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ELECTRONIC PROPERTIES OF SOLID

Size Effects on the Conditions of Edge State Formation in 1D Systems

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Abstract—A criterion for revealing edge states in the case when the size of a system is comparable with the localization length of these states has been proposed. The application of the algorithm for determining edge states in short systems has been demonstrated on examples of the Bernevig–Hughes–Zhang (BHZ) model in the cylindrical geometry, the Kitaev model, and a chain with the spin–orbit interaction and induced superconductivity. It has been shown that for finite-length 1D systems, there exist ranges of parameters in which the edge states are not formed, although the topological index is nontrivial; conversely, the emergence of the Majorana modes in regions with a trivial topological index has been demonstrated.

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1. INTRODUCTION

The properties of topologically nontrivial systems have attracted attention of researchers in recent decades [1–7]. Such systems are distinguished by the existence of topologically protected states in the dielectric gap, which ensure, among other things, the motion of a fermion without scattering by nonmagnetic impurities. The properties of such edge states are studied commonly using semi-infinite models with a single boundary, and the introduction of limited systems involves computation difficulties in most cases. The results obtained for semi-infinite systems are extended in this case to finite-size systems, and vice versa.

Additional interest in systems in which edge states are realized was induced by Kitaev's prediction of the existence of zero-energy edge (Majorana) modes in 1D systems with superconducting pairing [8]. The ranges of parameters ensuring the emergence of the Majorana modes in open systems are detected in most cases via the search of topologically nontrivial phases taking into account the periodic boundary conditions. The classification of such phases for noninteracting electrons was performed in [9, 10]. The systems were considered to be large enough for the size effects of the system to be disregarded. The limits of this approach were extended in [11, 12], where the emergence of lines of parameters corresponding to the formation of the Majorana modes separating the ground-state regions with different parities was demonstrated for 1D finite-size models.

Despite the huge number of features devoted to analysis of the properties of edge states in systems with a single boundary, the peculiarities in the realization of edge states in short chains have not been studied comprehensively [13–17]. All these publications were aimed at revealing the peculiar properties of edge states, which are associated with the finite size of such systems, while the size effects on the conditions for the emergence of edge states was not considered. This problem is exactly the subject of this study.

2. PROBLEM OF THE STATE TYPE INTERPRETATION IN FINITE-SIZE SYSTEMS

It is generally accepted that edge states are the states for which the wavefunction is mainly concentrated in the first atomic layers [18]. However, the decrease rate of the wavefunction amplitude can be indefinitely low, and the characteristic localization length can amount to hundreds of atomic layers. The energy of such one-electron state lies in the gap of the bulk spectrum, and its properties depend on the boundary conditions. Tamm [19, 20] and Shockley [21] emphasized in their publications that the location of the edge state energy in "forbidden" bands is an important characteristic of an edge state.

The problems associated with the above-mentioned identification from the localization length can be demonstrated on the following two examples. The first example is the state with zero excitation energy at special lines [11] of parameters in Kitaev's finite-length model (Fig. 1). In the case of a continuous variation of parameters along the special lines in the para-

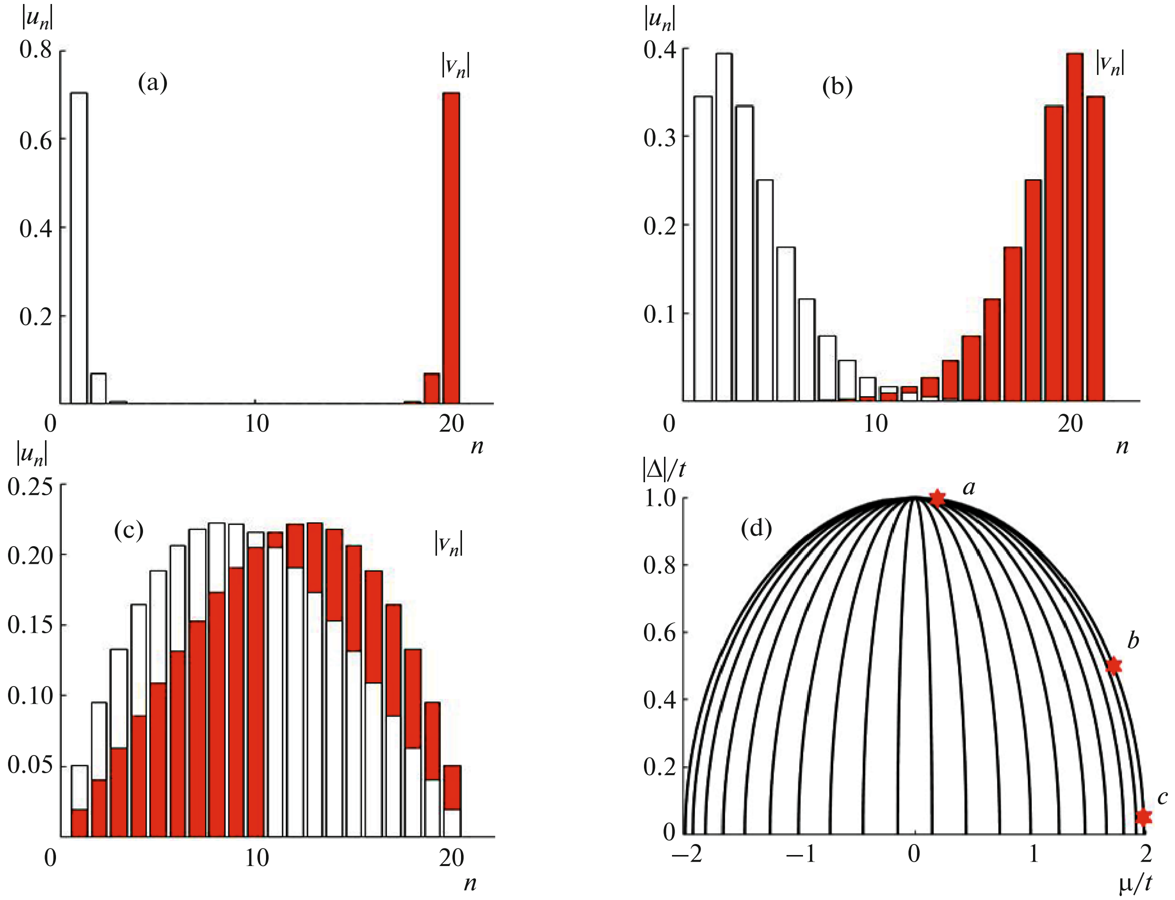

Fig. 1. (Color online) (a, b, c) Dependence of expansion coefficients (1) on the node number (d) for special lines of parameters in the Kitaev model for a finite-length chain. In spite of the fact that the expansion coefficient in (c) has a peak almost at the middle of the chain, this case corresponds to the edge mode.

metric space, the maximum of the expansion coefficient amplitude continuously shifts from the chain edge (Fig. 1a) to the center (Fig. 1c). Although (according to the amplitude graph in Fig. 1c) such an excitation is not of the edge type as regards the localization in the first atomic layers, it still exhibits the properties of an edge excitation. First, this excitation has energy $E = 0$, which is obviously in the gap of the bulk excitation spectrum. Second, this excitation appears only in the presence of open boundaries in the chain. Third, we must consider the analytic expression for the expansion coefficients of the annihilation operator for such an excitation in single-site operators. The expression for the Fermi operator corresponding to excitation energy $E = 0$ has the form

$$d_0 = \frac{1}{2\sqrt{A}}\sum_{n=1}^{N}[r^n \sin\phi_m n(c_{2n-1} + ic_{2N+2-2n})], \qquad (1)$$

$$\phi_m = \frac{\pi m}{N+1}, \qquad r = \sqrt{\frac{t-\Delta}{t+\Delta}},$$

$$\mu = 2\sqrt{t^2-\Delta^2}\cos\phi_m, \qquad m = 1,\dots,N,$$

where c_j are the Majorana operators. It can be seen that the expansion coefficients have a tendency toward an exponential decrease from the edges for any value of parameters as long as these parameters lie on a special line; however, in the case depicted in Fig. 1c, the chain length does not allow us to observe this decrease in view of its extremely small length of the chain.

Another example illustrating the problem emerging in finite-size systems is the Bernevig–Hughes–Zhang (BHZ) model with periodic boundary conditions along one direction and open boundary conditions along the other direction. Since it is possible in such geometry to introduce a classification of excitations according to the magnitude of the quasi-momentum in the direction along which the periodic boundary conditions are realized, the problem can be reduced to a 1D problem with parameters that are functions of this quasi-momentum k. Figure 2 shows the characteristic shape of the wavefunction amplitude at nodes along the direction in which the boundary conditions are open for the one-electron state that experiences a transition from the edge to a nonedge form upon a change in quasi-momentum k. We can see a continu-

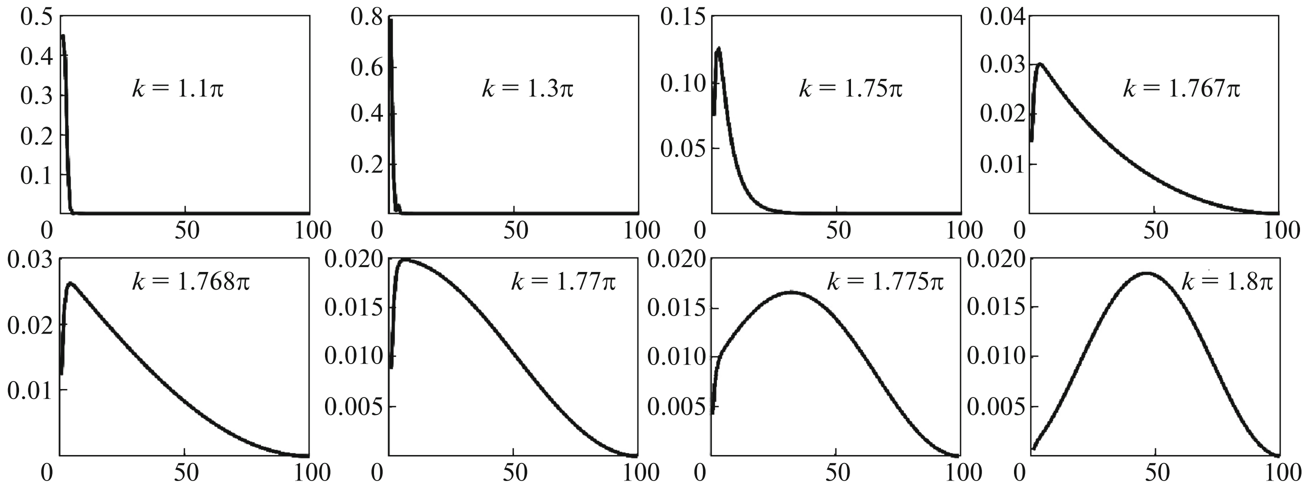

Fig. 2. Dependence of the probability amplitude on the node number for a state with spin projection $\sigma = \uparrow$ upon a transition from the edge to nonedge state in the BHZ model with a cylindrical geometry; $t = 0$, $\Delta t = 1$, $\alpha = 0.5$, $\Delta\varepsilon = 0.5$, and $N = 100$ for different values of quasi-momentum k. The state with $k = 1.767\pi$ (top right graph) is of the edge type, while the state with $k = 1.768\pi$ (bottom left graph) is of the nonedge type.

ous transition from the explicitly edge state to the nonedge state, which occurs most rapidly in the vicinity of $k = 1.76\pi$, but it is impossible to determine the value of the quasi-momentum at which the state stops being of the edge type from the degree of wavefunction localization.

3. GENERALIZATION OF THE CONCEPT OF EDGE STATES TO THE CASE OF 1D FINITE-SIZE SYSTEMS

The problem of determining the edge states for 1D finite-size systems was considered in [22], where an extended version of interpreting edge states was proposed and their properties were analyzed. It was proposed that the edge state in a finite-size 1D system be treated as a state existing only in the presence of a boundary, and the properties of this state are determined by the position of this boundary. It was demonstrated for a 1D system with a continuous periodic potential that the energies of the edge states lie in the gap of the bulk spectrum, and the wavefunction decrease rate for the edge state depends on the position of the edge state energy in the bulk spectrum gap: the energy at the middle of the gap corresponds to a rapid decrease, while the energy close to the bulk zone leads to a substantial expansion in the edge state localization region.

The criteria for the edge state were also considered in [23], where the BHZ model with periodic boundary conditions along one direction and with an open boundary along the other direction was analyzed. It was noted that the local density of state with the energy value in the gap of the bulk spectrum experiences space oscillations, as a result of which the peak in the local density of states shifts from the first atomic layer at the boundary to the bulk of the system. It was proposed that the range of parameters for which the edge state exists be determined from analysis of the indices of exponents appearing in the one-electron state wavefunction.

In this study, we confine our analysis to the concept of edge states in the tight binding approximation. The edge state can be rigorously determined only for a semi-infinite system with a single boundary;[1] an edge state is the state the local probability density of which tends to zero in a semi-infinite lattice:

$$\lim_{n\to\infty} |\Psi_n|^2 \to 0. \qquad (2)$$

The coefficients of wavefunction expansion for the one-electron state in single-site states can be represented as the sum of solutions to the equations for the coefficients disregarding boundaries (general equation). Such solutions to the general equation are also exponentials; if the Hamiltonian of an unbounded system exhibits inversion symmetry, these solutions appear in the expansion in pairs (as $e^{\lambda_j n}$ and as $e^{-\lambda_j n}$), the number of such pairs being equal to the number of equations at the system boundary:

$$\Psi = \sum_{n=1}^{\infty} u_n a_n^+ |0\rangle, \quad u_n = \sum_j (A_j e^{-\lambda_j n} + B_j e^{\lambda_j n}), \qquad (3)$$

where the sum over j implies the summation over the above-mentioned pairs of solutions, and u_n and a_n^+ can be the a row vector and a column vector with allowance for the spin and multiband structure of the system.

[1] The author is grateful to the reviewer who pointed out this fact.

Let us suppose that all solutions λ_j have a nonzero real part $\mathrm{Re}\lambda_j > 0$. Then the requirements of boundedness for a semi-infinite system wavefunction implies that all coefficients $B_j = 0$, and wavefunction (3) satisfies the definition of boundary state (2).

Let us now consider the case when the exponent index of one of general solutions λ_j is imaginary. Since the number of pairs of general solutions is equal to the number of equations at the boundary, it is impossible to simultaneously equate to zero the coefficients A_j and B_j corresponding to this pair of solutions. In such a case, the wavefunction has an undamped component, and such a state is not of the edge type. Obviously, in the case of a large number of purely imaginary exponential indices, the state will be penetrating by nature. Therefore, we can formulate an analytic criterion for the edge state in a 1D system.

Criterion

If all real parts of the indices of exponential functions that are the solution to the general equation for the coefficients of the wavefunction expansion in the nodes of the system for a preset state energy differ from zero, we have an edge state; otherwise, the state is a nonedge (penetrating) state:

$$\forall\lambda_j : \mathrm{Re}\,\lambda_j \neq 0. \tag{4}$$

This analytic criterion is in one-to-one correspondence with rigorous definition (2) of the edge state in a semi-infinite system. In contrast to the latter state, however, it does not require the unboundedness of the system and can be applied to finite-size 1D systems. Irrespective of the system size, the proposed criterion divides all states into two classes:

1. One-electron states with wavefunctions exponentially decreasing from the system edges. In a semi-infinite system, these are edge states in the rigorous sense of this word. The same class of solutions for a finite-size system exhibits the main properties of edge states (localization at the boundary and energy values lying in the bulk spectrum gap). In addition, these states appear only in the presence of boundaries and disappear when periodic boundary conditions are imposed. Therefore, such states in finite-size 1D systems should be referred to as edge states.

2. One-electron states with an undamped component in expansion (3), which should be referred to as nonedge or penetrating states.

Apart from the proposed criterion (4), an edge state in a 1D system can be determined from the energy of this state. If, for example, the energy value of a state lies in the bulk spectrum, at least one index of exponent λ_j for such a state must be purely imaginary, because the energies of bulk states are the solution to the eigenvalue problem of the same general equation, and such a state is penetrating. If an energy value falls into the bulk spectrum gap, none of the exponent indices can be imaginary, and we have an edge state.

4. EDGE STATES IN THE BHZ MODEL IN THE NARROW STRIPE GEOMETRY

Let us illustrate in detail the application of the proposed criterion of edge states for the BHZ model [2] with periodic boundary conditions along the x axis and open boundary conditions along the y direction. Following [24], we can write the BHZ model Hamiltonian in the tight binding approximation in the form

$$\begin{aligned}\mathcal{H}_{BHZ} &= \sum_{nm\sigma}[-\Delta\varepsilon a^{+}_{nm\sigma}a_{nm\sigma} + \Delta\varepsilon d^{+}_{nm\sigma}d_{nm\sigma}] \\ &+ \sum_{NN\sigma}[(t-\Delta t)a^{+}_{n'm'\sigma}a_{nm\sigma} + (t+\Delta t)d^{+}_{n'm'\sigma}d_{nm\sigma}] \\ &- i\alpha\sum_{nm\sigma}\sigma[d^{+}_{n+1m\sigma}a_{nm\sigma} - a^{+}_{nm\sigma}d_{n+1m\delta} \\ &- d^{+}_{n-1m\sigma}a_{nm\sigma} + a^{+}_{nm\sigma}d_{n-1m\sigma}] \\ &+ \alpha\sum_{nm\sigma}[d^{+}_{mn+1\sigma}a_{nm\sigma} + a^{+}_{nm\sigma}d_{nm+1\sigma} \\ &- d^{+}_{nm-1\sigma}a_{nm\sigma} - a^{+}_{nm\sigma}d_{nm-1\sigma}].\end{aligned} \tag{5}$$

Indices n and m here correspond to the node numbering along the x and y axes, respectively, and notation NN implies summation over the nearest neighbors.

The existence of periodic boundary condition makes it possible to pass to the effectively 1D case; in this case, the set of energy parameters is supplemented with quasi-momentum k along the x axis, which also affects the realization of the edge state. The wavefunction for the one-electron state with spin projection σ and quasi-momentum k has the form

$$\Psi_{k\sigma} = A\sum_{m}e^{ikm}\sum_{n=1}^{N}[u_{n\sigma}a^{+}_{nm\sigma} + v_{n\sigma}d^{+}_{nm\sigma}]|0\rangle, \tag{6}$$

where the expansion coefficients are the solutions to the general equation:

$$\begin{aligned}Eu_{n\sigma} &= (-\Delta\varepsilon + t^{-}_{k})u_{n\sigma} - s_{k\sigma}v_{n\sigma} \\ &+ t^{-}(u_{n+1m\sigma} + u_{n-1m\sigma}) + \alpha(v_{n+1\sigma} - v_{n-1\sigma}), \\ Ev_{n\sigma} &= (\Delta\varepsilon + t^{+}_{k})v_{n\sigma} - s_{k\sigma}u_{n\sigma} \\ &+ t^{+}(v_{n+1m\sigma} + u_{n+1m\sigma})v_{n\sigma} - \alpha(u_{n+1\sigma} - u_{n-1\sigma}), \\ t^{\pm}_{k} &= 2t^{\pm}\cos k; \quad t^{\pm} = t \pm \Delta t, \\ s_{k\sigma} &= 2\alpha\sigma\sin k, \quad \sigma = \pm 1.\end{aligned} \tag{7}$$

The general solution for the expansion coefficients can be written in the form

$$u_{n\sigma} = ue^{\lambda n}, \quad v_{n\sigma} = ve^{\lambda n}. \tag{8}$$

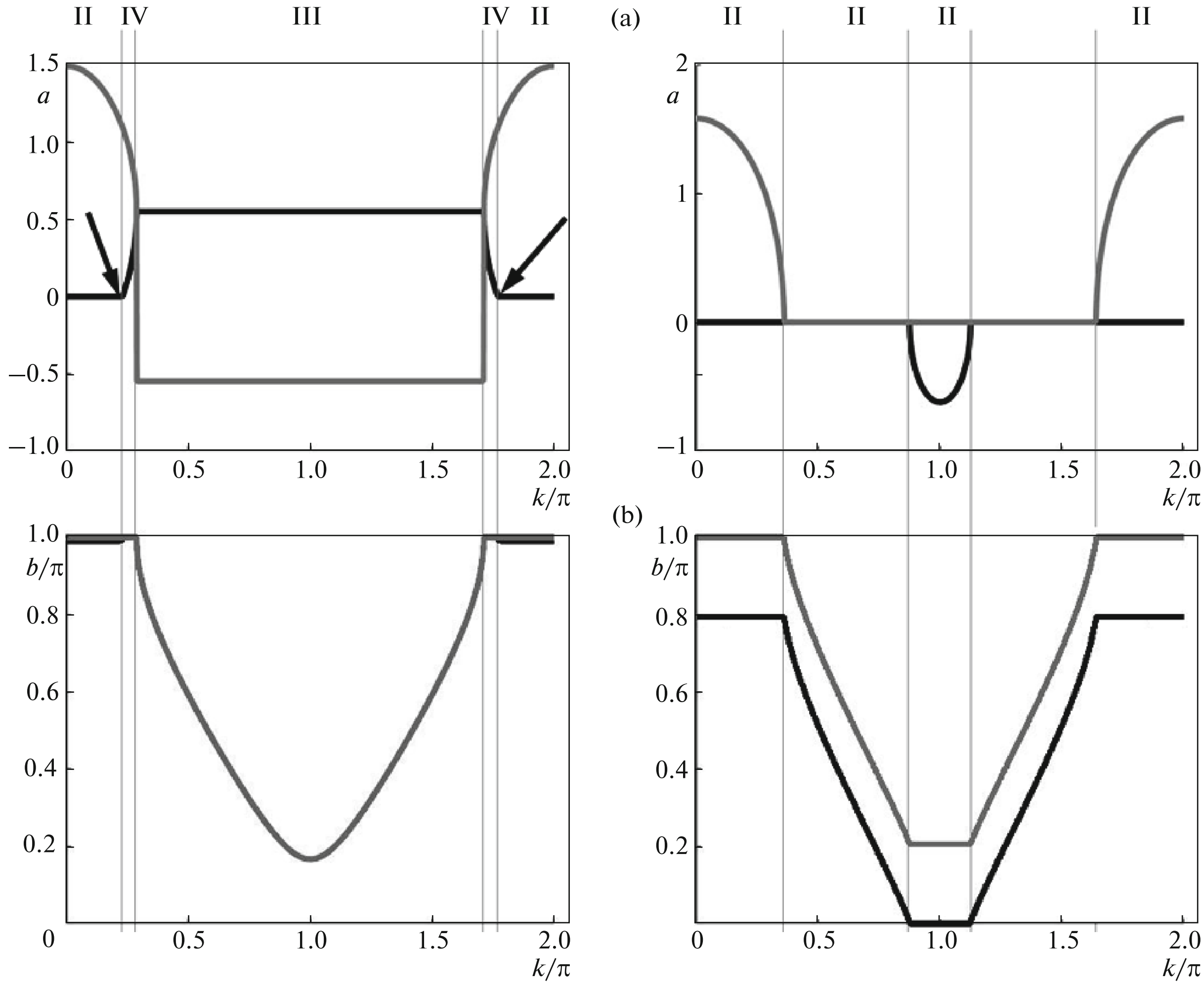

Fig. 3. Real (top) $a = \mathrm{Re}\lambda$ and imaginary (bottom) $b = \mathrm{Im}\lambda$ parts of the exponents for the solution changing from the edge to the nonedge type upon a change in quasi-momentum k (left) and being of the nonedge type in the entire range of k values (right) in the BHZ model with the cylindrical geometry; $t = 0$, $\Delta t = 1$, $\alpha = 0.5$, $\Delta\varepsilon = 0.5$, and $N = 100$. Roman numerals indicate the type of general solutions.

Here, if λ is a solution, $-\lambda$ and λ^* are also solutions. In this case, there exist four sets for $\lambda = a + ib$:

I. $\lambda = \pm ib_1, \pm ib_2$;

II. $\lambda = \pm a_1 + i\pi l, \pm ib_1$;

III. $\lambda = \pm a_1 \pm ib_1$;

IV. $\lambda = \pm a_1 + i\pi l_1, \pm a_2 + i\pi l_2$.

Here, a and b are real-valued nonzero quantities, and the correction $+i\pi l$, where l is an integer, has been introduced to take into account the solutions with sign-alternating real-valued solutions. Solutions of type I and II have a nondecreasing component, and their energies lie in the region of band solutions and, hence, cannot be of the edge type. Solutions of types III and IV are edge solutions, since all their components decrease either from the right or from the left edge, and their energies fall into the bulk spectrum gap. Numerical calculations show that bulk solutions of type II, which have an additional decreasing component, as well as edge solutions III inducing spatial oscillation of the probability density, are encountered quite often, which makes it difficult to distinguish between bulk and edge states from the degree of their localization at the boundary (Fig. 2).

Figure 3 shows a typical form of the dependence of λ on k for the state that changes its type from the edge to nonedge depending on k, as well as the state that is of the nonedge type for any value of k. It can be seen that there exists a clearly manifested point k_{cr} at which the state is no longer of the edge type and becomes a bulk state. In the case represented in Fig. 2, the quasi-momentum for which the edge state disappears is $k_{cr} = 1.7675\pi$. The same point corresponds to the splitting of the state energy from the band of bulk states. The behavior of the imaginary part of exponent $b = \mathrm{Im}\lambda$ is inessential.

An important result is the fact that the value of quasi-momentum k_{cr} at which edge states appear depends on

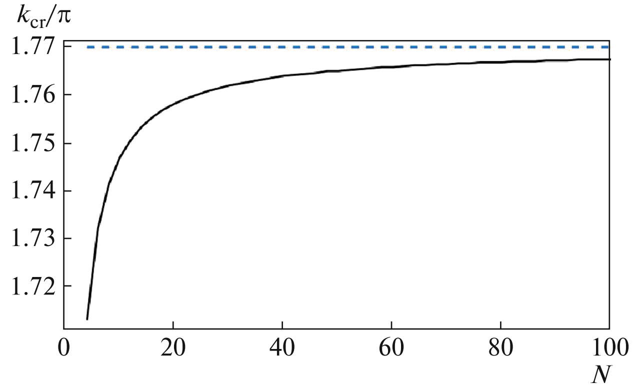

Fig. 4. Dependence of the value of k_{cr} corresponding to the point of transition from the edge to the nonedge state in the BHZ model in the cylindrical geometry on the cylinder length N; $t = 0$, $\Delta t = 1$, $\alpha = 0.5$, and $\Delta\varepsilon = 0.5$. Dashed line corresponds to the value of k_{cr} for $N \to \infty$.

chain length N. Such a dependence shown in Fig. 4 clearly demonstrates that the size of a 1D systems affects the conditions for the emergence of edge states.

5. EDGE STATES IN THE KITAEV FINITE-LENGTH MODEL

Let us illustrate the size effects on the conditions for the emergence of edge excitations using the Kitaev model as an example [8]. We can write the Hamiltonian in the form

$$\mathcal{H}_K = -\sum_{n=1}^{N} \mu a_l^\dagger a_l - t\sum_{l-1}^{N-1}(a_l^\dagger a_{l+1} + a_{l+1}^\dagger a_l) + \sum_{l=1}^{N-1}(\Delta a_l a_{l+1} + \Delta^* a_{l+1}^\dagger a_l^\dagger). \tag{9}$$

The ranges of parameters for which edge states appear in such a model are shown in Fig. 5. Apart from the above-mentioned realization of the zero-energy mode only on special lines [11], the finite size of the system leads to the following two effects. First, the lines bounding the region of realization of edge states and defined as $|\mu| = \pm 2|t|$ in an infinitely long chain become functions of superconducting pairing parameter $|\Delta|$, and the region is the smaller, the shorter the chain. Second, for small values of $|\Delta|$, pockets appear in the regions between the zero excitation energy lines, in which an edge state does not appear. This is due to the fact that strong overlapping of edge excitations striving to be localized at the opposite ends of the chain leads to the excitation energy falling into the bulk region and to a change of the excitation to the nonedge form. Figure 5 also clearly shows the relation between quantity $a = \mathrm{Re}\lambda$ and the depth of the position of the edge excitation in the gap; the maximum is attained in this case at the zero mode lines.

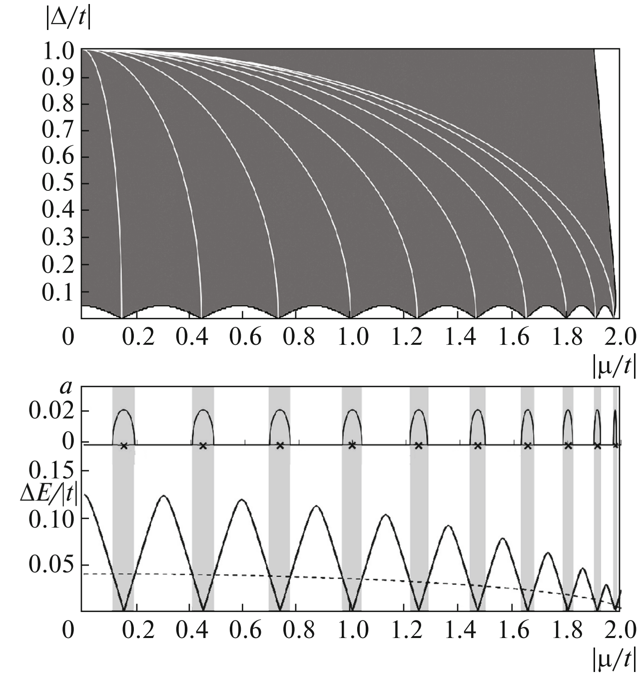

Fig. 5. (top) Domain of existence of edge states in the Kitaev model for chain length $N = 20$ (dark); white curves correspond to Majorana modes. (bottom) Dependences of $a = \mathrm{Re}\lambda$ and the minimal excitation energy on $|\mu/t|$ for $|\Delta/t| = 0.02$; dashed curve is the boundary of bulk excitation zone; crosses indicate the values of the chemical potential for which the Majorana mode is realized.

6. EDGE STATES IN A LIMITTED CHAIN WITH THE SPIN–ORBIT INTERACTION AND INDUCED SUPERCONDUCTIVITY

As another example, we consider a 1D chain with the spin–orbit interaction and induced superconductivity, which is placed into a magnetic field [25, 26]:

$$\mathcal{H}_{wire} = \sum_{n=1,\sigma}^{N}(-\mu + h\sigma)a_{n\sigma}^+ a_{n\sigma} - \sum_{n=1,\sigma}^{N-1}\left(\frac{t}{2}a_{n\sigma}^+ a_{n+1\sigma} + \frac{\alpha}{2}\sigma a_{n\sigma}^+ a_{n+1\bar{\sigma}}\right) + \sum_{n=1}^{N}\Delta a_{n\uparrow}a_{n\downarrow} + \mathrm{H.c.} \tag{10}$$

Figure 6 shows the regions on the diagram of chemical potential μ and magnetic field h, for which edge excitations appear. Like in the case with the Kitaev model, pockets without edge states in case of the finite chain length appear in the region of realization of edge states, which is obtained from analysis of the topological invariant for periodic boundary conditions. Conversely, in the case of a short chain in the range of parameters corresponding to the trivial Majorana number, there exist lines of parameters for which the Majorana modes appear.

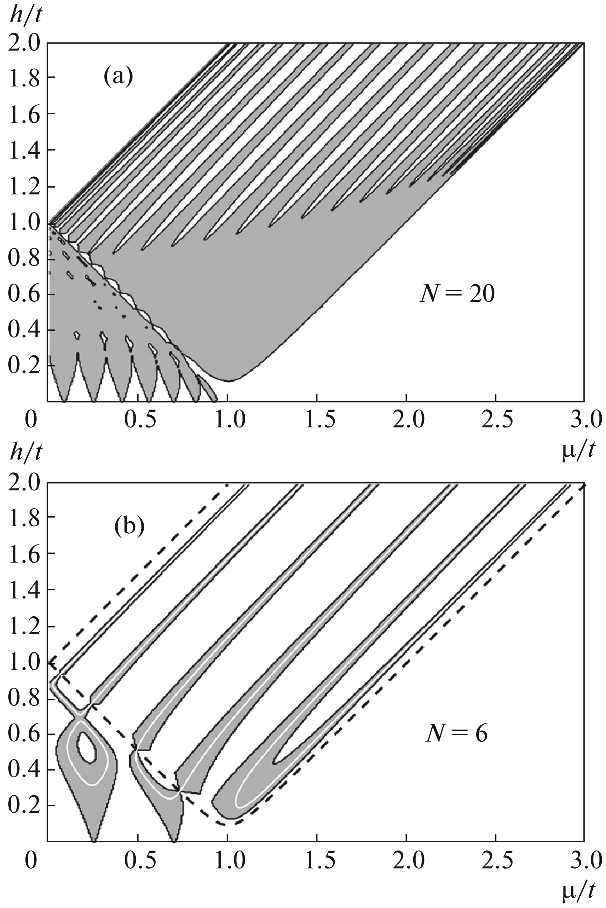

Fig. 6. Domain of realization of edge states in a chain with the spin–orbit interaction and induced superconductivity for (a) $N = 20$ and (b) $N = 6$. Dark regions correspond to parameters for which the edge state exists. White curves in the bottom figure mark the lines of parameters for which the Majorana modes are realized in the chain. The dashed line indicates the parameters for which the bulk gap is closed and the topological invariant changes; $\alpha = 0.5t$, $\Delta = 0.1t$.

In addition, in the range of parameters for $\mu < t$, there exists a region of localization of edge states, which cannot be determined from the topological invariant, because these states possess energy that is not exponentially low, although it is split from the bulk zone (Fig. 7). This region is larger and the excitation energy is split from the bulk zone more clearly, the longer the chain. It should be noted that the existence of a topological transition that is not associated with the Majorana modes in this range of energy parameters has been recently established in [27] from analysis of the spin and charge characteristics of a long chain. The possibility of penetration of edge states in the topologically trivial region has also been demonstrated earlier for a triangular lattice with a noncollinear magnetic order and chiral superconductivity of the d-wave type [28] in the cylindrical geometry. These results show that the method of

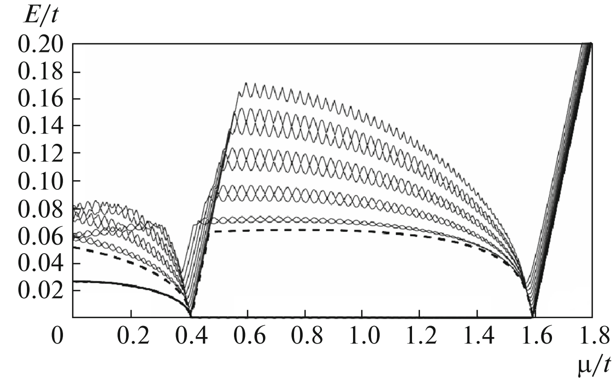

Fig. 7. Dependence of the first 10 energies of intrinsic excitations in a chain with the spin–orbit interaction and superconducting pairing on chemical potential μ. The lower excitation energy is shown by the bold solid curve; the boundary to the region of bulk one-particle excitations is shown by bold dashed curve; $\alpha = 0.5t$, $\Delta = 0.1t$, $h = 0.6t$, and $N = 100$.

topological invariant analysis is inapplicable for the search for the edge solutions in short systems with energy that is not exponentially low and with Majorana modes; other methods (in particular, the one proposed in this study) should be used.

7. CONCLUSIONS

In this study, an approach is proposed for determining the edge states in finite-size 1D systems. As the main criterion, the absence of the general solution with purely imaginary exponent is chosen for the preset energy of state, which is unambiguously related to the determination of energy of such a state beyond the range of allowed energies of bulk states. The effect of the finite chain length on the conditions for the emergence of edge solutions in 1D systems (and those that can be reduced to such systems) is demonstrated for the BHZ model, the Kitaev model, and a chain with the spin–orbit interaction and induced superconductivity. It is shown, in particular, that pockets without edge states appear in the range of parameters with a nontrivial topological index; the size and number of such pockets is determined by the chain length. The emergence of such pockets can also be expected in other effectively one-dimensional finite-size systems in which the lines of parameters corresponding to the realization of the Majorana modes appear. In the case of a chain with the spin–orbit interaction and superconducting pairing, the proposed algorithm for determining edge states has revealed a range of parameters corresponding to the emergence of edge excitations with finite energy in the chain; this range of parameters cannot be determined from analysis of the topological invariant.

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