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Majorana zero modes in the interacting fermion chain without pairing

A. A. Zvyagin

B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine Kharkiv 61103, Ukraine

V. N. Karazin Kharkiv National University, Kharkiv 61022, Ukraine

E-mail: zvyagin@ilt.kharkov.ua

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The ground state behavior of the spinless fermion chain with an interaction between fermions at neighboring sites is studied for free open boundaries. For the strong enough repulsion boundary gapless states (bound state of Majorana operators from opposite sites of the chain) can exist inside the gap for bulk excitations, i.e., in the topological insulator regime. We propose to use those Majorana zero modes as topological qubits, similar to the ones in one-dimensional topological superconductors. Possible physical realizations of the considered model are discussed.

Keywords: Majorana edge states, topological insulator, topological quantum computer.

During last years Majorana zero energy edge modes attract attention of researchers, for the review use, e.g., [1–3]. According to the original proposal [4] such modes can be used as the topological qubit. Such a qubit (a two-level system) can be formed by two Majorana fermions situated at different edges of the system. As such, by construction, the topological qubit is more stable with respect to local perturbations (local noise), than the local one. It will be more difficult to destroy the quantum coherence for the set of such topological qubits. As possible realizations, Majorana edge modes were proposed to be used in many condensed matter systems, including nanowires, topological insulator/superconductor heterostructures, helical liquids, two-leg ladders, Josephson junctions, etc. In experiments, a number of realizations of Majorana zero modes has been observed by now, see, e.g., [5–8].

To be distinguishable, Majorana edge modes must have energies lying inside the gap of bulk states. This is why, in the most of proposals related to Majorana edge modes, one uses the system of fermions with pairing. The latter yields the gap for bulk states, and Majorana edge modes exist (according to the special conditions on the parameters of the system, see [2–4]) with their energies inside that gap. In fact, Majorana edge modes, in that case, are the manifestation of the topological superconductivity. It is interesting, that Majorana state fixed at one edge can be observed [9].

Here we propose to consider a different situation: Let us study edge Majorana states in the (fermionic) system without pairing, however with interactions between fermions. For some conditions satisfied, bulk states of such systems can be gapped. On the other hand, there can exist Majorana edge states in such systems. It means that we propose to replace the one-dimensional topological superconductor of previous propositions by the one-dimensional topological insulator. In our contribution we study exactly, using the Bethe ansatz technique, the onset of Majorana edge modes, using as the prime example, following Kitaev [4], the one-dimensional model of spinless fermions with the interaction between fermions at neighboring sites of the lattice. Notice that unlike other studies, which consider interactions in fermion chains [10–16], we study systems without pairing. We consider open boundary conditions with free edges. For large enough repulsion between fermions (so that bulk excitations are gapped) there exist boundary bound states related to edge Majorana operators with zero (in the limit of infinite chain) energy. The model possesses two degenerate ground states. In addition to simple bound states for the noninteracting system (cf. Ref. 4), we point out that in our model of the topological insulator there exist a large number of boundary string bound states with zero energy, caused by the interaction. Finally, we discuss possible realization of the proposed model situation.

Consider the Hamiltonian of the open chain of spinless fermions, which interact being at neighbouring sites

$$\mathcal{H} = \sum_{j=1}^{L-1}\left(-\mu\left[n_j - \frac{1}{2}\right] - (ta_j^{\dagger}a_{j+1} - \Delta a_j a_{j+1} + \text{h.c.}) + V\left[n_j - \frac{1}{2}\right]\left[n_{j+1} - \frac{1}{2}\right]\right), \qquad (1)$$

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, $\Delta = |\Delta| \exp(i\theta)$ is the pairing amplitude, $\mu \geq 0$ is the chemical potential, V denotes the nearest-neighbor interaction, and L is the number of sites. Kitaev has suggested [4] (he considered the noninteracting chain $V = 0$) that one can replace standard Dirac operators $a_j^\dagger$ and a_j by other fermion operators, Majorana ones, c_j, $j = 1, \ldots, 2L$ according to the rule

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

with $j = 1, \ldots, L$. The following relations are satisfied for the Majorana operators $c_j^\dagger = c_j$, and $c_j c_m + c_m c_j = 2\delta_{j,m}$, $j, m = 1, \ldots, 2L$. Using the Majorana representation for the interacting case $V \neq 0$ we obtain, taking into account that $n_j - (1/2) = (i/2) c_{2j-1} c_{2j}$

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

For $V = 0$ Kitaev has pointed out 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., with the indices $2j$ and $2j-1$, see above), or to the neighboring sites

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

For the latter case, the Majorana operators c_1 and c_{2L} remain unpaired (for instance, they do not enter the Hamiltonian for $|\Delta| = t$ and $V = \mu = 0$). Kitaev has shown that for finite L in the noninteracting chain $V = 0$ for $2|t| > |\mu|$ and $\Delta \neq 0$ the system possesses two ground states with exponentially small energy difference between them and different fermionic parities $P = \prod_j (-ic_{2j-1} c_{2j})$. 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. 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 $L \to \infty$.

For $\Delta = 0$ and in the absence of interactions $V = 0$ the condition $2|t| > |\mu|$ just defines the region of a normal metal. In this case, there are no boundary states. Let us turn to the case $\Delta = 0$, however with nonzero interaction V. Our goal is to find, whether boundary modes can exist in this situation. For that purpose let us use the Jordan–Wigner transformation [17] for the Hamiltonian Eq. (3) (from now on let us consider for simplicity the case of real Δ, i.e., $\theta = 0$), which can be written as

$$c_{2j-1} = \sigma_j^x \prod_{k=1}^{j-1} \sigma_k^z , \quad c_{2j} = \sigma_j^y \prod_{k=1}^{j-1} \sigma_k^z , \qquad (5)$$

with $\sigma_j^{x,y,z}$ being the Pauli matrices. In the terms of Pauli matrices the Hamiltonian (1) or (3) exactly becomes the Hamiltonian of the effective spin chain. It reads

$$\mathcal{H} = \sum_{j=1}^{L-1} \left[\frac{1}{2} (J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z) - H \sigma_j^z \right], \qquad (6)$$

with $J_{x,y} = -(t \pm \Delta)$, $J_z = V/2$ and $H = -\mu/2$. Notice that after the nonlocal Jordan–Wigner transformation for $J_z = 0$ case (the XY model) in the phase $|J_x - J_y| > H$ the spin chain is ordered with the nonzero order parameter $\langle \sigma_j^x \rangle \neq 0$ in the ground state [19]. For the spin chain external fields can interact with the order parameter, breaking the phase coherence between two mentioned above ground states [4]. Notice that the ground state of the Hamiltonian (6) of the spin chain for $J_x = J_y$ (the XXZ model) for $J_z > J_x > 0$ with periodic boundary conditions is degenerate in the thermodynamic limit $L, M \to \infty$ with M/L fixed: There are two states with different energies for the finite chain, and the difference in their energies goes to zero for $L \to \infty$. The spontaneous magnetization $\langle \sigma_j^z \rangle$, defined as the modulus of the normalized matrix element of the z-projection of the local spin operator between these two states, is nonzero [20]. Notice that for the antiferromagnetic case the site spontaneous magnetization must be staggered. Then for the XXZ spin chain, as well as for the XY spin chain, external fields can interact with the order parameter, and break the phase coherence. However, we use the spin representation of the fermionic Hamiltonian only for analogy in calculation of the eigenvalues and eigenstates of the Hamiltonian Eqs. (1)–(3). To remind, after unitary transformations (the Jordan–Wigner transformation is the unitary one) the system has the same set of eigenvalues and eigenstates, and the Bethe ansatz describes the complete set of eigenstates and eigenvalues of the Hamiltonian (6), see, e.g., [18].

Each eigenvalue and eigenstate of the Hamiltonian Eqs. (1)–(3) for $\Delta = 0$ can be parametrized by the set of quantum numbers called rapidities, u_j, with $j = 1, \ldots, M$, 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 the strong enough repulsion between spinless fermions $V \geq 2|t|$, and denote $V/2|t| = J_z/J_x = \cosh(\eta) \geq 1$ (to remind, the case $\Delta = 0$ corresponds to the case $J_x = J_y$).

The rapidities u_j, $j = 1, \ldots, M$ satisfy the Bethe ansatz equations, cf. [21]

$$\left[\frac{\cosh[(iu_j + \eta)/2]}{\cosh[(iu_j - \eta)/2]}\right]^{2L}\left[\frac{\sinh[(iu_j - \eta)/2]}{\sinh[(iu_j + \eta)/2]}\right]^2 =$$
$$= \prod_{m=1,\, m\neq j}^{M}\frac{\sinh[(iu_j - iu_m + 2\eta)/2]}{\sinh[(iu_j - iu_m - 2\eta)/2]}\frac{\sinh[(iu_j + iu_m + 2\eta)/2]}{\sinh[(iu_j + iu_m - 2\eta)/2]}, \tag{7}$$

with the eigenvalue of the Hamiltonian

$$E = \frac{V(L-1)}{4} + 2|t|\sum_{j=1}^{M}\frac{\sinh^2(\eta)}{\cosh(\eta) + \cos(u_j)}. \tag{8}$$

The number M is determined by the value of the chemical potential for spinless fermions (or by the value of the homogeneous magnetic field in the spin representation). Consider for simplicity the case $\mu = 0$ $(H = 0)$, at which $M = L/2$ (half filling) in the ground state (nonzero μ case can be considered in a similar way; for example, for $\mu \le \mu_c = -(2|t| + V)$ one has $M = 0$ in the ground state; in that case boundary bound states do not contribute to the ground state energy, see below). The point with zero chemical potential for $V = 0$ $(J_z = 0)$ and $\Delta \neq 0$ according to Kitaev's analysis [4] also belongs to the interval where two edge Majorana operators are bound into the edge bound state.

Following [21–23] we can study the thermodynamic limit $L \to \infty$, $M \to \infty$ with M/L finite. We use the standard technique of the Bethe ansatz [24].

In the ground state in the main in L^{-1} approximation it corresponds to only real u_j being the roots of Eq. (7). Due to nonzero V there exist many other solutions to Eq. (7), namely bound states (called strings) [24], which are related to complex values of u_j. However, none of those solutions have negative energies, and, therefore, do not contribute to the ground state formation [24]. To remind, the ground state of the 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.

We can find using the standard Bethe ansatz technique for densities of roots of Bethe equations in the thermodynamic limit [24] that the main contribution in L^{-1} (the contribution from the bulk states) to the ground state energy is cf. [21, 23]

$$E^{(0)} = L\left[\frac{V}{4} - \sum_{n=-\infty}^{\infty}\frac{|t|\sinh(\eta)\,e^{-|n|\eta}}{\cosh(n\eta)}\right] \tag{9}$$

with the total charge of the ground state equal to $M = L/2$. Obviously it agrees with the ground state energy of the periodic spin chain [23].

The elementary 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)

$$e_h(u) = \sum_{n=-\infty}^{\infty}\frac{|t|\sinh(\eta)(-1)^n e^{-inu}}{\cosh(n\eta)}, \tag{10}$$

with the quasimomentum

$$p = -i\ln\left(\cosh[(iu + \eta)/2]/\cosh[(iu - \eta)/2]\right)$$

and the fractional charge $1/2$ with respect to the ground state. According to [25] physical excitations can carry only even number of holes, so the physical bulk excitation is the pair of holes. Such a state has the gap [23], i.e., 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.

However, we are interested in the (finite size) corrections to the energy $E^{(0)}$ of order of L^{-1}, which define the difference between the system with periodic boundary conditions and the one with the open boundary conditions. Their contribution is determined by the second multiplier in the l.h.s. of Eq. (7). Similar to [26] we can find the additional (with respect to the bulk ones) root of Eq. (7), namely with $u_0 = i\eta$. It is the solution to Eq. (7) because of the mutual cancellation of the decreasing modulus of the first multiplier in the l.h.s. of Eq. (7) and the increasing modulus of the second multiplier, when $L \to \infty$ and $u_j \to u_0$. That boundary bound state is localized at the edge of the chain: Its eigenfunction decays exponentially with the distance from the edge [27]. Such a boundary bound state has the energy

$$e_b = -\sum_{n=-\infty}^{\infty}\frac{|t|\sinh(\eta)(-1)^n e^{-n\eta}}{\cosh(n\eta)}, \tag{11}$$

and carries the fractional charge $-1/2$ with respect to the ground state of the periodic chain. This state has a negative energy, and, hence, it contributes to the Fermi sea of the open chain. The energy of the bound state is smaller than the energy of the minimal bulk excitation. It means that such a boundary bound state of the fermion chain with a neighboring repulsion has the energy, which value is inside the gap for bulk excitations. There can also exist boundary bound states, which correspond to complex boundary solutions to Eq. (7), similar to the string bound states of the bulk. They correspond to the roots of Eq. (7) of the form $u_0 - 2il\eta, u_0 - 2i(l-1)\eta, \ldots, u_0 + 2mi\eta$ with integer $m, l \ge 0$. However, it is easy to show similar to the analysis of [26] that their energies are either zero (for strings with nonzero m and $l = 0$, i.e., for strings with even number of poles), or they are equal to e_b for boundary strings with nonzero m and $l \ge 1$ (i.e., for boundary strings with odd number of poles). As bulk excitations, physical boundary excitations exist in pairs. However, the boundary state at the other edge of the chain has the energy $-e_b$ and carries charge $1/2$. Hence, the energy of the physical boundary edge state is zero, and it carries zero charge. This is why, our model Eqs. (1)–(3) in this regime $V > 2|t|$ describes one-dimensional topological insulator with gapped bulk eigenvalues and gapless boundary ones.

We can calculate the ground state surface energy, which is the difference between the ground state energy of the fermion chain with free open boundary conditions, and the one of the chain with periodic boundary conditions. As it must be, the ground state of the open fermion chain with free open boundaries also has the charge $M = L/2$. The ground state can be formed by any of two boundary bound states (at each edge), which means the degeneracy, cf. the analysis of Kitaev [4] for $\Delta \neq 0, V = 0$. The surface energy is

$$E_s = \frac{V}{4} - \sum_{n=-\infty}^{\infty} \frac{|t|\sinh(\eta)(e^{-2n\eta}-1)}{\cosh(2n\eta)} - \\ -|t|\sinh(\eta)\sum_{n=-\infty}^{\infty}(-1)^n\frac{e^{n\eta}-e^{-n\eta}}{\cosh(n\eta)}. \quad (12)$$

To stress the contribution of boundary bound states we have written the last term explicitly, which is caused by contribution from two boundary edge states, despite it is zero.

Hence, we can conclude that in the fermion chain without pairing, but with the strong enough repulsion $V > 2|t|$ at neighboring sites (insulator regime) with free boundaries for $\mu = 0$ there exist (topological) edge states (related to edge Majorana fermions) with zero energy in the thermodynamic limit. For

$$\mu < \mu_s = -2|t|\sinh(\eta)\sum_{n=-\infty}^{\infty}[(-1)^n/\cosh(n\eta)]$$

(at μ_s the gap for bulk excitations is closed) the situation remains similar, to what was described above. Then, for $\mu_c \le \mu \le \mu_s$ the bulk excitations become gapless, and it is difficult to distinguish boundary state(s) from bulk states. The boundary states become quasilocal, i.e., they renormalize the density of states inside the band of bulk excitations, but do not produce local levels. The system for those values of the chemical potential is in the normal metal regime. Finally, for $\mu < \mu_c$ such states do not contribute to the ground state energy, because their energy becomes positive.

Analysing the case with the strong enough attraction $V < -2|t|$, we can see that the ground state corresponds to $M = 0$. Therefore, solutions of Eq. (7) describing boundary bound states do exist. However they have positive energies (as well as for the strong repulsive case for $\mu < \mu_c$, see above), and do not renormalize the ground state energy of the chain.

We can also consider the case with a weak interaction, $-2|t| \le V \le 2|t|$ (related to the states of the XXZ spin chain with $-J_x \le J_z \le J_x$). We can parametrize $V/2|t| = \cos(\gamma)$. The Bethe ansatz equations for the set of rapidities v_j ($j = 1, \ldots, M$), which parametrize all eigenstates and eigenvalues of the Hamiltonian, are

$$\left[\frac{\sinh[(v_j+i\gamma)/2]}{\sinh[(v_j-i\gamma)/2]}\right]^{2L}\left[\frac{\cosh[(v_j-i\gamma)/2]}{\sinh[(v_j+i\gamma)/2]}\right]^2 = \\ = \prod_{\substack{m=1,\\ m\neq j}}^{M}\frac{\sinh[(v_j-v_m+2i\gamma)/2]}{\sinh[(v_j-v_m-2i\gamma)/2]}\frac{\sinh[(v_j+v_m+2i\gamma)/2]}{\sinh[(v_j+v_m-2i\gamma)/2]}, \quad (13)$$

with the eigenvalue of the Hamiltonian

$$E = \frac{-|t|(L-1)}{2}\cos(\gamma) - 2|t|\sum_{j=1}^{M}\frac{\sin^2(\gamma)}{\cos(\gamma)-\cosh(v_j)}. \quad (14)$$

The system is in the normal metal regime for $\mu_c < \mu$. Using the analysis similar to [28, 29] it is possible to show that there exist solutions of Eqs. (13), which describe boundary states, only for large enough boundary fields (no such states for free boundaries). One can check it, e.g., for the simplest case of noninteracting fermions, $V = 0$, see [24]. For that case, naturally, there are no string solutions, either bulk, or edge ones. For $\mu < \mu_c$ again $M = 0$, and boundary states do not contribute to the ground state.

How the considered model can be realized? First, one can study a one-dimensional 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 [31] with the device put on top of a ferromagnetic insulator to provide for the spin polarization [30]. On the other hand, the model can be realized in the spin-imbalanced ultracold gases of atoms confined to one-dimensional traps (tubes) [32]. Tubes can be regarded as isolated if the confinement by the laser beams is strong enough to suppress tunnelling between tubes. The scattering between atoms under transverse harmonic confinement is subject to a confinement-induced Feshbach-type resonance [33]. Then the strength of the interaction between fermions can be varied by the fine-tuning of that resonance [34]. Both of cases can be used to construct a topological qubit based on the boundary bound state for the open fermion chain. Of course, other realizations are possible, too.

In summary, we have shown that for the spinless interacting fermion chain with open free boundary conditions without pairing there can exist Majorana edge bound states. Those states define the ground state Fermi sea of the system for the strong enough repulsion between neighboring fermions. The energy of those Majorana edge modes is zero for the infinite chain, and there are degenerate ground states, similar to the one of the Majorana edge states of the open chain of noninteracting spinless fermions with pairing, considered by Kitaev. It means, that we predict Majorana edge states for the one-dimensional topological insulator, instead of one-dimensional topological superconductor.

We expect that similar states can be realized for higher-dimensional topological insulators also. Majorana edge zero modes, described in our work, can be used as topological qubits in topological quantum computation.

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Майоранівські нульові моди в ферміонному ланцюжку з взаємодією без спарювання

A. A. Zvyagin

Вивчається поведінка ланцюжка безспінових ферміонів з взаємодією між ферміонами у сусідніх вузлах без спарювання в основному стані для відкритих вільних границь. Для достатньо сильного відштовхування граничні безщільові стани (зв'язані стани майоранівських операторів з різних кінців ланцюжка) можуть існувати в щілині для об'ємних збуджень, тобто в режимі топологічного ізолятора. Запропоновано використовувати такі майоранівські нульові моди як топологічні кубіти, подібно модам в одновимірному топологічному надпровіднику. Дискутуються можливі фізичні реалізації моделі, що розглядається.

Ключові слова: майоранівські крайові стани, топологічний ізолятор, топологічний квантовий комп'ютер.