Charging of Majorana edge modes caused by interaction: Exact results

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The ground-state behavior of a spinless fermion chain with pairing (the Kitaev chain) and an interaction between fermions at neighboring sites is studied for free open boundaries. Using the exact quantum solution, it has been shown that there can exist boundary bound states for many values of the interaction. The interaction produces charging of the vacua of the model and charging of the boundary bound states. The theory also describes the behavior of an XYZ spin-1/2 chain with free open edges.

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I. INTRODUCTION

Recently, Majorana zero-energy edge modes have become a subject of interest to researchers; see, e.g., Refs. [1–3]. According to Ref. [4] those modes can be used as a topological qubit in quantum computers. The qubit is a two-level system, an elementary bit for a quantum computer. A topological qubit can be formed by two Majorana fermions situated at different edges of the system. The topological qubit is more stable with respect to local noise than the standard qubit. It is more difficult to destroy the quantum coherence for a set of such topological qubits. Majorana edge modes were proposed to be realized in many systems, and some realizations have been observed by now; see, e.g., Refs. [5–8].

Majorana edge modes must have energies lying inside the gap of bulk states, to distinguish them from the latter; that is, they are the manifestation of the topological superconductivity. A Majorana state fixed at one edge can be observed [9,10]. In the original contribution [4] and in most of the publications that followed (for a review, see, e.g., Refs. [2,3]), noninteracting fermions were considered. The question appears, How can interactions between fermions affect edge Majorana zero modes in quantum chains? In recent years several studies [11–26] considered such a situation. However, in those works the interaction was taken into account in the framework of, e.g., the density matrix renormalization group (numerically), the Luttinger liquid limit (which neglects higher-energy states), the variational matrix product state technique, or, perturbatively, using, e.g., the renormalization group (except for the exact result [21]; see below). In some works, special cases were studied, in which interacting models were mapped onto noninteracting ones. On the other hand, the theory of integrable models implies that there is a possibility to obtain exact results for the interacting chain. Motivated by that question, based on the exact quantum Bethe ansatz solution, in this paper it is shown that for the interacting Kitaev chain with free open boundaries there can exist boundary bound states equivalent to edge Majorana operators with zero (in the limit of an infinite-length chain) energy. It is also shown that the model possesses degenerate ground states. In addition to simple boundary bound states for the noninteracting system (cf. Ref. [4]), in the interacting case there exist boundary string bound states with zero energy in the infinite chain, caused by the interaction, which yield charged vacua and charged boundary bound states of the system.

II. CONSIDERED MODEL

Let us study the open Kitaev chain of spinless fermions, which interact at neighboring sites, with the Hamiltonian

$$\mathcal{H} = \sum_{j=1}^{L-1}(-\mu[n_j-(1/2)] - (ta_j^\dagger a_{j+1} - \Delta a_j a_{j+1} + \text{H.c.}) + V[n_j-(1/2)][n_{j+1}-(1/2)]) - \mu[n_L-(1/2)]. \quad (1)$$

Here, $a_j^\dagger$ (a_j) denotes the creating (destroying) operator of a spinless fermion at the site j, $n_j = a_j^\dagger a_j$, t denotes the hopping integral, $\Delta = |\Delta|\exp(i\theta)$ denotes the pairing amplitude, $\mu \geqslant 0$ is the chemical potential, V is the nearest-neighbor coupling parameter, and L is the number of sites in the chain. Kitaev [4] considered the noninteracting chain $V = 0$. He suggested that one can replace Dirac fermion operators $a_j^\dagger$ and a_j with other fermion operators, Majorana ones, c_j, $j = 1, \dots, 2L$, as

$$c_{2j-1} = e^{i\theta/2}a_j + e^{-i\theta/2}a_j^\dagger, \quad c_{2j} = -ie^{i\theta/2}a_j + ie^{-i\theta/2}a_j^\dagger, \quad (2)$$

where $j = 1, \dots, L$. Majorana operators satisfy the following relations: $c_j^\dagger = c_j$, and $c_jc_m + c_mc_j = 2\delta_{j,m}$, $j, m = 1, \dots, 2L$. In the representation of Majorana operators the considered Hamiltonian can be rewritten as

$$\mathcal{H} = \frac{i}{2}\sum_{j=1}^{L-1}\bigg(-\mu c_{2j-1}c_{2j} + (t+|\Delta|)c_{2j}c_{2j+1} + (-t+|\Delta|) \times c_{2j-1}c_{2j+2} + \frac{iV}{2}c_{2j-1}c_{2j}c_{2j+1}c_{2j+2}\bigg) - \frac{i}{2}\mu c_{2L-1}c_{2L}. \quad (3)$$

Kitaev has pointed out that the pair of Majorana operators, which forms the Dirac operator, can be connected to the same site of the original lattice, i.e., Majorana operators with the indices $2j$ and $2j-1$ [see Ref. (2)], or to the neighboring sites of the original lattice

$$\tilde{a}_j = (c_{2j} + ic_{2j+1})/2, \quad \tilde{a}_j^\dagger = (c_{2j} - ic_{2j+1})/2. \tag{4}$$

In that case the Majorana operators c_1 and c_{2L} remain unpaired (for instance, they do not enter the Hamiltonian for $|\Delta| = t$ and $V = \mu = 0$). For the chain without interactions $V = 0$, Kitaev has shown that for finite L for $2|t| > |\mu|$ and $\Delta \neq 0$ the system possesses two ground states with an exponentially small energy difference between them and different fermionic parities $P = \prod_j(-ic_{2j-1}c_{2j})$. Both states have the same bulk properties, but they have different boundary ones. It should be mentioned that two Majorana operators can be bonded into a boundary mode, constituting the phase coherence between two edges. Boundary modes are localized at either edge of the chain with zero energy for $L \to \infty$. For the noninteracting situation $V = 0$ the condition $2|t| < |\mu|$ defines the region of a normal superconductor, where there are no boundary states.

Now our goal is to find whether boundary modes can exist in the interacting case. From now on we consider for simplicity the case of real Δ, i.e., $\theta = 0$, and $\mu = 0$. According to Ref. [4], the case with zero chemical potential for $V = 0$ belongs to the interval where two edge Majorana operators are bound into the edge bound state. The Jordan-Wigner transformation [27] $c_{2j-1} = \sigma_j^x \prod_{k=1}^{j-1} \sigma_k^z$, $c_{2j} = \sigma_j^y \prod_{k=1}^{j-1} \sigma_k^z$, with $\sigma_j^{x,y,z}$ being the Pauli operators of the projections of spin 1/2 at the site j, can be applied. In the terms of spin operators, Hamiltonian (1) or (3) can be exactly rewritten as the Hamiltonian of the spin-1/2 XYZ chain with open free boundaries as

$$\mathcal{H} = (1/2)\sum_{j=1}^{L-1}\left(J_x\sigma_j^x\sigma_{j+1}^x + J_y\sigma_j^y\sigma_{j+1}^y + J_z\sigma_j^z\sigma_{j+1}^z\right), \tag{5}$$

with $J_{x,y} = -(t \pm \Delta)$, $J_z = V/2$. After unitary transformation the system has the same set of eigenvalues. Notice, however, that Kitaev has pointed out also that after the *nonlocal* Jordan-Wigner transformation for the $J_z = 0$ case (the XY spin-1/2 chain model) the spin chain is ordered with a nonzero order parameter $\langle\sigma_j^x\rangle \neq 0$ in the ground state [28]. For the spin chain, external fields can interact with the order parameter, breaking the phase coherence between the two mentioned ground states [4].

III. BETHE ANSATZ SOLUTION

In our solution the exact Bethe ansatz integrability [29] is used. In the Bethe ansatz scheme each eigenvalue and eigenstate of the Hamiltonian equations (1), (3), and (5) can be parametrized by the set of quantum numbers, rapidities, u_j. Let us write the parameters of the Hamiltonians (1), (3), and (5) as

$$J_x = -t - \Delta = \frac{e^{i\pi\eta}\vartheta_1[\eta + (\tau/2)]}{\vartheta_1(\tau/2)},$$
$$J_y = -t + \Delta = \frac{e^{i\pi\eta}\vartheta_1[\eta + (1+\tau)/2]}{\vartheta_1[(1+\tau)/2]},$$
$$J_z = \frac{V}{2} = \frac{\vartheta_1[\eta + (1/2)]}{\vartheta_1(1/2)}. \tag{6}$$

Here, $\vartheta_1(u,\tau) = i\exp(i\pi\tau/4)\sum_{m=-\infty}^{\infty}(-1)^m\exp\left(i\pi[(m^2+m)\tau + (2m+1)u]\right)$ is the elliptic theta function, so that the complex values η and τ totally determine the parameters of the Hamiltonians (1), (3), and (5) for any relations between $J_{x,y,z}$ (or between t, Δ, and V). In what follows we will use the standard shorthand notations $\vartheta_{1,2,3,4}(u,\tau) \equiv \vartheta_{1,2,3,4}(u)$, if theta functions are used for the same parameter τ. Here, one considers imaginary τ with $\mathrm{Im}\tau > 0$; sometimes one uses the notation $q = \exp(i\pi\tau)$.

Using the quantum inverse scattering method (the algebraic Bethe ansatz [29]), it is possible to show that Hamiltonian equation (5) [and hence Hamiltonian equations (1) and (3)] is the derivative (up to the constant multiplier; see below) of the logarithm of the transfer matrix $t(u)$ with respect to the spectral parameter u taken at $u = 0$, where

$$t(u) = \mathrm{Tr}_0[K_0^+(u)L_{0L}(u)L_{0L-1}(u)\cdots L_{01}(u) \times K_0^-(u)L_{10}(u)L_{20}(u)\cdots L_{L0}(u)]. \tag{7}$$

Here, 0 denotes the auxiliary subspace, and each L operator can be written as $L_{0j}(u) = \sum_{\alpha=0,x,y,z} w_j(u)\sigma_0^\alpha \otimes \sigma_j^\alpha$, with $\sigma^0 = I$ being the unity matrix. The following functions are used: $w_{x,y}(u) = [c(u) \pm d(u)]/2$ and $w_{0,z}(u) = [a(u) \pm b(u)]/2$, with

$$a(u) = \frac{\vartheta_4(u,2\tau)\vartheta_1(u+\eta,2\tau)}{\vartheta_4(0,2\tau)\vartheta_1(\eta,2\tau)},$$
$$b(u) = \frac{\vartheta_1(u,2\tau)\vartheta_4(u+\eta,2\tau)}{\vartheta_1(0,2\tau)\vartheta_4(\eta,2\tau)},$$
$$c(u) = \frac{\vartheta_4(u,2\tau)\vartheta_4(u+\eta,2\tau)}{\vartheta_4(0,2\tau)\vartheta_4(\eta,2\tau)},$$
$$d(u) = \frac{\vartheta_1(u,2\tau)\vartheta_1(u+\eta,2\tau)}{\vartheta_1(0,2\tau)\vartheta_1(\eta,2\tau)}, \tag{8}$$

where $\vartheta_4(u,\tau)$ is the elliptic theta function $\vartheta_4(u,\tau) = \exp\left(-i\pi[u + (1/2) + (\tau/4)]\right)\vartheta_1[u + (\tau/2)]$. L operators satisfy the Yang-Baxter equation [29–31]

$$L_{12}(u-v)L_{13}(u-w)L_{23}(v-w) = L_{23}(v-w)L_{13}(u-w)L_{12}(u-v). \tag{9}$$

The reflection matrices $K_0^\pm(u)$ for free open boundary conditions can be written as unitary 2×2 matrices I in the auxiliary subspace as

$$K^- = \frac{\vartheta_1(2u)}{2\vartheta_1(u)}I, \quad K^+ = \frac{\vartheta_1(-2u-2\eta)}{2\vartheta_1(-u-\eta)}I; \tag{10}$$

they satisfy the reflection equations [29,32,33]

$$L_{12}(u-v)K_1^-(u)L_{21}(u+v)K_2^-(v) = K_2^-(v)L_{12}(u+v)K_1^-(u)L_{21}(u-v),$$
$$L_{12}(v-u)K_1^+(u)L_{21}(-u-v-2)K_2^+(v) = K_2^+(v)L_{12}(-u-v-2)K_1^+(u)L_{21}(v-u). \tag{11}$$

Transfer matrices with different spectral parameters commute, $[t(u), t(v)] = 0$; this constitutes the exact integrability of the problem [31,34]. Then, the Hamiltonian of the open free chains, which can be presented as a function of the transfer matrix,

$$\mathcal{H} = \frac{\vartheta_1(\eta)}{2\vartheta_1'(u)_{u=0}}\left[\left(\frac{t'(u)}{t(u)}\right)_{u=0} - (L-1)\frac{\vartheta_1'(\eta)}{\vartheta_1(\eta)} - \frac{\vartheta_1'(2\eta)}{\vartheta_1(2\eta)}\right], \tag{12}$$

where $t'(u) = \partial t(u)/\partial u$ and $\vartheta_1'(u) = \partial\vartheta_1(u,\tau)/\partial u$, commutes with $t(u)$ and hence has the same set of eigenfunctions as the transfer matrix $t(u)$.

In the framework of the Bethe ansatz there are many ways to obtain the set of equations for rapidities. In this paper the procedure of the functional Bethe ansatz (also called T-Q relations [31,35]) is used. For instance, one can apply the result of the T-Q relations of the XYZ spin-1/2 chain with arbitrary boundary fields [36] to the case of free open boundaries. For odd L the rapidities $u_{j=1}^M$ satisfy the Bethe ansatz equations (BAEs)

$$X_{\eta/2}^{2L+1}(u_j)X_{\eta/2}^{-1}[u_j + (1/2)]X_{\eta/2}^{-1}[u_j - (1+\tau)/2] \times X_{\eta/2}^{-1}[u_j + (\tau/2)] = \prod_{k=1}^{M} X_\eta(u_j - u_k)X_\eta(u_j + u_k), \tag{13}$$

where $M = (L-1)/2$ and $X_\alpha(u) = \vartheta_1(u+\alpha)/\vartheta_1(u-\alpha)$. The eigenvalue of the Hamiltonian is

$$E = \frac{\vartheta_1(\eta)}{\vartheta_1'(u)_{u=0}}\left(-\frac{L-1}{2}\frac{\vartheta_1'(\eta)}{\vartheta_1(\eta)} + \sum_{j=1}^{M}\left[\frac{\vartheta_1'(u_j - [\eta/2])}{\vartheta_1(u_j - [\eta/2])} - \frac{\vartheta_1'(u_j + [\eta/2])}{\vartheta_1(u_j + [\eta/2])}\right]\right). \tag{14}$$

IV. LIMITING CASES

First, let us consider two known limiting cases of the BAEs and the energy. The case $J_x = J_y$ ($\Delta = 0$) corresponds to the limit $\tau \to = +i\infty$. For that limit we can use the first terms in the series for theta functions, $\lim_{\tau\to+i\infty}\vartheta_1(u) = -2\exp(i\pi\tau/4)\sin(\pi u) + \cdots$, and $\lim_{\tau\to+i\infty}\vartheta_4(u) = 1 - 2\exp(i\pi\tau)\cos(2\pi u) + \cdots$. In that case the expressions for the Hamiltonian, the energy (14), and the BAEs (13) coincide with the Hamiltonian, the energy, and the BAEs of the XXZ spin-1/2 chain, respectively (or the Hamiltonian and the energy of the interacting spinless fermions without pairing); see, e.g., Ref. [37]. Notice that for the easy-axis anisotropy case of the XXZ spin chain one uses imaginary values of η, while for the easy-plane case real values of η are used. That limiting case was studied in detail in Ref. [37]. It was shown there that for the open chain with free edges for the easy-axis anisotropy ($|J_x = J_y| < J_z$) of the XXZ antiferromagnetic spin chain related to the Mott insulator case $V > 2|t|$ of the spinless fermion chain there exist solutions of the BAEs localized at the boundary with zero energy at $L \to \infty$; the analysis is equivalent to the one presented below. In the simplest case they are related to zero Majorana modes; however, there are other boundary bound states (strings; see below) with zero energy at $L \to \infty$. On the other hand, for the easy-plane anisotropy ($|J_x = J_y| \geqslant J_z$) of the XXZ spin chain related to the metallic case $V \leqslant 2|t|$ of fermions there are no such boundary bound states for the chain with free boundaries. Similar results can be obtained for $J_x = J_z$ ($-t - \Delta = V/2$) or $J_y = J_z$ ($-t + \Delta = V/2$). In the former case, localized boundary bound states exist for $|J_x = J_z| < J_y$ [i.e., for $V = -2(t + \Delta)$ with $|-t-\Delta| < -t + \Delta$], while in the latter case they exist for $|J_y = J_z| < J_x$ [for $V = 2(\Delta - t)$ with $|-t+\Delta| < -t-\Delta$].

In the other known limiting case it is easy to see that the BAEs for the case in which any of the coupling constants $J_{x,y,z}$ is equal to zero [38] (such a limiting case can be reached by the choice of the parameter η) describe noninteracting quasiparticles: The right-hand sides of Eqs. (13) do not depend on u_k, i.e., each rapidity u_j is determined from its own equation, independent of other rapidities. Notice that specifically such a situation was studied in Refs. [20,23–26] for $t = \Delta$, related to $J_y = 0$ [it is reached for $\eta = -(1+\tau)/2$]. For example, for the noninteracting Kitaev chain $J_z = V/2 = 0$ [4] (or the XY spin-1/2 chain) the condition $\eta = 1/2$ can be applied. For that case, $J_x = J_y^{-1} = i\vartheta_1[(1+\tau)/2]/\vartheta_1(\tau/2) = \vartheta_3(0,\tau)/\vartheta_4(0,\tau)$, where $\vartheta_3(u,\tau) = \vartheta_4(u + [1/2], \tau)$ is the elliptic theta function. The BAEs are the quantization conditions for quasimomenta (the latter can be written as a function of the rapidities for any Bethe ansatz solvable model [29]) of noninteracting quasiparticles. In the general case of $\Delta \neq 0$ ($J_x \neq J_y$) there exist solutions of the BAEs, which describe boundary bound states. Physical eigenstates, related to those solutions, have zero energy for $L \to \infty$ and are nothing else than Majorana zero edge modes. On the other hand, taking then the limit $\tau \to +i\infty$, the situation without pairing of noninteracting fermions ($\Delta = 0$, $t = -1$), i.e., the spin-1/2 XX chain ($J_x = J_y = 1$), is obtained. In that case there are no boundary bound states and, thus, no edge Majorana modes in the system, in agreement with the analysis [4] for $\mu = 0$.

V. GENERAL CASE

Then, returning to the general case of the interacting Kitaev chain (or the XYZ spin-1/2 chain), the most important situation will be studied, namely, the so-called thermodynamic limit, in which one has $L \to \infty$, $M \to \infty$ with the finite ratio M/L. The standard technique of the Bethe ansatz is used [29]. Obviously, in the thermodynamic limit there must be no difference between even and odd L, while for the finite L such a difference exists. The ground state of any fermion system is formed by the total filling of the Fermi sea: All eigenstates with negative energies have a filling factor of 1, while for eigenstates with positive energies the filling factor is zero. Simple excitations of fermion systems are related to holes for eigenstates with negative energies and/or filling of eigenstates with positive energies, or combinations of such states. In the main contribution in the L^{-1} approximation ($E = LE_0 + E_1 + \cdots$; i.e., for E_0), the ground state of our system corresponds to only real roots of Eqs. (13) for u_j. Due to nonzero V there can exist many other solutions to Eqs. (13), namely, bound states (called strings) [29], which are related to complex values of u_j. Such states do not exist, obviously, for the noninteracting Kitaev chain or the XY spin-1/2 chain. However, none of those string solutions have negative energies, and therefore they do not contribute to the ground-state formation [31,34,35]. (Notice that for finite L the situation can be different.)

Using the known Bethe ansatz technique for densities of roots of BAEs in the thermodynamic limit [29], the main contribution in L^{-1} to the ground-state energy can be found (from now on the region of totally imaginary η with $0 < -i\eta < -i\pi\tau\vartheta_3^2(0)/8$ is considered [34]; it is possible to show [31,34,39] that other regions of parameters of the Hamiltonian can be obtained using that solution):

$$E_0 = \frac{\vartheta_1(\eta)}{\vartheta_1'(u)_{u=0}}\left[i\pi + 2i\pi\sum_{n=1}^{\infty}\frac{\sin[\pi n(\tau-\eta)]}{\sin(\pi n\tau)\cos(\pi n\eta)} - \frac{\vartheta_1'(\eta)}{2\vartheta_1(\eta)}\right]. \quad (15)$$

This coincides with the ground-state energy of the periodic spin-$1/2$ XYZ chain (in the thermodynamic limit) [31,34].

Elementary bulk excitations with respect to the ground state are related to holes in the distribution of real rapidities u_j, which form the Fermi sea (i.e., which have negative energies) [40]. The generic physical excitation, related to two holes, $u_{1,2}$, has the energy

$$e_e = i\pi\frac{\vartheta_1(\eta)}{\vartheta_1'(u)_{u=0}}\sum_{1,2}\sum_{n=-\infty}^{\infty}\frac{\exp[i\pi n u_{1,2}]}{\sin(\pi n\tau)\cos(\pi n\eta)}, \quad (16)$$

with the quasimomenta of each hole related to the rapidity via $p_{1,2} = -i\ln X_{\eta/2}(u_{1,2})$. Each hole carries the fractional charge $1/2$ with respect to the ground state. (Notice that for finite odd L there exist excitations related to one hole in the distribution of the rapidities situated at the edge of the band (real roots of the BAE u_j are distributed in the interval $[-1, 1]$), i.e., with $u = \pm 1$, which is gapless. However, it is possible to show that the eigenfunctions (see, e.g., Ref. [35]) of those states are exactly zero in the thermodynamic limit.) According to Ref. [41], physical excitations can carry only integer charge, i.e., they are formed by an even number of holes, so the elementary generic physical bulk excitation is formed by the pair of holes. Such a state has an activation (gap) [40] for any nonequal pairs of $|J_{x,y,z}|$ (nonequal $|-t-\Delta|, |-t+\Delta|, |V|/2$).

This work is interested in the finite-size corrections to the energy E_0 of the order of L^{-1} [29]. Those corrections determine, among other important properties, the difference between the system with periodic boundary conditions and the system with open boundary conditions. Edges of the chain in the limit $L \to \infty$ do not interact, so one can consider the effects of both edges separately. Let us first consider, for instance, the left edge of the chain. The most interesting contribution from open free edges is determined by the second, third, and fourth multipliers on the left-hand side of Eqs. (13), which are present in the BAEs for the open chain and absent for the ones for the periodic chain [31,34]. Let us investigate the effect of those terms separately. Consider the effect of the second term. Similar to Refs. [37,42], the additional (with respect to the bulk ones) root of Eqs. (13) can be found, namely, with $u_0^{(1)} = -(1/2) + (\eta/2)$ (imaginary η). It is the solution to Eqs. (13) because of the mutual cancellation of the increasing modulus of the first multiplier on the left-hand side of Eqs. (13) and the decreasing modulus of the second multiplier, when $L \to \infty$ and $u_j \to u_0^{(1)}$. That boundary bound state is localized at the left edge of the chain: Its eigenfunction decays exponentially with the distance from that edge. Such a boundary bound state has the energy

$$e_b^{(1)} = -\frac{\vartheta_1(\eta)}{\vartheta_1'(u)_{u=0}}\left(\frac{\vartheta_1'(\eta-[1/2])}{\vartheta_1(\eta-[1/2])} + 2\pi i[1+2\cot(2\pi\eta)]\right). \quad (17)$$

The second term in Eq. (17) is introduced to remove the solution $u_j = u_0^{(1)}$ from the right-hand side of the BAEs to keep the total number of solutions M. That procedure is often called the renormalization of the vacuum [42]. The boundary bound state has *negative* energy, and hence it contributes to the Fermi sea of the open chain. The boundary bound state carries the fractional charge $-1/2$ with respect to the ground state of the periodic chain. The energy of that bound state is smaller than the energy of the minimal bulk excitation. This means that such a boundary bound state of the interacting fermion chain has an energy whose value is inside the gap for bulk excitations. For the interacting chain there also exist boundary bound states, which correspond to complex boundary solutions to Eqs. (13), similar to the string bound states of the bulk. They correspond to the roots of Eqs. (13) of the form $u_0 - 2l\eta, u_0 - 2(l-1)\eta, \dots, u_0 + 2m\eta$ with integer $m, l \geqslant 0$ (the case $m = l = 0$ is the "pure" boundary bound state). They also carry fractional charges. However, it is possible to show, similar to the analysis of Refs. [37,42], that either their energies are zero for strings with nonzero m and $l = 0$ (they represent charged vacua) or they are equal to $e_b^{(1)}$ for boundary strings with nonzero m and $l \geqslant 1$ (they represent charged boundary excitations). There are no such string boundary states for the noninteracting case $V = 0$. Similar to bulk excitations, physical boundary excitations also should carry an integer charge. The analysis shows that the boundary state at the other (right) edge of the chain has the energy $-e_b^{(1)}$ (i.e., it is *positive*) and carries positive charge $1/2$. [The other possibility to keep the integer total charge of the Fermi sea of the system is to have the bulk excitation (the hole in the distribution of rapidities with real u_j) with the energy $-e_b^{(1)}$ and the charge $1/2$.] Hence the energy of the physical boundary edge states of this type is zero in the thermodynamic limit $L \to \infty$, and the physical boundary bound state carries zero charge. It does not matter at which edge the boundary bound state with the negative energy is situated; hence the doubly degenerate situation takes place, as in the noninteracting case [4].

A similar analysis can be applied to the third and fourth multipliers of the left-hand side of the BAEs (13). Boundary bound states at each edge with $u_0^{(2)} = (1+\tau)/2 + (\eta/2)$ and $u_0^{(3)} = -(\tau/2) + (\eta/2)$, respectively, and related boundary bound strings for the general case $V \neq 0$ are found. Those solutions also describe boundary bound states carrying fractional charges. However, their energies are positive, and hence these states do not contribute to the ground state.

In general our analysis shows that boundary bound states and strings with zero energy for $L \to \infty$ (the former are totally equivalent to pure Majorana edge states for the noninteracting case: They are located at the edges of the chain,

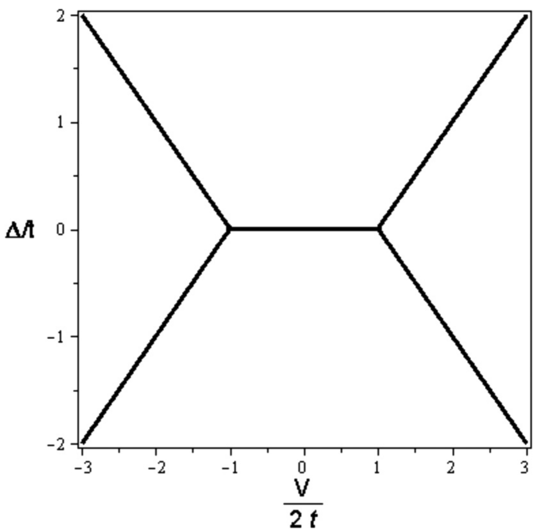

FIG. 1. The ground-state phase diagram of the interacting Kitaev chain.

they have zero energy, being inside the gap of bulk eigenstates, and they are doubly degenerate, according to the definition in Ref. [4]) in the Kitaev chain exist for any finite interaction V between fermions if $|-t-\Delta|$, $|-t+\Delta|$, and $|V|/2$ (or $|J_x|$, $|J_y|$, and $|J_z|$) are pairwise unequal to each other. For pairwise equal cases, pure boundary bound states exist, e.g., for the spinless fermion counterpart with strong coupling of the easy-axis magnetic (XXZ) spin-1/2 chain. In that case, bulk eigenstates are gapped, and there exist doubly degenerate pure boundary bound eigenstates with zero energy [37]: From those aspects they have the same properties as Kitaev's zero modes [4]. Notice that the XXZ gapped case belongs to the region of existence of so-called strong zero modes, studied exactly by Fendley [21]. In contrast, for $\Delta = 0$ and $|V| \leqslant 2|t|$, i.e., the normal metallic regime, the counterpart of the easy-plane spin chain, the localized boundary bound states do not exist. In Fig. 1 the zero-temperature phase diagram is presented. Boundary zero-energy modes exist everywhere except on the bold lines, which distinguish phases with different order parameters for the spin-1/2 XYZ chain counterpart. In the phases with large $|V|$ (left and right parts of the figure) the magnetic order parameter is directed along the z axis (the ordering is ferromagnetic for $V < 0$ and antiferromagnetic for $V > 0$), while the phases with large $|\Delta|$ (upper and lower parts of the figure) manifest the ordering with the magnetic order parameter directed along axes x and y, depending on the relative values of J_x and J_y. The region of the existence of boundary bound states obtained in this paper agrees with the exact result obtained in Ref. [21]. Fendley provided explicit expressions for the operators of strong zero modes in the XYZ spin-1/2 chain. With the BAE technique used in this paper, it is demanding to obtain such expressions for those operators. In the conclusion of Ref. [21], Fendley asks to what extent his results are related to the integrability of the model. From this viewpoint, the present results, based on the integrability, provide the complementary information about boundary zero-energy modes compared with Ref. [21]. However, the technique used in Ref. [21] does not permit one to study boundary strings, i.e., the charging of boundary modes (and vacua), which is shown here to be present in the considered model. Boundary strings, as well as other strings, appear as eigenstates *only* in interacting systems; hence they are the manifestation of the interaction present in the model compared with the noninteracting Kitaev case. While pure boundary bound states with zero energy, considered in this paper, have the same properties as Kitaev's zero-energy edge modes, the boundary bound strings differentiate the noninteracting case from the interacting one. In the field-theoretical approach the boundary bound strings can be interpreted as "breathing" of the pure boundary bound states. The fact that those boundary bound strings have the same (zero) energy as simple boundary bound states (which can be considered as strings of length 0) means that interaction in the Kitaev chain produces a much higher level of degeneracy of boundary bound states than is produced in the noninteracting Kitaev chain.

The ground-state behavior of the interacting spinless fermion periodic chain with pairing (related to the XYZ spin-1/2 chain) is reminiscent of that of the chain of fermions without pairing in the strong-interaction regime (easy-axis XXZ spin-1/2 chain). This is not a surprise, because already Gaudin pointed out that similarity [35]: For example, the density of real roots of the Bethe ansatz equation in the thermodynamic limit $L \to \infty$ for the ground state does not depend on τ. However, for the open chain there exists a difference, which results, e.g., in the boundary bound states of several types (though some of them do not contribute to the ground-state formation).

The ground-state surface energy E_s, which is the difference between the ground-state energy of the fermion chain with free open boundary conditions [related to $M = (L-1)/2$ for both situations in the thermodynamic limit] and the ground-state energy of the chain with periodic boundary conditions, is

$$E_s = \frac{\vartheta_1'(\eta)}{\vartheta_1'(0)} - \frac{\vartheta_1(\eta)}{\vartheta_1'(0)}\left(\frac{\vartheta_1'(\eta-[1/2])}{\vartheta_1(\eta-[1/2])} + \sum_{n=1}^{\infty}\frac{2\pi i}{\cos(\pi n\eta)}[\sin(\pi n[\tau-\eta-1]) - \sin(\pi n[\eta+1]) + \sin(\pi n[\eta-1])\cos(\pi n[2\eta-1])]\right). \quad (18)$$

VI. SUMMARY

In summary, using the exact integrability of the considered model, it has been shown that for the interacting spinless fermion chain with pairing for open free boundary conditions, edge bound states emerge. The regions of values of the interaction between nearest-neighbor fermions, at which they exist, have been analyzed. The energy of those edge modes is zero for the infinite chain, and there is a degeneracy of the ground state, similar to the noninteracting spinless fermions with pairing (Kitaev chain). On the other hand, we show that boundary string states for such a one-dimensional interacting topological superconductor can exist. Those strings charge the vacua and physical boundary bound states. This means that in the interacting Kitaev chain, zero-energy boundary bound states are highly degenerate. The developed theory also describes the behavior of the XYZ spin-1/2 chain with free open edges. The exact information about edge modes with zero energy, studied in this paper, can be used for the description of the behavior of topological qubits in topological quantum computation, because interaction effects (though perhaps small) have to be present in any realistic quantum devices. When constructing topological qubits, one needs to take into account the higher degeneracy of zero edge Majorana modes due to their charging caused by the interfermion interaction. It will take additional efforts to distinguish pure edge Majorana modes from other string boundary bound states.

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