\gamma}\)-quantization of the boundary charge as derived for the noninteracting case in Eq. (50) and discussed in connection with Fig. 5 can be found in Fig. 16. Thus, also this feature is robust against small interactions.
We can thus conclude that the interaction effects on the characteristic features (i)-(iv) of the boundary charge are weak and, most importantly, can fully be understood from the renormalized bulk properties. They are not altered by the interaction induced modulation of the onsite energies and hoppings close to the boundary. This must be contrasted to the number of “effective edge states” (in-gap δ-peaks of the single-particle spectral function) discussed in Sect. VI A. Therefore, the boundary charge might be the more appropriate indicator of a generalized BBC in the presence of two-particle interactions. We emphasize that it is only possible to show the generalized BBC of the boundary charge if in addition to the renormalization of the (low-energy) gap also the renormalization of the (high-energy) band width is properly captured. In contrast to low-energy field theories, which do not allow to compute the latter, the functional RG consistently provides the band width renormalization. This constitutes another advantage (besides the direct applicability to microscopic lattice models) of the functional RG over effective low-energy field theories.

Our result of the stability of the boundary charge against short-ranged two-particle interactions is a microscopic manifestation of the important property of insulators that local fields (either external or interaction-induced ones) of arbitrary size lead only to local charge redistributions, i.e., charges can not be displaced beyond a characteristic length scale (given roughly by $W/\Delta$ for our model). This principle, also called the nearsightedness principle (NSP) [79, 78], is responsible for many universal properties of topological insulators as, e.g., charge pumping [77, 76, 78], the orthodox BBC [27–34], and the exponential localization of the charge density at boundaries [79]. Recently, the NSP has also been used to derive the characteristic features (i), (ii) and (iv) of the boundary charge (see section II C). Therefore, the establishment of the NSP for an interacting microscopic lattice model is a very important step for a full understanding of the universal properties of insulators and their stability. In this regard the functional RG is a very useful tool as it can capture the microscopic details of the band structure and two-particle interactions on all energy scales. In contrast, other methods are either restricted to noninteracting systems (exact diagonalization) or to the regimes of small gaps (effective low-energy field theories). Computing the boundary charge for small gaps (low-energy limit) using the numerical DMRG is computationally very challenging. It requires the use of very large systems as the inverse system size sets a low-energy cutoff.

VI. SUMMARY AND OUTLOOK

We studied the local single-particle spectral function, the local density, as well as the boundary charge of the noninteracting and interacting RM model for periodic chains and such with open boundaries. For $U = 0$ our
main focus was on the boundary charge which currently experiences a revival as an indicator of a generalized BBC. We showed that results recently obtained in the low-energy limit $\Delta \ll W$ within an effective low-energy theory hold for surprisingly large gaps. In addition we found a universal $\frac{1}{\pi}$ quantization of the boundary charge for large gaps. We explicitly illustrated the four main characteristics of the boundary charge for the model under consideration which all follow from properties of the bulk Hamiltonian. We showed that this generalized BBC is robust towards small two-particle interactions employing a functional RG approach, which, for small interactions, provides reliable results on all energy scales. In contrast, interaction spoils the relation between the number of in-gap $\delta$-peaks, i.e. the number of “effective edge states”, and renormalized bulk properties. Novel interaction induced peaks are generated by the spatial variation of the self-energy close to the boundary. These also affect the local density close to the boundary. Our results provide a hint that the fractional part of the boundary charge might turn out to be the more appropriate indicator of a generalized BBC.

For noninteracting and clean systems the generalized BBC for the fractional part of the boundary charge is established via its relation to the Zak-Berry phase (also called “surface charge theorem”). It is also applied within density functional theory (DFT) and mean-field theories (MFT) under the restrictive assumption that two-particle interactions can be treated within such methods [40]. For 1d systems and in the limit of small gaps this assumption does not hold. The relation between the Zak-Berry phase and the fractional part of the boundary charge holds up to an unknown integer since there is a freedom of how to choose the gauge of the Bloch states. For systems with disorder or true many-body correlations, e.g. interacting 1d systems in the limit of small $\Delta$, the Zak-Berry phase is not defined and one should directly study the physical observable, namely the boundary charge. Therefore, its determination in terms of renormalized bulk parameters and the stability analysis of its universal properties is a central task of many-body methods. The functional RG is a very useful tool in this respect since it can capture true many-body correlations on all energy scales not accessible by DFT and MFT. This is of particular importance for 1d systems where Tomonaga-Luttinger liquid physics is very important for vanishing $\Delta$.

Furthermore, functional RG is very flexible and has the potential to be applied to a wide range of interesting systems. It will be of interest to study the validity range of universal low-energy results for larger values of the wavelength $Z$ of the external modulation (as compared to $Z = 2$ for the RM model) and for disordered systems. In addition one can study multi-channel systems with several orbitals per site. Besides the boundary charge, the interface charge is expected to have comparable universal properties [44] and can be directly calculated from the local density. Furthermore the functional RG can be used to study the density-density correlation function and the fluctuations of the boundary charge, and is in principle not restricted to one-dimensional systems. Therefore, we expect the functional RG to be a very useful tool to study topological properties in the presence of many-body correlations and disorder.

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Appendix: The noninteracting Rice-Mele model

In this Appendix we derive analytical expression for the density and the boundary charge of the noninteracting RM model. We start with the bulk density of the infinite system and prove Eq. (18). Using Eq. (17) we close the integration contour over $k$ in the upper half of the complex plane

$$\rho_{\text{bulk}}(j) = \frac{1}{2} + (-1)^j \frac{V}{4\pi} \oint_C dk \frac{1}{\epsilon_k}.$$  \hfill (A.1)

Here, $C$ is a closed curve defined via straight lines on the segments $-\pi \to \pi \to \pi + i\infty \to -\pi + i\infty \to -\pi$. This can be done since the additional segments do not contribute. The two segments $\pi \to \pi + i\infty$ and $-\pi + i\infty \to -\pi$ cancel each other due to periodicity under the shift of $k$ by $2\pi$. The segment $\pi + i\infty \to -\pi + i\infty$ is zero due to the infinite imaginary part of $k$. Using Eq. (13) for $\epsilon_k$, one finds a branch cut starting at the branching point $k_{bc}$ where $\epsilon_{k_{bc}} = 0$, leading to $k_{bc} = \pi + ik_{bc}$ and $\epsilon_{k_{bc}}$ given by Eq. (20). Choosing the branch cut in the direction of the positive imaginary axis and closing the integration contour around the branch cut, we find for the bulk density

$$\rho_{\text{bulk}}^{(bc)}(j) = \frac{1}{2} - (-1)^j \frac{V}{2\pi} \Im \int_0^{\infty} dk \frac{1}{\epsilon_{k_{bc} + i\kappa}}. \hfill (A.2)$$

Using

$$\epsilon_{k_{bc} + i\kappa} = i\sqrt{-R(\kappa)}.$$  \hfill (A.3)

with $R(\kappa)$ defined in Eq. (19), we arrive at Eq. (18).

To calculate the Friedel density from Eq. (27) we again close the integration contour over $k$ in the upper half of the complex plane

$$\rho_F(j) = -\frac{1}{2\pi} \oint_C dk \left[ \chi_k(i) \right]^2 e^{2i\kappa n}.$$  \hfill (A.4)
Using the form Eq. (15) of the Bloch states we find a pole of the integrand for \( \epsilon_k = -V \) and a branch cut starting at \( \kappa_{bc} \). The pole is only present for \( t_2 > t_1 \) and \( V < 0 \) and the residue can be shown to be such that the contribution to the integrand of Eq. (15) cancels the edge state density Eq. (26) for \( \mu = 0 \), see Ref. [48] for details. This proves Eq. (29). Closing the integration contour around the branch cut, we find for the branch cut contribution to the Friedel density

\[
\rho_F^{(bc)}(n, i) = \frac{1}{\pi} e^{-2\kappa_{bc} n} \text{Im} \int_0^\infty dk \chi_n^{(-)}(i) e^{-2k_n}.
\]

Inserting Eq. (15) and using

\[
\frac{N_n^{(-)}}{N_{k_n+i_{k}+\pm}} = 2R(k) + 2iV \sqrt{-R(k)},
\]

\[
\frac{\text{Im} \left( \frac{(V + \epsilon_{k_{bc}+i_{k}+\pm})^2}{N_{k_{bc}+i_{k}+\pm}} \right)}{V} = -\frac{2\sqrt{-R(k)} [V^2 - R(k)]^2}{\sqrt{R(k)}},
\]

we find Eqs. (30) and (31).

To prove the asymptotic behavior Eq. (36) of the branch cut contribution

\[
\rho_F^{(bc)}(n, i) \approx \frac{c_1}{\sqrt{n}} e^{-2\kappa_{bc} n}, \quad n \gg \frac{W}{\Delta} \gg 1,
\]

we consider the regime of small gap \( \Delta \ll W = 2t \) and note that \( \Delta \approx \frac{2t}{\Delta} \) in this case. Therefore, for \( n \gg \frac{W}{\Delta} = 2\kappa_{bc}^{-1} \), we get \( \kappa \sim \frac{1}{\kappa_{bc}} \) for the integration variable in Eqs. (30) and (31). Expanding \( R(k) \) for \( \kappa \ll \kappa_{bc} \) by using Eq. (19) we find

\[
R(k) \approx -W \Delta k.
\]

Inserting this result in Eq. (31) for \( \rho_F^{(bc)}(n, 2) \) and performing the integration we obtain Eq. (A.9) for \( i = 2 \) with

\[
c_2 = \frac{V}{\sqrt{\pi W \Delta}}.
\]

To prove Eq. (A.9) for \( i = 1 \), we consider the case \( V \ll \delta t \) such that \( V \sim \delta t \) and

\[
R(k) \sim W \Delta k \sim \frac{W \Delta}{n} \ll \Delta^2 \sim V^2.
\]

Therefore, we can use \( V^2 \equiv R(k) \approx V^2 \) in the integrand of Eq. (30) and, together with Eq. (A.10), we can calculate the integral with the result Eq. (A.9) for \( i = 1 \) and

\[
c_1 = \frac{(2\delta t - \Delta)^2}{V \sqrt{\pi W \Delta}}.
\]

To prove Eq. (42) for the boundary charge we split \( Q_B = Q_P + \delta Q_B \) via Eq. (39). To calculate \( Q_P \) we insert Eq. (18) in Eq. (40) and get

\[
Q_P = -\frac{V}{4\pi} \int_0^\infty dk \frac{1}{\sqrt{-R(k)}}.
\]

To obtain \( \delta Q_B \) we use Eq. (35) for \( \delta \rho(j) = \rho_F^{(bc)}(j) \) in Eq. (41), and use Eqs. (30) and (31) for the branch cut contribution of the Friedel density. Adding \( Q_P \) from Eq. (A.14), we find after a lengthy but straightforward calculation

\[
Q_B = I_1 + I_2,
\]

with

\[
I_1 = -\frac{V(t_2^2 - t_1^2)}{4\pi} \int_0^\infty dk \frac{1}{\sqrt{-R(k)}} [V^2 - R(k)],
\]

\[
I_2 = -\frac{V t_1 t_2}{2\pi} \int_0^\infty dk \frac{\sinh(\kappa_{bc} + k)}{\sqrt{-R(k)} [V^2 - R(k)]}.
\]

Inserting Eq. (19) for \( R(k) \), the integral \( I_2 \) can be analytically calculated with the result

\[
I_2 = -\frac{1}{4} \text{sign}(V).
\]

Taking Eqs. (A.15), (A.16), and (A.18) together we arrive at Eq. (42).

Alternatively, one can write Eq. (42) for the boundary charge also via an integration over the real axis

\[
Q_B = -\frac{1}{2} \Theta(t_2 - t_1) \text{sign}(V) + \tilde{I},
\]

with

\[
\tilde{I} = \frac{-WV\delta t}{8\pi\epsilon t_1 t_2} \int_0^\pi \frac{dk}{\epsilon k (\frac{2\delta t^2 + \epsilon k^2}{t_1 t_2} + 1 + \cos k)}
\]

\[
= \frac{-V \delta t}{\pi W \sqrt{4t_1 t_2 + \Delta^2}} \Pi \left( \frac{4t_1 t_2}{W^2}, \frac{2\sqrt{t_1 t_2}}{4t_1 t_2 + \Delta^2} \right),
\]

where \( \Pi \) is the complete elliptic integral of the third kind. Closing the integration contour of Eq. (A.20) in the upper half of the complex plane, we split this integral into a pole and a branch cut contributions

\[
\tilde{I} = \tilde{I}^{(\text{pole})} + \tilde{I}^{(bc)}.
\]

A straightforward calculation gives for the pole contribution

\[
\tilde{I}^{(\text{pole})} = \frac{1}{2} \Theta(t_2 - t_1) \text{sign}(V) - \frac{1}{4} \text{sign}(V),
\]

while the branch cut contribution \( \tilde{I}^{(bc)} \) is identical to \( I_1 \), see above. Taking all together we find the equivalence of Eqs. (A.19) and (42).
Using the representation Eq. (A.20) we study the limit $|V| \ll |\delta t|$. Approximating $\varepsilon_k \approx \sqrt{\delta t^2 + 2t_1t_2(1 + \cos k)}$, we immediately get

$$Q_B \approx -\frac{1}{2} \Theta(t_2 - t_1) \text{sign}(V) \frac{V}{4\pi \delta t} E \left(\frac{\sqrt{4t_1t_2}}{W}\right),$$  
(A.24)

where $E$ is the complete elliptic integral of the second kind. This proves Eq. (48). Assuming additionally $|\delta t| \ll W$, we can use the low-energy result Eq. (47) and get

$$Q_B \approx -\frac{1}{2} \Theta(t_2 - t_1) \text{sign}(V) \frac{V}{4\pi \delta t}. \quad (A.25)$$

For large $|V| \gg W, |\delta t|$ (atomic limit) we approximate

$$\varepsilon_k \approx \frac{1}{|V|} \frac{1}{\sqrt{1 + \frac{2t_1t_2(2\delta t^2 + 1 + \cos k)}{V^2}}},$$
(A.26)

It follows

$$\tilde{I} = -\frac{W}{8\pi t_1t_2} \int_{-\pi}^{\pi} \frac{dk}{\frac{2\delta t^2}{W^2} + 1 + \cos k} + \frac{W}{4V^2} \text{sign}(V) \delta t \frac{\text{sign}(\delta t)}{W} O \left(\frac{W^4}{V^4}\right).$$  
(A.27)

Evaluating Eq. (A.27) with the result

$$-\frac{\text{sign}(V) \text{sign}(\delta t)}{4},$$
(A.29)

we obtain for the boundary charge in this parameter regime

$$Q_B \approx -\frac{1}{4} \text{sign}(V) \left[1 - \frac{W}{2V^2} \right]. \quad (A.30)$$

This proves Eq. (50).

The case $|\delta t| \ll |V| \ll W$ is treated by approximating

$$\varepsilon_k \approx \frac{1}{\sqrt{V^2 + \frac{2}{W^2}(1 + \cos k)}},$$
(A.31)

and

$$\tilde{I} \approx -\frac{V \delta t}{4\pi W^2} \int_{-\pi}^{\pi} \frac{dk}{\frac{2\delta t^2}{W^2} + \frac{1}{2}(1 + \cos k)} \times \frac{1}{\sqrt{\frac{V^2}{W^2} + \frac{1}{2}(1 + \cos k)}}, \quad (A.32)$$

It is necessary to estimate the latter integral for the two small parameters $\frac{|\delta t|}{W} \ll \frac{|V|}{W} \ll 1$. The main contribution is received from the vicinity of $k = \pi$. Expanding $\frac{1}{2}(1 + \cos k) \approx \frac{1}{2} x$, with $x = k - \pi$, and extending the integration limits to infinities, we obtain

$$\tilde{I} \approx -\frac{2V \delta t}{\pi W^2} \int_{-\infty}^{\infty} \frac{dx}{1 + \frac{2\delta t^2}{W^2} + x^2} \left[\frac{1}{\frac{4V^2}{W^2} + x^2}\right].$$  
(A.33)

To perform this integral we deform the contour in the complex upper half-plane to embrace the pole $x = \frac{4\delta t}{W}$ and the branch cut starting at $x = \frac{4V}{W}$. Thus we obtain to the order $O(\delta t/W)$

$$\tilde{I} \approx -\frac{\text{sign}(V) \text{sign}(\delta t)}{4} + \frac{\delta t}{\pi W}. \quad (A.34)$$

Adding the other contributions, we obtain the result

$$Q_B \approx -\frac{1}{4} \text{sign}(V) + \frac{\delta t}{\pi W} \quad (A.35)$$

for this parameter regime. Together with Eq. (50) this proves Eq. (49).

Finally, to derive the low-energy result Eq. (47) for small gap $|\Delta| \ll W$, a convenient starting point is the representation Eq. (A.22) together with $I_1 = \tilde{I}^{(bc)}$ expressed as

$$I_1 = \frac{W^2 \sin 2\gamma}{16\pi t_1t_2 \sqrt{4t_1t_2}} \int_{-\pi}^{\pi} \frac{dk}{\cosh \kappa - \cosh \kappa_{bc}} + \frac{V^2}{2t_1t_2} \frac{1}{\cosh \kappa - \cosh \kappa_{bc}}.$$  
(A.36)

In particular, by introducing the new integration variable $x = \frac{\sqrt{2t_1t_2}}{\Delta} \cosh \kappa - \cosh \kappa_{bc}$ in Eq. (A.36), we cast it to

$$I_1 = \frac{W}{4\pi} \int_{0}^{\infty} \frac{dx}{x^2 + \cos^2 \gamma} \left[1 + \frac{1}{\sqrt{(x^2 + 1)(x^2 + 1 + \frac{4\Delta^2}{\Delta^2})}}\right]. \quad (A.37)$$

In the low-energy limit we have $W \approx \sqrt{4t_1t_2}$ as well as

$$I_1 \approx \frac{\sin 2\gamma}{4\pi} \int_{0}^{\infty} \frac{dx}{x^2 + \cos^2 \gamma} \frac{1}{\sqrt{x^2 + 1}} = \frac{\gamma}{2\pi} - \frac{1}{2} \Theta \left[\sin \gamma \frac{x}{2\pi} < \frac{3}{2}\pi - \Theta \left[\sin \gamma \frac{x}{2\pi} < \frac{3}{2}\pi\right]\right], \quad (A.38)$$

where the last equality holds for $0 < \gamma < 2\pi$. Combining this result with the other contributions, namely with

$$-\frac{1}{4} \text{sign}(V) = -\frac{1}{4} + \frac{1}{2} \Theta \left[\sin \gamma \frac{x}{2\pi} < \frac{3}{2}\pi\right], \quad (A.39)$$

we arrive at Eq. (47).

On the basis of Eq. (A.37) we also estimate the leading correction to Eq. (47), which amounts to

$$\frac{\sin 2\gamma}{8\pi} \left(\frac{\Delta}{W}\right)^2 \ln \frac{\Delta}{W}. \quad (A.40)$$

Due to the large denominator, this correction is negligible even for $\Delta \sim W$, and therefore the low-energy result Eq. (47) remains quantitatively accurate up to these gap values.
B.A. Volkov and O.A. Pankratov, Pisma Zh. Eksp. Teor. Fiz. 42, 145 (1985) [JETP Lett. 42, 178 (1985)].

O.A. Pankratov, S.V. Pakhomov, and B.A. Volkov, Solid State Commun. 61, 93 (1987).

C.L. Kane and E.J. Mele, Phys. Rev. Lett. 95, 146802 (2005).

B.A. Bernevig, T.L. Hughes, and S.-C. Zhang, Science 314, 1757 (2006).

L. Fu, C.L. Kane, and E.J. Mele, Phys. Rev. Lett. 98, 106803 (2007).

M. König, S. Wiedmann, C. Brune, A. Roth, H. Buhmann, L.W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).

J.K. Asbóth, L. Oroszlány, and A. Pályi, J. Phys.: Condens. Matter 24, 085426 (2012).
Note that Ref. [51] contains several typos in relevant formulas for the exponent. The same holds for H. B. Thacker, Rev. Mod. Phys. 53, 253 (1981) in which the details of the Bethe ansatz solution of the massive Thirring model are presented.

For generic tight-binding models in 1d see Ref. [44], where it was shown that the boundary charge changes generically by $\bar{\rho} \mod(1)$ under the translation by one lattice site towards the boundary.

J. Zak, Phys. Rev. Lett. 48, 359 (1982); J. Zak, Phys. Rev. Lett. 62, 2747 (1989).

S. Ryu, A. P. Schnyder, A. Furusaki, and A. W. W. Ludwig, New J. Phys. 12, 065010 (2010).

W. Kohn, Phys. Rev. Lett. 76 3168 (1996).

E. Prodan and W. Kohn, PNAS 102, 11638 (2005).

D. J. Thouless, Phys. Rev. B 27, 6083 (1983).

Q. Niu and D. J. Thouless, J. Phys. A 17, 2453 (1984).

C. Kallin and B. I. Halperin, Phys. Rev. B 29, 2175 (1984).