Boundary fidelity and entanglement in the symmetry protected topological phase of the SSH model

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Abstract. We present a detailed study of the fidelity, the entanglement entropy and the entanglement spectrum, for a dimerized chain of spinless fermions—a simplified Su–Schrieffer–Heeger (SSH) model—with open boundary conditions which is a well-known example for a model supporting a symmetry protected topological (SPT) phase. In the non-interacting case the Hamiltonian matrix is tridiagonal and the eigenvalues and vectors can be given explicitly as a function of a single parameter which is known analytically for odd chain lengths and can be determined numerically in the even length case. From a scaling analysis of these data for essentially semi-infinite chains we obtain the fidelity susceptibility and show that it contains a boundary contribution which is different in the topologically ordered than in the topologically trivial phase. For the entanglement spectrum and entropy we confirm predictions from massive field theory for a block in the middle of an infinite chain but also consider blocks containing the edge of the chain. For the latter case we show that in the SPT phase additional entanglement—as compared to the trivial phase—is
Boundary fidelity and entanglement in the symmetry protected topological phase of the SSH model present which is localized at the boundary. Finally, we extend our study to the dimerized chain with a nearest-neighbour interaction using exact diagonalization, Arnoldi and density-matrix renormalization group methods and show that a phase transition into a topologically trivial charge-density wave phase occurs.

**Keywords:** solvable lattice models, topology and combinatorics, density matrix renormalization group calculations, entanglement in extended quantum systems (theory)

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1. Introduction

The Su–Schrieffer–Heeger (SSH) model has been introduced as a tight-binding model to describe conducting polymers such as polyacetylene \cite{1,2}. A simplified version of the SSH Hamiltonian for spinless fermions and a static lattice dimerization is given by

\[
H = -t \sum_{j=1}^{N-1} \left[ 1 + (-1)^j \delta \right] (c_{j+1}^\dagger c_j + \text{h.c.}) + U \sum_{j=1}^{N-1} (n_j - 1/2)(n_{j+1} - 1/2)
\]

(1.1)

where \( t \) is the hopping amplitude, \( \delta \) the dimerization parameter, \( U \) the nearest-neighbour repulsion and \( N \) the number of lattice sites. The creation operator for a spinless fermion at site \( j \) is denoted by \( c_{j}^\dagger \) and \( n_j = c_j^\dagger c_j \) is the occupation number operator. The model possesses time reversal symmetry \( T \) and particle-hole symmetry \( C \) with \( T^2 = 1 \) and \( C^2 = 1 \) and thus, for \( U = 0 \), belongs into the BDI class in a classification scheme of single-particle Hamiltonians \cite{3}.

We will concentrate first on the non-interacting case, \( U = 0 \) and postpone a discussion of the interacting case to section 6. For half-filling and any finite \( \delta \) (dimerized case) the excitation spectrum is then gapped with a gap \( \Delta_E \propto |\delta| \) in the thermodynamic limit. It has also been realized early on that the excitations in the dimerized case are topological solitons and anti-solitons (domain walls between the two possible dimerization patterns) which carry exactly half an electron charge \cite{2,4}.

In recent years, the SSH model has also attracted interest as one of the simplest examples for a model with a symmetry protected topological (SPT) phase \cite{5,6}. The topologically non-trivial phase for the Hamiltonian (1.1) with \( N \) even is realized for \( \delta > 0 \). It can only be transformed into a topological trivial phase by either breaking the symmetries which protect it or by closing the excitation gap. Thus gapless edge modes have to be present at the boundary of an SSH chain with \( \delta > 0 \) and the topologically trivial vacuum. An open SSH chain with \( \delta < 0 \), on the other hand, is topologically trivial and there are no edge modes. Instead of distinguishing the two phases by the presence or absence of edge modes, one can equivalently consider the Zak-Berry phase \( \gamma \) (bulk-boundary correspondence) which is a \( \mathbb{Z}_2 \) bulk invariant with \( \gamma = \pi \) in the SPT phase and \( \gamma = 0 \) in the topologically trivial phase \cite{7–10}.

The complexity of the ground state of a quantum many-body system and its response to changes in the microscopic parameters of the Hamiltonian can be characterized by its entanglement properties and by the fidelity, respectively. An interesting question is the relation between these quantum information measures and SPT order. For model (1.1) without interactions the von-Neumann entanglement entropy \( S_{\text{ent}} \) as a function of dimerization \( \delta \) in a periodic chain, obtained after tracing out one half of the system, has been investigated in \cite{9}. A detailed study of the entanglement entropy and spectrum as a function of the block size in the SPT and topological trivial phases has, however, not been performed yet. While it is clear that the ground state in the SPT phase is still only short-ranged entangled so that the bulk entanglement properties are the same as in the trivial phase\(^6\), additional entanglement can arise at the boundaries. Studying these boundary contributions to the entanglement is one of the main goals of our study.

\(^6\) Note, however, that tracing out part of the system creates virtual edges so that the entanglement spectra will have different degeneracies depending on whether a strong or a weak bond is cut. The degeneracies of the entanglement spectrum can be used to classify topological phases in one-dimensional interacting systems \cite{11–13}.
The fidelity susceptibility $\chi$ near phase transitions has also been studied in various models with topological phases [14,15], however, these studies concentrated on the bulk contribution $\chi_0$. For an open system there will in addition also be a boundary contribution, $\chi = \chi_0 + \chi_B/N$, where $N$ is the number of lattice sites, which to the best of our knowledge has not been investigated for models with SPT phases before. It is exactly this boundary contribution $\chi_B$ which should be sensitive to the presence or absence of edge states.

Our paper is organized as follows: In section 2 we review the exact solution of the SSH chain for periodic boundary conditions (PBC) and open boundary conditions (OBC). In section 3 we calculate the fidelity susceptibility and analyze the boundary contribution $\chi_B$ both in the SPT and in the topologically trivial phase. In section 4 we first briefly review known results for the entanglement entropy in critical and gapped quantum chains and the general formalism to calculate the entanglement spectrum for free fermion models. In the analysis of the obtained data for the SSH model we then show, in particular, that predictions from massive field theory for the scaling of $S_{\text{ent}}$ with block size are not valid in the SPT phase. In section 5 we study the entanglement spectra and compare with known analytical results in the limit of large block sizes. By using exact diagonalization, Arnoldi and density-matrix renormalization group methods we then extend our investigations in section 6 to the SSH model with a nearest-neighbour Coulomb repulsion. On the basis of the entanglement properties we identify, in particular, a transition into a topologically trivial charge-density wave phase. In section 7 we summarize our main results and conclude.

2. Diagonalization of the SSH model

We will briefly review the steps required to diagonalize the SSH model with periodic and open boundary conditions and give the eigenenergies and eigenvectors. For OBC we will consider both the case where the number of sites $N$ is even and the case where it is odd. The calculations to obtain the fidelity susceptibility and the entanglement spectrum and entropy are then explained in sections 3–5, respectively.

2.1. Periodic boundary conditions and $N$ even

This is the simplest case to handle. Taking the doubling of the unit cell due to the dimerization into account and performing a Fourier transform, the Hamiltonian (1.1) can be written as

$$H = -2t \sum_k \begin{pmatrix} c_{1k}^\dagger & c_{2k}^\dagger \end{pmatrix} T \begin{pmatrix} 0 & \cos k + i\delta \sin k \\ \cos k - i\delta \sin k & 0 \end{pmatrix} \begin{pmatrix} c_{1k} \\ c_{2k} \end{pmatrix}$$

(2.1)

where $k = 2\pi n/N$ and $n = 1, \cdots, N/2$. This is straightforwardly diagonalized. The eigenvalues are

$$\lambda_k^\pm = \pm 2t \sqrt{\cos^2 k + \delta^2 \sin^2 k} = \pm \sqrt{2t\sqrt{1 + \delta^2 + (1 - \delta^2) \cos 2k}}$$

(2.2)
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with a gap at the Fermi points \( k_F = \pm \pi/2 \) given by \( \Delta_E = 4|t|\delta \). The new operators in which the Hamiltonian is diagonal,

\[
H = - \sum_k \lambda_k^+ (\alpha_k^\dagger \alpha_k - \beta_k^\dagger \beta_k),
\]

are given by

\[
\alpha_k = \frac{1}{\sqrt{2}}(\mathcal{A}c_{k1} + c_{k2}), \quad \beta_k = \frac{1}{\sqrt{2}}(-\mathcal{A}c_{k1} + c_{k2})
\]

with \( \mathcal{A} = \lambda_k^+/2t(\cos k + i\delta \sin k) \). The ground state of the Hamiltonian (2.3) at half-filling is obtained by filling up the valence band, \( |\Psi_0\rangle = \prod_k \alpha_k^\dagger |0\rangle \).

2.2. Open boundary conditions and \( N \) odd

While in the PBC case only two momentum modes are coupled so that we are left with the diagonalization of a \( 2 \times 2 \) matrix, see equation (2.1), open boundary conditions instead lead to a coupling of all momentum modes so that a Fourier transform does not diagonalize the problem.

In real space, on the other hand, the Hamiltonian is a symmetric tridiagonal matrix with zero diagonal elements and superdiagonal and subdiagonal elements which alternate between \( 1 \pm \delta \). The eigenvalues and -vectors are explicitly known if the number of lattice sites is odd [16]. The eigenvalues are

\[
\lambda_0 = 0, \quad \lambda_k^\pm = \pm \sqrt{2t} \sqrt{1 + \delta^2 + (1 - \delta^2) \cos \theta_k}
\]

where

\[
\theta_k = \frac{2\pi k}{N + 1}
\]

and \( k = 1, \cdots, (N - 1)/2 \). The spectrum thus contains a single zero energy mode, see figure 1(a). If we parametrize each eigenvector as

\[
|\psi_k\rangle = (x_1^k, x_2^k, \ldots, x_N^k)^T,
\]

then the not-normalized elements of the eigenvector for the zero energy mode are

\[
x_{2n-1}^0 = \left(\frac{1 - \delta}{1 + \delta}\right)^{n-1}, \quad n = 1, \cdots, \frac{N + 1}{2}; \quad x_{2n}^0 = 0, \quad n = 1, \cdots, \frac{N - 1}{2}.
\]

For the other modes one finds

\[
x_{2n-1}^k = \frac{1 + \delta}{1 - \delta} \sin \left(\frac{2\pi k(n - 1)}{N + 1}\right) + \sin \left(\frac{2\pi kn}{N + 1}\right), \quad n = 1, \cdots, \frac{N + 1}{2}
\]

\[
x_{2n}^k = \frac{\lambda_k^\pm}{1 - \delta} \sin \left(\frac{2\pi kn}{N + 1}\right), \quad n = 1, \cdots, \frac{N - 1}{2}.
\]

Depending on the sign of the dimerization \( \delta \) the edge mode is thus localized either at the right or the left end of the chain.

2.3. Open boundary conditions and \( N \) even

For an even number of lattice sites we expect two edge states for \( \delta > 0 \) and no edge states for \( \delta < 0 \). The eigenenergies \( \lambda_k^\pm \) can still be written as in equation (2.5), however, the doi:10.1088/1742-5468/2014/10/P10032 5
parameters $\theta_k$ are no longer known analytically and instead have to be determined by numerically solving the implicit equation [16]

$$
(1 - \delta)T(\theta_k, N/2) + (1 + \delta)T(\theta_k, N/2 - 1) = 0,
$$

with

$$
T(\theta_k, n) = \frac{\sin[(n + 1)\theta_k]}{\sin \theta_k}.
$$

The eigenvector corresponding to each of the $N$ solutions $\theta_k$ of equation (2.10) is then given by

$$
x_{2n-1}^k(\delta) = \frac{1 + \delta}{1 - \delta} T(\theta_k, n - 2) + T(\theta_k, n - 1)
$$

$$
x_{2n}^k(\delta) = \frac{\lambda_{k}^{\pm}}{1 - \delta} T(\theta_k, n - 1),
$$

where $n$ takes values from $1, 2, \ldots N/2$.

While for $\delta < 0$ all $N$ states are extended, localized edge states are possible for $\delta > 0$ corresponding to complex solutions of equation (2.10). More precisely, we find that the system has $N - 2$ real solutions and two complex solutions if $\delta > \delta_c$ where

$$
\delta_c = \frac{1}{1 + N},
$$

while all solutions are real if $\delta < \delta_c$. Physically, this can be understood as follows: The extended states in a finite system are protected against a small dimerization by the finite size gap $\Delta_E$ of order $1/N$. Only if the gap $\Delta_E \sim |\delta|$ induced by the dimerization overcomes the finite size gap can the spectrum change qualitatively. Alternatively, one can also think about this problem in terms of the localization length $\xi_{\text{loc}} \sim 1/\delta$ of the edge state, see

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equation (2.8), which has to become smaller than the system size in order to allow for localized states. In the thermodynamic limit, $N \to \infty$, we have $\delta_c \to 0$ so that the phase transition between the topological trivial and the SPT phase occurs, as expected, at $\delta = 0$. The eigenspectrum for a finite system as a function of dimerization shown in figure 1(b) makes it clear that there is always a small gap between the two edge modes which will only go to zero for all $\delta > 0$ in the thermodynamic limit.

3. Bulk and boundary fidelity susceptibility

At a quantum phase transition between different states of matter we expect the many-body wave function to change. A measure for this change is the fidelity $F(\delta, \epsilon) = |\langle \Psi(\delta) | \Psi(\delta + \epsilon) \rangle|$ where $\epsilon$ parameterizes the difference in dimerization between the two states with $F(\delta, 0) \equiv 1$. Similar to the Anderson orthogonality catastrophe [17] we expect the overlap between the two many-body wave functions to vanish exponentially with system size $N$ for $\epsilon \neq 0$. It is therefore appropriate to consider the fidelity density defined as

$$f(\delta, \epsilon) = -\frac{1}{N} \ln F(\delta, \epsilon).$$  (3.1)

Since $f(\delta, 0) \equiv 0$ is a minimum, the fidelity has the small $\epsilon$ expansion $f(\delta, \epsilon) = \chi(\delta) \epsilon^2 + \mathcal{O}(\epsilon^3)$ where

$$\chi(\delta) = \frac{1}{2} \frac{\partial^2 f}{\partial \epsilon^2} \bigg|_{\epsilon=0}$$  (3.2)

is the fidelity susceptibility. At a quantum phase transition, this quantity shows universal scaling behaviour [18–21] and can thus be used to characterize the transition.

Here we want to use the fidelity susceptibility to characterize the transition from the topologically trivial into the SPT phase in the SSH model (1.1). In an expansion in $1/N$ we can write $\chi = \chi_0 + \chi_B/N + \mathcal{O}(N^{-2})$. While the bulk contribution $\chi_0 = \lim_{N \to \infty} \chi$ will be the same in both phases, we expect that the boundary fidelity susceptibility $\chi_B$ is different.

For a system of non-interacting electrons, the many-body wave functions are simple Slater determinants of the single particle eigenstates. The fidelity $F(\delta, \epsilon)$ can thus be expressed as

$$F(\delta, \epsilon) = |\det A_{kl}(\delta, \epsilon)|,$$  (3.3)

with the $M \times M$ single particle overlap matrix

$$A_{kl}(\delta, \epsilon) = \langle \psi_k(\delta) | \psi_l(\delta + \epsilon) \rangle,$$  (3.4)

where $M$ is the number of particles in the ground state. The fidelity susceptibility can now be obtained as

$$\chi(\delta) = -\frac{1}{N} \lim_{\epsilon \to 0} \frac{\ln F(\delta, \epsilon)}{\epsilon^2}$$  (3.5)

and thus does not require taking numerical derivatives.

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3.1. Periodic boundary conditions

In this case there is no boundary so that $\chi_B = 0$. Furthermore, we expect $\chi(\delta) = \chi(-\delta)$ for $N$ even because changing the sign of $\delta$ is in this case equivalent to a simple relabelling of the lattice sites.

Using the results of section 2.1, the analytic calculation of the fidelity at half-filling is straightforward

$$|\langle \Psi(\delta) | \Psi(\delta + \epsilon) \rangle| = \prod_{k,k'} |\langle 0 | \alpha_k \tilde{\alpha}_{k'}^\dagger | 0 \rangle|$$

where $\tilde{\alpha}_k$ and $\tilde{A}$ are obtained by replacing $\delta \to \delta + \epsilon$. For the fidelity density this leads to

$$f = -\frac{1}{N} \sum_k \ln \frac{|\tilde{A} \tilde{A}^* + 1|}{2} \left( \frac{1}{\pi} \int_0^{\pi/2} \ln \frac{|\tilde{A} \tilde{A}^* + 1|}{2} \, dk \right).$$

The bulk fidelity susceptibility can now be calculated in closed form

$$\chi_0 = \frac{1}{32\pi} \int_0^{\pi/2} \frac{dk}{(\cos^2 k + \delta^2 \sin^2 k)^2} = \frac{1}{32|\delta|(1 + |\delta|)^2}.$$  

The finite size corrections in the gapped phase are exponentially small, $\chi(N) - \chi_0 \sim N \exp(-N/\xi)$ for $N \gg 1$, where $\xi$ is the correlation length, see equation (4.14). At the critical point $\delta = 0$ the fidelity susceptibility thus diverges as $\chi_0 \sim 1/|\delta|$. This is consistent with the general scaling theory at a critical point $\delta_c$ which predicts $\chi_0 \sim |\delta - \delta_c|^{d \nu - 2}$ where $d$ is the spatial dimension and $\nu$ the critical exponent related to the divergence of the correlation length at the critical point. In the case considered here we have $\delta_c = 0$, $d = 1$ and $\nu = 1$.

3.2. Open boundary conditions and $N$ odd

In the open chain case, we expect a $1/N$ boundary contribution $\chi_B$ (surface term) to the fidelity susceptibility. According to the bulk-boundary correspondence, a symmetry protected topological phase as indicated by a bulk invariant Zak-Berry phase is related to the presence of edge modes. We thus expect that $\chi_B$ is a measure which can distinguish between a topologically trivial and a non-trivial phase.

We start by considering the case of an odd number of sites $N$ where the single particle eigenstates are known exactly, see section 2.2. Note that in this case a single edge mode is present both for $\delta < 0$ and for $\delta > 0$. In order to obtain both the bulk and the boundary contribution, we use equations (3.3)–(3.5) with the exact single particle eigenstates given by equations (2.8) and (2.9). We are interested in the half-filled case, however, for $N$ odd we can only put either $(N - 1)/2$ or $(N + 1)/2$ particles into the system. This means that the zero energy edge mode is either empty or occupied. Because the Hamiltonian is particle-hole symmetric, the fidelity is, however, exactly the same in both cases.
Figure 2. Fidelity susceptibility for the SSH chain with OBC and an odd number of sites (symbols). The lines are linear fits for $1/N$ small. Note that the next-leading corrections become more important with decreasing $|\delta|$ with the expansion in $1/N$ breaking down at the critical point $\delta = 0$.

Figure 3. Symbols denote (a) the bulk susceptibility and (b) the boundary susceptibility for $N$ odd extracted from the scaling in figure 2. The data in (a) are compared with the analytical solution (lines), equation (3.8). In (b) the lines represent $\chi_B \approx 0.033 |\delta|^{-1.988}$ obtained by fitting the data for $|\delta| \leq 0.2$.

In figure 2 we show exemplarily the scaling of the fidelity susceptibility for different dimerizations, demonstrating that the leading correction to the bulk susceptibility is indeed of order $1/N$. The bulk and boundary susceptibilities extracted from the scaling are shown in figure 3. Note that both are symmetric in $\delta$ as they should be because $\delta \rightarrow -\delta$ is—up to a relabelling of the lattice sites—a symmetry of the Hamiltonian (1.1) if $N$ is odd. The bulk contribution $\chi_0$ is independent of the boundary conditions and agrees with the analytical solution (3.8) obtained using periodic boundary conditions. For the boundary contribution $\chi_B$ we numerically find a behaviour close to the critical point which is consistent with $\chi_B \sim 1/|\delta|^\eta$ with $\eta \approx 2$. Note, however, that we have two different
Figure 4. (a) \(\chi_B\) in the thermodynamic limit for an even number of sites (circles). Lines are a guide to the eye. (b) Fits of the data (circles) for (1) \(N\) even, \(\delta < 0\): \(|\chi_B^{(1)}| \approx 0.0177/|\delta|^{2.073}\), (2) \(N\) even, \(\delta > 0\): \(\chi_B^{(2)} \approx 0.0928/|\delta|^{1.979}\) and (3) \(N\) odd: data and function \(\chi_B^{(3)} = (\chi_B^{(1)} + \chi_B^{(2)})/2\), see equation (3.9). For the fits the data with \(|\delta| \leq 0.1\) have been used.

3.3. Open boundary conditions and \(N\) even

In the \(N\) even case we can again calculate the overlap matrix (3.4) from the single particle eigenstates, equation (2.12). However, this time the parameters \(\theta_k\) have to be determined by the implicit equation (2.10). Especially for the bound states where \(\theta_k\) becomes imaginary this requires a high accuracy making the calculations numerically challenging for large system sizes.

The boundary susceptibility obtained in this case is shown in figure 4. Note that \(\chi_B\) in the topological trivial phase (\(\delta < 0\)) is qualitatively different from \(\chi_B\) in the SPT phase (\(\delta > 0\)). In particular, the sign is different. The data in figure 4(b), furthermore, indicate that also the exponents of, what seems to be a power-law divergence at the critical point, are different by about 5%. The presence or absence of edge states is thus clearly visible in \(\chi_B\).

For large chain lengths \(N\) the edges should become independent so that \(\chi_B\) is simply the sum of the contributions from each of the two edges. In particular, this implies that

\[
\left[\chi_B^{N\ even\rightarrow\infty}(\delta) + \chi_B^{N\ even\rightarrow\infty}(-\delta)\right] / 2 = \chi_B^{N\ odd\rightarrow\infty}(\pm\delta).
\tag{3.9}
\]

This behaviour is confirmed by the fits shown in figure 4(b). The data for the \(N\) odd case are thus better fitted by the sum of two power laws with different exponents rather than by the single power law used in figure 3.
Finally, we can also study the finite size scaling of the fidelity susceptibility right at
the critical point, see figure 5. While both data sets for \( N \) even and \( N \) odd show a scaling
\( \chi \sim N \) consistent with the general scaling prediction \( \chi \sim N^{2/d_{\nu}-1} \) [20], the prefactors are
different.

To summarize, we have established that the boundary susceptibility \( \chi_{B} \) behaves
qualitatively different in the SPT (\( \delta > 0 \)) than in the topologically trivial phase (\( \delta < 0 \)).
In particular, \( \chi_{B}(\delta < 0) < 0 \) and \( \chi_{B}(\delta > 0) > 0 \).

4. Entanglement entropy

The entanglement entropy is the von-Neumann entropy of a reduced density matrix
\[ S_{A} = -\text{Tr}(\rho_{A} \ln \rho_{A}) \] (4.1)
with \( \rho_{A} = \text{Tr}_{B} \rho \) where \( \rho = |\Psi\rangle\langle\Psi| \) is the full density matrix with \( |\Psi\rangle \) being the ground
state of the many-body Hamiltonian. The system has been divided up into two blocks
\( A \) and \( B \). It is easy to prove that \( S_{A} = S_{B} \equiv S_{\text{ent}} \). The entanglement entropy is an
effective measure to characterize the ground states of many-body systems. A gain in
entanglement entropy can, furthermore, be a driving force for a Peierls transition [22]
leading to a dimerization of the chain as considered here. For one-dimensional critical
quantum systems it has been shown that \( S_{\text{ent}} \) shows a universal dependence on the length
\( \ell \) of the block \( A \). For a system of size \( N \) with PBC one finds
\[ S_{\text{ent}}^{\text{CFT}} = \frac{c}{3} \ln \left[ \frac{N}{\pi} \sin \frac{\pi \ell}{N} \right] + s_{1} \] (4.2)
where \( c \) is the central charge of the underlying conformal field theory (CFT) in the scaling
limit and \( s_{1} \) a non-universal constant [23]. In the thermodynamic limit \( N \to \infty \), the CFT
formula (4.2) reduces to
\[ S_{\text{ent}}^{\text{CFT}} = \frac{c}{3} \ln \ell + s_{1} . \] (4.3)

Figure 5. Finite size scaling of \( \chi \) at the critical point \( \delta = 0 \) for \( N \) even (circles) and \( N \) odd (squares) with open boundary conditions. The lines are fits with
\( \chi \approx 0.01791N \) (\( N \) even) and \( \chi \approx 0.03123N \approx N/32 \) (\( N \) odd).
By a conformal mapping one can show that a similar relation also holds for a system at small but finite temperatures [24]. For the undimerized chain of spinless fermions, equation (1.1) with $\delta = 0$, one finds $c = 1$ and $s_1 \approx 0.726$ [25].

These results are altered though if one changes the boundary conditions from periodic to open. In this case the entanglement entropy of a block which includes the end of the chain reads [23]

$$S^\text{CFT}_{\text{ent}} = \frac{c}{6} \ln \left[ \frac{2N \sin \frac{\pi \ell}{N}}{\pi} \right] + \ln g + s_1/2$$

(4.4)

where $\ln g$ is the boundary entropy related to the ground state degeneracy of the considered system [26]. For the critical undimerized chain we have $g = 1$. In numerical studies the scaling law for OBC, equation (4.4), is, however, often obscured by corrections coming from leading operators of the underlying CFT [27]. For critical systems described by Luttinger liquid theory one finds, for example, $S_{\text{ent}} \sim S^\text{CFT}_{\text{ent}} + \cos(2k_F \ell)\ell^{-K}$ (4.5)

where $k_F$ is the Fermi momentum and $K$ the Luttinger liquid parameter [28–32].

In a massive phase one expects, on the other hand, that the entanglement entropy saturates once the block size become larger than the correlation length $\xi$. If the system is in a massive phase but close to a critical point then also the leading corrections can be calculated and one finds for a block in an infinite chain

$$S_{\text{ent}} = \frac{c}{3} \ln(\xi_1/a) + U - \frac{1}{8} \sum_{\alpha=1} K_0(2\ell/\xi_\alpha)$$

(4.6)

where $U$ and $a$ are non-universal constants, $\xi_\alpha$ the correlation lengths (with $\xi_1$ being the largest) and $K_0$ the modified Bessel function [33]. This type of scaling behaviour has recently been confirmed numerically for certain spin models [34].

4.1. General setup

In the following, we want to study the entanglement entropy of the SSH model (1.1). We will consider two cases: First, a block in an infinite chain. Here we can simply use PBC which makes it possible to perform the thermodynamic limit exactly. This case will provide a numerical check of the formula (4.6). Second, we will consider the case of a block at the end of a semi-infinite chain. Here we can use either odd chain lengths where the eigenstates are known explicitly, or even chain lengths. The odd chain length has an edge state which is either filled or empty, which are equivalent by particle-hole symmetry. In contrast at half-filling a finite open system with an even number of sites in the SPT phase has two edge states, only one of which is occupied at half filling. However, the boundary states at the edges in the thermodynamic limit are a superposition of states localized at the left and the right edge. Thus we can also consider a semi-infinite chain with a partially occupied edge state. Since the correlation length $\xi \sim |\delta|^{-1}$ is finite for $\delta \neq 0$ it suffices to consider chain lengths $N \gg \xi$ in order to be effectively in the thermodynamic limit. We are particularly interested in the difference in entanglement entropies with and without a localized state being present at the boundary of the chain.

For a free fermion model there is a general setup to obtain the eigenvalues of the reduced density matrix $\rho_A$ [35,36]. The main observation is that $\rho_A$ can be represented as
the exponential of a free-fermion operator $\mathcal{H}_A$—the so-called entanglement Hamiltonian—with

$$
\rho_A = \frac{1}{Z} \exp(-\mathcal{H}_A) = \frac{1}{Z} \exp \left( -\sum_{k=1}^{\ell} \epsilon_k a_k^\dagger a_k \right)
$$

(4.7)

and $Z = \text{Tr} \exp(-\mathcal{H}_A)$. On the other hand, all properties of a free-fermion system can be obtained from the matrix $C$ of two-point correlation functions because all higher correlation functions can be expressed through the two-point functions by using Wick’s theorem. The matrix elements of $C$ for all two-point functions within the considered block $A$ are, in particular, determined by the reduced density matrix $\rho_A$, i.e. matrix elements are given by

$$
C_{ij} = \text{Tr}(\rho_A c_i^\dagger c_j).
$$

(4.8)

The eigenvalues $\zeta_k$ of the correlation matrix can then be related to the eigenvalues $\epsilon_k$ of the entanglement Hamiltonian in equation (4.7) and one finds

$$
\zeta_k = (e^{\epsilon_k} + 1)^{-1}.
$$

(4.9)

According to equation (4.7) the $2^\ell$-many eigenvalues $z_p$ of $\rho_A$ itself are now obtained by considering all possible fillings of the $\ell$-many levels $\epsilon_k$

$$
z_p = \frac{1}{Z} \prod_k \exp \left( -\epsilon_k n_k^{(p)} \right)
$$

(4.10)

where $n_k^{(p)} \in \{0, 1\}$ are fixed single-level occupation numbers, and $Z = \sum_p z_p$. The entanglement entropy is then given by

$$
S_{\text{ent}} = -\sum_p z_p \ln z_p.
$$

(4.11)

4.2. A block in an infinite chain

Using the results from section (2.1) for a chain with PBC at half-filling, the two-point correlation function can be easily calculated and the thermodynamic limit performed exactly. For even distances one finds $C_{ij} = \delta_{ij}/2$, i.e. only the onsite correlation function (occupation number) is nonzero. For odd distances the result is

$$
\langle c_{2n}^\dagger c_{2m+1} \rangle = \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} dk \frac{\cos k \cos k(2m + 1 - 2n) + \delta \sin k \sin k(2m + 1 - 2n)}{\sqrt{\cos^2 k + \delta^2 \sin^2 k}}
$$

(4.12)

and the correlation function $\langle c_{2n+1}^\dagger c_{2m} \rangle$ is obtained by replacing $\delta \to -\delta$. For the non-dimerized case, this reduces to the well-known result

$$
\langle c_n^\dagger c_m \rangle = \frac{1}{\pi} \sin \left( \frac{\pi}{2} (m - n) \right) \frac{1}{m - n}.
$$

(4.13)

By methods of steepest descent we can also obtain the asymptotic behaviour of the correlation function (4.12) at large distances. In particular, we find that the dominant correlation length is given by

$$
\xi_n^{-1} \equiv \xi_{\ell}^{-1} = \frac{1}{2} \left| \ln \frac{1 + \delta}{1 - \delta} \right|.
$$

(4.14)
There should now be three different regimes depending on the ratio of block size $\ell$ and largest correlation length $\xi \equiv \xi_1$: (1) For $\xi \gg \ell \gg 1$ the entanglement entropy will essentially follow the scaling law for a critical system, equation (4.2), as obtained by CFT. Exemplarily, we present in figure 6 results for $S_{\text{ent}}$ for small dimerizations and odd block lengths $\ell$. Indeed, we see that the smaller the dimerization is the longer equation (4.2) approximately holds as a function of block size. (2) For $\xi \ll \ell$, on the other hand, the entanglement entropy will settle to a constant value $S_{\text{ent}} = \frac{\xi}{3} \ln(\xi/a) + U$ where both constants $a$ and $U$ are non-universal. This behaviour is shown exemplarily in figure 7(a). In figure 7(b) we show, furthermore, that the saturation value depends on whether two weak bonds ($\ell$ even), a weak and a strong bond ($\ell$ odd), or two strong bonds ($\ell$ even) are cut. We have chosen the block for $\ell$ even in such a way that $\delta < 0$ corresponds to cutting two weak and $\delta > 0$ to cutting two strong bonds. For block sizes $\ell \gg \xi$ each non-trivial edge—caused by the cutting of a strong bond—gives an independent contribution $S_{\text{edge}}$ to the entanglement entropy. More precisely, we can define the edge contribution as

$$S_{\text{edge}} = \lim_{\ell \to \infty} |S_{\text{ent}}(\ell, \ell \text{ odd}) - S_{\text{ent}}(\ell + 1, \ell + 1 \text{ even})|,$$

which is shown as a function of dimerization in figure 8. In particular, in the limit $|\delta| \to 1$ the entanglement entropy will be dominated entirely by the edge contribution so that $S_{\text{ent}}^{\delta - 1}(\ell \text{ even}) = 2S_{\text{edge}}^{\delta - 1}$, $S_{\text{ent}}^{\delta - 1}(\ell \text{ odd}) = S_{\text{edge}}^{\delta - 1}$ and $S_{\text{ent}}^{\delta - 1}(\ell \text{ even}) \equiv 0$ with $S_{\text{edge}}^{\delta - 1} = \ln 2$. The insets of figure 8 are consistent with a power law behaviour of $S_{\text{edge}}$ for small $\delta$ and for $\delta \to 1$.

(3) Finally, there is also the regime $\xi \lesssim \ell$ where the formula (4.6) should hold which gives the leading correction to the constant value obtained in the limit $\xi \ll \ell$. In the case of the dimerized model considered here, the leading correlation length $\xi$ will show up twice: once with wave vector $k = \pi/2$ and once with wave vector $k = -\pi/2$ [37, 38]. Therefore, to leading order, we expect the entanglement entropy to scale as

$$S_{\text{ent}} = S_{\text{ent}}(\ell \to \infty) - \frac{1}{4} K_0(2\ell/\xi)$$

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Figure 7. (a) $S_{\text{ent}}$ for a block with an odd number of sites in an infinite chain and large dimerizations. (b) $S_{\text{ent}}$ for $\ell$ even and $\delta = -0.2$ (circles), $\ell$ odd (squares) and $\ell$ even and $\delta = +0.2$ (triangles). Each non-trivial edge gives a contribution $S_{\text{edge}}$ to $S_{\text{ent}}$. The dashed lines are a guide to the eye.

Figure 8. Edge contribution (4.15) to the entanglement entropy of a block in an infinite chain. The line marks the limiting value $S_{\text{edge}}^{\delta \to -1} = \ln 2$. The dashed line is a guide to the eye. Inset (a): fit for $|\delta| \ll 1$ with $S_{\text{edge}} \approx 1.339 |\delta|^{0.694}$. Inset (b): fit for $|\delta| \lesssim 1$ with $S_{\text{edge}} \approx \ln 2 - 0.273(1 - |\delta|)^{1.909}$.

with $\xi$ as given in equation (4.14). Fixing $S_{\text{ent}}(\ell \to \infty)$ by the numerical data for large block sizes, there is thus no free fitting parameter. The comparison in figure 9 with data for $|\delta| = 0.02$, in which case $\xi \approx 25$, confirms this scaling prediction. For large arguments, the Bessel function asymptotically scales as $\mathcal{K}_0(x) \sim \sqrt{\frac{2}{\pi x}} \exp(-x)$. The inset of figure 9 demonstrates that this is indeed the correct scaling of the entanglement entropy for large block sizes. The data for the three different cuts, in particular, collapse onto a single line after subtracting the constant part $S_{\text{ent}}(\ell \to \infty)$.

4.3. A block at the end of a semi-infinite chain

To calculate the entanglement entropy for a block which includes the end of a semi-infinite chain, we can use the analytic results for the single-particle eigenstates of a chain with OBC and $N$ odd given in section 2.2 and the numerical results for $N$ even from section 2.3.
In both cases, the matrix elements of the correlation matrix $C_{ij}$, see equation (4.8), can be expressed as

$$C_{ij} = \sum_{k \text{ occupied}} (\Psi^k_i)^* \Psi^k_j$$

(4.17)

with the sum running over all occupied single-particle states. Diagonalizing the correlation matrix then gives access to the single-particle eigenenergies $\epsilon_k$ of the entanglement Hamiltonian using the relation (4.9).

Results for small dimerizations are shown in figure 10. While the entanglement entropy for $\delta < 0$, where a strong bond terminates the semi-infinite chain, behaves qualitatively similar to the case of a block in an infinite chain (see figure 6) we find a much more complicated scaling for $\delta > 0$ and $N$ odd. In this case a localized boundary state is present leading to a competition between an increase of the boundary contribution to $S_{\text{ent}}$ with increasing $\delta$ and a decrease of the bulk contribution due to the decreasing correlation length $\xi \sim 1/\delta$. As a result, the curves for different dimerizations cross, see figure 10(b).

The final possibility is to consider the semi-infinite chain with a localized edge state which is not fully occupied, as realized in a chain $N$ even at half-filling, see figure 10(c). As for the fully occupied edge state there is a competition between the increasing boundary entropy and decreasing bulk entropy with $\delta$. However, due to the higher degeneracy associated with the partially occupied edge state, see also the entanglement spectra in the following section, the curves for the same dimerizations will cross at a much larger sub-block size, than for a fully occupied edge state. Therefore we show in figure 10(c) data for dimerizations which are an order of magnitude larger than in the other two cases shown in figures 10(a) and (b).

For large block size $\ell$ and finite dimerization we again expect that $S_{\text{ent}}$ saturates. Let us first concentrate on the case $\delta < 0$ shown in figure 11. In this case $S_{\text{ent}}$ is monotonically
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Figure 10. $S_{\text{ent}}$ for a block at the end of a semi-infinite chain at small dimerizations with $\ell$ even for (a) $\delta < 0$ where the boundary is trivial, (b) $\delta > 0$ where a localized boundary state is present and filled and (c) $\delta > 0$ for $N$ even where a localized boundary state is present but only half-filled. In all cases the CFT result (4.4) in the non-dimerized case with $s_1 = 0.726$ has been subtracted. The dashed lines are a guide to the eye.

Figure 11. $S_{\text{ent}}$ for a block at the end of a semi-infinite chain with $\ell$ even, fitted by equation (4.18) with the fitting parameter $\tilde{\xi}$ given in table 1. The inset shows that the scaling is still roughly consistent with the Bessel function asymptotics.

increasing. We can thus try to fit the data for large block sizes by

$$S_{\text{ent}} = S_{\text{ent}}(\ell \to \infty) - \frac{1}{8} K_0(2\ell / \tilde{\xi})$$

(4.18)

similar to the quantum field theory result (4.6) but with $\tilde{\xi}$ as a free parameter. Doing so we obtain very good fits with parameters as given in table 1. The correlation length $\tilde{\xi}$ obtained from the fits seems to be about a factor $\sqrt{2}$ smaller than the bulk correlation length $\xi$ given in equation (4.14). Note, however, that the heuristic fitting formula (4.18) is

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Table 1. Parameters in equation (4.18) used to fit the data for large block sizes shown in figure 11.

| $\delta$ | $S_{\text{ent}}(\ell \to \infty)$ | $\tilde{\xi}$ | $\xi$ | $\xi/\tilde{\xi}$ |
|----------|-----------------------------------|--------------|------|------------------|
| -0.02    | 0.838                             | 34.80        | 49.99| 1.44             |
| -0.04    | 0.696                             | 17.59        | 24.99| 1.42             |
| -0.06    | 0.605                             | 11.89        | 16.65| 1.40             |

Figure 12. $S_{\text{ent}}$ for a block at the end of a semi-infinite chain with $\delta > 0$ and a fully occupied boundary state. Shown are data for even (circles) and odd block sizes (squares).

too naive to be able to fully capture the behaviour of $S_{\text{ent}}$. A two-point correlation function near a boundary does not only depend on the distance between the two operators but also on the distance of the operators from the boundary so that a third length scale has to appear.

Let us now return to the case $\delta > 0$ with the fully occupied boundary state where figure 10(b) already indicates that the scaling behaviour of the entanglement entropy with block size is completely changed. Figure 12 shows that the competition between boundary and bulk contributions leads to a maximum in $S_{\text{ent}}$ which becomes sharper and whose position shifts to smaller block sizes with increasing dimerization. Consequently, the constant value $S_{\text{ent}}(\ell \to \infty)$ is now approached from above. Clearly a scaling as in (4.18) is no longer valid.

To verify that the additional entanglement entropy is indeed caused by the boundary state we can define

$$S_{\text{bound}}(\ell) = S_{\text{ent}}^{\delta > 0}(\ell, \ell \text{ odd}) - S_{\text{ent}}^{\delta < 0}(\ell + 1, \ell + 1 \text{ even}).$$

(4.19)

For both entropies in equation (4.19) a weak bond is cut so that for large block sizes $\ell$ any remaining difference is directly related to the localized boundary state present for $\delta > 0$. Figure 13 shows that $S_{\text{bound}}(\ell)$ is exponentially decaying with block size. According to equation (2.8) a non-trivial boundary leads to an exponentially localized zero energy state with a localization length

$$\xi_{\text{loc}}^{-1} = \ln \left( \frac{1 + \delta}{1 - \delta} \right).$$

(4.20)
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Figure 13. $S_{\text{bound}}$ as defined in equation (4.19) for different $\delta > 0$ where the boundary state is fully occupied. The lines display $S_{\text{bound}} = a \exp(-\ell/\xi_{\text{loc}})$ with the localization length (4.20) and $a$ used as the only fitting parameter.

Figure 14. $S_{\text{ent}}$ for $\delta > 0$ and a partially filled boundary state. Shown are data for even block sizes (circles). The lines are exponential fits, see equation (4.21).

The exponential fits in figure 13 using this correlation length are indeed in excellent agreement with the data for $S_{\text{bound}}(\ell)$ confirming that the boundary state leads to additional entanglement which is exponentially localized at the boundary.

For $\delta > 0$, $N$ even and half-filling the boundary state is only half-filled. As shown in figure 14 this qualitatively changes the behaviour of $S_{\text{ent}}$ as compared to the case where the edge state is completely filled. In particular, there is no longer a maximum yet the scaling with block size is also not described by a modified Bessel function as was the case for $\delta < 0$. Instead, the scaling seems purely exponential

$$S_{\text{ent}}(\ell) = S_{\text{ent}}(\ell \to \infty) - a \exp(-2\ell/\xi) \quad (4.21)$$

with $\xi$ being the leading correlation length, see equation (4.14) and $a$ a fitting parameter. The boundary contribution of the partially filled edge state can again be calculated from equation (4.19) and is exponentially decaying with block size similar to the case of the

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Figure 15. $S_{\text{bound}}$ as defined in equation (4.19) for $\delta > 0$ with a partially filled boundary state. The lines display $S_{\text{bound}} = a \exp(-\ell/\xi_{\text{loc}})$ with the localization length (4.20) and $a$ used as the only fitting parameter.

completely filled edge state, see figure 15. To summarize, we have shown that the presence of localized boundary states in a massive phase completely changes the scaling of $S_{\text{ent}}(\ell)$ with block size $\ell$ for a block at the end of a semi-infinite chain. The boundary state leads, in particular, to additional entanglement which is exponentially localized. Further insight into the different entanglement properties of a block with or without a localized boundary state can be gained by directly investigating the entanglement spectrum.

5. Entanglement spectra

Instead of just considering the entanglement entropy, which is a map from the $2^\ell$ dimensional space of eigenvalues of $\rho_A$ into the real numbers, it is often instructive to consider the spectrum of $\rho_A$—the so-called entanglement spectrum—directly.

5.1. A block in an infinite chain

As for the entanglement entropy we can use the analytical result for the elements of the correlation matrix in the thermodynamic limit to determine the spectrum of the reduced density matrix. In figure 16 the logarithm of the eigenvalues $z_p$ of the reduced density matrix, see equation (4.10), for the three different cuts possible are shown. The pictograms in the figure show whether the block size is even or odd (but not the actual block size!) and if strong (double lines) or weak (single dashed lines) bonds are cut. While the structure is complicated for finite block sizes $\ell$, the distribution of eigenvalues becomes very simple in the limit $\ell \to \infty$. In this case, the single particle energies $\epsilon_k$ of the entanglement Hamiltonian (4.7) become equally spaced and the level spacing $\epsilon$ can be obtained analytically using corner transfer methods [24,39]. One finds

$$\epsilon = \pi I(x')/I(x) \quad \text{with} \quad x = (1 - \delta)/(1 + \delta),$$

(5.1)
Figure 16. Entanglement spectrum for a block in an infinite chain at $|\delta| = 0.1$ with (a) odd block size, (b) even block size cutting two weak bonds and (c) even block size cutting two strong bonds. The black stars are data for $\ell = 19$ ($\ell = 20$), the red crosses for $\ell = 69$ ($\ell = 70$). The dashed lines are the single particle levels in the thermodynamic limit, the numbers in brackets give the degeneracy $d_k$ of each level.

$x' = \sqrt{1 - x^2}$ and $I(x)$ being the elliptic integral of the first kind. This is the correct level spacing for odd block size as well as for even block size if two weak bonds are cut. Cutting two strong bonds, on the other hand, leads to a level spacing $2\epsilon$, see figure 16.

The eigenvalues $z_p$ of the reduced density matrix in the thermodynamic limit can then be obtained by filling up the single particle levels. The dominant eigenvalue of $\rho_A$ is obtained by filling up the ‘Fermi sea’ of negative eigenvalues $\epsilon_k$. In the case shown in figure 16(b)—where the block size is even and two weak bonds are cut—this leads to a unique dominant eigenvalue. In the case where either one (figure 16(a)) or two (figure 16(c)) strong bonds are cut the lowest eigenvalue is, however, degenerate. This can be understood as follows: Cutting a strong bond leads to an edge spin. For the case $\ell$ odd where one strong bond is cut this leads to an eigenenergy $\epsilon_{(\ell+1)/2} \equiv 0$. This level can now either be empty or filled leading to a two-fold degeneracy of the leading eigenvalue. For the case $\ell$ even where two strong bonds are cut, eigenvalues $\epsilon_{\ell/2} = -\epsilon_{\ell/2+1}$ appear which approach zero in the thermodynamic limit. Consequently, the dominant eigenvalue of $\rho_A$ becomes four-fold degenerate. Thus the low-energy entanglement spectrum allows to directly identify the number of ‘edge states’ caused by cutting a strong bond.

Equation (5.1) only gives the level spacing. In order to obtain the allowed values for the eigenvalues $z_p$ of $\rho_A$ one has to use, in addition, the normalization condition

$$1 = \text{Tr}\rho_A = \sum_p z_p = \sum_{k=0}^{\infty} d_k e^{-\epsilon_0 - k\epsilon} \Rightarrow \epsilon_0 = \ln \left( \sum_{k=0}^{\infty} d_k e^{-k\epsilon} \right).$$ (5.2)
Figure 17. Entanglement spectrum for a block at the end of a semi-infinite chain at $\delta = -0.1$ with (a) even block size and (b) odd block size. The black stars are data for $\ell = 19$ ($\ell = 20$), the red crosses for $\ell = 69$ ($\ell = 70$). The dashed lines are the single particle levels in the thermodynamic limit, the numbers in brackets give the degeneracy of each level.

Here $d_k$ is the number of degenerate eigenvalues $\{z_p\}$ for which $z_p = \exp(-\epsilon_0 - k\epsilon)$ with $k$ fixed. The levels $\epsilon_0 + k\epsilon$ or $\epsilon_0 + 2k\epsilon$, respectively, with $k = 0, 1, 2, 3, \ldots$ are shown as dashed lines in figure 16.

5.2. A block at the end of a semi-infinite chain

While the case of a block in an infinite chain is well understood, the interesting case of the entanglement spectrum for a block at the end of a dimerized semi-infinite chain with or without a localized boundary state has not been considered so far. We have already shown that a localized boundary state causes additional entanglement which is also localized at the boundary, see figure 13. Here we want to further investigate this case by directly looking at the entanglement spectrum.

For $N$ odd, we can distinguish four cases now: $\delta < 0$ (topological trivial case) or $\delta > 0$ (SPT case) with $\ell$ either even or odd. In addition, we have to consider the two cases $\ell$ even or odd with $N$ even and $\delta > 0$, where the edge state is only partially filled, separately. We start with the topological trivial case $\delta < 0$. Data for even and odd block sizes with $\delta = -0.1$ are shown in figure 17. For even block sizes, see figure 17(a), the leading eigenvalue is unique and the separation of the single-particle levels is given by equation (5.1) as in the case of an even block in an infinite chain where two weak bonds are cut, see figure 16(b). However, the degeneracy structure of the higher levels is different which explains the differences in the entanglement entropy discussed in the previous subsection. For the case of an odd block size, shown in figure 17(b), the degeneracy structure of the spectrum is the same as for a block of odd length in an infinite chain, see...
Figure 18. Entanglement spectrum for a block at the end of a semi-infinite chain at $\delta = 0.1$ with a fully occupied boundary state for (a) odd block size and (b) even block size. The black stars are data for $\ell = 19$ ($\ell = 20$), the red crosses for $\ell = 69$ ($\ell = 70$). The dashed lines are the single particle levels in the limit $\ell \to \infty$, the numbers in brackets give the degeneracy of each level.

figure 16(a), however, the level spacing in the semi-infinite chain is $2\epsilon$ instead of $\epsilon$ for the infinite chain. Note that the finite size corrections for a block at the end of a semi-infinite chain in the topological trivial case are of similar magnitude as for the infinite chain, i.e. for the lowest single-particle levels the data for the smaller block sizes $\ell = 19, 20$ and the larger ones, $\ell = 69, 70$, hardly deviate from each other.

This is completely different in the SPT phase—the case $\delta = 0.1$ with $N$ odd is shown as example in figure 18—where finite size corrections are much larger. In the limit $\ell \to \infty$, on the other hand, both the level spacing and the degeneracies agree between the cases $\delta < 0$, $\ell$ even (figure 17(a)) and $\delta > 0$, $\ell$ odd (figure 18(a)) as well as $\delta < 0$, $\ell$ odd (figure 17(b)) and $\delta > 0$, $\ell$ even (figure 18(b)). This means that the localized boundary state present for $\delta > 0$ does not play any role in the limit $\ell \to \infty$ and that the spectra in the trivial and the SPT phase become identical in this limit.

The dramatic change in the entanglement spectra for small block sizes if a localized state is present—which leads to the non-monotonic behaviour of the entanglement entropy shown in figure 12—can be understood as follows: The non-trivial edge leads to an exponentially localized zero energy state, equation (2.8), with a localization length as given in equation (4.20).

For the case $\delta = 0.1$ considered here the localization length is $\xi_{\text{loc}} \approx 1/2\delta = 5$ lattice sites. The low-energy part of the entanglement spectrum will thus become similar to the one without the localized state if $\ell \gg \xi_{\text{loc}}$ while it will be substantially modified for $\ell \lesssim \xi_{\text{loc}}$. The modification of the entanglement spectrum and the entanglement entropy is thus an effect of finite block size which is directly tied to the appearance of localized states in the SPT phase.
The final possibility is to consider the case $N$ even, $\delta > 0$ where the boundary state is only partially filled, see figure 19. In this case the degeneracy of the levels is doubled compared to the case with a fully occupied boundary state, shown in figure 18. Furthermore, corrections to the $\ell \to \infty$ limit for finite blocks are smaller, explaining the different behaviour seen in the entanglement entropy.

To summarize, we have shown that the presence of a localized boundary state significantly alters the entanglement spectra for small block sizes. In the limit $\ell \to \infty$, on the other hand, a free fermion spectrum with an equidistant level spacing is recovered. While creating virtual edges by considering a block in an infinite chain gives the same degeneracy of the lowest level than a physical edge for a corresponding block at the end of a semi-infinite chain, the degeneracies of higher levels as well as the level spacing are, in general, different. This explains the different scaling properties of $S_{\text{ent}}(\ell)$ for a block at the end as compared to a block in the middle.

6. The SSH model with nearest-neighbour repulsion

Finally, we will investigate the effects of interactions by adding a nearest-neighbour repulsion term, see the Hamiltonian in equation (1.1). It has been shown that topological phases of interacting one-dimensional quantum systems can be classified by their entanglement properties [11–13]. Interaction effects in one-dimensional dimerized fermionic systems with SPT phases have already been studied in [40]. However, in this work a spinful dimerized Hubbard model was considered where for $\delta \to 1$ (SPT phase),
even in the limit of infinite onsite Hubbard repulsion, one can still remove an electron from
the edge site without any energy cost. Thus the cases $\delta < 0$ and $\delta > 0$ remain topologically
distinct in the presence of a Hubbard interaction. For the spinless model with nearest-neighbour repulsion considered here, the situation is different. For $U \rightarrow \infty$ the system
will be forced into a charge-density-wave (CDW) state with every second site occupied so
that, even for $\delta \rightarrow 1$, the edges are no longer decoupled from the rest of the chain. We
therefore expect a phase transition in the model (1.1) as a function of interaction $U$ where
the fidelity and the entanglement measures will change. We focus first on open chains with
an even number of sites and use exact diagonalization and Arnoldi algorithms to calculate
the ground state properties for system sizes up to $N = 24$. In order to firmly establish the
change of the entanglement properties at the phase transition we, furthermore, present
light cone renormalization group (LCRG) [41] results for infinite chains.

6.1. Fidelity susceptibility
In figure 20 we show the fidelity susceptibility at different interaction strengths $U$ for
$\delta = 0.5$ (topological phase for $U = 0$) and $\delta = -0.5$ (trivial phase for $U = 0$). For
$U = 0.5$ and $U = 2.5$ the fidelity susceptibility behaves qualitatively similar to the non-interacting case with the bulk susceptibility $\chi_0$ being reduced with increasing interaction
strength. Furthermore, we still find $\chi_B(\delta < 0) < 0$ and $\chi_B(\delta > 0) > 0$ with $\chi_B$ given
by the slope of the curves in figure 20 for $1/N$ small. This is an indication that the two
cases remain topologically distinct even for intermediate interaction strengths. For $U = 5$,
however, a drastic change is observed. In this case $\chi_B$ is negative both for $\delta < 0$ and
for $\delta > 0$. Apparently the boundaries now behave qualitatively similar suggesting that
a phase transition has occurred and edge states no longer exist. We will provide further
evidence that this is indeed the case in the following. $\chi_B$ can thus be used as a measure
to distinguish between phases with and without edge states also in interacting systems.

Figure 20. Fidelity susceptibility for the interacting SSH chain (1.1) with an
even number of sites where (a) $\delta = 0.5$ and (b) $\delta = -0.5$.
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Figure 21. Entanglement spectrum for a block centered at the middle of a chain with length \( N = 20 \) at \( |\delta| = 0.5 \) with (a) odd block size \( \ell = 5 \), (b) even block \( \ell = 4 \) size cutting two weak bonds and (c) cutting two strong bonds. The blue circles are data for \( U = 0 \), the black stars for \( U = 0.5 \), the green pluses for \( U = 2 \) and the red crosses for \( U = 10 \). The numbers in parenthesis give the degeneracy of the levels for the non-interacting system in the limit \( \ell \to \infty \).

6.2. Entanglement spectra

We now turn to the entanglement spectra in the interacting case. We concentrate on large dimerizations (as an example, data for \( |\delta| = 0.5 \) are shown throughout this section) where the correlation length is small so that effects caused by the finite chain length can be neglected for the low-energy part of the spectrum. As in the non-interacting case, we start by choosing a block from the middle of the chain, cutting (a) a weak and a strong bond, (b) two weak bonds and (c) two strong bonds, see figure 21. For weak and intermediate interaction strengths, \( U = 0.5 \) and \( U = 2 \) respectively, the degeneracy of the lowest level is not altered while for \( U = 10 \) a twofold degeneracy starts to emerge in all three cases. This can be understood as follows: For \( U/t \to \infty \) the ground state of the chain will become a superposition of the two degenerate product states, \( |\Psi\rangle = (|1010\cdots10\rangle + |0101\cdots01\rangle)/\sqrt{2} \), i.e. the system is driven into a symmetrized CDW state (‘cat state’). The reduced density matrix for any cut has then two eigenvalues \( 1/2 \) while all other eigenvalues are zero. The corrections for non-zero \( t/U \ll 1 \) can be calculated perturbatively similar to the case of the XXZ chain considered in [24,42]. The entanglement spectrum will then become equidistant again—though not all levels are necessarily occupied—with degeneracies which depend on the way the block is chosen and which are different from the non-interacting case. We thus expect an evolution with increasing \( U \) from an equidistant spectrum at \( U = 0 \) through some intermediate regime into a different equidistant spectrum at \( U/t \gg 1 \). Such an evolution is indeed observed, see in particular figure 21(b), where already at \( U = 10 \) the spectrum becomes again almost equidistant.

Next we plot the entanglement spectrum for a block at the end of a chain, a measure which is sensitive to the presence of localized edge states. First, we consider the evolution...
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Figure 22. Entanglement spectrum for a block at the end of a chain of length $N = 20$ at $\delta = -0.5$ with (a) even block size $\ell = 4$ and (b) odd block size $\ell = 5$. The blue circles are data for $U = 0$, the black stars for $U = 0.5$, the green pluses for $U = 2$ and the red crosses for $U = 10$. The numbers in parenthesis give the degeneracy of the $U = 0$ spectra.

of the spectrum in what is the topological trivial phase for $U = 0$, see figure 22, cutting (a) a weak bond and (b) a strong bond. Again we find that the degeneracy of the lowest level is stable up to intermediate interactions, $U = 2$, while a new level structure with a twofold degenerate ground state emerges in both cases for $U = 10$.

For a block at the end of a chain in the SPT phase, shown in figure 23, the picture is qualitatively similar. The boundary susceptibility and entanglement spectra for $\delta < 0$ and $\delta > 0$ thus remain distinct from each other even if nearest-neighbour interactions of intermediate strength are added. In particular, we still find numerically a twofold (fourfold) degeneracy of the lowest level for a block with $\ell$ odd ($\ell$ even) at the end of a chain in the SPT phase, see figure 23. For $U = 0$ this is directly related to an edge state which is shared between the two boundaries and which is thus, for an infinite separation of the boundaries, only partially filled.

6.3. LCRG results for infinite chains

The LCRG algorithm is a variant of the density-matrix renormalization group [41, 43]. Originally proposed to study the real time evolution after a quantum quench, it is also possible to consider an imaginary time evolution starting from an initial product state. In this case the initial state is projected onto the ground state of the Hamiltonian used in the time evolution and ground state properties of infinite chains can be studied. Here we will use this algorithm to investigate the entanglement spectrum and entropy of an essentially infinite block within the infinite chain as a function of dimerization $\delta$ and interaction $U$. We choose our block in such a way that two strong bonds are cut so that the largest eigenvalue of the reduced density matrix for $U = 0$ will be fourfold degenerate. In figure 21 we have
seen that this fourfold degeneracy changes into a twofold degeneracy at large interaction strengths. In order to find the point where this change occurs, we order the eigenvalues of the reduced density matrix by magnitude and plot LCRG results for $3z_1 - 2z_2 - z_3 - z_4$ in figure 24(a). This quantity is zero as long as the largest eigenvalue is fourfold degenerate while it should become non-zero in the CDW phase. Indeed, a very sharp transition is observed numerically with $U_c \approx 4$ at $\delta = 0.1$ and $U_c \approx 8$ for $\delta \rightarrow 1$. Since the symmetries which protect the SPT phase are not violated by the interaction, the excitation gap should close at the phase transition. To confirm a closing of the energy gap at the transition, we show the numerically calculated entanglement entropy as a function of $U$ for various dimerizations $\delta$ in figure 24(b). The entanglement entropy evolves in all cases shown from $S_{\text{ent}} \approx 2 \ln 2$ at $U = 0$ to $S_{\text{ent}} = \ln 2$ for $U \rightarrow \infty$. At $U$ values consistent with those where we find an abrupt change of the degeneracy of the largest eigenvalue, see figure 24(a), the entanglement entropy has a sharp maximum. Here a comment about the numerical calculations is in order: We time evolve the initial product state up to imaginary times $\tau = 50$. For all $U$ values apart from the small region where $S_{\text{ent}}$ is peaked the projection

Figure 23. Same as figure 22 but for $\delta = 0.5$ with (a) $\ell = 5$ and (b) $\ell = 4$.

Figure 24. (a) Degeneracy of the lowest level, measured by $3z_1 - 2z_2 - z_3 - z_4$ and (b) entanglement entropy $S_{\text{ent}}$ of the reduced density matrix for an effectively infinite block in an infinite chain obtained by LCRG.
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converges and the values shown in figure 24(b) are the finite fully converged entropies of the gapped ground states. At the phase transition, however, we find $S_{\text{ent}} \sim \ln \tau$ consistent with a diverging entanglement entropy for $\tau \to \infty$ as expected for a gapless state. In this case the projection is not fully converged and the values for $S_{\text{ent}}$ shown are simply the values obtained at our maximal simulation time $\tau = 50$.

7. Summary and conclusions

A system in a symmetry protected topological (SPT) phase is an insulator with short-range entanglement. The scaling of the bulk entanglement entropy with block size for a block in an infinite chain as well as the bulk fidelity are therefore not any different from those of a topologically trivial insulator. SPT phases, however, have localized edge states so that the entanglement properties for a block at the end of a chain with SPT order as well as the boundary fidelity susceptibility are expected to deviate from those in a topological trivial phase.

To investigate these boundary contributions we have considered a well-known example: a chain of non-interacting spinless fermions with a dimerized hopping in which an SPT phase is realized for $\delta > 0$ while the phase for $\delta < 0$ is topologically trivial. We have confirmed that the bulk fidelity only depends on the absolute value of the dimerization $\delta$, i.e. it cannot be used to distinguish between the SPT and the trivial phase. For the boundary contribution $\chi_B$, on the other hand, we have found that $\chi_B(\delta < 0) < 0$ while $\chi_B(\delta > 0) > 0$. Furthermore, the divergence of $\chi_B$ at the critical point $\delta = 0$ seems to follow a power law with exponents which are different in the two phases.

For a block in an infinite chain we have tested a prediction from massive field theory [33] for the scaling of the entanglement entropy with block size $\ell$ for the case $\ell \lesssim \xi$ where $\xi$ is the correlation length. Apart from a recent numerical study of spin models [34] this is the second independent numerical confirmation of this formula for a different class of gapped models. Again, SPT and trivial phase show exactly the same properties. This is different if a block at the end of a semi-infinite chain is considered instead. In this case we have shown that the scaling with block size in the trivial phase is still apparently of the same functional form as for a block in an infinite chain while the scaling is drastically altered in the SPT phase. If the boundary state is completely filled we find, in particular, a maximum in $S_{\text{ent}}(\ell)$ at a finite block size $\ell$, i.e. the saturation value $S_{\text{ent}}(\ell \to \infty)$ is now approached from above. We have explained this maximum as a direct consequence of additional entanglement caused by the boundary state which is exponentially localized on the scale of the localization length of this state. In the entanglement spectrum this qualitatively different behaviour in the SPT phase is reflected by a rather smooth spectrum for $\ell \lesssim \xi$ while only for $\ell \gg \xi$ the equidistant spectrum, obtained by corner transfer methods for a large block in an infinite system, is recovered. In the latter limit the spectra in the SPT and in the trivial phase for a block at the end of a semi-infinite chain thus become identical again.

Finally, we have used exact diagonalization and Arnoldi algorithms to investigate in how far the distinct boundary fidelity and entanglement properties in the SPT phase survive if interactions are included. To this end, we have considered the dimerized chain with a nearest-neighbour repulsion, which, in the limit $U/t \to \infty$, will drive the system into...
a charge-density-wave state. Our results show that both the different sign of the boundary susceptibility in the SPT as compared to the trivial phase as well as the exponentially localized additional entanglement for a block at the end of a chain in an SPT phase are stable features up to the phase transition into the topological trivial CDW phase. Using a density-matrix renormalization group algorithm for infinite chains we have, furthermore, shown that the phase transition can be located precisely by finding the point where the degeneracy of the largest eigenvalue of the reduced density matrix changes.

For the future it would be of interest to develop a massive field theory approach to explain the scaling of the entanglement entropy found in this work for a block at the end of a semi-infinite chain both in topologically trivial as well as in SPT phases.

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