Expectation value of the edge Majorana fermion in an interacting fermion chain

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The expectation value of the edge Majorana operator is calculated for the one-dimensional model of spinless fermions with nearest-neighbor interactions and with open boundary conditions. The consideration is performed for the regime of the topological insulator (gapped bulk excitations and edge modes inside the gap), and for the normal metal regime (gapless bulk excitations). We show that the expectation value of the edge Majorana operator can be formed by two contributions, from the bulk states, and from the localized edge modes.

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I. INTRODUCTION

Majorana fermions [1], especially Majorana edge states, are of great interest for researchers past years. Kitaev has proposed to use those states as a topological qubit [2]. The latter is a two-level system (the Dirac fermion), composed of two Majoranas, situated, e.g., at opposite edges of a fermionic chain. By construction, the topological qubit is more stable than the standard bulk fermion, because local noises perturb only parts of that composite qubit. Local interactions cannot yield decoherence because they cannot distinguish between the computational basis states, constituting the topological protection of qubit operations. Since that time, a number of scenarios of existent Majorana edge modes in real systems were proposed, and many experiments, see, e.g., Refs. [3–6], reported the observation of Majorana zero modes.

To be distinguishable from other eigenstates, Majorana edge modes must have energies lying inside the gap of bulk states. This is why, in the most of studies connected with Majorana edge modes, the system of fermions with pairing was used. Naturally, we discuss only edge Majorana modes, not, e.g., Andreev bound states, which can exist inside the gap of a superconducting system also. The important property of the edge Majorana modes is that, unlike, e.g., Andreev states, they have zero energy, i.e., they are bound at the Fermi energy. The pairing yields the gap for bulk states, and Majorana edge modes exist (according to the special conditions for the parameters of the system, see Refs. [2,7,8]) with their energies inside that gap. In fact, Majorana edge modes in that case are the manifestation of the topological superconductivity. Topological qubits due to the mentioned topological protection are expected to have long coherence times, growing exponentially with the distance between Majoranas, permitting manipulation with them and reading the information from them, however without a strong effect of the randomly fluctuating environment, for the recent reviews see, e.g., Refs. [9–11].

In this contribution we consider a different situation: We study edge Majorana states in the gapped fermionic system *without pairing*, however, with interactions between fermions, which causes the gap for bulk eigenstates, but with the gapless edge states, i.e., the topological insulator instead of the topological superconductor of previous propositions [2,7,8]. As the main subject of our study, we consider the one-dimensional system of spinless fermions with open boundary conditions. The advantage of the proposed model is the possibility of obtaining exact results, because the model is integrable. Unlike previous work where interactions in the spinless fermion chains with pairing were considered [12–18], here we study systems without pairing. To govern the state of the edge Majorana fermions, for example, for manipulating topological qubits the gates (which are in quantum mechanics local unitary transformations) acting on the edge Majorana modes, are used. Notice that only Clifford gates (e.g., Hadamard or phase ones) can be implemented directly to a single topological qubit [19], while other important gates, e.g., CNOT gates imply the involvement of additional topological qubits. One needs to know, among other things, how the expectation value of those edge Majorana fermions depends on external governing parameters and the parameters of the system. In quantum computation it is important to initialize the register of the qubit in the well-defined state. One of the possibilities of such an initialization of the topological qubit based on the Majorana edge operators, forming the Majorana zero mode, is the application of local fields to edge Majorana operators. For that purpose the knowledge of the expectation values of the edge Majorana operators is highly desirable. For the standard Kitaev chain (noninteractiong spinless fermions with pairing), such a program was realized [20]. Possible realizations of the proposed model situation is also discussed.

II. CONSIDERED SYSTEM

Let us study the properties of the interacting spinless fermion chain with open boundaries, the Hamiltonian of which has the form

$$\mathcal{H} = \sum_{j=1}^{L-1}\biggl(-\mu\biggl[n_j - \frac{1}{2}\biggr] - t(a_j^\dagger a_{j+1} + \text{H.c.}) + V\biggl[n_j - \frac{1}{2}\biggr]\biggl[n_{j+1} - \frac{1}{2}\biggr]\biggr) + h(a_1^\dagger + a_1) - \mu\biggl[n_L - \frac{1}{2}\biggr], \tag{1}$$

where $a_j^\dagger$ (a_j) creates (destroys) a spinless fermion at the site j, $n_j = a_j^\dagger a_j$, t is the hopping integral, $\mu \geqslant 0$ is the chemical potential, V denotes the nearest-neighbor interaction, and L is the number of sites of the chain. The Lagrange multiplier $h \geqslant 0$ is introduced to describe the expectation value of the edge Majorana fermion, see below. It can be considered also as the external governing parameter. One can replace [2] $2L$ Dirac operators $a_j^\dagger$ and a_j by $2L$ Majorana ones, c_n, as

$$c_{2j-1} = a_j + a_j^\dagger, \quad c_{2j} = -ia_j + ia_j^\dagger, \tag{2}$$

with $j = 1, \dots, L$ ($c_j^\dagger = c_j$). Majorana operators satisfy the fermion commutation relations $c_j c_m + c_m c_j = 2\delta_{j,m}$ $j, m = 1, \dots, 2L$. Using the Majorana representation for the interacting case $V \neq 0$ we obtain ($n_j - (1/2) = (i/2)c_{2j-1}c_{2j}$) the expression for the Hamiltonian

$$\mathcal{H} = \frac{i}{2}\sum_{j=1}^{L-1}\biggl(-\mu c_{2j-1}c_{2j} + t(c_{2j}c_{2j+1} - c_{2j-1}c_{2j+2}) + \frac{iV}{2}c_{2j-1}c_{2j}c_{2j+1}c_{2j+2}\biggr) - \frac{i}{2}\mu c_{2L-1}c_{2L} + hc_1\,. \tag{3}$$

Then from the basics of quantum mechanics it is clear that the expectation value of the edge Majorana operator $\langle c_1\rangle$ is the derivative of the free energy of the system with the Hamiltonian (3) with respect to h.

Kitaev has pointed out for the spinless fermion chain that for the formation of Dirac operators, the pair of Majorana operator can be related to the same site of the original lattice (i.e., to the indices $2j$ and $2j-1$, see above), or to the neighboring sites of the original lattice

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

In that representation the Majorana operators c_1 and c_{2L} remain unpaired. Kitaev has shown that for finite L in the noninteracting chain $V = 0$ for $2|t| > |\mu|$ and nonzero pairing amplitude the system possesses two ground states with exponentially small energy difference between them and different fermionic parities $P = \prod_j(-ic_{2j-1}c_{2j}) \equiv \prod_j(2n_j - 1)$. Both states have the same bulk properties, however, different edge ones. One of these phases can be transformed into the other one and vice versa by the permutation of Majorana operators. The mentioned 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 $L \to \infty$. In the absence of interactions $V = 0$ without pairing the condition $2|t| > |\mu|$ just defines the region of a normal metal. In this case there are no boundary states. For the case without pairing, however with nonzero interaction V and $h = 0$, i.e., for free edges, we have shown recently that for the case $V \geqslant 2|t| \geqslant 0$ there can exist Majorana edge localized modes inside the gap of bulk eigenstates [21]. There are also two degenerate ground states, i.e., the situation is similar to the one of the Majorana edge states of the open chain of noninteracting spinless fermions with pairing, considered by Kitaev.

III. EXACT SOLUTION

In this contribution our aim is to find the expectation value of Majorana edge operator c_1 (the consideration of the operator c_{2L} can be performed in a similar, however, more complicated way). For simplicity reasons we limit ourselves with the case $\mu = 0$.

To find the exact quantum mechanical solution of the system with the Hamiltonian (1) we can use the quantum inverse scattering method (or the algebraic Bethe ansatz) [22]. Using the Jordan-Wigner transformation [23] $c_{2j-1} = \sigma_j^x \prod_{k=1}^{j-1}\sigma_k^z$, $c_{2j} = \sigma_j^y \prod_{k=1}^{j-1}\sigma_k^z$, with $\sigma_j^{x,y,z}$ being the Pauli matrices, the Hamiltonian (1) can be *exactly* rewritten as

$$\mathcal{H} = \sum_{j=1}^{L-1}\biggl[\frac{1}{2}\biggl(J\bigl(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\bigr) + J_z\sigma_j^z\sigma_{j+1}^z\biggr)\biggr] + h\sigma_1^x, \tag{5}$$

with $J = -t$ and $J_z = V/2$. Notice that the static properties of the system with the Hamiltonian (5) are the same for $J \to -J$ [24], hence in what follows we consider $|t|$ instead of $\pm t$. In the framework of the algebraic Bethe ansatz one can show [25] that the Hamiltonian (5) is the derivative of the logarithm of the transfer matrix $\tau(u)$ with respect to the spectral parameter u, where

$$\tau(u) = \text{Tr}_0[K^+(u)L_{0L}(u)L_{0L-1}(u)\cdots L_{01}(u) \times K^-(u)L_{01}(u)L_{02}(u)\cdots L_{0L}(u)]. \tag{6}$$

Here 0 denotes the auxiliary subspace, the L operator can be written as

$$L_{0j} = \frac{1}{2\sinh(\eta)}\bigl[\sinh(u+\eta)\bigl(1 + \sigma_j^z\sigma_0^z\bigr) + \sinh(u)\bigl(1 - \sigma_j^z\sigma_0^z\bigr)\bigr] + \frac{1}{2}\bigl(\sigma_j^x\sigma_0^x + \sigma_j^y\sigma_0^y\bigr)\,, \tag{7}$$

were $\cosh(\eta) = V/2|t|$. It satisfies the Yang-Baxter equation [26,27]

$$L_{12}(u-v)L_{13}(u-w)L_{23}(v-w) = L_{23}(v-w)L_{13}(u-w)L_{12}(u-v). \tag{8}$$

The reflection matrices $K^\pm(u)$ can be written as a 2×2 matrix in the auxiliary subspace with the coefficients

$$K_{11}^- = K_{22}^- = \frac{2|t|\sinh(\eta)\cosh(u)}{h},\ K_{12}^- = K_{21}^- = \sinh(2u),$$
$$K_{11}^+ = K_{22}^+ = 2\cosh(u+\eta), \quad K_{12}^+ = K_{21}^+ = 0. \tag{9}$$

The reflection matrices satisfy the reflection equations [25,28]

$$L_{12}(u-v)K_1^-(u)L_{21}(u+v)K_2^-(v) = K_2^-(v)L_{12}(u+v)K_1^-(u)L_{21}(u-v),$$
$$L_{12}(v-u)K_1^+(u)L_{21}(-u-v-2)K_2^+(v) = K_2^+(v)L_{12}(-u-v-2)K_1^+(u)L_{21}(v-u). \tag{10}$$

As usual for Bethe ansatz integrable models, each eigenvalue and eigenfunction of the Hamiltonian Eqs. (1), (3), and (5) is parametrized by the set of quantum numbers, called rapidities, u_j, with $j = 1, \dots, M$, where M is related to the total charge (total number) of spinless fermions (or to the z-projection of the total spin moment of the chain in the spin representation). Let us consider first the strong repulsion between spinless fermions $V > 2|t|$. The case $V = 2|t|$ is related to the isotropic spin-1/2 chain, and the behavior of the expectation value of the boundary spin was studied in detail in Ref. [29]. The rapidities u_j satisfy the Bethe ansatz equations

$$\prod_{m=1, m\neq j}^{M} \frac{\sinh[(iu_j - iu_m + 2\eta)/2]}{\sinh[(iu_j - iu_m - 2\eta)/2]} \frac{\sinh[(iu_j + iu_m + 2\eta)/2]}{\sinh[(iu_j + iu_m - 2\eta)/2]}$$
$$= -\left[\frac{\cosh[(iu_j + \eta)/2]}{\cosh[(iu_j - \eta)/2]}\right]^{2L} \left[\frac{\sinh[(iu_j - \eta)/2]}{\sinh[(iu_j + \eta)/2]}\right]^2$$
$$\times \frac{\cosh[(iu_j + \eta)/2 + \alpha]}{\cosh[(iu_j - \eta)/2 - \alpha]}, \quad (11)$$

where $\sinh(\alpha) = |t|\sinh(\eta)/h$, with the eigenvalue of the Hamiltonian

$$E = \frac{V(L-1)}{2} - |t|\sinh(\eta)\coth(\alpha) + 2|t|\sum_{j=1}^{M} \frac{\sinh^2(\eta)}{\cosh(\eta) + \cos(u_j)}. \quad (12)$$

For $\mu = 0$ the number M is equal to $L/2$ (half filling).

We consider the thermodynamic limit $L \to \infty$, $M \to \infty$ with their ratio M/L finite. We use the standard technique of the Bethe ansatz [22]. In the main, in the L^{-1} approximation, the ground state corresponds to only real u_j being the roots of Eqs. (11). Due to nonzero V there exist many other solutions to Eqs. (11), namely bound states (called strings) [22], which are related to complex values of roots u_j. However, none of those solutions of Bethe ansatz equations (11) have negative energies, and, therefore, do not contribute to the ground state formation [30,31]. To remind the reader, the ground state of any fermionic system is formed by the total filling of the Fermi sea: All eigenstates with negative energies have the filling factor 1, while for eigenstates with positive energies the filling factor is 0. Excitations of fermion systems are related to holes for eigenstates with negative energies and/or filling of eigenstates with positive energies. For $V > 2|t|$ bulk excitation with the rapidity u with respect to the ground state is the hole in the distribution of real rapidities u_j, which form the Fermi sea (i.e., which have negative energies)

$$e_h(u) = \sum_{n=-\infty}^{\infty} \frac{|t|\sinh(\eta)e^{-inu}}{\cosh(n\eta)}, \quad (13)$$

with the quasimomentum $p = -i\ln(\cosh[(iu + \eta)/2]/\cosh[(iu - \eta)/2]$ and the fractional charge $-1/2$ with respect to the ground state. One can see that the state has a gap. According to Ref. [32] physical excitations of the integrable one-dimensional system can carry only even number of holes, so the physical bulk excitation is the pair of holes. Energies of physical excitations have to be larger than the gap value. So, in the regime $V > 2|t|$ at $\mu = 0$ the Hamiltonian (1) or (3) describes the one-dimensional Mott insulator.

For the chain with open boundaries there can exist additional solutions, see, e.g., Refs [33–38] to Bethe ansatz equations, which can appear due to free boundaries themselves, or due to nonzero boundary potential h. Those solutions are localized at each boundary. Their eigenfunctions decay exponentially with the distance from the edge. Depending on the value of the boundary potential, those modes, totally analogous to Majorana edge states of the noninteracting spinless fermion chain with pairing [2], can have negative or positive energies. For example, the energy of the boundary localized state is zero for $\alpha > \eta/2$ (in particular for $\alpha \to \infty$, i.e., for the free boundary $h = 0$ [21]), and for $-\eta/2 < \alpha < \eta/2$ the energy of the edge localized state is

$$e_b = \frac{|t|\sinh^2(\eta)}{\sinh(2(\alpha+\eta))\sinh(\alpha)} + |t|\sinh(\eta)\sum_{n=-\infty}^{\infty} \frac{e^{-2\eta|n|}\cosh((2\alpha+\eta)n)}{\cosh(\eta n)}. \quad (14)$$

Those boundary localized states carry charge $\pm 1/2$, depending of the value of h. Physical eigenstates should carry integer charge [32]. Hence, boundary localized states can exist in pairs, or one boundary state with an additional bulk hole state, to keep the charge integer. Unlike the situation for noninteracting fermions with pairing [2], for the interacting fermion chain there can exist not only simple localized boundary states, but also localized boundary strings [21,35,36]. However, it is possible to show that their energies are either zero for strings with an even number of poles, or their energies are equal to e_b for boundary strings with an odd number of poles.

For $h = 0$ boundary localized states have zero energy in the limit $L \to \infty$ [21]. In that sense they are totally analogous to Majorana zero modes of the noninteractiong chain with pairing [2], because they carry zero energy (for the infinite chain) being inside the gap for bulk excitations, the Dirac operator of the localized state is formed by the Majorana fermions from both edges of the chain, and the ground state is doubly degenerate [21].

IV. RESULTS FOR THE EXPECTATION VALUE

Now we determine the ground state expectation value of the edge Majorana operator $\langle c_1\rangle$ as the derivative of the h-dependent part of the ground state energy of the chain $\langle c_1\rangle = \partial E(h)/\partial h$, where

$$E(h) = \sqrt{h^2 + (|t|\sinh(\eta))^2} - |t|\sinh(\eta)\sum_{n=-\infty}^{\infty} \frac{e^{-|n|(2\alpha+\eta)}}{\cosh(n\eta)}. \quad (15)$$

The latter, obviously, is defined by the finite size correction to the ground state energy [22]. We stress that depending on the value of h (keeping the ground state half-filling value $M = L/2$) both bulk states and localized states contribute to $E(h)$, and, hence, determine the expectation value $\langle c_1\rangle$, similar to the case of the chain of noninteracting spinless fermions with

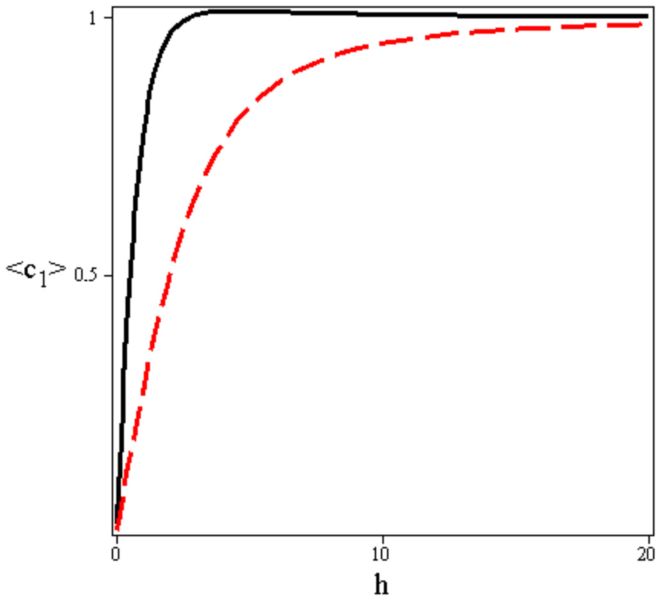

FIG. 1. The ground state expectation value of the edge Majorana fermion as a function of h for the topological insulator with $|t| = 1$ and $\eta = 1$ (black solid line); $\eta = 2$ (red dashed line).

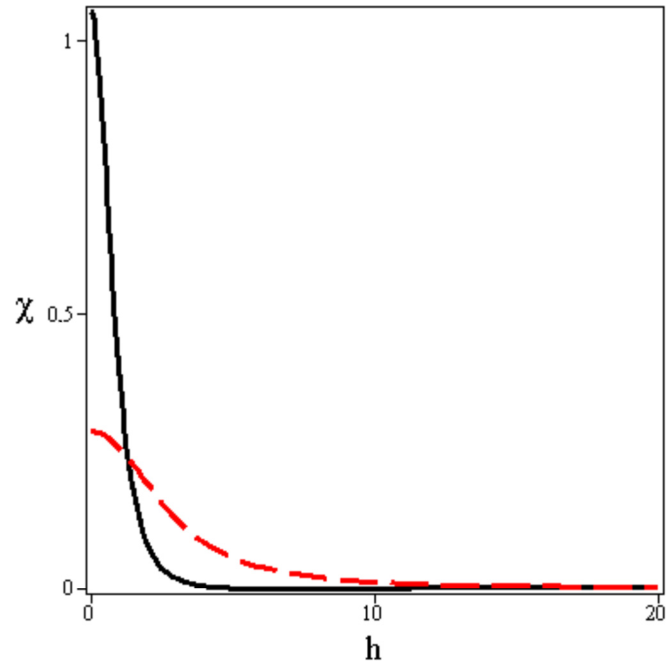

FIG. 2. The ground state local susceptibility χ of the expectation value of the edge Majorana fermion as a function of h. Parameters are the same as in Fig. 1.

pairing [20]. We get

$$\langle c_1\rangle = \frac{h}{\sinh(\eta)\sqrt{h^2 + (|t|\sinh(\eta))^2}} + \frac{2|t|^2\sinh^2(\eta)}{h\sqrt{h^2 + (|t|\sinh(\eta))^2}}\sum_{n=1}^{\infty}\frac{nx^{(2|n|+1)}e^{-|n|\eta)}}{\cosh(n\eta)}, \quad (16)$$

where $x = h/[|t|\sinh(\eta) + \sqrt{(|t|\sinh(\eta))^2 + h^2}]$. We can see that the expectation value $\langle c_1\rangle$ is zero at $h = 0$ and reaches 1 only at $h \to \infty$: In the presence of the last term in Eqs. (1) and (3) the total number of fermions [the z projection of the total spin of the spin chain (5)] is not conserved. The ground state behavior of the expectation value of the edge Majorana operator is illustrated for $|t| = 1$ and $\eta = 1$ and $\eta = 2$ in Fig. 1. We can also determine the derivative of the expectation value $\langle c_1\rangle$ with respect to h, $\chi = \partial\langle c_1\rangle/\partial h$, which plays the role of the local edge susceptibility of the chain [29,35]. It is finite for $h = 0$, and decays monotonously to zero at $h \to \infty$. The ground state behavior of the local susceptibility of the edge Majorana fermion is shown in Fig. 2. It turns out, that depending on the value of h, the edge localized modes and bulk eigenstates can both contribute to the values of $\langle c_1\rangle$ and χ, similar to the case of noninteracting spinless fermions with pairing [20].

In the case of $0 < V < 2|t|$ (it is related to imaginary η and α) analogous analysis of the Bethe ansatz solution shows that bulk excitations are gapless, i.e., the model describes the metallic situation. Localized boundary states can have negative energies only for $h \neq 0$. For free edges $h = 0$ there are no Majorana zero edge modes in the metallic case [21,36]. Figure 3 shows the ground state behavior of the expectation value $\langle c_1\rangle$ for that case. The behavior of the expectation value is reminiscent of the one for the topological insulator case $V > 2|t|$. Similar behavior persists for the weak attraction $-|t| < V < 0$. However for the strong attraction $V < -|t|$, the ground state for free open boundaries corresponds to $M = 0$, and there are no boundary edge modes. We see that the dependences of $\langle c_0\rangle$ and χ on h are similar for the metallic and insulator situations of the interacting fermion chain as well as for the one obtained for the expectation value and the local susceptibility for the one-dimensional topological superconductor [20], and in all cases the contribution to $\langle c_0\rangle$

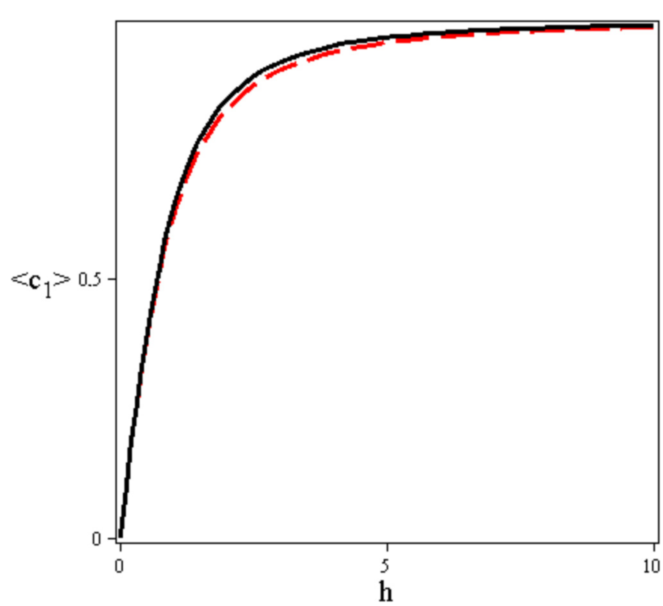

FIG. 3. The ground state expectation value of the edge Majorana operator $\langle c_1\rangle$ as a function of h for the metallic case $|t| = 1$, $\eta = i\pi/4$ (the solid black line) and $\eta = i\pi/3$ (the dashed red line).

comes from both boundary bound states and bulk states. In all cases the expectation value is zero at $h = 0$, and monotonically grows with h till the nominal value reached at $h \to \infty$. The latter feature is related to the fact that the total number of fermions is not conserved for $h \neq 0$. The differences between the behaviors of the expectation value in the mentioned models is only quantitative.

Using the thermodynamic Bethe ansatz technique [22] it is possible to show that for high temperatures $T \gg |t|, V$, the expectation value of the Majorana edge operator is

$$\langle c_1 \rangle = \frac{h}{T}. \tag{17}$$

At low temperatures we have to distinguish two cases. For $V > 2|t|$, in the topological insulator case, at low temperatures only exponentially small in T corrections to the expectation value of the edge Majorana operator exist. As for the metallic case, $-2|t| < V < 2|t|$, the nonzero temperature corrections to the ground state energy can be calculated in the framework of the Luttinger liquid (or conformal field theory) approach [22]. Such an approach produces h-independent part of the low-temperature correction to the ground state energy [39].

One can realize one-dimensional spinless fermions as the spin-polarized interacting electron system (which is described by fermions with only one spin projection), using a quantum wire patterned in a semiconductor quantum well [40] with the device put on top of a ferromagnetic insulator to provide for the spin polarization of electrons [41]. Depending on the applied homogeneous (electrostatic) potential the system can be turned to the insulator phase. Then the application of the local electric field acting on the edge electric dipole of the wire can be described by h. The other realization of the model can be performed in the spin-imbalanced ultracold gases of atoms confined to one-dimensional traps (tubes) [42]. Tubes can be regarded as isolated if the confinement by the laser beams is strong enough to suppress tunneling between tubes. The scattering between atoms under transverse harmonic confinement is subject to a confinement-induced Feshbach-type resonance [43]. Then the strength of the interaction between fermions can be varied by the fine tuning of that resonance [44]. Again, the local electric field acting on the dipole at the edge of the tube yields h. The considered model can also be realized in the chain of coupled cavities with strong in-cavity photon-photon interaction (photons being in resonance with cavities) in the cavity quantum electrodynamics [45]. The multiplier h is then related to the interaction of the edge cavity with light. All these cases can be used to manufacture a topological qubit based on the boundary bound state for the open fermion chain.

V. SUMMARY

In summary, we have studied the model of the one-dimensional topological insulator, in which edge Majorana zero modes exist together with gapped bulk excitations. For that situation we have calculated analytically, using the exact integrability of the problem, the expectation value of the edge Majorana operator. Several realizations of the proposed model have been discussed.

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