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Topological properties of superconducting junctions

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Motivated by recent developments in the field of one-dimensional topological superconductors, we investigate the topological properties of s-matrix of generic superconducting junctions where dimension should not play any role. We argue that for a finite junction the s-matrix is always topologically trivial. We resolve an apparent contradiction with the previous results by taking into account the low-energy resonant poles of s-matrix. Thus no common topological transition occur in a finite junction. We reveal a transition of a different kind that concerns the configuration of the resonant poles.

Superconducting junctions, including superconducting-normal (SN) ones where dissipative conduction can take place and superconducting-superconducting (SS) ones where a discrete spectrum of bound Andreev states is formed, have been in focus of condensed-matter research for almost fifty years [1, 2]. An indispensable compact approach to superconducting junctions employs a scattering matrix that relates incoming and outgoing wave amplitudes that obey the Bogolyubov–deGennes (BdG) equation [3, 4, 5]. The beauty and power of this approach stems from its ability to incorporate numerous microscopic details in a compact form of the scattering amplitudes. Straightforward extensions permit to include magnetism, spin-orbit interaction, non-trivial superconducting pairing [6]. The s-matrix approach can be easily combined with semiclassical treatment of electron transport in the framework of a quantum circuit theory [2].

Recent developments in the field of superconductivity require revision of the common assumptions concerning the structure and properties of the scattering matrix of a superconducting junction. Kitaev in 2000 has suggested a model $1d$ p-wave superconductor [7] that exhibits a topological order. It has been shown recently that the same topological order can be realized in more realistic systems that combine spin magnetic field [8] with strong spin-orbit interaction [9, 10]. Similar situation would occur in a superconductor on the top of topological insulator or half-metal [11]. The relevance of these developments for generic superconducting junctions is not immediately obvious. Indeed, the general properties of those are not supposed to depend on dimension [12], while topological ordering considered is specific for one dimension [13] thus suggesting that the topological properties are not at all manifested in junctions. However, a number of spectacular predictions and device schemes that relate the topology and junction properties has appeared in the last years. Those include: prediction of so-called 4π periodic Josephson effect [9, 10, 14, 15], formulation of a criterion for topological transition in terms of reflection matrix of a junction [16], proposals of topological qubits based on majorana bound states [7, 15] as well as their readout with qubits of different type [17].

This motivated us to focus on a general BdG scattering matrix that bears no information on such details as dimensionality, absence/presence of disorder and concrete values of parameters responsible for the lifting of spin and time-reversal degeneracies. We have performed a topological analysis of such matrix concentrating on energy dependence of its eigenvalues. This rather elementary analysis shows that *i.* there are topologically non-trivial s-matrices (TNTM) characterized by real eigenvalues at zero energy, *ii.* there are topologically non-trivial trajectories (TNTT) in the space of topologically trivial s-matrices (TTM), that pass a matrix with real eigenvalues at $E = 0$ odd number of times.

TNTM would correspond to a "topological" SN-junction [18], while TNTT would explain 4π-periodicity of Josephson effect in SS-junctions [9, 10, 14]. However, if we proceed with the same topological arguments we are able to prove the topological triviality of all physical (i.e. describing finite junctions) s-matrices. *There are no TNTM neither TNTT*. This brings about a paradox that requires an explanation. We resolve it by recognizing a potentially sharp energy dependence of a s-matrix near zero energy. Such energy dependence is due to resonant poles [19] that manifest formation and coupling of zero-energy quasilocalized states. With this, we reconcile the predictions of [9, 10, 14], show the absence of a common topological transition and reveal topological transitions related to the resonant poles.

We illustrate these results with two minimal setups, SN- and SS-junctions (Fig. 1), where a single-channel

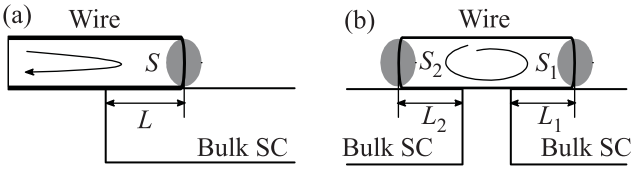

Fig. 1. Setups to illustrate general topological properties of BdG s-matrices. (a) – Finite-length wire with strong spin-orbit coupling on the top of superconducting lead forming a SN-junction. (b) – Finite-length wire between two superconductors forming SS-junction. Grey ellipses indicate "buried" zero-energy states

wire with strong spin-orbit coupling and subject to magnetic field is brought in contact with a bulk superconductor. The Hamiltonian description of this situation is found in [9]. In distinction from [9], we assume finite length of the contact. The solutions of BdG-equation for a single channel encompass spin and electron-hole degree of freedom so that the minimal single-channel scattering matrix is 4×4. The parameter space of the model that includes the superconducting gap, chemical potential, strength of spin-orbit interaction, and magnetic field, can be separated into two ranges: "topological" and " non-topological".

Let us consider a general s-matrix of a SN-junction assuming no symmetries. The only constraint on such matrix stems from the structure of BdG-equation: its Hamiltonian satisfies $\hat{H}^* = -\tau_1 \hat{H} \tau_1$, where the operator τ_1 switches electrons and holes. The constraint is convenient to represent in so-called Majorana basis [20] where the Hamiltonian is antisymmetric and the scattering matrix satisfies $S(E) = S^*(-E)$, E being energy counted from the chemical potential of the superconductor. We will consider only energies E within the energy gap of the bulk superconductor. In this case, there are no scattering waves in the bulk of superconductor, the matrix $\hat{S}$ is in the basis of normal-metal scattering waves satisfying unitary condition.

Let us concentrate on (continuous) energy dependence of the matrix eigenvalues $e^{i\chi(E)}$. That can be represented as a manifold of curves in $\chi - E$ plane (Fig. 2). The BdG-constraint implies that if a point (χ, E) belongs to the manifold, the inverted point $(-\chi, -E)$ belongs to it as well. These two points can belong to either the same curve or to two distinct curves. In the first case, the curve is topologically distinct: it is forced to pass either $\chi = 0$ or $\chi = \pm\pi$ at zero energy. If two such curves pass the same point, they can be deformed by continuous change of Hamiltonian parameters into a pair of trivial curves. However, a single curve is topologically stable: the fact it passes the point cannot be changed by Hamiltonian variations. We note that the dimension of the physical s-matrices can be always chosen even. With all this, all s-matrices can be separated onto two classes. Topologically trivial matrices (TTM) have no topologically distinct curves while topologically non-trivial (TNTM) have two topologically distinct curves passing respectively $\chi = 0$ and $\chi = \pm\pi$ at $E = 0$. Indeed, at zero energy s-matrices are real forming O(2N) group. TTM belong to SO(2N) subgroup of O(2N), while TNTM belong to the rest of O(2N). The matrices from these distinct submanifolds cannot be continuously deformed into one another: indeed, at $E = 0$ $\det(\mathrm{TTM}) = 1$ while $\det(\mathrm{TNTM}) = -1$.

This classifies s-matrices of SN-junction. An SS-junction is characterized by a combination of two s-matrices (Fig. 3). The spectrum of Andreev states of the junction as function of superconducting phase difference ϕ is obtained from the equation [4]

$$0 = \det\left(\hat{1} - \hat{S}\right); \; \hat{S} = \hat{s}_1 e^{i\phi\tau_3/2} \hat{s}_2 e^{-i\phi\tau_3/2}, \qquad (1)$$

τ_3 being Nambu matrix distinguishing electrons and holes. It is instructive to note that the unitary matrix $\hat{S}(\phi)$ satisfies the same BdG-constraint as an SN s-matrix. Therefore, the above topological classification applies to SS-junctions as well.

In this respect it is crucial to note another topological property that concerns continuous one-parameter closed manifolds of TTM (trajectories). Intuitively, eigenvalues of a generic matrix "repel" each other and never come together. This applies to BdG-matrices expect a special situation: $E = 0$ and real eigenvalues. Owing to this peculiarity, a trajectory in matrix space can in principle pass a matrix where two eigenvalues, say, $+1$, are the same. It turns out that the trajectories of the kind can be separated onto two topological classes that differ by parity of the number of passes (Fig. 4) to see the possibility for odd number of passes, let us take a closed trajectory with a single pass and concentrate on two eigenvectors corresponding to the eigenvalue $+1$. In this situation, if the parameter cycles over the trajectory, a given eigenvector is transformed not to itself but rather to its orthogonal counterpart, this guarantees the stability of this topologically non-trivial trajectory (TNTT).

Let us understand the results of [9, 15, 14] in terms of the above classification. Without going into details, we enunciate that TNTM are realized in the "topological" parameter range. The TNTT give the topological explanation of the 4π Josephson effect described in these articles. The trajectory parameter in this case is the superconducting phase difference ϕ.

However, similar topological considerations show that *no* physical s-matrix belongs to TNTM-class, *neither* any closed trajectory in parameter space is a TNTT. "Physical" in this case means a finite junction

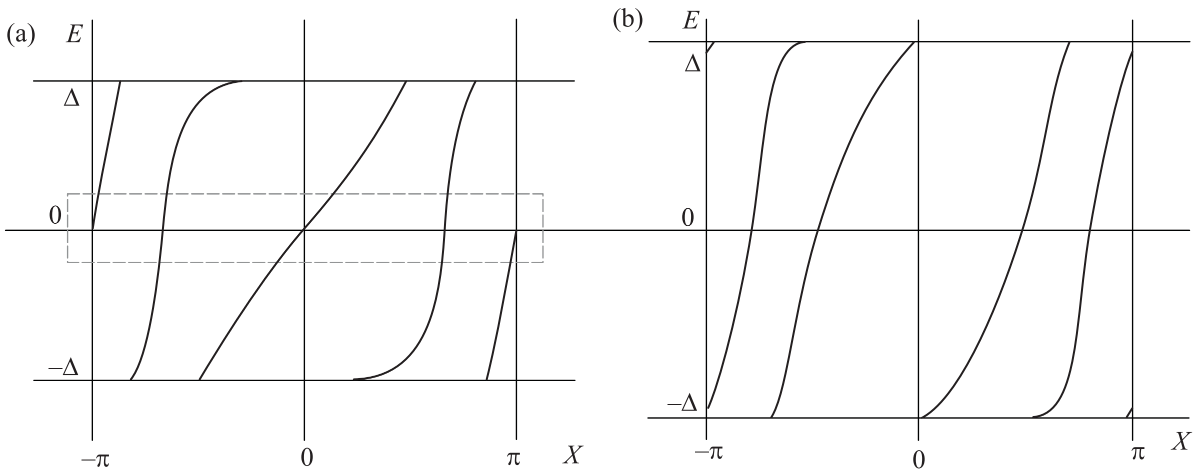

Fig. 2. Energy dependence of s-matrix eigenvalues. (a) – Topologically non-trivial (TNTM) case, corresponding to the "topological" parameter range in [9]. (b) – Generic topologically trivial (TTM) case. (Numerical results for the setup in Fig. 1a in the limit $L \to \infty$.)

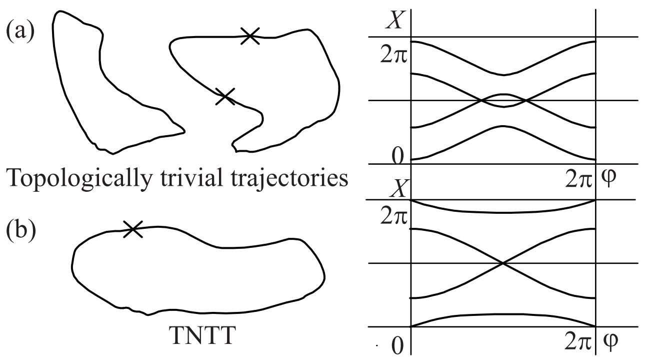

Fig. 3. Topological classes of trajectories in the space of TTM. A trajectory is topologically non-trivial (TNTT) provided it passes the matrix with two degenerate real eigenvalues *odd* number of times. Illustration: the dependencies of eigenvalues of the scattering matrix characterizing the SS-junction on superconducting phase difference ϕ at zero energy for (a) "non-topological" and (b) "topological" parameter ranges

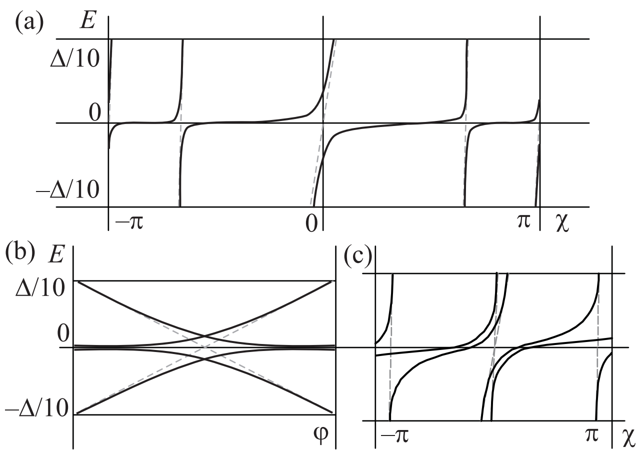

Fig. 4. (a) – Energy dependence of eigenvalues for NS-junction in a narrow energy interval illustrates the topological triviality of s-matrix for finite length of the contact ($L = 7$ in units of [9]). Dashed lines: "high"-energy TNTM eigenvalues. We see the reconnection of neighboring eigenvalues. (b) – Andreev levels in SS-junction versus superconducting phase difference at $L_1 = L_2 = 7$ (solid lines) as compared to TNTT-case at $L_{1,2} = \infty$ (dashed lines). (c) – Energy dependence of eigenvalues for case (b) and $\phi = \pi$. Dashed lines: TNTT-case

between infinite leads where the "topological" [9, 10, 14] transition is necessary smoothed. To prove, let us start with a common junction manifesting no exotic properties. For our examples, this may correspond to a junction in zero magnetic field and zero spin-orbit interaction. The s-matrix at this parameter choice as well as all trajectories are topologically trivial. Since there is no continuous way to tune scattering matrix from TTM- to TNTM-class, and the transition is smoothed, the s-matrix will stay trivial at any strength of magnetic field/spin-orbit interaction, even after the "topological" transition. This proof is in a seeming contradiction with the predictions mentioned [9, 10, 14]. This "*paradox*" motivated us for the deeper research.

Prior to presenting the solution of the paradox, let us mention that the absence of TNTT resolves an annoying problem that concerns the parity of particle number of the ground state of the SS-junction. The level crossings at $E = 0$ are known in the context of ferromagnetic SS-junctions. Upon passing the crossing, it becomes energetically favourable to put a single polarized quasiparticle to the junction [21]. Therefore, the parity of the ground state must be different at two sides of the crossing. In this work, we concentrate on the properties of the ground state. However, the odd number of crossings at a closed curve suggest that the parity of this ground state cannot be unambiguously defined: a situation that is annoyingly difficult to comprehend.

To see how the paradox is resolved, let us consider numerical results for a finite SN-junction in "topological" parameter range(Fig. 4a). If the results are plotted at energy scale of the superconducting gap, the pattern of energy dependent eigenvalues is apparently of TNTM-type as in Fig. 2a. However, replotting the results near $E=0$ at smaller scale reveals topological triviality (cf. Fig. 4a and Fig. 2b). The eigenvalues move fast in the vicinity of $E=0$ reconnecting the branches visible at larger energy scale in a rather unexpected way. The typical energy scale of such reconnection is small depending exponentially on the contact length L, and shrinks to zero at $L\to\infty$. Therefore, the ground state is always of even parity and its energy is 2π-periodic. The 4π-periodicity may only be observed if the phase is swept fast enough to get the setup to an excited state (of the same parity).

The adequate description of the situation combines a smooth energy dependence of s-matrix at $E\simeq\Delta$ with a pole or poles that are anomalously close to $E=0$. Let us consider a single pole. The BdG-constraints restrict it to purely imaginary energy, $-i\Gamma\ll\Delta$. The s-matrix reads

$$\hat{s}=\left[\hat{1}+\left(\frac{\epsilon-i\Gamma}{\epsilon+i\Gamma}-1\right)|\Psi\rangle\langle\Psi|\right]\hat{S}_0, \qquad (2)$$

where Ψ is the eigenvector associated with the resonant level and $\hat{S}_0$ is the matrix, with smooth energy dependence to disregard at $E\simeq\Gamma$. The eigenvalues in this energy range are determined from equation $\epsilon/\Gamma=\sum_k|\Psi_k|^2\cot(\chi_k-\chi_k^{(0)})$, $\exp(i\chi_k^{(0)})$ being "high-energy" ($|E|\gg\Gamma$) eigenvalues of S_0. They follow the pattern in Fig. 4 connecting neighboring "high-energy" eigenvalues, $\exp(i\chi_k^{(0)})\to\exp(i\chi_{k+1}^{(0)})$. This guarantees that the total shift of phases of all eigenvalues upon crossing a single pole equals 2π. Physically, the pole is associated with a quasi-localized zero-energy state being formed at the far end of the wire. If the contact length exceeds the localization length, this state is efficiently "buried" ($\Gamma\ll\Delta$) in the superconductor and hardly accessible for incoming electron or hole waves except $E=0$ when the scattering of the waves become resonant. Andreev conductance of the junction is expressed as $G_A=G_Q\mathrm{Tr}\left(\tau_3\hat{s}\tau_3\hat{s}^\dagger\right)$. In the resonant energy interval, the energy dependence of the conductance assumes a universal form $G_A(E)=G_A+\frac{\Gamma^2}{E^2+\Gamma^2}[G_A(0)-G_A]$, $G_A(0), G_A$ being its values at $E=0, |E|\gg\Gamma$ that depend on details of the junction.

Let us turn to the SS-junction in the "topological" parameter range. Solving Eq. (1) gives the spectrum of Andreev states (Fig. 5b). We observe the level crossing at $E=0,\phi=\pi$ being lifted in a narrow energy interval. Strikingly, we observe another pair of levels with energies remaining small in the whole range of phase. These levels are absent in TNTT picture and emerge as a consequence of topological triviality of the s-matrix. Since there is no level crossing at $E=0$, the parity of the ground state is always even.

The situation can be comprehended if we notice that each matrix $\hat{s}_1,\hat{s}_2$ forming the resulting $\hat{s}$ brings a resonant pole corresponding to a "buried" zero-energy state at far end of each wire. The $\hat{s}$ thus has two resonant poles. The mixing of the two "buried" states results in their (phase-dependent) energy splitting and formation of the pair of low-energy Andreev levels. The eigenvalues of s-matrix move in the narrow energy interval reconnecting next-to-nearest (two poles) neighbour "high-energy" eigenvalues (Fig. 3b). This brings four rather than two states in the vicinity of the crossing point $E=0,\phi=\pi,\chi=0$, all being involved in the lifting of the degeneracy. The detailed theory of the crossing point will be presented elsewhere.

Since the s-matrix remains topologically trivial, there seem to be no sharp transition in its characteristics that would correspond to the "topological" transition in the (rather unphysical) limit of infinite wire. However, a BdG-s-matrix with resonant poles is characterized by a topological number that can change sharply upon changing the parameters. This, not directly connected to the limit of the infinite wire, transition happens near the point of "topological" transition in the finite wire.

Let us illustrate this with a two-pole scattering matrix corresponding to the fork setup in Fig. 5a. Here the scattering matrices s_1, s_2 of fork tines bring a resonant pole each. The BdG symmetry leaves two distinct possibilities for the poles of the total scattering matrix: i, both poles lie on the imaginary energy axis ($E=-i\Gamma_1$, $-i\Gamma_2$), ii. they form a pair symmetric with respect to reflection $\mathrm{Re}E\to-\mathrm{Re}E$ ($E=\pm\varepsilon-i\Gamma$). One can now change the s-matrix $\check{S}_0$ describing the normal scattering in the fork. If the tines are open to the lead states, the pole configuration should be like one for two parallel SN-junctions: the possibility ii is realized. If the tines are isolated, the "buried" states mix resulting in an energy spitting: the possibility i is realized. We thus expect the transition at intermediate coupling.

Generally, one can characterize a BdG-s-matrix of arbitrary dimension with a topological number that is just the number of poles lying precisely on the imaginary axis. We expect this number to change by 2 upon changing the parameters, this gives a series of "topological" transitions. (Fig. 5b, c) Two poles are degenerate at the

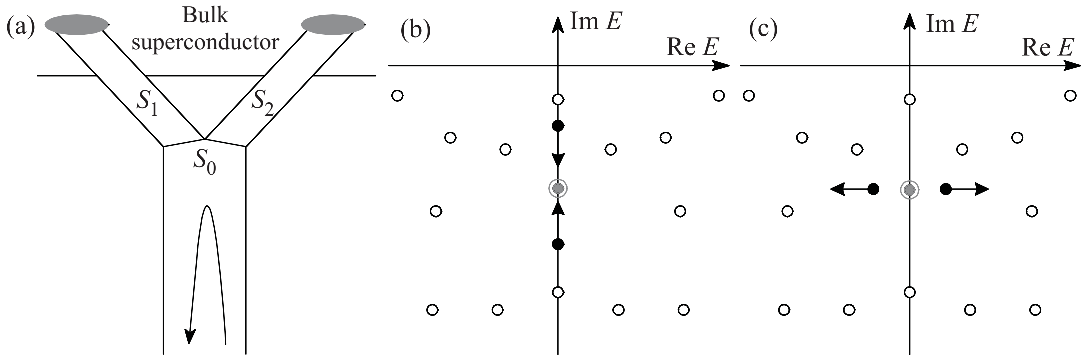

Fig. 5. (a) – Fork SN junction to illustrate topological transitions concerning the resonant poles. (b), (c) – Configurations of the resonant poles in the complex energy plane (b) before and (c) after a transition. At the transition point, the poles are degenerate (double gray circle)

transition point. However, since in general the degenerate poles are at finite imaginary energy Γ, the manifestations of the transitions in transport properties are limited. The energy-dependent Andreev conductance does not seem to have a singularity at the transition point.

We have performed the topological analysis of the properties of SN- and SS-junctions characterized by BdG-s-matrices. We have proven topological triviality of physical matrices that describe finite-size junctions: there is neither TNTM, nor TNTT. This implies the absence of a sharp "topological" transition upon crossing to "topological" parameter range as well as the absence of 4π-periodic Josephson effect. We have resolved the apparent contradiction with results of [9, 10, 15, 14] by considering the low-energy poles of s-matrices. The resulting sharp energy dependence at $E \approx 0$ leads to Lorentian energy dependence of Andreev conductance. We have demonstrated a topological transition (or a series of transitions) of a different kind associated with a change of the configuration of the resonant poles in complex energy plane.

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