Detection of topological phases by quasilocal operators

Wing Chi Yu,[1] P. D. Sacramento,[2,3,*] Yan Chao Li,[4,3] Dimitris G. Angelakis,[1,5] and Hai-Qing Lin[3]

[1]*Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, Singapore 117543*

[2]*CeFEMA, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais, 1049-001 Lisboa, Portugal*

[3]*Beijing Computational Science Research Center, Beijing 100193, China*

[4]*College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 100049, China*

[5]*School of Electrical and Computer Engineering, Technical University of Crete, Chania, Crete, 73100 Greece*

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It was proposed recently by some of the authors that the quantum phase transition of a topological insulator like the Su-Schrieffer-Heeger (SSH) model may be detected by the eigenvalues and eigenvectors of the reduced density matrix. Here we further extend the scheme of identifying the order parameters by considering the SSH model with the addition of triplet superconductivity. This model has a rich phase diagram due to the competition of the SSH "order" and the Kitaev "order," which requires the introduction of four order parameters to describe the various topological phases. We show how these order parameters can be expressed simply as averages of projection operators on the ground state at certain points deep in each phase and how one can simply obtain the phase boundaries. A scaling analysis in the vicinity of the transition lines is consistent with the quantum Ising universality class.

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I. INTRODUCTION

In condensed-matter physics, the order parameter plays an important role in the study of phase transitions. It characterizes the order of a phase and helps to detect the critical point. People usually rely on physical intuition or resort to methods such as group theory and the renormalization group analysis to identify the order parameters of a many-body system. However, those methods require prior knowledge of the symmetries of the Hamiltonian and do not always apply, especially for systems exhibiting topological phase transitions. A general and systematic scheme to derive the order parameters without the aid of such empirical knowledge will thus be highly constructive to the field.

Recently, a proposal based on using the dominant eigenstates of the reduced density matrix of a many-body system was established by some of the authors [1,2]. Unlike the other schemes proposed [3–5], the approach is nonvariational. Our scheme has also been extended to the detection of the topological phase of topological insulators [6,7] such as the Su-Schrieffer-Heeger (SSH) model [8] and, equivalently, the Schockley model [9].

In our original proposal, one has to first determine the minimum size of the reduced density matrix that captures the extended correlations in the system by calculating the mutual information. Then the dominant states (with relatively larger eigenvalues) of the reduced density matrix are used to construct the order parameter. For example, in the Mott insulator phase of the fermion Hubbard model, the single-site reduced density matrix has the largest eigenvalues for the local state spin up and spin down. One can then define the order operator as a linear combination of the projectors of these two states, which turns out to be the Pauli matrix in the z direction, as expected [2]. However, in some cases such as the topological phase of the SSH model, several eigenstates of the reduced density matrix with comparable weights contribute and lead to an undetermined combination in the order parameter [6].

In this work, we introduce a fundamental extension of our previous proposal [6] to overcome the above-mentioned issue by considering the projector of a subset of the system's ground state. The order parameter is then defined as the expectation value of this projector in the original representation. We apply the method to the SSH model with the addition of triplet pairings between the fermionic states. The phase diagram of the model consists of a trivial phase, two topological phases of the Kitaev type, and one topological phase of the SSH type. The four order parameters that describe the various phases of the model are obtained. In comparison to the previously adopted methods of calculating topological invariants or the entanglement spectrum [10] to characterize a topological phase, the order parameters obtained here provide additional physical insight into the phases in real space. Unlike the topological invariants, our approach does not require the analysis of the symmetry of the underlying lattice and order structure. We also identify the phase transition points from the crossing of the derived order parameters. The approach thus provides an alternative way to obtain information on the topological transitions.

This paper is organized as follows. In Sec. II we recap our original scheme of deriving the order parameter and introduce the fundamental extension of the method. We then apply the method to obtain the order operators in the SSH model with triplet pairing in Sec. III and calculate the order parameters (ground-state average of the order operators) in Sec. IV. We also study the universality class of the model from finite-size

*pdss@cefema.tecnico.ulisboa.pt

scaling analysis of the derived order parameters in Sec. V. In Sec. VI, we mention that the application of the method to the Kitaev model leads to a quasilocal operator that may be identified with the local Hamiltonian. It is shown for both the Kitaev model and the SSH-Kitaev model that the local Hamiltonian may also be used to detect the topological transitions. Finally, a conclusion is given in Sec. VII.

II. THE METHOD

The first step in our original proposal [1] to derive the order parameter is to determine the minimum size of the block (or subsystem) for which the mutual information does not vanish at a long distance. The mutual information is defined as

$$S(i,j) = S(\rho_i) + S(\rho_j) - S(\rho_{i\cup j}), \tag{1}$$

where $S(\rho_i) = -\mathrm{tr}(\rho_i \ln \rho_i)$ is the von Neumann entropy of block i. The reduced density matrix ρ_i is obtained by tracing out all other degrees of freedom except those of block i, i.e., $\rho_i = \mathrm{tr}|\Psi_0\rangle\langle\Psi_0|$, where $|\Psi_0\rangle$ is the ground state of the system. If and only if the mutual information is nonvanishing at a long distance does a long-range order (or quasi-long-range order) exist in the system [11,12].

The next step is to calculate the eigenvalues and eigenstates of the reduced density matrix of the desired block size. The order operator is then defined as the linear combination of the dominant eigenstates [1], i.e.,

$$\hat{O}_i = \sum_{\mu\leqslant\xi} w_\mu a_{i\mu}^\dagger a_{i\mu}, \tag{2}$$

where $a_{i\mu}^\dagger$ ($a_{i\mu}$) is the creation (annihilation) operator of state μ at site i and ξ is the rank of ρ_i. It can be proved that for any $\mu > \xi$, the operator $a_{i\mu}^\dagger a_{i\mu}$ does not correlate. The coefficients w_μ can be fixed by the traceless condition $\mathrm{tr}(\rho_i\hat{O}_i) = 0$ and the cutoff condition $\max(\{w_\mu\}) = 1$.

In some cases, the basis of the reduced density matrix may not be ideal because of degeneracies, making it hard to determine the coefficients ω_μ in Eq. (2). In our previous work [6] where the SSH model is considered, we demonstrated that such a difficulty can be overcome by a transformation into a Majorana basis. This allows a diagonal representation of the Hamiltonian in terms of fermionic operators, which are nonlocal combinations of the original fermion operators, at some specific points in the phase diagram. The dominant eigenstate of the reduced density matrix in this diagonal basis is then simply a subset of the system's ground state.

This suggests one may try a different approach and motivates us to introduce a variation of our original scheme as used in this work. Consider a Hamiltonian which can be expressed in terms of some quasilocal Hamiltonian H_j that couples sites with a finite separation in real space. The quasilocal Hamiltonian is, in general, a function of a set of parameters, i.e., $H_j(g_1, g_2, \dots)$. We may identify inside a phase in the phase diagram a point $(G_1, G_2, \dots)$ where we can diagonalize the Hamiltonian. Call $|G_1, G_2, \dots\rangle$ the ground state of H_j at this point. Define an operator

$$\hat{O}_j = |G_1, G_2, \dots\rangle\langle G_1, G_2, \dots|, \tag{3}$$

which is a projector to a subset of the system's ground state. We may now define the order parameter as the average value of this operator in the ground state of $H_j(g_1, g_2, \dots)$.

Note that

$$\begin{aligned} O_j &= \langle g_1, g_2, \cdots|\hat{O}_j|g_1, g_2, \cdots\rangle \\ &= |\langle g_1, g_2, \cdots|G_1, G_2, \cdots\rangle|^2. \end{aligned} \tag{4}$$

Physically, this is like a measure of the overlap between the ground state at two points in the phase diagram. However, unlike the conventional fidelity approach to quantum phase transitions [13–15], the two points $(g_1, g_2, \dots)$ and $(G_1, G_2, \dots)$ are, in general, far apart. See also, for instance, [16,17]. In the next section, we illustrate the method in more detail by applying it to the SSH model with triplet pairing (SSH-Kitaev model).

III. ORDER OPERATORS OF THE SSH MODEL WITH TRIPLET PAIRING

A. Model

This model may be viewed as a dimerized Kitaev superconductor [18]. The dimerization is parametrized by η, and the superconductivity is parametrized by Δ.

This model is given by the Hamiltonian

$$\begin{aligned} H = &-\mu\sum_j (c_{j,A}^\dagger c_{j,A} + c_{j,B}^\dagger c_{j,B}) \\ &- t\sum_j [(1+\eta)c_{j,B}^\dagger c_{j,A} + (1+\eta)c_{j,A}^\dagger c_{j,B} \\ &+ (1-\eta)c_{j+1,A}^\dagger c_{j,B} + (1-\eta)c_{j,B}^\dagger c_{j+1,A}] \\ &+ \Delta\sum_j [(1+\eta)c_{j,B}^\dagger c_{j,A}^\dagger + (1+\eta)c_{j,A}c_{j,B} \\ &+ (1-\eta)c_{j+1,A}^\dagger c_{j,B}^\dagger + (1-\eta)c_{j,B}c_{j+1,A}], \end{aligned} \tag{5}$$

where t is the hopping, Δ is the pairing amplitude, and μ is the chemical potential. The anisotropies in the hopping term and the pairing term are assumed to be the same since both of them are associated with the spontaneous dimerization of the lattice as a result of the coupling to the phonons. The model with no superconductivity ($\Delta = 0$) is related to the Schockley model by taking $t_1 = t(1+\eta)$ and $t_2 = t(1-\eta)$. The region of $\eta > 0$ corresponds to $t_1 > t_2$ and vice versa for $\eta < 0$. The Hamiltonian in real space mixes nearest-neighbor sites and also has local terms. We consider a system with $j = 1, \dots, N$ (N A sites and N B sites). The local terms can be grouped in the matrix

$$H_{j,j} = \begin{pmatrix} -\mu & -t(1+\eta) & 0 & -\Delta(1+\eta) \\ -t(1+\eta) & -\mu & \Delta(1+\eta) & 0 \\ 0 & \Delta(1+\eta) & \mu & t(1+\eta) \\ -\Delta(1+\eta) & 0 & t(1+\eta) & \mu \end{pmatrix}. \tag{6}$$

The nonlocal terms of the nearest neighbors can be written as

$$H_{j,j+1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -t(1-\eta) & 0 & -\Delta(1-\eta) & 0 \\ 0 & 0 & 0 & 0 \\ \Delta(1-\eta) & 0 & t(1-\eta) & 0 \end{pmatrix} \tag{7}$$

and

$$H_{j,j-1} = \begin{pmatrix} 0 & -t(1-\eta) & 0 & \Delta(1-\eta) \\ 0 & 0 & 0 & 0 \\ 0 & -\Delta(1-\eta) & 0 & t(1-\eta) \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{8}$$

The Hamiltonian matrices are the matrix elements in the basis

$$\begin{pmatrix} c_{j,A} \\ c_{j,B} \\ c^{\dagger}_{j,A} \\ c^{\dagger}_{j,B} \end{pmatrix}. \tag{9}$$

In general, a fermion operator may be written in terms of two Hermitian operators, γ_1, γ_2, in the following way:

$$\begin{aligned} c_{j,\sigma} &= \tfrac{1}{2}(\gamma_{j,\sigma,1} + i\gamma_{j,\sigma,2}), \\ c^{\dagger}_{j,\sigma} &= \tfrac{1}{2}(\gamma_{j,\sigma,1} - i\gamma_{j,\sigma,2}). \end{aligned} \tag{10}$$

The index σ represents internal degrees of freedom of the fermionic operator, such as the spin and/or sublattice index, and the γ operators are Hermitian and satisfy the Clifford algebra

$$\{\gamma_m, \gamma_n\} = 2\delta_{nm}. \tag{11}$$

In terms of Majorana operators the Hamiltonian is written as

$$\begin{aligned} H = &-\frac{\mu}{2}\sum_{j=1}^{N}(2 + i\gamma_{j,A,1}\gamma_{j,A,2} + i\gamma_{j,B,1}\gamma_{j,B,2}) \\ &-\frac{it}{2}(1+\eta)\sum_{j=1}^{N}(\gamma_{j,B,1}\gamma_{j,A,2} + \gamma_{j,A,1}\gamma_{j,B,2}) \\ &-\frac{it}{2}(1-\eta)\sum_{j=1}^{N-1}(\gamma_{j+1,A,1}\gamma_{j,B,2} + \gamma_{j,B,1}\gamma_{j+1,A,2}) \\ &+\frac{i\Delta}{2}(1+\eta)\sum_{j=1}^{N}(\gamma_{j,A,1}\gamma_{j,B,2} + \gamma_{j,A,2}\gamma_{j,B,1}) \\ &+\frac{i\Delta}{2}(1-\eta)\sum_{j=1}^{N-1}(\gamma_{j,B,1}\gamma_{j+1,A,2} + \gamma_{j,B,2}\gamma_{j+1,A,1}). \end{aligned} \tag{12}$$

Taking from now on $\mu = 0$, we have four special points, three corresponding to topological phases and one corresponding to a trivial phase (Fig. 1): (i) Taking $\eta = -1$ and $\Delta = 0$, we have a state similar to that in the SSH and Schockley models with two fermioniclike zero-energy edge states since the four operators $\gamma_{1,A,1}$, $\gamma_{1,A,2}$, $\gamma_{N,B,1}$, $\gamma_{N,B,2}$ are missing from the Hamiltonian. (ii) $\eta = 0, t = \Delta$, and (iii) $\eta = 0, t = -\Delta$ are Kitaev like states since there are two Majorana operators missing from the Hamiltonian, such as $\gamma_{1,A,1}$ and $\gamma_{N,B,2}$, one from each end. (iv) An example of a trivial phase is the point $\eta = 1$ and $\Delta = 0$, in which case there are no zero energy edge states. This model provides a testing ground for the comparison of fermionic and Majorana edge modes.

The order parameters (also called topological correlators in Ref. [7]) can be determined separately for each phase.

B. The $\eta = -1$, $\Delta = 0$ topological phase

At the point $\mu = 0, \eta = -1, \Delta = 0$ shown in Fig. 1, the Hamiltonian reduces to

$$H = it\sum_{j=1}^{N-1}(\gamma_{j,B,2}\gamma_{j+1,A,1} - \gamma_{j,B,1}\gamma_{j+1,A,2}). \tag{13}$$

Let us define nonlocal fermionic operators [19]

$$\begin{aligned} d_j &= \tfrac{1}{2}(\gamma_{j,B,2} + i\gamma_{j+1,A,1}), \\ d^{\dagger}_j &= \tfrac{1}{2}(\gamma_{j,B,2} - i\gamma_{j+1,A,1}), \end{aligned} \tag{14}$$

and

$$\begin{aligned} f_j &= \tfrac{1}{2}(\gamma_{j,B,1} - i\gamma_{j+1,A,2}), \\ f^{\dagger}_j &= \tfrac{1}{2}(\gamma_{j,B,1} + i\gamma_{j+1,A,2}). \end{aligned} \tag{15}$$

We can show that

$$\begin{aligned} i\gamma_{j,B,2}\gamma_{j+1,A,1} &= 2d^{\dagger}_j d_j - 1, \\ -i\gamma_{j,B,1}\gamma_{j+1,A,2} &= 2f^{\dagger}_j f_j - 1. \end{aligned} \tag{16}$$

In terms of these new operators we can write that

$$H = t\sum_{j=1}^{N-1}(2d^{\dagger}_j d_j - 1 + 2f^{\dagger}_j f_j - 1), \tag{17}$$

and therefore the Hamiltonian is diagonalized. It is now clear that the ground state is obtained by taking $d^{\dagger}_j d_j = 0$ and $f^{\dagger}_j f_j = 0$ at each site. This new Hamiltonian in terms of the d and f operators is like a Hamiltonian with no hopping and just a chemical potential $\tilde{\mu} = -2t$.

The new operators can be related to the original ones in terms of a nonlocal transformation as

$$\begin{aligned} d_j &= \frac{i}{2}(c^{\dagger}_{j,B} - c_{j,B} + c_{j+1,A} + c^{\dagger}_{j+1,A}), \\ f_j &= \frac{1}{2}(c^{\dagger}_{j,B} + c_{j,B} - c_{j+1,A} + c^{\dagger}_{j+1,A}). \end{aligned} \tag{18}$$

Also

$$\begin{aligned} c_{j,A} &= \tfrac{1}{2}[-i(-d^{\dagger}_{j-1} + d_{j-1}) - (f_{j-1} - f^{\dagger}_{j-1})], \\ c_{j,B} &= \tfrac{1}{2}[f^{\dagger}_j + f_j + i(d_j + d^{\dagger}_j)]. \end{aligned} \tag{19}$$

Note that the index j of the d and f operators refers to the bond connecting the j, B and $j+1, A$ sites in the original representation. At the special point we are considering, we may also write

$$H = -2t\sum_{j}(c^{\dagger}_{j+1,A}c_{j,B} + c^{\dagger}_{j,B}c_{j+1,A}). \tag{20}$$

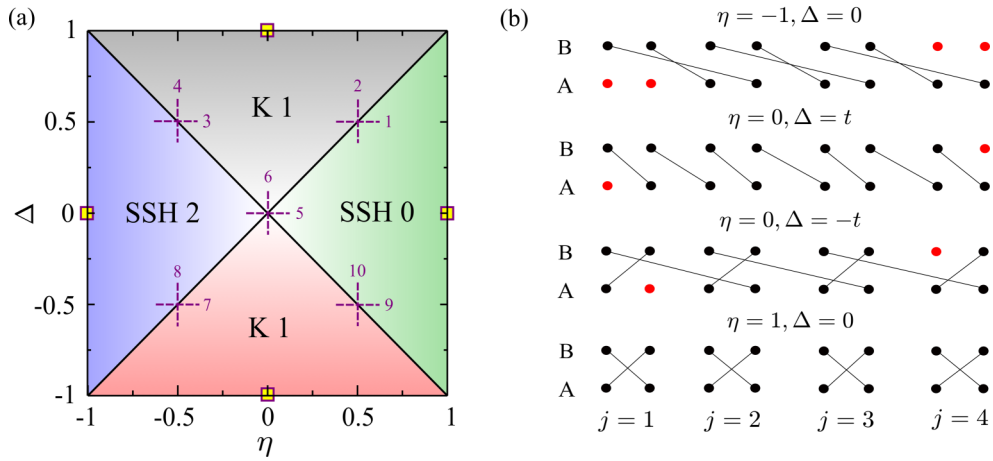

FIG. 1. (a) Phases of the SSH-Kitaev model for zero chemical potential. When $\Delta = 0$, the model reduces to the SSH model, and for negative η the model is topologically nontrivial, with edge states represented by the decoupled Majorana operators. As in the Schockley model, since at each end site there are two decoupled Majoranas, they combine to form edge fermionic modes. This constitutes phase SSH2 with $\eta = -1$, $\Delta = 0$, and two edge modes. If superconductivity is present and there is no dimerization, $\eta = 0$, the model reduces to the Kitaev model. Phase K1 with $\eta = 0$, $\Delta = t$ has two decoupled Majorana operators, one at each end, and therefore there is one Majorana mode at each edge. The model interpolates between Majorana modes and fermionic modes as the parameters change. There is also a trivial phase with no zero-energy modes denoted SSH0 which is similar to the trivial phase of the Schockley model. The Hamiltonian in terms of Majoranas simplifies at the four points marked with yellow squares, and (b) shows an illustration of the Majorana modes at these four points. At each of the lattice sites j, the two dots represent the Majorana operators $\gamma_{j,\sigma,1}$ and $\gamma_{j,\sigma,2}$ ($\sigma = A$ or B). The lines represent the links between the Majorana operators.

In the diagonalized basis, the ground state is a product state of $|00\rangle$. Using Eq. (3), the order operator is

$$\begin{aligned}\hat{O}_-^{\mathrm{SSH}} &= |00\rangle\langle 00| \\ &= I - |10\rangle\langle 10| - |01\rangle\langle 01| - |11\rangle\langle 11| \\ &= 1 - f_j^\dagger f_j(1 - d_j^\dagger d_j) - d_j^\dagger d_j(1 - f_j^\dagger f_j) - f_j^\dagger f_j d_j^\dagger d_j \\ &= (1 - f_j^\dagger f_j)(1 - d_j^\dagger d_j). \end{aligned} \tag{21}$$

Note that the same expression can also be obtained using Eq. (2) by considering the reduced density matrix in the diagonalized basis, which is solely contributed by the eigenstate $|00\rangle$ [6]. The above expressions are local in space. We may now use the relation between the d and f operators and the original operators in Eq. (18). This is a nonlocal transformation since it couples site j with the nearest-neighbor site $j+1$. The operator may now be obtained as

$$\begin{aligned}\hat{O}_-^{\mathrm{SSH}} &= \tfrac{1}{2}(c_{j+1,A}^\dagger c_{j,B} + c_{j,B}^\dagger c_{j+1,A}) - n_{j,B} n_{j+1,A} \\ &\quad + \tfrac{1}{2}(n_{j,B} + n_{j+1,A}). \end{aligned} \tag{22}$$

C. The $\eta = 0$, $\Delta = t$ topological phase

Consider now the special point of the SSH-Kitaev model given by $\eta = 0$, $\Delta = t$. This point is deep inside the Kitaev-like phase, as shown in Fig. 1. At this point the Hamiltonian simplifies to

$$H = t \sum_j (i\gamma_{j,A,2}\gamma_{j,B,1} + i\gamma_{j,B,2}\gamma_{j+1,A,1}). \tag{23}$$

Write

$$\begin{aligned} i\gamma_{j,B,2}\gamma_{j+1,A,1} &= 2d_j^\dagger d_j - 1, \\ i\gamma_{j,A,2}\gamma_{j,B,1} &= 2g_j^\dagger g_j - 1. \end{aligned} \tag{24}$$

Here the operator d_j is defined in Eq. (14), and the operator g_j is given by

$$g_j = \tfrac{1}{2}(\gamma_{j,B,1} - i\gamma_{j,A,2}). \tag{25}$$

Therefore

$$g_j = \tfrac{1}{2}(c_{j,B}^\dagger + c_{j,B} - c_{j,A} + c_{j,A}^\dagger). \tag{26}$$

The ground state is obtained by taking $n_{d,j} = 0$ and $n_{g,j} = 0$. Therefore let us define the new operator in the basis of these occupation numbers as

$$\begin{aligned}\hat{O}_+^{SK} &= |00\rangle\langle 00| \\ &= 1 - d_j^\dagger d_j - g_j^\dagger g_j + d_j^\dagger d_j g_j^\dagger g_j. \end{aligned} \tag{27}$$

Using their expressions in terms of the original operators, one obtains

$$\begin{aligned}\hat{O}_+^{SK} &= \tfrac{1}{4}[c_{j,B}^\dagger(c_{j,A} + c_{j+1,A}) + (c_{j,A}^\dagger + c_{j+1,A}^\dagger)c_{j,B} \\ &\quad + c_{j,B}(c_{j,A} - c_{j+1,A}) + (c_{j,A}^\dagger - c_{j+1,A}^\dagger)c_{j,B}^\dagger] \\ &\quad - \tfrac{1}{4}(2n_{j,B} - 1)(c_{j+1,A}^\dagger c_{j,A} + c_{j,A}^\dagger c_{j+1,A} \\ &\quad + c_{j+1,A}c_{j,A} + c_{j,A}^\dagger c_{j+1,A}^\dagger) + \tfrac{1}{4}. \end{aligned} \tag{28}$$

D. The $\eta = 0$, $\Delta = -t$ topological phase

Taking $\eta = 0$, $\Delta = -t$, the Hamiltonian reduces to

$$H = -it \sum_j (\gamma_{j,A,1}\gamma_{j,B,2} + \gamma_{j,B,1}\gamma_{j+1,A,2}). \tag{29}$$

Define two new operators

$$f_j = \tfrac{1}{2}(\gamma_{j,B,1} - i\gamma_{j+1,A,2}), \tag{30}$$

$$h_j = \tfrac{1}{2}(\gamma_{j,A,1} - i\gamma_{j,B,2}). \tag{31}$$

In terms of the original fermion operators,

$$f_j = \tfrac{1}{2}[c_{j,B} + c^\dagger_{j,B} - (c_{j+1,A} - c^\dagger_{j+1,A})],$$
$$h_j = \tfrac{1}{2}[c_{j,A} + c^\dagger_{j,A} - (c_{j,B} - c^\dagger_{j,B})]. \tag{32}$$

The Hamiltonian at this point can be written as

$$H = t\sum_j (2h^\dagger_j h_j - 1 + 2f^\dagger_j f_j - 1). \tag{33}$$

Again, the ground state is obtained by taking the state of no occupation of number operators of the f and h operators. So let us define a new operator valid for negative Δ as

$$\begin{aligned}\hat{O}^{SK}_- &= |00\rangle\langle 00| \\ &= 1 - f^\dagger_j f_j - h^\dagger_j h_j + f^\dagger_j f_j h^\dagger_j h_j \qquad (34)\\ &= \tfrac{1}{4}[c^\dagger_{j,B}(c_{j,A} + c_{j+1,A}) + (c^\dagger_{j,A} + c^\dagger_{j+1,A})c_{j,B} \\ &\quad + c_{j,B}(-c_{j,A} + c_{j+1,A}) + (-c^\dagger_{j,A} + c^\dagger_{j+1,A})c^\dagger_{j,B}] \\ &\quad - \tfrac{1}{4}(2n_{j,B} - 1)(c^\dagger_{j+1,A}c_{j,A} + c^\dagger_{j,A}c_{j+1,A} \\ &\quad - c_{j+1,A}c_{j,A} - c^\dagger_{j,A}c^\dagger_{j+1,A}) + \tfrac{1}{4}. \qquad (35)\end{aligned}$$

E. The $\eta = 1$, $\Delta = 0$ trivial phase

For $\eta > 0$, the mutual information is exponentially vanishing, and the correlation is not captured by considering the single-site block with A and B atoms. However, one could take the block consisting of a B atom at site j and an A atom at site $j+1$. The mutual information obtained would be the mirror image of that in Fig. 4 of Ref. [6] along $\eta = 0$. The eigenspectrum of the reduced density matrix in this case is shown in Fig. 5(b) of the same reference. Carrying out a similar analysis as above, the order parameter takes the form of Eq. (22), but with the indices $\{j+1, A\}$ and $\{j, B\}$ being replaced by $\{j, B\}$ and $\{j, A\}$, respectively. We have

$$\hat{O}^{\rm SSH}_+ = \tfrac{1}{2}(c^\dagger_{j,B}c_{j,A} + c^\dagger_{j,A}c_{j,B}) - n_{j,A}n_{j,B} + \tfrac{1}{2}(n_{j,A} + n_{j,B}). \tag{36}$$

IV. PHASE DIAGRAM AND ORDER PARAMETERS

A. Calculation method

We may now calculate the order parameters (or topological correlators) as the ground-state average values of the operators $\hat{O}^{\rm SSH}_+$, $\hat{O}^{\rm SSH}_-$, $\hat{O}^{SK}_+$, $\hat{O}^{SK}_-$ defined in the previous section.

The average values may be obtained, for instance, using exact diagonalization, using the density matrix renormalization group [20–22] (particularly useful if one introduces interactions between the original fermions), or via the solution of the Bogoliubov–de Gennes (BdG) equations in the absence of interactions. This last method allows the solution for large systems (suitable for the finite-size scaling analysis carried out below). We consider open boundary conditions in the following. The results obtained using exact diagonalization and the BdG method agree.

We may write that

$$c_{j,A} = \sum_n \left(u^n_{j,A}\gamma_n + v^n_{j,A}\gamma^\dagger_n\right),$$
$$c_{j,B} = \sum_n \left(u^n_{j,B}\gamma_n + v^n_{j,B}\gamma^\dagger_n\right), \tag{37}$$

where γ_n are the fermionic operators that diagonalize the Hamiltonian. The Bogoliubov–de Gennes equations are written in real space as

$$\sum_{j'} H_{j,j'}\begin{pmatrix} u_{j',A} \\ u_{j',B} \\ v_{j',A} \\ v_{j',B}\end{pmatrix} = \epsilon_n \begin{pmatrix} u_{j,A} \\ u_{j,B} \\ v_{j,A} \\ v_{j,B}\end{pmatrix}, \tag{38}$$

where ϵ_n are the energy eigenvalues, $u_{A,B}$ and $v_{A,B}$ are the components of the eigenfunctions, and j' is restricted to $j = j'$ and $j = j' \pm 1$.

The averages of the order parameters may then be obtained by solving the BdG equations and determining the wave functions. Considering a finite system of size N, the problem requires the diagonalization of a $(4N) \times (4N)$ matrix.

B. Results

We may now consider cuts in the phase diagram and calculate the order parameters. With open boundary conditions it is better to take the average over alternating lattice sites [7]. Specifically,

$$O = \frac{2}{N}\sum_{j=2i+1} O_j. \tag{39}$$

In the top panel of Fig. 2 we consider three cuts for $\eta = -0.5$, $\eta = 0$, $\eta = 0.5$, and in the bottom panel we consider cuts for $\Delta = -0.5$, $\Delta = 0$, $\Delta = 0.5$. We calculate the average order parameter, and the results shown are for a large system size of $N = 100$. The results for the two types of cuts are quite symmetrical if we change η to Δ and vice versa, also changing the order parameters appropriately. The order parameters clearly identify various phases in the model, and we observe the following:

(i) At the points where each order parameter is defined the order parameter is normalized to 1 since it is the ground-state average value of the projector to that state.

(ii) At each phase the order parameter characteristic of that phase has the largest value.

(iii) The order parameters cross at the transition lines.

V. SCALING AND CRITICAL EXPONENTS

We may now determine the scaling properties of the order parameters. The scaling allows us to determine the critical exponents and the universality class of the system.

We recall that the order parameters defined above do not vanish at the transition points as usual. Also the order parameter does not separate a disordered phase with a vanishing order parameter from an ordered phase with finite values of the order parameter. The various averages of the order operators that represent the various topological phases cross at the driving parameter $g = g_c(N)$ with finite values $O_c(N)$.

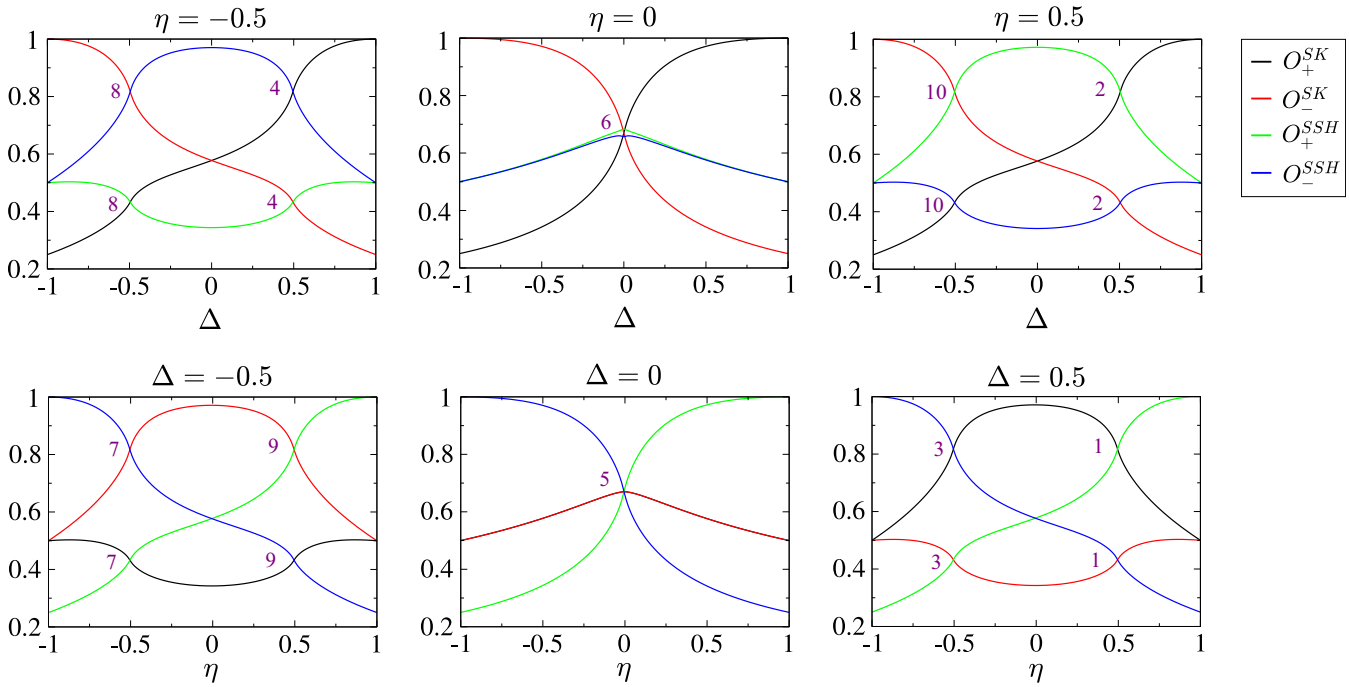

FIG. 2. Top: Order parameters as a function of Δ for constant values of $\eta = -0.5, 0, 0.5$. Bottom: Order parameters as a function of η for constant values of $\Delta = -0.5, 0, 0.5$. We consider open boundary conditions and a system size $N = 100$. The numbers in purple next to where the order parameters cross correspond to the cuts through the phase boundaries labeled in Fig. 1(a).

The scaling is then expected to have the form

$$N^{\beta/\nu}(O - O_c) = f(N^{1/\nu}(g - g_c)). \tag{40}$$

Here β is the usual critical exponent associated with an order parameter, and ν is the exponent associated with the correlation length. The function f is the scaling function. In comparison to the standard scaling relation that describes a continuous phase transition [23], O is replaced by $O - O_c$ to make the equation consistent in the thermodynamic limit. Plotting the left-hand side of the above scaling relation against the argument of the scaling function, we expect that the curves for different system sizes should collapse into a single curve near the critical point. Note that the scaling function is independent of the system size at the crossing point $g = g_c$, and the size dependence of each order parameter is such that in the thermodynamic limit the order parameter should converge to a value $O_c \neq 0$ in our problem.

Consider first a single-band Kitaev model. The model is not expected to have some form of quasi-long-range order. The correlation functions decay exponentially with a correlation length that indeed diverges at the topological transition with an exponent $\nu = 1$. This may be obtained using the scaling behavior of the energy gap $E_g \sim (g - g_c)^{\nu z}$, where z is the dynamical critical exponent. Since the energy spectrum is linear, we have $z = 1$, and the gap scales linearly, which leads to $\nu = 1$ (as shown, for instance, in [24]). Generalizing the Kitaev model to a multiband model with an antisymmetric coupling between the two bands leads to a rich phase diagram that displays a topological transition between a Weyl-like phase and a conventional superconductor that turns out to be in a different universality class of the Kitaev model [25]. The dispersion relation near the transition points turns out to be quadratic, leading to a dynamical critical exponent $z = 2$, and since the gap as a function of the driving parameter (the chemical potential) vanishes linearly, this leads to $\nu = 1/2$ [also using the hyperscaling relation $2 - \alpha = \nu(d + z)$, where d is the spatial dimension, leads to $\alpha = 3/2$, while in the Kitaev universality class $\alpha = 0$].

Consider now the SSH model with no superconductivity. In Ref. [7] a mapping was established in some regime between the Schwinger model on a lattice and the SSH model. Using the order parameter O_-^{SSH}, it was shown that the model is in the universality class of the $d = 2$ classical Ising model or the quantum Ising model in a transverse field (recall that a mapping exists between a quantum model in d dimensions and a classical model in $d + z$ dimensions; therefore if $z = 1$, there is a mapping from a quantum one-dimensional model and a classical two-dimensional model). Note that the two-dimensional Ising model displays a true phase transition and it makes sense to define an order parameter. In this class the critical exponents are given by $\nu = 1, \beta = 1/8$. The results are consistent with previous treatments of the massive Schwinger model [26–28].

A. Scaling in the Ising universality class

Let us now consider the SSH model with triplet pairing and consider open boundary conditions (ignoring the small discontinuity at the transition points observed for small system sizes yields similar results in the case of periodic boundary conditions). In order to consider the scaling we must choose the critical exponents and perform the analysis with different system sizes.

Consider some cuts in the phase diagram as indicated by the purple dashed segments in Fig. 1(a). In Fig. 3, we show results for the scaling of the order parameters for some of the

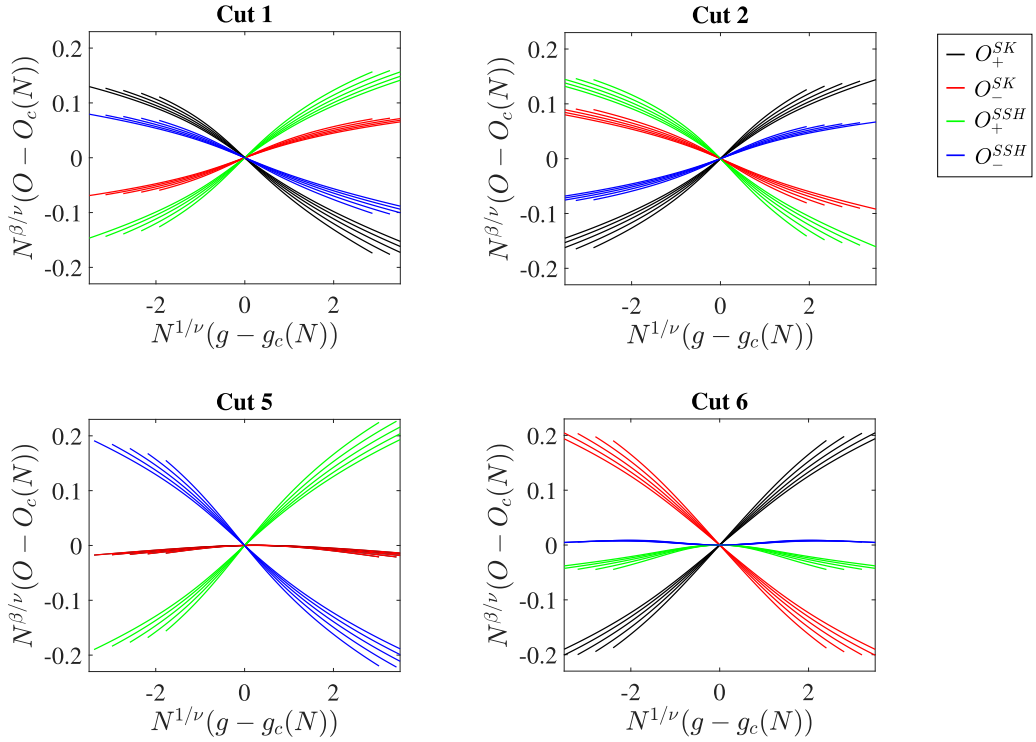

FIG. 3. Scaling of various order parameters for cuts 1, 2, 5, and 6 with $\nu = 1$, $\beta = 1/8$. The black, red, green, and blue curves correspond to O_+^{SK}, O_-^{SK}, O_+^{SSH}, and O_-^{SSH}, respectively. Here we use open boundary conditions (OBCs), and order parameters are averaged over all odd sites (or even sites) as defined in Eq. (39). We consider system sizes $N = 24, 28, 32, 36, 40$.

various cuts considered. Here we use the Ising universality class with $\nu = 1$ and $\beta = 1/8$, as obtained before for the SSH model. The scaling seems to work approximately well for the various cases since the curves near the transition points collapse basically into a single curve.

B. Optimizing the scaling

While the choice of critical exponents above describes well the scaling of the various order parameters near the various transition lines, we may find a pair of critical exponents that best fit the scaling ansatz in Eq. (40). A criterion may be used such that the deviations between the various curves for different system sizes in the vicinity of the critical point are minimized. One may also minimize the squares of these deviations. The logarithm of this deviation D is shown in Fig. 4 for the scaling of the order parameter O_+^{SK} across the transition associated with cut 1. Specifically, for each value of the driving parameter around the critical point (in this case η), the squared differences between the minimum and maximum values of the order parameter for the various system sizes (taken here as $N = 24, 40, 60, 100, 200$) are considered. The result shown in Fig. 4 is the logarithm of the sum of this differences squared at each η value. The results obtained suggest that the universality class may be different from the Ising class. We may also fit a polynomial function to the results for the various system sizes and use the least-squares method for a given scaling function. This leads to similar results. Similar results are also found for the other cuts considered in Fig. 1(a) and for the various order parameters and therefore are not shown here.

As we can see, the deviation is minimized if we keep increasing ν and decreasing β. So a value of $\nu = 1$ is a large value, and $\beta = 1/8$ is small, but the agreement becomes better (but slowly varying) if we change along the lines mentioned. Note that $\beta = 0$ and a very large ν lead to a scaling of the type

$$O - O_c = f((g - g_c)) \tag{41}$$

with no system size dependence at all. Clearly, in the infinite system limit this holds.

The exponent $\nu = 1$ has also been obtained by other methods. In one-dimensional systems of the Dirac type of class *AIII* it has been shown [29] that, in general, $\gamma = \nu$. Considering the case of the SSH model it was explicitly shown [29] that $\nu = 1$. Our results for cut 5 (with $\Delta = 0$ and changing η as in the SSH model) as for the other cuts

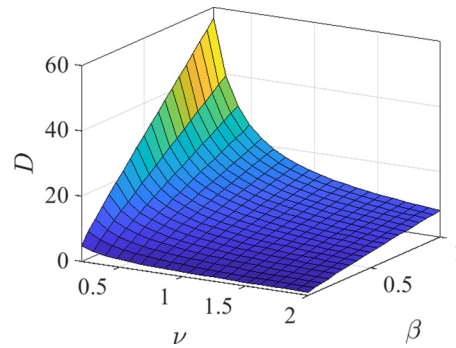

FIG. 4. Minimization of spreading of scaled curves of O_+^{SK} around the critical point of cut 1.

are not inconsistent with the analytical behavior for the SSH model since the optimization shows a very slow change of the least-squares deviation.

VI. LOCAL HAMILTONIAN AS THE "ORDER PARAMETER"

A. Single-band Kitaev model

Consider the single-band Kitaev model at a zero chemical potential described by the Hamiltonian

$$H = -t\sum_j (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}) + \Delta\sum_j (c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger). \tag{42}$$

The Hamiltonian takes a simple form at points $\Delta = t$ and $\Delta = -t$, as discussed above for the generalization of the model to two sublattices. A similar procedure allows us to determine two operators associated with the diagonalization of the Hamiltonian at these two points. The order parameters are simply given by the average of the projectors to a single-site zero occupation of the d_j operators defined in Eq. (14) (and the f operators defined in Eq. (15) for the case of $\Delta = -t$). We obtain then that

$$\begin{aligned}\hat{O}^K_{j,+} &= |0\rangle\langle 0| = 1 - d_j^\dagger d_j \\ &= \tfrac{1}{2} - \tfrac{1}{2}H_j(t = \Delta = 1)\end{aligned} \tag{43}$$

and

$$\hat{O}^K_{j,-} = \tfrac{1}{2} - \tfrac{1}{2}H_j(t = -\Delta = 1), \tag{44}$$

where H_j is the contribution from site j to the Hamiltonians

$$H_j(t = \Delta = 1) = -c_{j+1}^\dagger c_j - c_j^\dagger c_{j+1} + c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger \tag{45}$$

and

$$H_j(t = -\Delta = 1) = -c_{j+1}^\dagger c_j - c_j^\dagger c_{j+1} - c_j c_{j+1} - c_{j+1}^\dagger c_j^\dagger, \tag{46}$$

respectively. Diagonalizing the full Hamiltonian at an arbitrary point in the phase diagram, we may write

$$\begin{aligned}\hat{O}^K_{j,+} &= \frac{1}{2} + \sum_n v_j^n\left(u_{j+1}^n + v_{j+1}^n\right), \\ \hat{O}^K_{j,-} &= \frac{1}{2} + \sum_n v_j^n\left(-u_{j+1}^n + v_{j+1}^n\right).\end{aligned} \tag{47}$$

In Fig. 5 we calculate the order parameters as a function of Δ and take the average over odd sites as in the previous section. The order parameters cross at the transition point. Since these operators are basically the local Hamiltonian plus a constant, this suggests that the local Hamiltonian itself may be used as an order parameter. While in the case of the single-band Kitaev model the procedure to determine the projectors leads to the local Hamiltonian at that specific point in the phase diagram, this does not occur in the SSH-Kitaev model, as shown in Sec. III.

In any case, let us consider the local Hamiltonian of the SSH-Kitaev model to see if it can be used as a suitable operator that leads to an order parameter.

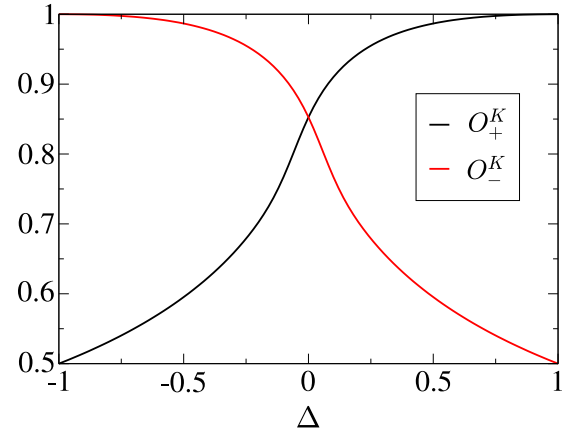

FIG. 5. Order parameters for the single-band Kitaev model as a function of Δ for $N = 32$.

B. SSH-Kitaev model

Write the Hamiltonian in Eq. (5) as $H = \sum_j H_j$, and then define four operators as the local Hamiltonian H_j at the points indicated in Fig. 1(a). We calculate their averages at an arbitrary point of the phase diagram using the eigenstates of the Hamiltonian at this arbitrary point. Note that, in general, these states are not the eigenstates of the Hamiltonians at the special points marked in Fig. 1(a). As an example let us consider that we fix $\Delta = 0.5$ and change η from -1 to 1. The results for other ranges of values lead to similar conclusions. In Fig. 6 we show the results for this cut in the phase diagram for the four local Hamiltonians. The results are strikingly similar to the ones obtained using the order parameters O_+^{SK}, O_-^{SK}, O_+^{SSH}, O_-^{SSH}, and the transitions are clearly signaled by the crossings of the various order parameters defined from the local Hamiltonians.

We may as well identify the phase transitions considering only one of the order parameters, and actually, we do not have to limit their definition to the special points where a diagonalization of the Hamiltonian can be performed analytically (as is easily done using the Majorana representation). Let us consider the local Hamiltonian H_j in an arbitrary point in the phase diagram of the SSH-Kitaev model (this should hold

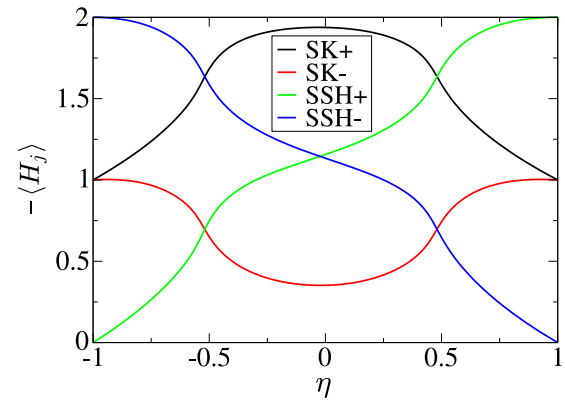

FIG. 6. Local Hamiltonian order parameters for the SSH-Kitaev model as a function of η at $\Delta = 0.5$, using OBCs and taking $N = 32$.

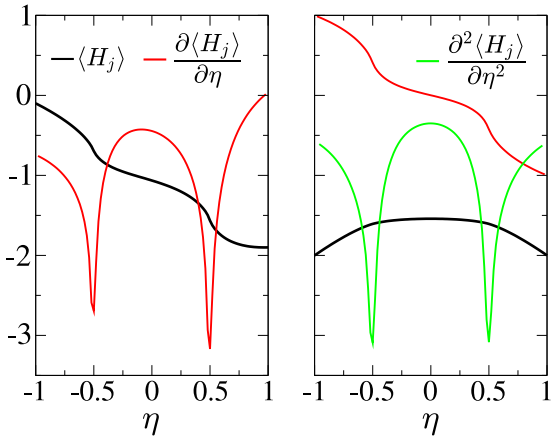

FIG. 7. Local Hamiltonian order parameters for the SSH-Kitaev model and its derivatives with respect to η as a function of η at $\Delta = 0.5$, using OBC and taking $N = 100$. In the left panel, the local Hamiltonian at the point $\eta = 0.9$ and $\Delta = -0.1$ is considered. In the right panel we take the local Hamiltonian at $\Delta = 0.5$ and at the sequence of values of η along the cut. Therefore in the right panel it is the energy per site.

for an arbitrary Hamiltonian). Let us now consider a cut in the phase diagram that crosses some transition or transition lines (points). We will show now that the derivative of the average of this local Hamiltonian in the basis of the eigenstates of the full Hamiltonian at each point along the cut with respect to the parameter that defines the cut detects the transition lines. We will focus on a specific example, but the result can be checked for arbitrary examples.

Consider, for example, the same cut as above, where $\Delta = 0.5$ and we change η from -1 to 1. There are two transition points at $\eta = -0.5$ and $\eta = 0.5$. Consider the local Hamiltonian at the point $\eta = 0.9$, $\Delta = -0.1$, some arbitrary point in the phase diagram and not on the cut that we choose. We also calculate the average energy per site. The results are shown in Fig. 7. While the transitions are detected by calculating the second derivative of the energy per site with respect to the driving parameter η (this is like a susceptibility or related to the fidelity susceptibility), it is enough to calculate the first derivative of the average of the local Hamiltonian at an arbitrary point in the phase diagram not necessarily located in a point on the cut.

VII. CONCLUSIONS

With the method introduced, we obtained the order parameters that clearly signal the various phase transitions in the SSH model with triplet pairing. Also the magnitudes of the various order parameters are in complete agreement with the sequence of phases in the sense that the larger order para meter corresponds to the dominant characteristic of each phase.

The finite-size scaling analysis results with exponents $\nu = 1$ and $\beta = 1/8$ seem to support the model belonging to the quantum Ising universality class. This is consistent with previous results obtained for the SSH model. However, the least-squares optimization analysis also showed that ν and β can be values larger than 1 and $1/8$, respectively. This suggests some nontrivial scaling relations may be required to describe the quantum criticality in the model since we have competing order parameters. One possibility is related to the existence of more than one order parameter, as discussed, for instance, in Ref. [30]. Another possibility is the existence of more than one correlation length, as discussed in Ref. [31].

We expect the method we proposed here can also be applied to other symmetry-protected topological systems, in which the topological order is expected to be short range and a deformation to a quasilocal Hamiltonian is possible as long as the gap does not close in the procedure, for example, the multiband hybridized superconductors [25,32], which have a diagonal representation of the Hamiltonian at specific points of the phase diagram. For future works, it will be interesting to examine how the method can be extended to Hamiltonians with long-range terms or a true topological ordered system with long-range entanglement. In the latter case, we believe that our method will also work with a suitable modification and the order parameter, instead of being limited to a few neighbors, may extend farther throughout the system.

ACKNOWLEDGMENTS

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