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Classical impurities and boundary Majorana zero modes in quantum chains

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ABSTRACT

We study the response of classical impurities in quantum Ising chains. The $\mathbb{Z}_2$ degeneracy they entail renders the existence of two decoupled Majorana modes at zero energy, an exact property of a finite system at arbitrary values of its bulk parameters. We trace the evolution of these modes across the transition from the disordered phase to the ordered one and analyze the concomitant qualitative changes of local magnetic properties of an isolated impurity. In the disordered phase, the two ground states differ only close to the impurity, and they are related by the action of an explicitly constructed quasi-local operator. In this phase the local transverse spin susceptibility follows a Curie law. The critical response of a boundary impurity is logarithmically divergent and maps to the two-channel Kondo problem, while it saturates for critical bulk impurities, as well as in the ordered phase. The results for the Ising chain translate to the related problem of a resonant level coupled to a 1d p-wave superconductor or a Peierls chain, whereby the magnetic order is mapped to topological order. We find that the topological phase always exhibits a continuous impurity response to local fields as a result of the level repulsion of local levels from the boundary Majorana zero mode. In contrast, the disordered phase generically features a discontinuous

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magnetization or charging response. This difference constitutes a general thermodynamic fingerprint of topological order in phases with a bulk gap.

1. Introduction

In recent years there was a substantial boost in the search for signatures of Majorana zero modes (MZM) that may emerge as localized quasiparticles in various condensed matter realizations because of their potential for quantum computation [1,2]. MZMs occurring at boundaries or defects (domain walls and vortices) in low-dimensional topological superconductors are of particular importance because of their non-Abelian anyonic statistics that uncovers new prospects for storage and manipulation of quantum information [3,4].

In his seminal paper Kitaev [5] proposed a one-dimensional model of a spinless p-wave superconductor (1DPS)

$$H = -\mu \sum_{n=1}^{N} (a_n^\dagger a_n - 1/2) + \frac{1}{2} \sum_{n=1}^{N-1} \left(t a_n^\dagger a_{n+1} + \Delta a_n^\dagger a_{n+1}^\dagger + \text{h.c.} \right) \tag{1}$$

(the usual negative sign of the hopping term can be obtained by the transformation $a_n \to (-1)^n a_n$, which changes the signs of t and Δ). This model has a topologically non-trivial massive phase that supports localized Majorana modes at the ends of the chain. For a macroscopically large system these boundary modes can be regarded as unpaired, in which case they represent a non-local realization of a doubly degenerate fermionic zero-energy state. The spatial separation of the two MZMs ensures the immunity of the topologically degenerate ground state of the 1DPS against weak local perturbations (as long as quasi-particle poisoning can be neglected, and thus fermion parity is conserved), making such a system potentially useful for the needs of quantum computation. Thus it is of great theoretical interest and practical importance to identify the physical properties of the edge of such a 1D system that can serve as evidence for the existence of boundary MZMs.

It has soon been realized that principal features of the Kitaev 1D model [5] can be reproduced experimentally using a quantum wire with a strong spin–orbit coupling in the presence of an external magnetic field and the proximity effect with a conventional s-wave superconducting substrate [6,7]. Much theoretical and experimental effort is currently going into finding unambiguous signatures of MZMs in various set-ups. Important steps forward in this direction include tunneling spectroscopy experiments [8,9], whose findings, in particular, the zero-bias conductance peak observed in one-dimensional semiconductor–superconductor contacts, were consistent with theoretical predictions (see Ref. [1] for a recent review).

Closely related to the 1DPS model is the quantum Ising chain (QIC), described by the Hamiltonian:

$$H = -J \sum_{n=1}^{N-1} \sigma_n^x \sigma_{n+1}^x - h \sum_{n=1}^{N} \sigma_n^z . \tag{2}$$

Here σ_n^α are Pauli matrices, $J > 0$ is the exchange interaction and h is a transverse magnetic field which endows the spins with quantum dynamics. The model possesses a $\mathbb{Z}_2$-symmetry associated with the global transformation $P_S \sigma_n^x P_S^{-1} = -\sigma_n^x$, where $P_S = \prod_{j=1}^{N} \sigma_j^z$, $[H, P_S] = 0$. This is an exactly solvable quantum 1D model which, by virtue of the transfer matrix formalism, is related to the classical 2D Ising model [10–12]. The Jordan–Wigner (JW) transformation maps the many-body problem (2) onto a quadratic model of spinless fermions, the latter actually being a particular realization of the 1DPS (1) with a fine-tuned pairing amplitude $\Delta = \pm t$. Close to criticality, in the field-theoretical limit, the QIC represents a $(1+1)$-dimensional theory of a massive Majorana fermion [12]. The topological phase of the 1DPS corresponds to the ordered phase of the QIC, which (in the thermodynamic limit) is characterized by spontaneously broken symmetry and a two-fold degeneracy of the ground state (up to an exponentially small splitting). The ordered phase ($J > h$) is separated from the topologically trivial, disordered phase ($J < h$) by a quantum critical point ($J = h$). As follows from the Kramers–Wannier duality [11,12], the two massive phases of the QIC (2) have identical bulk spectrum; however, they differ in the boundary conditions at the edges of a finite chain, reflecting their topological distinction.

This difference is clearly seen from the Kitaev–Majorana (KM) representation of the QIC [5,13]: the N-site spin chain (2) is equivalent to a $2N$-site tight-binding model of real (Majorana) fermions with nearest-neighbor couplings, as will be briefly reviewed below:

$$H = i\sum_{j=1}^{N}\left(hc_{2j-1}c_{2j} + Jc_{2j}c_{2j+1}\right), \qquad c_i^\dagger = c_i, \qquad \{c_i, c_j\} = 2\delta_{ij}. \tag{3}$$

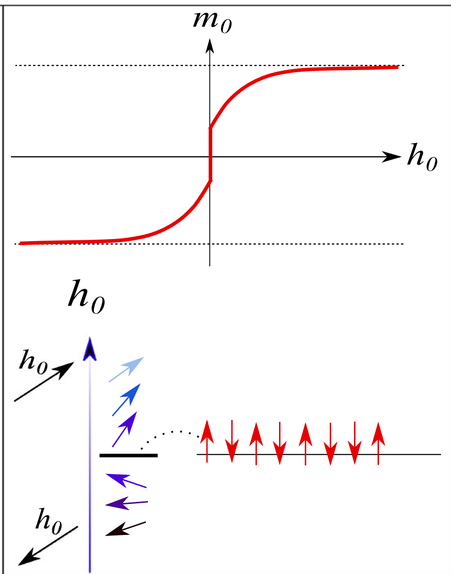
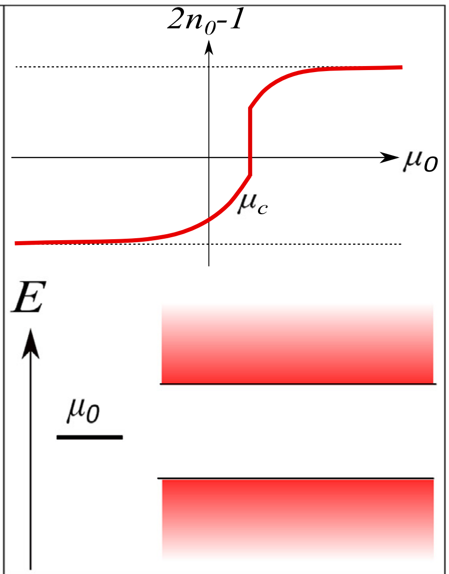
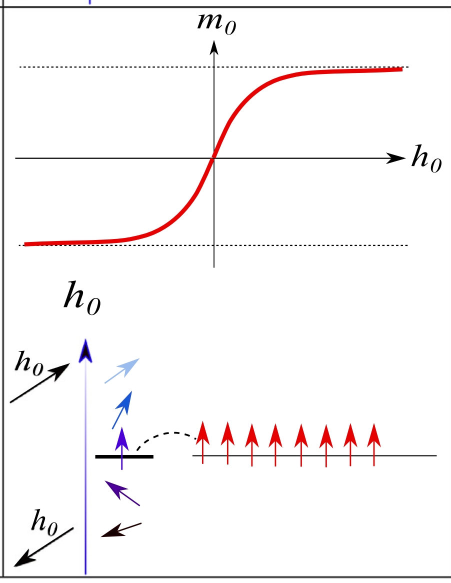
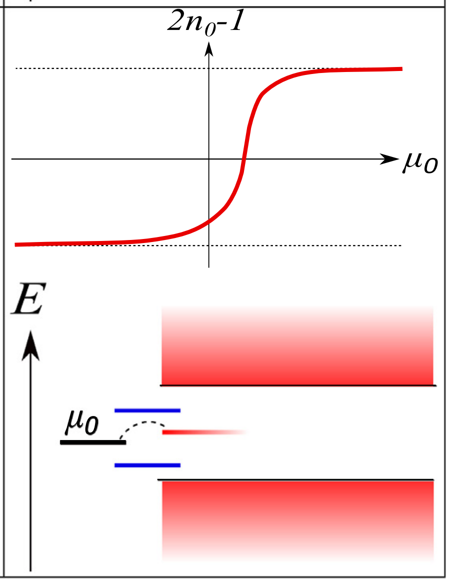
In the representative limits $h/J \to 0$ and $J/h \to 0$ a greatly simplified qualitative picture emerges. For $h \to 0$ one finds two decoupled boundary MZMs, c_1 and c_{2N}, in the otherwise dimerized chain, implying a two-fold degeneracy of the ground state, while for $J \to 0$ the KM lattice has a full dimer covering and the ground state is unique. At finite $h/J < 1$ the exact degeneracy between the two boundary MZMs in the ordered phase is removed. In spin language, the level splitting is caused by quantum tunneling between the two classical Ising vacua caused by the propagation of a magnetization kink from one end of the chain to the other. For a macroscopically long chain, the tunneling amplitude is exponentially small, $t_{\mathrm{eff}} \sim J\exp(-L/\xi)$ (L and ξ being the length of the chain and the correlation length, respectively). However, within this accuracy the two boundary Majorana modes remain true zero modes, and their existence implies the two-fold degeneracy of the ground state in the ordered phase of the QIC.

It is worth mentioning that the usefulness of the Majorana fermions in the QIC hinges on the exact $\mathbb{Z}_2$ symmetry of the spin model (2). Local terms (in the σ^x or σ^y) which break the Ising symmetry induce non-local couplings among the Majoranas and spoil the degeneracy of the edge modes. In contrast, the topological phase of the 1DPS is robust against any local perturbations in the fermionic basis. Nevertheless, within the symmetry protected sector, the QIC exhibits very similar physical properties as the 1DPS.

In this paper we aim at identifying clear physical differences associated with the presence or absence of Majorana edges modes in the topologically ordered or non-ordered phases, respectively. We focus on the effects of an impurity that interrupts an otherwise homogeneous 1d chain, or terminates it. We study its spectral weight and its response to locally applied external fields. Our main result is the finding summarized in Table 1: the local susceptibility of such an impurity can serve as a probe for Majorana edges modes in the adjacent bulk phase(s). In particular, we find that the non-topological phase is characterized by a discontinuity in the polarization response of the impurity to an external field, and a concomitant divergence of the susceptibility. In contrast, topological order and the associated MZMs quench such a divergence. This effect may serve as a *thermodynamic*, *equilibrium* tool in the search for direct traces of Majorana edge modes, which so far have been sought mostly in transport properties at zero bias.

For illustrative purposes and analytical convenience we focus on the QIC model in which the presence of impurities of a certain kind enforces all energy levels of the system to be two-fold degenerate even for a finite system. The impurities we have in mind represent lattice sites where the local transverse magnetic field vanishes. The spins residing at these sites are unable to flip and, therefore, are classical. The $\mathbb{Z}_2$ degeneracy of the ground state makes the existence of two decoupled Majorana modes at zero energy an exact property of a *finite* system at *arbitrary* values of the bulk parameters J and h. The goal of this work is to trace the evolution of the associated MZMs across the transition from the disordered phase to the ordered one and describe the corresponding qualitative changes of measurable quantities—the spectral weight (density of states) of the impurity spin and the local magnetic susceptibility defined as the linear response to a small transverse magnetic field. For a 1D p-wave superconductor the equivalent quantities are the average occupancy of the impurity fermionic level and the local charge susceptibility.

Table 1
The response of an impurity to local fields reveals the nature of the chain that it couples to. Ising spin chains and spinless p-wave superconductors are closely analogous. At $T = 0$, the spin σ_0 undergoes a discontinuous flip at $h_0 = 0$ in the paramagnetic phase, where a dressed free spin remains localized at the edge. On the ferromagnetic side, the spontaneously broken symmetry in the ground state generates a longitudinal field on the impurity and renders the transverse magnetization response $m_0(h_0)$ smooth. Upon JW transformation the Ising system maps to a single-level quantum dot which couples to a 1d p-wave superconductor. Thereby the dot's occupation n_0 as a function of the local potential μ_0 takes the role of $m_0(h_0)$. In the topologically trivial phase the level localized on the quantum dot can be driven through zero energy, inducing a discontinuous jump in $n_0(\mu_0)$. In this case, generic local couplings will shift the jump to arbitrary μ_c. In contrast, in the topological phase the coupling to the boundary Majorana zero mode repels the energy of the localized boundary state away from zero and thus renders $n_0(\mu_0)$ smooth. This paper analyzes the impurity response in the various phases, especially close to the degeneracy point ($h_0 = 0$ or $\mu_0 = \mu_c$). The susceptibility has Curie-like divergence in the disordered phase, while it saturates in the ordered phase. At criticality, the problem maps to the 2-channel Kondo effect, and accordingly, the susceptibility is a logarithmically diverging function of temperature.

	Quantum Ising chain	1d p-wave superconductor
Disordered phase		
Ordered phase (magnetic/topological)		

The paper is organized as follows. In Section 2 we briefly overview the QIC in the KM representation, which in Section 3 is used to qualitatively describe the main features of a quantum Ising chain containing classical-spin impurities: the presence of a free local spin with a local Curie susceptibility in the disordered phase, its delocalization at the phase transition and the transformation of the spectral degeneracy from locally differing ground states to globally differing Ising symmetry-broken states.

In Section 4 we explicitly construct a triplet of conserved operators which obey the standard spin 1/2 algebra, and are quasi-local in the disordered phase. We relate their existence to the integrable character of the considered models, and compare with similar conserved operators in many-body localized systems.

In Section 5 we consider a single classical impurity in an Ising chain close to criticality. Taking the scaling limit, we establish the connection with massive versions of previously studied resonant-level models where the impurity couples to two channels of Majorana fermions, and we explain how to compute the observables of interest using the Green's functions of the auxiliary Majorana fermions. Section 6 contains our central results for a boundary impurity. We evaluate the impurity spectral weight in both phases and calculate the temperature dependence of the transverse susceptibility of the impurity spin finding a rich behavior across the quantum critical window. At criticality, the QIC with a boundary impurity coincides with the Majorana resonant-level model discussed earlier by Emery and Kivelson [14] in their studies of the two-channel Kondo problem. In this regime the impurity spin has a logarithmically divergent low-temperature susceptibility. This is intermediate between the Curie asymptotics of the disordered phase and the saturating susceptibility in the ordered phase. Section 8 establishes the connection with the one-dimensional p-wave superconductors to which the QIC maps under JW transformation. In particular, we find that the local compressibility of an impurity site (a quantum dot coupled to a superconducting wire) provides a thermodynamic signature of the presence or absence of topological order in the superconductor: The topological phase with its boundary Majorana zero mode forces the charge occupation of the quantum dot to be a smooth function of local potential acting on the dot. This is in contrast to the topologically trivial superconducting phase of the wire, in the presence of which the occupation of the dot generically undergoes discrete jumps as a function of applied gate voltage. Section 7 analyzes an impurity in the bulk and summarizes the salient features of the susceptibility, and how it differs from a boundary impurity. The symmetrically coupled impurity is shown to map to a semi-infinite Peierls chain coupled to a boundary impurity. The concluding Section 9 summarizes the main results, and discusses how generally topological order in 1 dimension may be detected by the absence of discontinuous response to local fields acting on impurities.

2. Quantum Ising chain in Kitaev–Majorana representation

We start our discussion with a brief overview of the KM representation of the QIC [5,13]. The non-local JW transformation expresses the lattice spin-1/2 operators $S_n^\alpha = (1/2)\sigma_n^\alpha$ in terms of spinless fermionic operators a_n and $a_n^\dagger$:

$$\sigma_n^+ = \sigma^x + i\sigma^y = 2(-1)^n a_n^\dagger \exp\left(i\pi \sum_{j=1}^{n-1} a_j^\dagger a_j\right), \qquad \sigma_n^z = 2a_n^\dagger a_n - 1. \tag{4}$$

The Hamiltonian (2) then transforms to a quadratic form

$$\begin{aligned} H &= \sum_n [J(a_n^\dagger - a_n)(a_{n+1}^\dagger + a_{n+1}) - h(a_n^\dagger - a_n)(a_n^\dagger + a_n)] \\ &= J\sum_n \left(a_n^\dagger a_{n+1} + \text{h.c.}\right) + J\sum_n \left(a_n^\dagger a_{n+1}^\dagger + \text{h.c.}\right) - 2h\sum_n \left(a_n^\dagger a_n - 1/2\right). \end{aligned} \tag{5}$$

It does not conserve the particle number $N_F = \sum_i a_i^\dagger a_i$, but only the fermionic number parity: $P_S = (-1)^{N_F}$. The latter is simply the fermionic expression for the Ising flip operator. Notice that (5) is a 1DPS model (1) with a fine-tuned amplitude of the Cooper pairing Δ equaling the hopping strength t. The underlying Majorana structure of the Hamiltonian (5) is manifest. A physical site j of the original lattice, shown as a box in Fig. 1, is associated with a local Fock space of the complex fermion $(a_j, a_j^\dagger)$. Each physical site can then be split into a pair of "Majorana" sites, shown by crosses in Fig. 1, where real fermion operators $\{c_j\}$ are defined,

$$c_{2j-1} = a_j^\dagger + a_j, \qquad c_{2j} = -i(a_j^\dagger - a_j), \qquad \{c_j, c_l\} = 2\delta_{jl}. \tag{6}$$

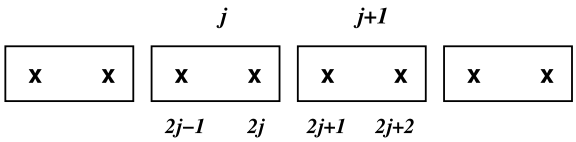


Fig. 1. Kitaev–Majorana chain with twice as many lattice sites as the Ising spin chain. Boxes indicate the Ising spin degrees of freedom which are split into two Majoranas.

The Hamiltonian (5) then transforms into the $2N$-site KM lattice model (3). At $J \neq h$ the translational invariance of the KM lattice (3) is broken, entailing a spectral gap. For later purposes, it is crucial to keep in mind that the transverse field h tends to pair the c-fermions belonging to the same physical site, while the exchange interaction J couples fermions belonging to neighboring boxes.

The Kramers–Wannier duality [11,12] transforms the original set of spin operators σ_n^α to the so-called disorder operators μ_n^α associated with the links $\langle n, n+1\rangle$,

$$\mu_n^x = \prod_{j=1}^{n-1} \sigma_j^z, \qquad \mu_n^x \mu_{n+1}^x = \sigma_n^z, \qquad \mu_n^z = \sigma_n^x \sigma_{n+1}^x. \tag{7}$$

Thereby it maps the Hamiltonian (2) into the same model, but with J and h interchanged, up to boundary terms. In the KM representation (3), the non-local transformation (7) simply reduces to a translation by one lattice spacing.

3. Classical impurity spins in quantum Ising chain: qualitative picture

Consider the ordered phase of an inhomogeneous QIC with locally varying transverse magnetic fields h_n. Imagine that a magnetization kink, separating two classical Ising vacua with opposite spin polarizations, travels along the chain from its left end to the right one, with each elementary step being associated with a spin reversal caused by a nonzero local field h_n. For $h_n \ll J$ the vacuum–vacuum tunneling amplitude is proportional to (one can always assume that $h_n \geq 0$)

$$t_{\mathrm{eff}} \approx J \prod_{n=1}^{N} \left(\frac{h_n}{J} \right). \tag{8}$$

Therefore, if at some lattice site the local field vanishes, t_{eff} vanishes as well implying that the boundary Majorana modes become true degenerate zero modes, *even for finite N*. Physically, this follows from the fact that at the impurity site spin reversal is impossible. The spin localized at such a site is classical, i.e., unable to flip. For a kink moving along the chain the zero-field site represents an infinitely high barrier which blocks its further propagation. Mixing of the boundary Majorana states located at the opposite boundaries thus becomes impossible; hence an exact $\mathbb{Z}_2$ degeneracy of the ground state.

Let us make this statement more precise. Consider a QIC with a zero-h impurity, say at $n = 0$:

$$H = -J \sum_n \sigma_n^x \sigma_{n+1}^x - h \sum_{n \neq 0} \sigma_n^z. \tag{9}$$

There are two operators, σ_0^x and $P_S = \prod_{n=1}^{N} \sigma_n^z$, which commute with the Hamiltonian, but anticommute with each other. Each of these operators squares to unity. If ψ_σ is an eigenstate of both H and σ_0^x,

$$H\psi_\sigma = E\psi_\sigma, \quad \sigma_0^x \psi_\sigma = \sigma\psi_\sigma \quad (\sigma = \pm 1)$$

then the anticommutation relation $\{\sigma_0^x, P_S\} = 0$ implies that the state $\psi'_{\sigma'} = P_S \psi_\sigma$ is also an eigenstate of H with the same energy E but with $\sigma' = -\sigma$. Hence all energy levels of the system are two-fold degenerate at *arbitrary* J/h. This conclusion remains obviously valid for an arbitrary number N_i of zero-field impurities in which case the Hamiltonian has the form:

$$H = -J \sum_n \sigma_n^x \sigma_{n+1}^x - h \sum_{n \notin \mathcal{J}} \sigma_n^z, \tag{10}$$

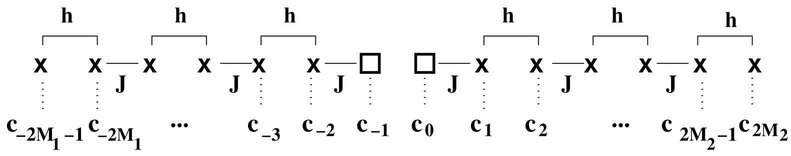


Fig. 2. KM representation of QIC with $h_j = h(1 - \delta_{j0})$.

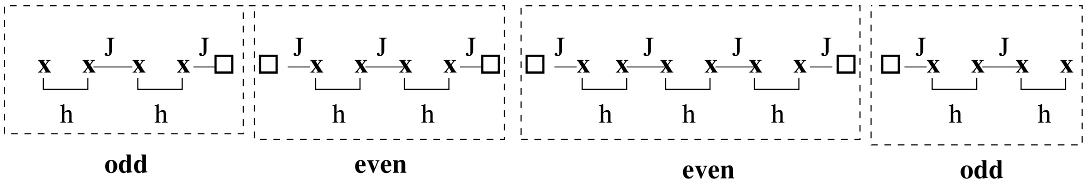


Fig. 3. QIC with several classical (zero-field) impurities in the KM representation.

where $\mathcal{J}$ is the set of all impurity sites. Obviously, H commutes with P_S and the N_i operators σ_m^x ($m \in \mathcal{J}$). The operators σ_m^x commute among each other, whereas all of them anticommute with P_S. Since P_S simultaneously inverts the signs of the eigenvalues of all impurity spins σ_m^x, by the same argument as before one concludes that the energy levels of the many-impurity model are also two-fold degenerate (but generically there is no higher degeneracy). Thus, irrespective of the nature of the bulk phase, ordered or disordered, the ground state of a QIC with classical impurity spins is $\mathbb{Z}_2$-degenerate.

To understand how this degeneracy is physically realized in the disordered and ordered bulk phases, let us look at the KM representation of a finite QIC with a zero-field impurity at the origin. Let M_1 and M_2 be the numbers of the lattice sites to the left and to the right of the impurity site, the total number of physical sites being $N = M_1 + M_2 + 1$. The pattern of pairings of neighboring c-operators on the corresponding KM lattice is displayed in Fig. 2. The operators c_{-1} and c_0 shown by two squares originate from the impurity site $n = 0$. As opposed to all other c-operators, these two operators are unpaired, $\langle c_{-1}c_0\rangle = 0$, because $h_0 = 0$. As a consequence, the impurity cuts the KM chain in Fig. 2 into two disconnected pieces containing $2M_1 + 1$ and $2M_2 + 1$ sites, respectively. Since these numbers are odd, the emerging situation is special because a piece of a Majorana lattice with an odd number of sites does not represent a segment of the original physical lattice where the spins σ_n^α are defined.

Local fluctuations of the Hamiltonian parameters can indeed cut the KM lattice into disconnected pieces. This can be due to vanishing local values of J or h at certain links or sites. The former case is trivial: randomly distributed links with vanishing exchange couplings cut the original spin chain into segments, each representing a smaller-size chain with open boundaries. On the KM lattice, each disconnected segment contains an even number of sites. This picture should be contrasted with the situation emerging in a QIC containing sites with vanishing local magnetic fields. An example is shown in Fig. 3. For a spin chain with N_i impurities, the corresponding KM lattice decouples into $N_i + 1$ pieces: $N_i - 1$ of them contain even numbers of c-sites and two more pieces with odd numbers of sites are attached to the boundaries.

Now, a finite KM chain with an odd number of sites necessarily contains an exact MZM. Indeed, the Hamiltonian of such a chain is a quadratic form $\mathcal{H} = i\sum_{jk} A_{jk}c_jc_k$, where A_{jk} is a real, antisymmetric $N \times N$ matrix, where N is odd. Consequently, $\det \hat{A} = 0$ and so the set of eigenvalues of $\hat{A}$ necessarily contains a zero eigenvalue. So a finite QIC with a classical-spin impurity should have two exact MZMs. To understand where these zero modes are located, it is instructive to turn again to the limiting cases $h = 0, J \neq 0$ and $J = 0, h \neq 0$. Considering for instance the right segment of the KM chain in Fig. 2, one finds that a KM chain with an odd number of sites contains a zero mode at the right boundary if $J > h$ or at the left boundary if $J < h$. For the left segment of the KM chain the situation is just inverted. The boundary MZM will have a finite localization radius at any $J \neq h$ and move from one boundary to the other as the critical point is crossed.

We thus arrive at the following physical picture for a QIC with an impurity spin in the bulk. In the disordered phase the two MZMs are located close to the impurity site. In this phase, the free impurity

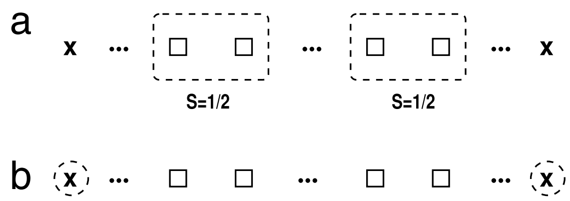


Fig. 4. Majorana zero modes in a many-impurity system. (a) Disordered phase: $2N_{imp}$ Majorana quasi-zero modes; (b) ordered phase: no localized free spins left, two exact MZMs at the end-points of the chain.

spin of the limit $J \to 0$ retains its identity, despite getting dressed and delocalizing over a finite length scale ξ: the local transverse spin susceptibility, defined as the linear response to a small transverse field h_0, follows a Curie law: $\chi_0 \sim T^{-1}$. The impurity zero modes are fragile because they are not spatially separated: application of a small transverse local field h_0 will produce Zeeman splitting of the zero-energy levels and polarize the impurity spin in the z-direction.

Once the system passes over to the ordered phase, the exact $\mathbb{Z}_2$ degeneracy becomes a non-local property of the ground state. The free impurity spin "disappears" because it gets strongly coupled to the rest of the system by the classical Ising exchange. The local spin susceptibility χ_0 is finite in the zero-temperature limit. However, in agreement with the Kitaev's picture [5], the disappearance of the impurity spin in the ordered phase is accompanied, in the fermionic language, by the appearance of two spatially separated MZMs at the end-points of the chain. In other words, these boundary zero modes represent what the spectral weight of the local impurity spin transforms into when the system undergoes the quantum phase transition from the disordered to the ordered phase. Let us stress again that these are *exactly degenerate* boundary MZMs in a *finite* quantum Ising chain—an effect caused by the zero-field impurity, which kills the tunneling between the Ising vacua.

Consider now the case of a finite number N_i of classical-spin impurities. As already explained, there should again be two exact MZMs in the ground state. In the ordered phase, the Kitaev's picture [5] of two boundary MZMs at the end-points of the chain is intact. In the disordered phase there are $2N_i$ boundary Majorana modes localized in the vicinity of N_i impurity spins. However, as follows from Fig. 3, only two of them are exact MZMs, namely those located at the right and left ends of the left and right odd-number segments of the KM chain, respectively. The Majorana modes residing at the boundaries of the inner (even-site) pieces of the KM chain overlap and split. Nevertheless, in the dilute limit of rare impurities separated by distances much larger than the correlation length, the level splitting of the boundary modes of each even-site inner segment is exponentially small, and one can think of $2N_i$ MZMs in the disordered phase, forming N_i nearly free spins. This is the limit in which the interaction between the impurity spins can be neglected and the symmetry of the disordered phase gets approximately promoted to $[\mathbb{Z}_2]^{N_i}$.

The difference between the numbers of the Majorana (quasi-)zero modes in the ordered and disordered phase of the dilute impurity system (see Fig. 4) originates from the non-trivial topological property of the inner pieces of the KM lattice. In spite of having even numbers of c-sites, these pieces do *not* represent parts of the original spin chain defined in terms of the σ_n^α operators. Indeed, the sequence of Majorana links in a finite QIC is $[hJhJ \cdots hJh]$, whereas in all inner even-site pieces the sequence of links is different: $[JhJh \cdots JhJ]$. For these pieces it is impossible to form local spin operators by pairing the c-operators according to the usual rule $[12]$ $[34]$ $\cdots [2M-1, 2M]$. It can be readily seen that, for the inner pieces of the KM lattice, the pattern of pairing neighbors actually corresponds to the *dual* lattice of links, i.e., the lattice of the disorder μ_n^α-operators, Eq. (7). Thus the inner even-site segments of Fig. 3 can be treated as "physical" only in the dual (μ_j^α) representation. In this sense, zero-field impurities favor a description using the Kramers–Wannier duality transformation of the original quantum spin chain.

As a consequence of this curious fact, in the inner regions of the QIC separated by zero-field impurities, the zero boundary modes appear only in the disordered phase. Therefore for these regions it is the spin disordered phase (being ordered in the dual representation) which is topological. This is consistent with the observation that for $J < h$ the boundary zero modes of neighboring regions will combine and form local, free $S = 1/2$ degrees of freedom.

4. Conserved, free spin operator

As was discussed in the preceding section, in a Quantum Ising model the presence of a classical impurity with vanishing transverse field leads to an exact degeneracy of the entire spectrum, all eigenstates coming in pairs of equal energy, $|E_n, \pm\rangle$, where $\pm$ indicates the eigenvalue of σ_0^x. Formally one can thus define a set of three "spin operators" $S^{x,y,z}$ by their action in this basis:

$$S^z|E_n, \pm\rangle = |E_n, \mp\rangle, \tag{11}$$

$$S^y|E_n, \pm\rangle = \mp i|E_n, \mp\rangle, \tag{12}$$

$$S^x|E_n, \pm\rangle = \pm|E_n, \pm\rangle. \tag{13}$$

They all commute with the Hamiltonian and satisfy the standard SU(2) commutation relations. These operators thus represent a free spin 1/2 degree of freedom. Note however, that these latter properties do not uniquely determine the operators $S^{x,y,z}$. Indeed, we could have chosen the labeling of eigenstates such that $\pm$ refers instead to the eigenvalue of $\tau_n\sigma_0^x$ with τ_n being a random sign (± 1), chosen independently for each n. The same construction then yields a different triplet of free spin operators. However, almost all of these choices would result in highly non-local operators, which have no practical interest. The above choice (11) with $\tau_n \equiv 1$ is singled out by the further requirement that the resulting operators be local in the ordered phase of the QIC.

It is not difficult to construct the operators $S^{x,y,z}$ explicitly using the Majorana zero modes on either side of the impurity. In terms of the notation introduced in Eq. (28) (see the next section), those zero modes have the explicit expressions

$$\Xi_a = \sqrt{1-(J/h)^2}\left(\beta_a + \sum_{j\geq 1}^{L} \eta_{aj}\left(\frac{J}{h}\right)^j\right), \quad a = 1, 2, \tag{14}$$

where for simplicity we consider the case of homogeneous Ising couplings, $\tilde{J}_{1,2} = J_{1,2} = J$. The zero Majorana modes commute with the Hamiltonian (28), and for $h > J$ are normalized to satisfy $\Xi_a^2 = 1$ in the thermodynamic limit. In finite size systems the zero modes still exist even in the ordered phase, $h < J$, but there, the corresponding operators are dominated by the last terms in the sum (14) and thus act primarily on the far ends of the finite chains.

The bilinear

$$S^z \equiv i\Xi_1\Xi_2 \tag{15}$$

is obviously conserved, too, and squares to 1. Since in the product of two Majorana operators the JW tails cancel, S^z is a quasi-local operator in spin degrees of freedom for $h > J$, with the explicit representation

$$S^z = \left[1-\left(\frac{J}{h}\right)^2\right]\left[\sigma_0^z - \sum_{j\leq 0\leq k;\,(j,k)\neq(0,0)} \left(\frac{J}{h}\right)^{k-j} \sigma_j^y\sigma_k^y \prod_{m=j+1}^{k-1} \sigma_m^z\right]. \tag{16}$$

Defining

$$S^x \equiv \sigma_0^x, \tag{17}$$

one easily checks the anticommutation relation $\{S^z, S^x\} = 0$. Defining eventually

$$S^y \equiv iS^xS^z, \tag{18}$$

one obtains a third conserved operator. It completes the triple of SU(2) operators which satisfies the spin algebra $\{S^i, S^j\} = 2\delta_{ij}$ and $[S^i, S^j] = 2i\epsilon_{ijk}S^k$. The presence of this quasi-local free spin operator in the disordered phase implies not only the Curie form of the local susceptibility, but the two-fold degeneracy of the entire spectrum. Furthermore, to obtain the partner state of a given eigenstate which is simultaneously an eigenstate of σ_0^x, it suffices to act with S^z or S^y on that state. This establishes a specific local relationship between *all* many-body states, throughout the entire spectrum. Below we will use this property to estimate the local transverse susceptibility in the disordered phase, but close to criticality.

4.1. The existence of conserved quasi-local spin operators is tied to integrability

It is natural to ask whether the existence of a quasi-local, conserved $S = 1/2$ spin operator is already implied by the mere presence of a classical impurity in the QIC model. In any Ising model such an impurity always implies the two-fold degeneracy of the entire spectrum and, by the abstract construction above, the existence of some conserved operators $S^{x,y,z}$ which obey SU(2) commutation relations. However, we believe that these operators are generically non-local, except in models with strong disorder or with an integrable structure (as for the QIC). Indeed, consider the perturbative construction of the operator S^z according to the following formal recipe. Consider the general Ising model,

$$H = -\sum_i h_i\sigma_i^z - \sum_{i,j} J_{ij}\sigma_i^x\sigma_j^x \equiv H_0 + H_1, \tag{19}$$

with the transverse field term being described by $H_0 \sim h$ and the exchange term by $H_1 \sim J \ll h$. The couplings J_{ij} are non-zero only for spins i and j that are spatially close, but not necessarily restricted to nearest neighbor pairs. Now make the perturbative ansatz

$$S^z \equiv S^{z,(0)} + S^{z,(1)} + \sum_{k\geq 2} S^{z,(k)} = \sigma_0^z - \sum_i \frac{J_{0i}}{h_i}\sigma_0^y\sigma_i^y + O((J/h)^2), \tag{20}$$

where the norm of the operator $S^{z,(k)}$ scales as $(J/h)^k$, as $J \to 0$. We may now try to find the $S^{z,(k)}$ iteratively by solving the conservation constraint $[H, S^z] = 0$ order by order:

$$[H_0, S^{z,(k)}] + [H_1, S^{z,(k-1)}] = 0. \tag{21}$$

This recipe has been followed in the context of many-body localized systems to construct quasi-local integrals of motion [15]. It has been argued that for sufficiently strong disorder ($\mathrm{Var}(h_i) \gg J^2$, where J is the typical nearest neighbor exchange coupling), the formal perturbation series defined by Eq. (21) can be resummed and leads to quasi-local integrals of motion. In this strongly disordered case, the construction actually works irrespectively of the value of h_0. The existence of such quasi-local conserved operators was proven almost rigorously for one-dimensional Ising spin chains [16].

However, for this procedure to work, it is essential that sums and differences of sets of different h_i do not vanish, and that they yield small values only with sufficiently low probability, since such terms appear in the denominators of the coefficients that multiply products of spin operators in $S^{z,(k)}$. In a homogeneous system, where all h_i are equal (except for $h_0 = 0$), this requirement is maximally violated, and the above procedure is very likely to fail. In fact, one faces an extreme case of a small denominator problem, since many denominators of the formal perturbation theory will exactly vanish as $h_i \to h =$ const. This problem arises because the conjugation with H_0, $C(X) = [H_0, X]$ is not surjective as a linear map in operator space. For the case of generically disordered h_i its kernel is however small enough, such that one can prove that a solution to (21) can be found at every step [15].

However, for $h_i =$ const, the kernel of C is much larger, so that after a few steps of perturbation theory one cannot ensure that $[H_1, S^{z,(k-1)}]$ lies in the image of C. This issue appears at the earliest in the 4th order of perturbation theory, if triangles formed by exchange bonds are present. At this point, one would have to track back and seek for conserved operators using degenerate perturbation theory, remembering that the exponentially large set of all polynomials in σ_i^z's is conserved by H_0. They are thus all zero-eigenvectors under conjugation with H_0 and therefore, in general, perturbation theory has to be carried out starting from an appropriate linear combination of those degenerate eigen-operators. In view of the non-local nature of most of those polynomials, it seems very unlikely that such a procedure can be engineered to result in a local conserved operator S^z.

Also from physical considerations there are good reasons not to expect the existence of such a local conserved operator in general. A converging, quasi-local S^z could be viewed as the creation operator of a sharp, quasi-local excitation with zero energy, that is, an exact zero-energy quasiparticle with infinite life time. In a non-integrable, non-localized system it is not conceivable that such infinitely long-lived excitations should exist. Indeed, at any finite temperature there is a finite phase space for the decay of that quasiparticle, upon scattering from excited delocalized modes above the spectral gap. Of course, the cross-section of these processes decreases exponentially to zero as $T \to 0$. This ensures that ultimately, at $T = 0$, there will still be a sharp excitation localized close to the impurity, and this will still give rise to a Curie susceptibility in the low T limit.

However, for classical impurities in very special, non-disordered Ising models such as a chain with only nearest neighbor interactions, the above-discussed problem of perturbation theory does not arise because of a lot of exact cancellations that kill the dangerous terms. A non-trivial example is given below. The existence of such local operators in these systems is presumably tightly linked to the integrability of the transverse field Ising model in strictly 1d systems. Related issues in more complex, but integrable spin chains have recently been analyzed in Ref. [17].

Local conserved operators S^z appear to exist only in fine-tuned systems, unless one considers strongly disordered, many-body localized systems. Nevertheless, having the explicit form of conserved S^z in such fine-tuned systems helps us to visualize the physical properties associated with a classical impurity, especially at low T. Furthermore, we expect those properties to be more general than the existence of the local S^z operator itself. Since S^z takes one ground state to another, the spatial extent of the operator makes precise the notion that the ground states differ only locally, a fact that should be generically true, independent of integrability or localization. Below, the structure of S^z will also help us to understand the scaling of the low T susceptibility upon approaching criticality. The fact that in specific models S^z as an operator is quasi-local implies additionally that *all* degenerate pairs of states are similar up to local modifications, not only the ground state.

4.2. *Exact conserved spin operators in junctions of transverse field Ising chains*

It is interesting to note that conserved free spin operators also exist in the case where the classical impurity sits at the junction of an arbitrary number n of 1d chains—a situation in which integrability is not as obvious as in the cases of an impurity at the end or in the bulk of a simple chain, which correspond to $n = 1, 2$. Labeling the junction spin by 0, one can check that the operator

$$S^z = \left(1 - \frac{J^2}{h^2}\right)^{n/2} \sum_{k=0}^{n} (-i\sigma_0^x)^k \sigma_0^z \sum_{j_1,\dots,j_k \geq 1} \prod_{a=1}^{k} \left[\left(\frac{J}{h}\right)^{j_a} \sigma_{j_a}^y \prod_{i_a=1}^{j_a-1} \sigma_{i_a}^z \right] \tag{22}$$

is indeed conserved by the Ising Hamiltonian on such a junction structure if $h_0 = 0$. This expression generalizes Eq. (16), to which it reduces for $n = 2$. This operator also squares to 1. Again one obtains a full triplet of spin operators by completing S^z with the conserved operators $S^x = \sigma_0^x$ and $S^y = iS^xS^z$.

In the low temperature limit, the Lehmann representation of the local spin susceptibility $\chi_0 = \lim_{h_0 \to 0} \left(\partial \langle \sigma_0^z \rangle\right) \partial h_0$ leads to the Curie law

$$\chi_0(T) = \mu_{\rm eff}^2/T, \tag{23}$$

where the effective magnetic moment $\mu_{\rm eff}$ is defined as the matrix element of σ_0^z between the two degenerate ground states $|0, \pm\rangle$,

$$\mu_{\rm eff} = \langle 0, -|\sigma_0^z|0, +\rangle = \langle 0, +|S^z \sigma_0^z|0, +\rangle. \tag{24}$$

The states $|0, \pm\rangle$ are eigenstates of σ_0^x with eigenvalues ± 1, respectively. Inserting the explicit expression (22) we see that the contribution from the leading term is simply

$$\mu_{\rm eff} = \left(1 - \frac{J^2}{h^2}\right)^{n/2} \Big|_{h-J\sim m\to 0} \sim m^{n/2}. \tag{25}$$

Assuming that the matrix elements of higher spin operator products come with random signs, one finds that they contribute with the same scaling to $\mu_{\rm eff}$. Close to criticality, in the continuum limit, one thus expects the scaling

$$\chi_0(T \to 0) \sim \frac{m^n}{T}. \tag{26}$$

This conjecture is confirmed by the explicit calculations for the cases $n = 1$ and $n = 2$, see Eqs. (74) and (107).

5. Impurity in a weakly non-critical QIC

5.1. Reduction to a two-channel resonant-level model of massive Majorana fermions

In the rest of this paper we will be dealing with a single impurity in a weakly non-critical QIC. In this section we set up a formalism based on a continuum, field-theoretical description of the bulk degrees of freedom to treat effects caused by the impurity spin. The impurity is located at the origin. The right and left parts of the chain, supplied with subscripts 1 and 2, respectively, are assumed to be homogeneous, but may represent different quantum Ising chains characterized by two sets of parameters, (J_1, h_1) and (J_2, h_2). In the KM representation, the Hamiltonian of the system reads:

$$\begin{aligned} H = &-ih_0\beta_1\beta_2 + i\tilde{J}_1\beta_1c_1 + i\tilde{J}_2c_{-2}\beta_2 \\ &+ iJ_1(c_2c_3 + c_4c_5 + \cdots) + ih_1(c_1c_2 + c_3c_4 + \cdots) \\ &+ iJ_2(c_{-4}c_{-3} + c_{-6}c_{-5} + \cdots) + ih_2(c_{-3}c_{-2} + c_{-5}c_{-4} + \cdots). \end{aligned} \tag{27}$$

The pair of Majorana operators, β_1 and β_2 (previously denoted c_0 and c_{-1}, respectively) describes the impurity spin $\sigma_0^z = i\beta_1\beta_2$ located at the origin. h_0 is the transverse magnetic field at the impurity site which must be kept small but finite to calculate the local response function. The coupling constants $\tilde{J}_1$ and $\tilde{J}_2$ parametrize hybridization between the impurity Majorana fermions and the bulk degrees of freedom.

Before passing to the continuum limit, it is convenient to distinguish between even and odd sites of the KM lattice. For the right part of the chain we set $c_{2j-1} = \zeta_j$, $c_{2j} = \eta_j$ $(1 \le j \le N)$ with a minor modification for the left part, $c_{2j-1} = \eta_j$, $c_{2j} = -\zeta_j$ $(-N \le j \le -1)$. In the new notations the Hamiltonian reads

$$\begin{aligned} H = &-ih_0\beta_1\beta_2 + i\tilde{J}_1\beta_1\zeta_1 + i\tilde{J}_2\beta_2\zeta_{-1} + i\sum_{j\ge1}\left(h_1\zeta_i\eta_j + J_1\eta_j\zeta_{j+1}\right) \\ &- i\sum_{j\ge1}\left(h_2\eta_{-j}\zeta_{-j} + J_2\zeta_{-j-1}\eta_{-j}\right). \end{aligned}$$

Mapping the negative semi-axis to the positive one, as shown in Fig. 5, and introducing two species of Majorana operators, $\eta_j \equiv \eta_{1j},\ \zeta_j \equiv \zeta_{1j},\ \eta_{-j} \equiv \eta_{2j},\ \zeta_{-j} \equiv \zeta_{2j}$, we transform the Hamiltonian as follows

$$H = -ih_0\beta_1\beta_2 + i\sum_{a=1,2}\tilde{J}_a\beta_a\zeta_{a1} + i\sum_{a=1,2}\sum_{j\ge1}\left(J_a\eta_{aj}\zeta_{a,j+1} - h_a\eta_{aj}\zeta_{aj}\right). \tag{28}$$

The last term in (28) represents a sum of two semi-infinite QIC models. Assuming that each chain is close to criticality, $|h_a - J_a| \ll J_a$ $(a = 1, 2)$, one can pass from the lattice Majorana operators to continuum fields using the correspondence

$$\eta_{aj} \to \sqrt{2a_0}\,\eta_a(x), \qquad \zeta_{aj} \to \sqrt{2a_0}\,\zeta_a(x). \tag{29}$$

The fields satisfy the algebra

$$\{\eta_a(x), \eta_b(x')\} = \{\zeta_a(x), \zeta_b(x')\} = \delta_{ab}\delta(x - x'), \qquad \{\eta_a(x), \zeta_b(x')\} = 0. \tag{30}$$

In the continuum limit, the Hamiltonian (28) takes the form

$$\begin{aligned} H = &-ih_0\beta_1\beta_2 + i\sqrt{2a_0}\sum_{a=1,2}\tilde{J}_a\beta_a\zeta_a(0) \\ &+ \sum_{a=1,2}\int_0^L \mathrm{d}x\ \left[iv_a\eta_a(x)\partial_x\zeta_a(x) - im_a\eta_a(x)\zeta_a(x)\right]. \end{aligned} \tag{31}$$

In (31) the bulk degrees of freedom of the system are described in terms of two (formally Lorentz-invariant) free massive Majorana fields with group velocities $v_a = 2J_aa_0$ and masses $m_a = 2(h_a - J_a)$.

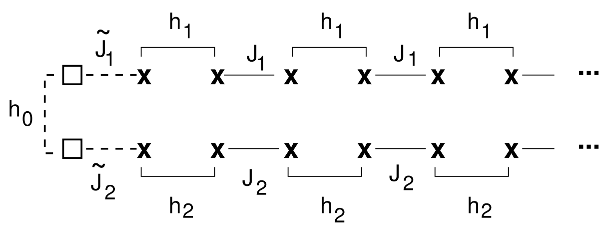


Fig. 5. Folded KM chain with an impurity.

In the continuum limit, the Majorana fields at the open end must satisfy boundary conditions which are obtained as follows. Take a semi-infinite KM lattice $(\zeta_1, \eta_1), (\zeta_2, \eta_2), \ldots$ and add an extra site $j = 0$ requiring that the pairing between η_0 and ζ_1 is absent. For the degrees of freedom on the chains this is equivalent to having a finite coupling, but imposing the constraint $\eta_0 = 0$. Thus, in the continuum description, which captures the relevant low-energy subspace of the model, the boundary conditions are

$$\eta_a(0) = 0, \quad (a = 1, 2). \tag{32}$$

The original model is thus equivalently represented as a Majorana version of the two-channel, massive resonant-level model on a semi-infinite (for $N \to \infty$) axis with an impurity at the boundary. It is crucial that different bulk channels ($a = 1, 2$) are coupled to different Majorana components of the impurity spin (β_1 and β_2). Note that if $h_0 = 0$ the channels decouple.

The massless limit of the model (31) has been thoroughly studied long ago in the context of the overscreened Kondo effect. Indeed, at $m_1 = m_2 = 0$ and $v_1 = v_2$, Eq. (31) represents the Majorana resonant-level model introduced and solved by Emery and Kivelson [14] in their bosonization treatment of the two-channel Kondo problem with XXZ exchange anisotropy (see e.g. Ref. [18] for a review). The correspondence between the critical point of the model (31) and the two-channel resonant-level model is briefly discussed in Appendix A. When one of the two bulk-impurity couplings, $\tilde{J}_1$ or $\tilde{J}_2$, vanishes, one has a problem of massive Majorana fermions on a single semi-infinite chain with an impurity at the open end. In the related two-channel Kondo model, this case corresponds to the channel-symmetric situation describing the overscreened Kondo effect. For two identical massless chains and coinciding coupling constants ($\tilde{J}_1 = \tilde{J}_2$) the Hamiltonian (31) acquires an enhanced, $O(2)$, symmetry associated with global planar rotations of the first and second Majorana species. In this case the Hamiltonian (31) represents the usual resonant-level model for complex fermions, in which the total particle number is conserved and which is relevant to the single-channel Kondo problem [19].

At $m_1 = m_2 \neq 0$, $v_1 = v_2$ the model (31) describes a semi-infinite Peierls insulator (PI) chain with an impurity fermionic d-state at the open boundary whose energy is $\varepsilon_d = -2h_0$ (see Appendix D).

5.2. Diagonalized bulk spectrum and the total Hamiltonian

To diagonalize the bulk part of the Hamiltonian (31), one first performs a chiral rotation of the Majorana fields (η_a, ζ_a):

$$\eta_a(x) = \frac{\xi_{aR}(x) + \xi_{aL}(x)}{\sqrt{2}}, \qquad \zeta_a(x) = \frac{-\xi_{aR}(x) + \xi_{aL}(x)}{\sqrt{2}}. \tag{33}$$

The new Majorana fields satisfy the algebra:

$$\{\xi_{aR}(x), \xi_{bR}(x')\} = \{\xi_{aL}(x), \xi_{bL}(x')\} = \delta_{ab}\delta(x - x'), \qquad \{\xi_{aR}(x), \xi_{bL}(x')\} = 0. \tag{34}$$

The boundary conditions (32) translate to

$$\xi_{aR}(0) = -\xi_{aL}(0). \tag{35}$$

In terms of the fields $\xi_{a;R,L}(x)$ the Hamiltonian takes the form

$$H - ih_0\beta_1\beta_2 - 2i\sqrt{a_0}\sum_{a=1,2}\tilde{J}_a\beta_a\xi_{aR}(0) + \sum_{a=1,2}\int_0^L \mathrm{d}x\left[\frac{iv_a}{2}\left(\xi_{aL}(x)\partial_x\xi_{aL}(x) - \xi_{aR}(x)\partial_x\xi_{aR}(x)\right) - im_a\xi_{aR}(x)\xi_{aL}(x)\right]. \tag{36}$$

The diagonalization of a massive Majorana model on a semi-axis is discussed in Appendix B. The spectrum contains a continuum of extended states with the energy $\varepsilon_k = \sqrt{k^2v^2 + m^2}$ and, for a negative mass only ($m < 0$), a normalizable zero-energy state localized at the boundary of the chain within a characteristic length $\xi = a_0/|\ln(h/J)| \simeq a_0/(1-h/J) = v/|m|$. The normal-mode expansion of a single massive Majorana spinor field operator is given by formula (B.14). Using this expansion one rewrites the Hamiltonian as follows:

$$H = -ih_0\beta_1\beta_2 + \sum_{k>0}\sum_a \varepsilon_{ak}\hat{\gamma}^\dagger_{ak}\hat{\gamma}_{ak} - i\sum_a \lambda_0^a\beta_a\gamma_{a0} - i\sqrt{\frac{2}{N}}\sum_a\beta_a\sum_{k>0}\lambda_k^a(\gamma_{ak} + \gamma^\dagger_{ak}). \tag{37}$$

Here $\gamma_k,\ \gamma_k^\dagger$ are fermionic quasiparticle operators related to the continuum part of the spectrum, $\gamma_0 = \gamma_0^\dagger$ is the operator describing the boundary MZM, and

$$\lambda_0^a = 2\theta(-m_a)\sqrt{\frac{|m_a|a_0}{v}}\tilde{J}_a, \qquad \lambda_k^a = \tilde{J}_a\frac{kv}{\varepsilon_{ak}} \tag{38}$$

are the coupling constants. In the last term of (37) the local Majorana operators β_a couple to a Hermitian combination of the band operators, $\gamma_{ak} + \gamma^\dagger_{ak}$. Therefore we can "majoranize" the bulk part of the spectrum as well. Represent the quasiparticle operator $\gamma_k^\dagger$ as a linear combination of two real operators: $\gamma_k^\dagger = (b_k + if_k)/2$. The algebra $\{\gamma_k, \gamma^\dagger_{k'}\} = \delta_{kk'}$ implies that $\{b_k, b_{k'}\} = \{f_k, f_{k'}\} = 2\delta_{kk'}$ with all remaining anticommutators vanishing. The kinetic energy becomes

$$\sum_{k>0}\varepsilon_k\gamma_k^\dagger\gamma_k = -\frac{i}{2}\sum_{k>0}\varepsilon_k b_k f_k + \text{const}.$$

Thus the total Hamiltonian can be represented entirely in terms of Majorana degrees if freedom:

$$H_M = -ih_0\beta_1\beta_2 - \frac{i}{2}\sum_{k>0,a}\varepsilon_{ak}b_{ak}f_{ak} - i\sum_a\lambda_0^a\beta_a\gamma_{a0} - i\sqrt{\frac{2}{N}}\sum_a\sum_{k>0}\lambda_k^a\beta_a b_{ak}. \tag{39}$$

As we shall show below, the coupling of the impurity Majorana operators β_a to the Majorana boundary MZM operators γ_{a0}, parametrized by the constants λ_0^a, plays a crucial role in the low-temperature asymptotics of the local spin susceptibility in the ordered bulk phase.

5.3. Physical quantities in terms of Green's functions

The Hamiltonian H_M in (39) represents a one-particle, exactly solvable model. Our goal is to calculate the impurity parts of the physical quantities: the spectral weight of the impurity spin, the local magnetization and spin susceptibility defined as the linear response to the local transverse magnetic field. All calculations are straightforward and can be done using the formalism of Matsubara Green's functions (GF) [20].

Here we provide basic definitions. The impurity spin is described in terms of a complex (Jordan–Wigner) spinless d-fermion:

$$\sigma_0^z = 2d^\dagger d - 1 \equiv 2n_d - 1, \qquad \sigma_0^+ = 2d^\dagger\exp[i\pi N_2], \qquad \sigma_0^- = 2d\exp[i\pi N_2], \tag{40}$$

or equivalently, a pair of Majorana operators, β_1 and β_2: $d^\dagger = \beta_2 + i\beta_1$, $\sigma_0^z = i\beta_1\beta_2$

$$N_2 = \sum_{j=1}^{\infty} a_{2,j}^\dagger a_{2,j}. \tag{41}$$

A local magnetic field h_0 determines the Zeeman energy of the impurity spin, $H_0 = -h_0\sigma_0^z$. Accordingly, the local magnetization and spin susceptibility are defined as

$$m_0(h_0, T) = \langle \sigma_0^z \rangle = 2(\langle n_d \rangle - 1/2), \qquad \chi_0(T) = \frac{\partial m_0}{\partial h_0}\Big|_{h_0=0}. \tag{42}$$

In the context of a 1DPS, the local magnetization of the impurity in a QIC translates to the average occupation number of the d-fermionic state, $m_0 \to 2(\langle n_d \rangle - 1/2)$, the magnetic field h_0 transforms to the local energy of the d-fermion, $\mu_0 = 2h_0$, and the local spin susceptibility χ_0 becomes the local charge susceptibility ("compressibility") of the impurity site.

An important characteristics of free fermionic models which determines local thermodynamic properties of the impurity is the spectral weight (or local density of states) of the boundary complex fermion:

$$A(\omega) = -\frac{1}{\pi}\Im m\, \mathcal{G}(\omega + i\delta), \qquad \int_{-\infty}^{\infty} \mathrm{d}\omega\, A(\omega) = 1. \tag{43}$$

Here the retarded GF $\mathcal{G}(\omega + i\delta)$ is the analytic continuation of the Fourier transform $G(\varepsilon_n)$ of the Matsubara single-fermion GF

$$G(\varepsilon_n) = \int_0^{1/T} \mathrm{d}\tau\, e^{i\varepsilon_n\tau} G(\tau), \quad G(\tau) = -\langle T_\tau d(\tau) d^\dagger \rangle, \quad \varepsilon_n = (2n+1)\pi T \tag{44}$$

where T_τ is the imaginary-time ordering operator and $d(\tau) = e^{\tau H} d e^{-\tau H}$. Using the integral representation for $G(\varepsilon_n)$

$$G(\varepsilon_n) = \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{A(\omega)}{i\varepsilon_n - \omega}, \tag{45}$$

one obtains the expressions for m_0 and $\langle n_d \rangle$ [20]

$$m_0(h_0, T) = -\int_{-\infty}^{\infty} \mathrm{d}\omega\, A(\omega; h_0) \tanh\frac{\omega}{2T}, \qquad \langle n_d \rangle = \int_{-\infty}^{\infty} \mathrm{d}\omega\, A(\omega; h_0) f(\omega) \tag{46}$$

where $f(\omega) = (e^{\omega/T} + 1)^{-1}$ is the Fermi distribution function.

Thus, the spectral weight determines the local magnetization m_0 and average occupation $\langle n_d \rangle$ of the impurity site, both being experimentally accessible quantities. However, when describing the impurity spin dynamics in terms of the local d-fermion, one should pay attention to the important difference between the cases of a boundary impurity in a semi-infinite QIC and an impurity in the bulk of the spin chain. In the former case, the impurity spin is located at the open end of the chain, so the boundary spin operators $\sigma_0^\pm$ do not contain the JW exponentials and are *locally* expressed in terms of d and $d^\dagger$: $\sigma_0^+ = 2d^\dagger$, $\sigma_0^- = 2d$. In this case the d-fermion Green's function $G_d(\tau)$ coincides with the spin–spin correlation function,

$$G_d(\tau) = -\frac{1}{4}\langle \sigma_0^-(\tau)\sigma_0^+(0) \rangle, \tag{47}$$

and the spectral function $A(\omega)$ measures the fluctuation spectrum of the impurity spin.

This is not so for an impurity coupled to both Ising chains, $\tilde{J}_1, \tilde{J}_2 \neq 0$. In this case, only the total fermion number parity $P_S = \exp[i\pi(N_1 + N_2)]$ is conserved, while the parities of each chain, $P_{1,2}$, are not. Therefore, in the definition (40), the JW "tail" operator $P_2 = \exp(i\pi N_2)$ has a nontrivial dynamics, implying that for an impurity in the bulk of the QIC, the impurity spin components $\sigma_0^\pm$ are essentially nonlocal objects in terms of the JW fermions. In this case $A(\omega)$ cannot be expressed in terms of simple local spin–spin correlators and thus only has the meaning of a density of states for the d-fermion.

At $h_0 = 0$ the Hamiltonian (39) has an exact sub-chain symmetry: it remains invariant under the transformations

$$\begin{aligned} &\beta_1 \to -\beta_1, \qquad \gamma_{10} \to -\gamma_{10}, \qquad b_{1k} \to -b_{1k}, \qquad f_{1k} \to -f_{1k}, \\ &\beta_2 \to \beta_2, \qquad \gamma_{20} \to \gamma_{20}, \qquad b_{2k} \to b_{2k}, \qquad f_{2k} \to f_{2k}. \end{aligned} \tag{48}$$

In particular, the transformation (48) swaps $d \leftrightarrow d^\dagger$, implying that at $h_0 = 0 G(\varepsilon_n) = -G(-\varepsilon_n)$ and, according to (45), $A(\omega; 0) = A(-\omega; 0)$. Therefore at any finite temperature $m_0 \to 0$ as $h_0 \to 0$. However, the limit $h_0 \to 0$ does in general not commute with the limit $T \to 0$, in which $\tanh(\omega/2T)$ acquires a discontinuity at $\omega = 0$. The result of the integration in (46) thus becomes ambiguous if $A(\omega)$ has a δ-function singularity at $\omega = 0$. This singularity reflects the two-fold degeneracy of the impurity ground state. The local zero-temperature magnetization will exhibit a discontinuity as h_0, and with it the δ-function singularity of $A(\omega)$, cross zero. A free spin 1/2 is a simple example of this kind: when the external magnetic field is switched off, the magnetization $m_0(h_0) = \mathrm{sgn}(h_0)$ keeps track of its original orientation. Switching on a finite magnetic field h_0 generates an antisymmetric part of the spectral weight which yields a nonzero contribution to the integral (46). The spin susceptibility can then be obtained using the definition (42). Formula (46) for m_0 will be used extensively below.

The zero-field local susceptibility $\chi_0(T) = [\partial m_0/\partial h_0]_{h_0=0}$ has an equivalent representation in terms of the response function

$$\chi^{zz}(\omega) = i \int_0^\infty \mathrm{d}t\, e^{i\omega t} \langle [\sigma_0^z(t), \sigma_0^z(0)] \rangle. \tag{49}$$

Its Matsubara counterpart

$$X_0^{zz}(\omega_m) = \int_0^{1/T} \mathrm{d}\tau\, e^{i\omega_m \tau} \langle T_\tau \sigma_0^z(\tau) \sigma_0^z(0) \rangle, \quad (\omega_m = 2m\pi T),$$

represents a "polarization loop" of two impurity Majorana GFs:

$$X_0^{zz}(\omega_m) = T \sum_{\varepsilon_n} [D_{11}(\varepsilon_n) D_{22}(\omega_m - \varepsilon_n) - D_{12}(\varepsilon_n) D_{21}(\omega_m - \varepsilon_n)].$$

$\chi_0(T)$ is defined as the static limit of the local dynamical spin susceptibility:

$$\chi_0(T) = X_0^{zz}(\omega_m = 0) = T \sum_{\varepsilon_n} [D_{11}(\varepsilon_n) D_{22}(-\varepsilon_n) - D_{12}(\varepsilon_n) D_{21}(-\varepsilon_n)]. \tag{50}$$

In the model (39), at $h_0 = 0$ the Majorana fields β_1 and β_2 are decoupled, and in (50) one should set $D_{12} = D_{21} = 0$. The representation (50) will prove useful in the next section when we analyze the susceptibility close to criticality.

6. Boundary impurity in a semi-infinite quantum Ising chain

In the remainder of this paper we primarily deal with a situation displaying rich physics at the boundary: the model of a single non-critical semi-infinite QIC with an impurity spin at the open end. It is obtained from the Hamiltonian (27) by cutting off the coupling of the impurity Majorana fermion β_2 to the second channel ($\tilde{J}_2 = 0$). We will first gain some intuition about the MZMs in the two phases in the discrete version of this model and then turn to a continuum description assuming that massive phases of the semi-infinite QIC are only weakly non-critical.

A qualitative picture of the MZMs can be inferred from Fig. 5 where the lower KM chain should be completely ignored. Set $h_0 = 0, \tilde{J}_1 \neq 0$ and consider the limiting cases $J/h \to 0$ and $h/J \to 0$. In the former case, the impurity degrees of freedom are represented by two MZMs: one being the decoupled Majorana fermion β_2 and the other contained in the spectrum of the 3-site complex, $H_3 = i\tilde{J}_1 \beta_1 c_1 + ihc_1 c_2$. Therefore in the disordered phase ($J > h \neq 0$) there are two zero-energy bound states attached to the boundary: one of them localized just at the impurity site while the other one has a finite penetration into the bulk. The two MZMs describe a well-defined local spin degree of freedom.

In the ordered phase, there remains only one MZM (β_2) localized exactly at the boundary. The second impurity Majorana (β_1) couples with a nonzero binding energy to the bulk fermion c_1, which, in the impurity-bulk decoupling limit ($\tilde{J}_1 = 0$), represents the boundary MZM of an isolated QIC in its ordered phase [5]. In this phase no local spin 1/2 remains at the impurity site. As we will see in what follows, the bound state between the impurity Majorana fermion and the boundary zero mode of the bulk plays a crucial role in quenching the transverse susceptibility of the impurity spin in the topological (ordered) phase of the QIC.

6.1. Spectral weight of the impurity spin

Now we turn to a continuum model describing a semi-infinite, weakly non-critical QIC with an impurity spin at the open end. Such a model is obtained from (39) by removing the coupling of the Majorana fermion β_2 to the second channel ($\lambda_{20} = \lambda_{2k} = 0$):

$$H = -ih_0\beta_1\beta_2 - \frac{i}{2}\sum_{k>0}\varepsilon_k b_k f_k - i\lambda_0\beta_1\gamma_0 - i\sqrt{\frac{2}{N}}\sum_{k>0}\lambda_k\beta_1 b_k. \tag{51}$$

Here $\lambda_0 = \lambda_{10}$, $\lambda_k = \lambda_{1k}$, $b_k = b_{1k}$, $f_k = f_{1k}$. The GF $G(\varepsilon_n)$ is calculated in Appendix C:

$$G(\varepsilon_n, h_0) = \frac{1}{2i\varepsilon_n}\left[1 - \frac{(i\varepsilon_n - 2h_0)^2}{\Delta(\varepsilon_n) + 4h_0^2}\right]. \tag{52}$$

Here

$$\Delta(\varepsilon_n) = \varepsilon_n^2 + \Gamma\left(\sqrt{\varepsilon_n^2 + m^2} - m\right),$$

where $\Gamma = 4\tilde{J}^2 a_0/v = 2\tilde{J}^2/J$ is the hybridization width of the impurity level.

Analytic continuation $G(\varepsilon_n) \to \mathcal{G}(\omega + i\delta)$ should be done according to the prescription: under $i\varepsilon_n \to \omega + i\delta$ ($\varepsilon_n > 0$)

$$\begin{aligned}\sqrt{\varepsilon_n^2 + m^2} &\to -i\sqrt{\omega^2 - m^2}\,\mathrm{sgn}\,\omega, \quad \text{if } \omega^2 > m^2,\\ &\to \sqrt{m^2 - \omega^2}, \quad \text{if } \omega^2 < m^2.\end{aligned} \tag{53}$$

This yields the following expressions for the retarded GF at high and low frequencies:

$$\omega^2 > m^2 : \ \mathcal{G}_>(\omega + i\delta; h_0) = \frac{1}{2(\omega + i\delta)}\left[1 + \frac{(\omega - 2h_0)^2}{\omega^2 + \Gamma m - 4h_0^2 + i\Gamma\sqrt{\omega^2 - m^2}\,\mathrm{sgn}\,\omega}\right], \tag{54}$$

$$\begin{aligned}&\omega^2 < m^2 : \ \mathcal{G}_<(\omega + i\delta; h_0)\\ &= \frac{1}{2(\omega + i\delta)}\left[1 + \frac{(\omega - 2h_0)^2}{\omega^2 + \Gamma m - 4h_0^2 - \Gamma\sqrt{m^2 - \omega^2} + i\delta\,\mathrm{sgn}\,\omega}\right].\end{aligned} \tag{55}$$

Separating the imaginary parts of the GFs (54) and (55) we find that, at $h_0 = 0$, for a non-critical semi-infinite QIC the impurity spectral weight has the following form:

$$A(\omega) = \frac{1}{2}\delta(\omega) + \frac{1}{2}A_f(\omega). \tag{56}$$

Here the δ-function term is the contribution of the impurity Majorana fermion β_2, which is completely decoupled at $h_0 = 0$. On the other hand, $A_f(\omega)$ alone represents the impurity spectral weight for two identical QICs symmetrically coupled to the impurity, in which case the model maps onto the standard massive semi-infinite resonant-level model. In particular, such a model emerges in a continuum description of a 1D spinless Peierls insulator which also possesses topological and trivial massive phases [21] (see Appendix D). The explicit expressions for the impurity spectral weight $A_f(\omega)$ at $h_0 = 0$ are:

$$m > 0: \; A_f(\omega) = Z\delta(\omega) + \theta\,(\omega^2 - m^2)\frac{\Gamma}{\pi}\frac{\sqrt{\omega^2 - m^2}}{|\omega|\left(\omega^2 + 2\Gamma m + \Gamma^2\right)}; \tag{57}$$

$$\begin{aligned} m < 0: \; A_f(\omega) \;&=\; \theta(|m| - \Gamma)\left(\frac{|m| - \Gamma}{2|m| - \Gamma}\right)[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)] \\ &+ \theta(\omega^2 - m^2)\frac{\Gamma}{\pi}\frac{\sqrt{\omega^2 - m^2}}{|\omega|\left(\omega^2 - 2\Gamma|m| + \Gamma^2\right)}; \end{aligned} \tag{58}$$

where

$$Z = \frac{2m}{\Gamma + 2m}, \quad (m > 0), \tag{59}$$

$$\omega_0 = \sqrt{\Gamma(2|m| - \Gamma)} < |m|, \quad (m < 0 \text{ and } |m| > \Gamma). \tag{60}$$

Below we split the susceptibility into contributions from the discrete δ-functions, $\chi_<$, and from the continuum ($\omega^2 > m^2$) above the gap, $\chi_>$, respectively,

$$\chi_0 = \chi_< + \chi_>. \tag{61}$$

For a critical Majorana resonant level model (the case $m = 0$) the additive structure of the spectral weight $A(\omega)$ given by the sum (56) was first obtained by Emery and Kivelson [14]. As we see, the immunity of the decoupled Majorana fermion β_2 keeps the structure (56) valid in the massive case as well. It shows that only one half of the boundary spin degrees of freedom is hybridized with the gapless bulk excitations while the other half is decoupled from the rest of the system.

The representation (56) is no longer valid at $h_0 \neq 0$. The spectral weight at a small nonzero h_0 will be discussed separately in the sequel.

6.2. Local magnetization and spin susceptibility

6.2.1. Critical state, $m = 0$

At $m = 0$ the Hamiltonian (51) coincides with the resonant-level model introduced and solved by Emery and Kivelson [14] in their treatment of the two-channel Kondo problem. For the sake of completeness and later comparison with massive cases, we reproduce their main findings here.

The spectral weight of the d-fermion is given by formula (56). Setting $m = 0$ in Eq. (57) or (58) one obtains [14] ($h_0 = 0$)

$$A(\omega) = \frac{1}{2}\delta(\omega) + \frac{1}{2}\frac{\Gamma}{\pi}\frac{1}{\omega^2 + \Gamma^2}. \tag{62}$$

The zero-temperature entropy of the impurity spin, $S = (1/2)\ln 2$, is a half of its value for an isolated spin 1/2. This is a direct effect of the decoupled boundary Majorana β_2-fermion. Applying a small local magnetic field h_0 induces an antisymmetric part of $A(\omega)$ which can be easily obtained from (54). According to the definition (46), this leads to the following result for the zero-field local susceptibility

$$\chi_0(T) = \frac{4\Gamma}{\pi}\int_0^\infty \frac{d\omega}{\omega}\frac{\tanh(\omega/2T)}{\omega^2 + \Gamma^2}. \tag{63}$$

At $T \gg \Gamma$ the susceptibility follows the Curie law, $\chi_0 = 1/T$, as expected. In contrast, at low temperatures, $T \ll \Gamma$, it has a logarithmic temperature dependence typical for the two-channel, overscreened Kondo impurity in the channel-symmetric case [14]:

$$\chi_0(T) = \frac{4}{\pi\Gamma}\ln\frac{\Gamma}{T}. \tag{64}$$

It is instructive to make a comparison with the case of two (instead of one) identical critical Majorana chains coupled to the boundary spin. This reduces to the standard resonant-level model describing a semi-infinite metallic chain with a d-fermion state at its boundary. Such a model with two attached critical Ising chains maps identically to a U(1)-symmetric spin-1/2, semi-infinite XX chain with a boundary spin 1/2 in a transverse magnetic field h_0. This model is known to be related to the standard, one-channel Kondo problem at the Toulouse point (see e.g. Ref. [18]). In this case the impurity spectral weight and the local charge susceptibility at $T/\Gamma \to 0$,

$$A_{\mathrm{f}}(\omega) = \frac{\Gamma}{\pi} \frac{1}{\omega^2 + \Gamma^2}, \qquad \chi = \frac{1}{\pi \Gamma}, \tag{65}$$

describe a local "Fermi-liquid" regime at the boundary. The impurity spin is totally screened and its ground state is non-degenerate: at $T = 0$ the local boundary magnetization smoothly vanishes as $h_0 \to 0$.

As follows from the Emery–Kivelson solution, the logarithmic divergence of the local susceptibility (64) is weaker than the Curie law. This is a signature of non-Fermi-liquid character of the local response. The logarithmic asymptotics of the boundary susceptibility (64) are the *hallmark of Majorana physics at the edge of a single chain*. As discussed below, these asymptotics hold in the massive case as well when the quantum critical regime $|m| \ll T \ll \Gamma$ is considered.

6.2.2. *Disordered phase, $m > 0$*

As we already know, there are two boundary MZMs in the disordered phase. One of them (β_2) is completely decoupled whereas the other Majorana mode (β_1) hybridizes with the bulk degrees of freedom. The behavior of the thermodynamic quantities at the edge in various temperature regimes will depend on the ratio m/Γ, or equivalently, on the relation between two length scales—the correlation length $\xi_m \sim v/m$ and the hybridization length $\xi_\Gamma \sim v/\Gamma$. At $\xi_m \ll \xi_\Gamma$ $(m \gg \Gamma)$ both boundary MZMs are well localized, and one expects a Curie law for the local susceptibility, $\chi_0 = C/T$, with a slightly reduced Curie constant ($C \lesssim 1$). In the other limit, $\xi_m \gg \xi_\Gamma$ $(m \ll \Gamma)$, hybridization effects are dominant. If $m \ll T \ll \Gamma$, the mass gap can be ignored and the logarithmic regime (64) is seen. However, upon further decreasing the temperature, $T \ll m \ll \Gamma$, a low-T Curie behavior of the impurity reappears, albeit with a strongly reduced Curie constant.

With this qualitative picture in mind, let us now turn to the spectral weight at $m > 0$ given by Eq. (57). At $h_0 = 0$, its evolution on decreasing the mass m is shown in Fig. 6. The low-frequency part of $A(\omega)$ contains a δ-function singularity

$$A_{\mathrm{sing}}(\omega) = A_0 \delta(\omega), \qquad A_0 = \frac{1}{2}(1 + Z) = \frac{1 + (\Gamma/4m)}{1 + (\Gamma/2m)} \tag{66}$$

where Z is given by (59). Its amplitude A_0 interpolates between the free-spin value $A_0 = 1$ in the strong localization limit ($\Gamma/m \to 0$) and the "two-channel Kondo" value $A_0 = 1/2$ (see Eq. (62)) in the strong hybridization limit ($\Gamma/m \to \infty$). To calculate $m(h_0, T)$ at $h_0 \to 0$ we need to know the low-frequency part of $A(\omega; h_0)$ at a small nonzero h_0. Using (55) at $|\omega|, h_0 \ll m$ we obtain

$$A_<(\omega; h_0) \simeq \frac{(\omega - 2h_0)^2}{4|\tilde{h}_0|} Z \delta\left(\omega^2 - 4\tilde{h}_0^2\right),$$

where $\tilde{h}_0 = h_0\sqrt{Z}$. Here we only need the antisymmetric part of $A(\omega)$:

$$A_<^{(\mathrm{as})}(\omega; h_0) = -\frac{1}{2}\sqrt{Z}\left[\delta(\omega - 2\tilde{h}_0) - \delta(\omega + 2\tilde{h}_0)\right]. \tag{67}$$

Substituting (67) into (46) we obtain

$$m_{0;<}(h_0, T) = -\int_{-\infty}^{\infty} \mathrm{d}\omega\, A_<^{(\mathrm{as})}(\omega; h_0) \tanh\frac{\omega}{2T} = \sqrt{Z} \tanh\frac{\sqrt{Z} h_0}{T}. \tag{68}$$

This expression yields the picture of a boundary spin $\mu_{\mathrm{eff}}\sigma_0^z$, where $\mu_{\mathrm{eff}} = \sqrt{Z}$ is the effective magnetic moment. If the temperature is kept finite and $h_0 \to 0$, $m_{0;<}$ follows a Curie law, $m_{0;<} = \chi_<(T) h_0$,

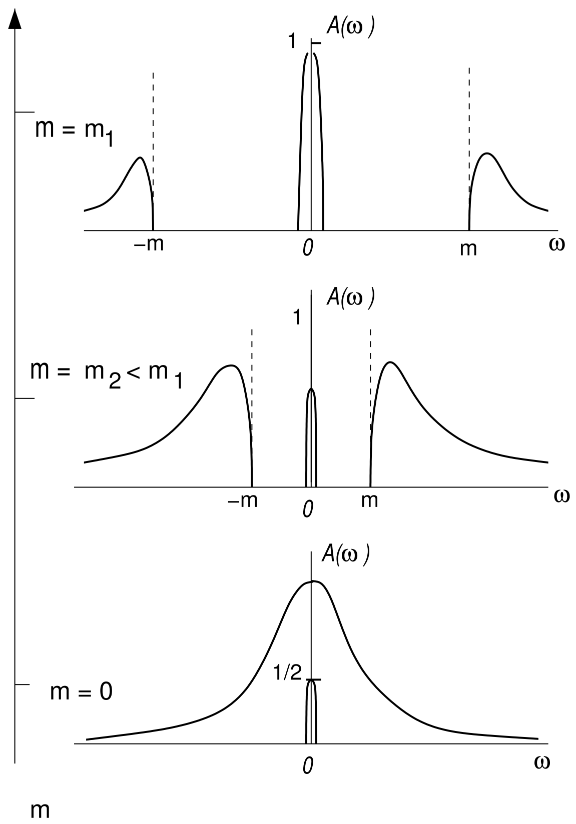


Fig. 6. Evolution of the spectral weight in the disordered phase ($m > 0$) upon decreasing m. The lowest plot corresponds to $m = 0$, where the continuum shoulders tend to $\omega \to 0$. In this case the continuum spectral function is to be understood as contributing only to the principal part when appearing in an integral, on top of which there is still a δ-function contribution from $\omega = 0$.

where $\chi_<(T)$ is given by (23). The zero-temperature value of $m_{0;<}$ displays the expected discontinuity at $h_0 \to \pm 0$: $m_{0;<} = \mu_{\rm eff}\,{\rm sgn}(h_0)$.

The high-frequency part of the spectral weight features a broad continuum of states at $\omega^2 > m^2$ with a non-singular behavior at the thresholds $\omega = \pm m$: $A(\omega) \sim \sqrt{\omega \mp m}$. To estimate the contribution of this frequency region to the boundary spin susceptibility we proceed from the expression (54) for $\mathcal{G}_>(\omega)$, find in the leading order in h_0 the antisymmetric part of the spectral weight and, using formula (46), obtain the high-frequency contribution to the local susceptibility:

$$\chi_> = \frac{4\Gamma}{\pi}\int_m^\infty {\rm d}\omega\, \tanh\left(\frac{\omega}{2T}\right)\cdot \frac{\sqrt{\omega^2 - m^2}}{\omega^2(\omega^2+\Omega_1^2)}, \tag{69}$$

where $\Omega_1^2 = \Gamma(2m+\Gamma) > 0$. At temperatures $T \ll m$ and arbitrary Γ/m, $\chi_>(T)$ can be replaced by its zero-temperature value

$$\chi_>(T=0) = \frac{4\Gamma}{\pi}\int_m^\infty {\rm d}\omega\, \frac{\sqrt{\omega^2 - m^2}}{\omega^2(\omega^2+\Omega_1^2)} \simeq \frac{4}{\pi(2m+\Gamma)}\ln\left(\frac{m+\Gamma}{m}\right). \tag{70}$$

In the regime $m \gg \Gamma$ when the impurity spin is strongly localized, the high-frequency part of the impurity spectral weight gives only a small correction compared to the contribution of the already considered low-frequency part, $\chi_<(T)$, the relative correction being of the order of $T\Gamma/m^2$ for $T \ll m$, or of order Γ/m for $T \gg m \gg \Gamma$.

The situation changes in the strong hybridization limit, $m \ll \Gamma$. As the ratio m/Γ tends to zero, the effective magnetic moment $\mu_{\rm eff}$ vanishes and, at the same time, the high-frequency contribution to the local susceptibility, Eq. (70), logarithmically diverges. This means that at $m \ll \Gamma$ this contribution becomes dominant if $T > m$. Indeed, replacing Ω_1 by Γ in (69) we obtain:

$$\chi_>(T) = \frac{1}{T}, \quad T \gg \Gamma, \tag{71}$$

$$= \frac{4}{\pi\Gamma} \ln \frac{\Gamma}{\{T, m\}}, \quad T \ll \Gamma, \tag{72}$$

where $\{a, b\} \equiv \max(a, b)$. We see that at $m \ll \Gamma \ll T$, the Curie-law behavior of the local susceptibility is contributed by the incoherent, high-energy continuum of states. At lower temperatures, $T, m \ll \Gamma$, $\chi_>$ follows the logarithmic two-channel-Kondo asymptotics [14], so that the total local susceptibility is given by the sum

$$\chi_0(T) = \chi_<(T) + \chi_>(T) = \left(\frac{2m}{\Gamma}\right)\frac{1}{T} + \frac{4}{\pi\Gamma} \ln \frac{\Gamma}{\{T, m\}}. \tag{73}$$

Therefore, at temperatures $T \ll m/\ln(\Gamma/m)$ a Curie regime with a small Curie constant is recovered:

$$\chi_0(T) = \frac{C}{T}, \quad C = \mu_{\text{eff}}^2 \simeq \frac{2m}{\Gamma}. \tag{74}$$

The high-temperature and low-temperature Curie behaviors of χ_0 "sandwich" the intermediate-temperature ($m \ll T \ll \Gamma$) logarithmic asymptotics (64).

Thus, at any *finite* $m > 0$ (i.e. $Z \neq 0$) there exists a well defined spin-1/2 degree of freedom localized at the open boundary of the chain and characterized by the effective magnetic moment μ_{eff} which depends on the ratio m/Γ. The effective moment takes the value $\mu_{\text{eff}} = 1$ at $\Gamma/m \to 0$ and decreases upon increasing the ratio Γ/m, vanishing at criticality ($m = 0$). In the strong localization limit, $m \gg \Gamma$, the Curie law $\chi_0 \simeq 1/T$ is valid at any temperature. Delocalization of the impurity fermion β_1 across the whole chain in the critical state of the system is concomitant with the disappearance of the boundary spin-1/2 degree of freedom ($\mu_{\text{eff}} \to 0$ as $m \to 0$). This is consistent with the emerging non-Curie, logarithmic temperature dependence of the local susceptibility, Eq. (72). Exactly at criticality ($m = 0$), the local magnetization at $T = 0$ is a non-analytic function of h_0 [14]: $m(h_0) = (8h_0/\pi\Gamma)\ln(\Gamma/h_0)$.

6.2.3. Effective moment of the Curie law: a probe of similarity of degenerate ground states

It is useful to look at the effective magnetic moment μ_{eff} from a different perspective, using a Lehmann representation as in Eq. (24), where μ_{eff} was expressed as the matrix element of the operator σ_0^z between the two degenerate ground states. A renormalized but finite local free-spin susceptibility (23) in the disordered phase reflects the fact that the two ground states only differ locally, that is, in a finite number of degrees of freedom. This shows that in this phase the origin of the exact spectral degeneracy is purely local, and accordingly, cannot be seen in measurements which only probe degrees of freedom far from the impurity. The vanishing of μ_{eff} upon tuning to the critical point and in the ordered phase can be interpreted as an emerging orthogonality between the ground states for $h_0 = 0\pm$. It is this orthogonality at the degeneracy point $h_0 = 0$, which protects the susceptibility from diverging in the ordered (topological) phase.

To put this result into a more general context, it is useful to switch to the eigenbasis, in which the parity operator P_S has a definite eigenvalue. Since P_S commutes with H irrespective of the value of the transverse field h_0, this basis is better adapted to discuss the crossing of the degeneracy point $h_0 = 0$. In the QIC model it is easy to prove that the ground states associated with transverse fields h_0 and $-h_0$ have opposite parity. This follows immediately from the fact that conjugation with σ_0^x ($H \to \sigma_0^x H \sigma_0^x$, $P_S \to \sigma_0^x P_S \sigma_0^x$) flips both the sign of h_0 and the parity operator. This implies that at $h_0 = 0$ the ground state is degenerate and that its parity flips, as h_0 is tuned across 0.

Let us now analyze a generic system in which the ground state is tuned to a point where it becomes doubly degenerate or has exponentially small level splitting δ, while the remaining states are separated by a finite gap Δ. Let the two-dimensional ground state manifold be spanned by the orthogonal eigenstates $|\alpha\rangle$ and $|\beta\rangle$. At temperatures $\delta \ll T \ll \Delta$, the density matrix is simply proportional to unity in this subspace,

$$\rho = \frac{|\alpha\rangle\langle\alpha| + |\beta\rangle\langle\beta|}{2}. \tag{75}$$

The susceptibility of an observable A, defined as the linear response to its conjugate field, is easily calculated to have the low temperature asymptotics of a Curie law,

$$\chi_A = \int_0^{1/T} d\tau \, \left[\langle A(\tau)A(0)\rangle - \langle A\rangle^2\right] = \frac{1}{T}\left[|A_{\alpha\beta}|^2 + \frac{1}{4}(A_{\alpha\alpha} - A_{\beta\beta})^2\right], \tag{76}$$

where $A_{\nu\nu'} = \langle\nu|A|\nu'\rangle$. This expression is manifestly basis-independent when rewritten as $\chi_A = \mu_{\rm eff}^2/T$ with

$$\mu_{\rm eff}^2 = \left[\frac{{\rm Tr}(A_{\gamma\eta})}{2}\right]^2 - {\rm Det}(A_{\gamma\eta}) = \frac{(\lambda_1 - \lambda_2)^2}{4}, \tag{77}$$

where $\lambda_{1,2}$ are the eigenvalues of the restriction of A to the ground state manifold.

In the quantum Ising model, the degeneracy occurs at $h_0 = 0$ and the local transverse susceptibility corresponds to the operator $A = \sigma_0^z$. If $|\alpha\rangle, |\beta\rangle$ are chosen to be the eigenstates $|+\rangle, |-\rangle$ of σ_0^x, then only the off-diagonal elements are nonzero, and one recovers Eq. (24) for $\mu_{\rm eff}$. Choosing instead the parity eigenbasis, $|P_S = \pm 1\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$, only the diagonal elements can be nonzero by symmetry. As follows from (77), in the disordered phase $\mu_{\rm eff}$ can assume any value ≤ 1. However, anywhere in the ordered phase, $\mu_{\rm eff}$ becomes exponentially small in the system size, because of spontaneous symmetry breaking: The parity-even and -odd ground states are equal weight superpositions of the symmetry breaking ground states $|\pm\rangle$ (magnetization aligned or anti-aligned with x), with equal or opposite signs, respectively. This implies equality of the diagonal matrix elements in the parity basis, up to an exponentially small difference given by the matrix element $\langle -|\sigma_0^z|+\rangle$, which connects the two symmetry breaking sectors.

After the JW transformation, the symmetry-related degeneracy translates into the topological degeneracy of the Majorana Hamiltonian, with parity-even and -odd sectors being degenerate up to exponentially small perturbations. The latter feature is generic in topological phases, and essentially constitutes their defining property—topological protection: The action of any local observables, such as A, restricted to the topologically degenerate manifold is that of a unit operator, up to corrections which are exponentially small in the system size. From this and formula (77) it follows immediately that the Curie weight $\mu_{\rm eff}^2$ is exponentially suppressed in a topological phase. This is the case even at exact degeneracy points, where the parity of the ground state switches (as happens, e.g., for $h_0 = 0$ in the fermionic version of the QIC in its ferromagnetic phase). We will see in Section 8 a non-trivial example of a 1d p-wave superconductor, where the suppression of a Curie-like divergence of the low temperature charge susceptibility is found everywhere in the topological phase, independent of the fine-tuning of the local potential μ_0 acting on an impurity site. As we will argue, the only generic exact ground state degeneracy occurs when the ground state switches parity within the topologically degenerate manifold. To bring about further degeneracies within the same parity sector requires a high degree of fine-tuning. Such degeneracies will thus generically not be encountered upon moving along a single parameter family of Hamiltonians, such as varying a local potential or field.

6.2.4. *Ordered phase, $m < 0$*

The physical picture emerging in the ordered phase ($m < 0$) is qualitatively different from the disordered phase. As follows from (56), the completely decoupled MZM β_2 gives a contribution $(1/2)\delta(\omega)$ to the spectral weight which remains intact upon varying the ratio $|m|/\Gamma$ and is immune against application of external fields. The transformation of the incoherent high-frequency background on increasing the mass gap $|m|$ is shown in Fig. 7. As long as $|m| < \Gamma$, the behavior of $A(\omega)$ is qualitatively the same as in the disordered phase. At $|m| = \Gamma$ the spectral weight acquires new features. Precisely at this point the thresholds at $\omega = \pm|m|$ transform from non-singular to singular:

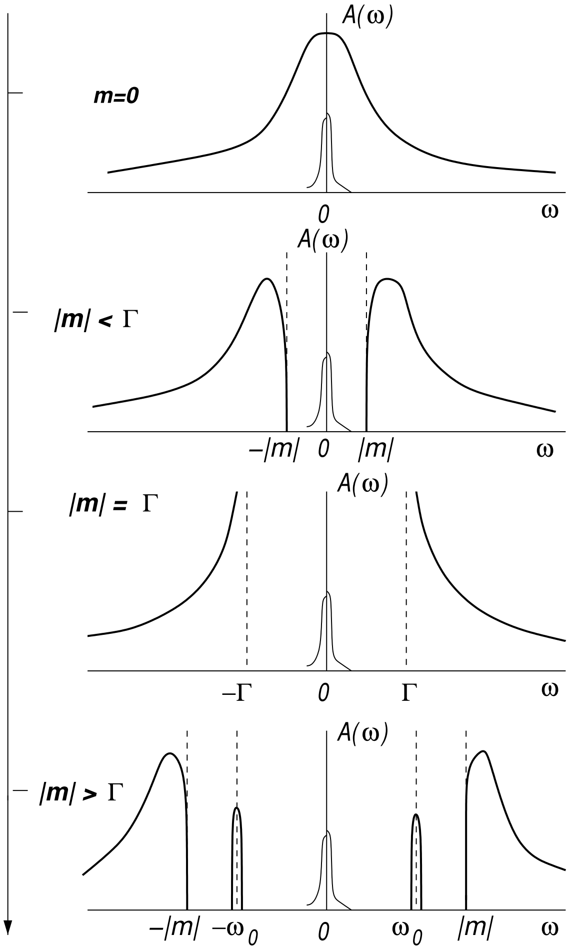


Fig. 7. Evolution of the spectral weight in the ordered phase ($m < 0$) upon increasing $|m|$. As the bulk gap $|m|$ crosses Γ, a pair of discrete subgap states emerges.

$A(\omega) \sim 1/\sqrt{\omega \mp |m|}$. This feature comes together with the "birth" of a particle in the spectrum: at $|m| = \Gamma + 0$ two symmetric δ-function peaks, $\delta(\omega \mp \omega_0)$, emerge just below the thresholds. They belong to new levels with energies inside the gap, which split from the incoherent continuum of states. They are mainly due to the hybridization between two zero modes—the impurity β_1-Majorana fermion and the zero mode γ_0, which is present in the spectrum of the Dirac Hamiltonian at $m < 0$. These discrete sub-gap states exist provided that the localization of γ_0 is strong enough (the condition $|m| > \Gamma$). The effective Hamiltonian describing this splitting in the limit $|m| \gg \Gamma$ simply coincides with the λ_0-mixing term in the model (51): $H' = -i\lambda_0\beta_1\gamma_0$, where $\lambda_0 \sim \sqrt{\Gamma|m|} \sim \omega_0$. Notice that as soon as $|m| > \Gamma$ the spectra at the thresholds $\omega = \pm|m|$ return to a non-singular form.

The main features of the spectral weight $A(\omega)$ in the strong localization limit, $|m| > \Gamma$, shown schematically in the last plot of Fig. 7, are in a qualitative agreement with the results of a recent numerical work [22], where the spectrum of a resonant level attached to the edge of a 1D triplet superconductor was calculated. However, local thermodynamic properties of this system have not been addressed in Ref. [22].

Let us determine the effect of these subgap states on the susceptibility of the impurity spin. At $h_0 \ll \omega_0$ the positions of the peaks $\delta(\omega \mp \omega_0)$ change only by an amount $\sim O(h_0^2)$, which can be safely neglected. As a result the antisymmetric part of the low-frequency ($\omega^2 < m^2$) spectral weight $A_<(\omega)$ is simply proportional to h_0:

$$A_<^{(\mathrm{as})}(\omega) = -\frac{2h_0}{\omega_0}\theta(|m| - \Gamma)\left(\frac{|m| - \Gamma}{2|m| - \Gamma}\right)[\delta(\omega - \omega_0) - \delta(\omega + \omega_0)], \quad m < 0. \tag{78}$$

Accordingly, $\chi_<$ is equal to

$$\chi_<(T) = \theta(|m| - \Gamma)\frac{4}{\omega_0}\left(\frac{|m| - \Gamma}{2|m| - \Gamma}\right)\tanh\frac{\omega_0}{2T}. \tag{79}$$

At $T \gg \omega_0$ the δ-function contribution to the susceptibility follows a Curie law $\chi_<(T) = \bar{\mu}_{\rm eff}^2/T$, where the effective boundary magnetic moment $\bar{\mu}_{\rm eff} = [2(|m| - \Gamma)/(2|m| - \Gamma)]^{1/2}$ varies from $\bar{\mu}_{\rm eff} = 1$ at $|m|/\Gamma \gg 1$ to $\bar{\mu}_{\rm eff} = 0$ as $|m| \to \Gamma + 0$. As follows from (79), at lower temperatures, $T \ll \omega_0$, $\chi_<(T)$ crosses over to a constant, temperature independent value

$$\chi_<(T = 0) = 4\theta(|m| - \Gamma)\left(\frac{|m| - \Gamma}{2|m| - \Gamma}\right)\frac{1}{\sqrt{\Gamma(2|m| - \Gamma)}}. \tag{80}$$

In particular, at strong inequality, $|m| \gg \Gamma$, we have

$$\chi_<(T = 0) = \frac{2}{\sqrt{2\Gamma|m|}}, \tag{81}$$

for which we will give a simple heuristic explanation below.

Estimating the effect of the high-frequency spectral function on the susceptibility χ_0, we find that the expression for $\chi_>$ for the ordered phase is obtained similarly as in the disordered phase:

$$\chi_>(T) = \frac{4\Gamma}{\pi}\int_{|m|}^{\infty} \mathrm{d}\omega\, \tanh\left(\frac{\omega}{2T}\right)\frac{\sqrt{\omega^2 - m^2}}{\omega^2(\omega^2 - 2|m|\Gamma + \Gamma^2)}. \tag{82}$$

Using (82) one can easily check that at the threshold $|m| = \Gamma$ where the spectral weight becomes singular, the local susceptibility remains analytic. Turning to the strong localization regime, $|m| \gg \Gamma$, we find that the $T = 0$ value of $\chi_>$ is given by

$$\chi_>(T = 0) = \frac{4\Gamma}{\pi}\int_{|m|}^{\infty} \mathrm{d}\omega\, \frac{\sqrt{\omega^2 - m^2}}{\omega^2(\omega^2 - \omega_0^2)} \simeq \frac{4\Gamma}{\pi}\int_{|m|}^{\infty} \mathrm{d}\omega\, \frac{\sqrt{\omega^2 - m^2}}{\omega^4} \sim \frac{\Gamma}{m^2},$$

where we have used the fact that $\omega_0 = \sqrt{2\Gamma|m|} \ll |m|$. In the same limit $\chi_<$ is given by (81). Therefore $\chi_>/\chi_< \sim (\Gamma/|m|)^{3/2} \ll 1$.

Thus we conclude that in the strong localization limit ($|m| \gg \Gamma$), the dominant contribution to the local susceptibility $\chi_0 = \chi_< + \chi_>$ comes from its low-frequency part $\chi_<$, Eqs. (79)–(81).

The result (81) can be understood as follows. The impurity spin σ_0^x couples by an exchange interaction $\tilde{J}$ to the spin σ_1^x located at the boundary site $j = 1$ of the semi-infinite QIC: $H_{01} = -\tilde{J}\sigma_0^x\sigma_1^x$. In the ordered phase σ_1^x acquires an expectation value, and in the leading order the impurity spin experiences a local magnetic field $h_x = \tilde{J}\langle\sigma_1^x\rangle$. Adding a local transverse field $\mathbf{h}_0 = (0, 0, h_0)$, we write the total energy of the impurity spin as $H_{01} = -h_x\sigma_0^x - h_0\sigma_0^z$. In the limit $h_0 \to 0$, the transverse spin susceptibility is equal to $\chi_0 = 1/h_x \sim 1/\sqrt{\Gamma}\langle\sigma_1^x\rangle$, where $\Gamma \sim \tilde{J}^2/v$. The crucial point is that the scaling (i.e., the mass dependence) of the boundary magnetization in a slightly non-critical (ordered) QIC is different from that in the bulk [23]: $\langle\sigma^x\rangle_{\rm bound} \sim \sqrt{|m|}$. This leads to $\chi_0 \sim 1/\sqrt{\Gamma|m|}$.

It remains to consider the regime $|m| \ll \Gamma$, which is entirely contributed by the high-frequency part of the impurity spectral weight. In this regime the role of the mass gap $|m|$ reduces to an infrared cutoff in the logarithmic temperature dependence of the local susceptibility, and the sign of the mass is completely unimportant. Therefore, replacing m by $|m|$, the formulae (71), (72) of the preceding subsection can be used in this case as well:

$$|m| \ll \Gamma \ll T: \ \chi_0 = \frac{1}{T}, \tag{83}$$

$$|m|, T \ll \Gamma: \ \chi_0 = \frac{4}{\pi\Gamma}\ln\frac{\Gamma}{\{T, |m|\}}. \tag{84}$$

The zero-temperature local susceptibility is given by

$$\chi_0(T=0;|m|\ll\Gamma)=\frac{4}{\pi\Gamma}\ln\frac{\Gamma}{|m|}. \tag{85}$$

The results obtained in this subsection lead us to the conclusion that the state of the boundary impurity in the ordered phase is nondegenerate.

The asymptotic behavior of the impurity spin susceptibility in different temperature regimes is summarized in the tables below:

Disordered phase: $m>0$

$$\begin{aligned}
m\gg\Gamma:\quad &\chi_0=\frac{1}{T}\quad \text{at all } T,\\
m\ll\Gamma:\quad &\chi_0=\frac{1}{T}\quad \text{at } T\gg\Gamma,\\
&\chi_0=\frac{4}{\pi\Gamma}\ln\frac{\Gamma}{T}\quad \text{at } \frac{m}{\ln(\Gamma/m)}\ll T\ll\Gamma,\\
&\chi_0=\left(\frac{2m}{\Gamma}\right)\frac{1}{T}\quad \text{at } T\ll\frac{m}{\ln(\Gamma/m)}.
\end{aligned} \tag{86}$$

Ordered phase: $m<0$

$$\begin{aligned}
m\gg\Gamma:\quad &\chi_0=\frac{1}{T}\quad \text{at } T\gg\sqrt{\Gamma|m|},\\
&\chi_0=\frac{2}{\sqrt{2\Gamma|m|}}\quad \text{at } T\ll\sqrt{\Gamma|m|},\\
m\ll\Gamma:\quad &\chi_0=\frac{1}{T}\quad \text{at } T\gg\Gamma,\\
&\chi_0=\frac{4}{\pi\Gamma}\ln\frac{\Gamma}{T}\quad \text{at } |m|\ll T\ll\Gamma,\\
&\chi_0=\frac{4}{\pi\Gamma}\ln\frac{\Gamma}{|m|}\quad \text{at } T\ll|m|.
\end{aligned} \tag{87}$$

To conclude our discussion of a boundary impurity in the topological phase of a wire, let us consider a more general situation in which the end of the wire is essentially described by an odd number $(2N-1)$ Majorana modes, $c_{2,\ldots,2N}$, with the remaining degrees of freedom being treated as sufficiently strongly gapped and therefore irrelevant for the low energy sector. The impurity is again described by two Majoranas, c_0 and c_1. The most general quadratic Hamiltonian then takes the form

$$\mathcal{H}=i\sum_{jk}A_{jk}c_jc_k, \tag{88}$$

where A_{jk} is a real, antisymmetric $(2N+1)\times(2N+1)$ matrix.

Since the number of Majoranas is odd and the spectrum has a particle–hole symmetry, the presence of at least one exact zero mode is guaranteed. We now show that all other levels are generically repelled from zero. This is most conveniently seen from the characteristic polynomial of the matrix iA,

$$p_{iA}(E)\equiv\det(iA-E)=\sum_{i=1}^{N}c_i(A)E^{1+2i}, \tag{89}$$

where only odd powers of the energy variable E appear with coefficients $c_i(A)$. In order to find a fermionic level at $E=0$ further to the guaranteed Majorana zero mode, the characteristic polynomial must have a triple zero at $E = 0$. This requires $c_1(A) = 0$, which can be expressed in terms of the diagonal minors of A,

$$c_1(A) = (-1)^{N+1} \sum_{i=0}^{2N} \det(\hat{A}_{ii}) = (-1)^{N+1} \sum_{i=0}^{2N} [\mathrm{Pf}(\hat{A}_{ii})]^2 = 0, \tag{90}$$

where $\hat{A}_{ii}$ is the matrix with the i'th row and the i'th column eliminated, and $\mathrm{Pf}(\hat{A}_{ii})$ is its Pfaffian. Due to the antisymmetry of A, the minors $\det(\hat{A}_{ii})$ are squares of Pfaffians, which must all vanish simultaneously for any other level to cross $E = 0$. It is clear that it requires a high degree of fine-tuning to circumvent the level repulsion from the guaranteed zero mode. The only obvious way to achieve this is by completely decoupling one or several sites from the rest and driving a zero-crossing in that decoupled part of the system. However, a generic variation of local parameters at the impurity or at the end of the chain will not lead to an extra zero crossing.

6.2.5. Qualitative difference of the boundary response in topologically ordered and disordered phases

As discussed above, the local response of the system to a boundary transverse magnetic field is qualitatively different in the topologically disordered and ordered phases: in the disordered phase the response function $\chi_0(T)$ follows a singular Curie asymptotics in the $T \to 0$ limit, whereas in the ordered phase it is finite. It is instructive to look again at this qualitative difference by approaching it from the "polarization-loop" representation of $\chi_0(T)$, Eq. (50).

Using the explicit form of the Majorana Green's functions $D_{aa}(\varepsilon_n)$ $(a = 1, 2)$ at $h_0 = 0$ (see Appendix C) one represents $\chi_0(T)$ as a sum over Matsubara frequencies

$$\chi_0(T) = 4T \sum_{\varepsilon_n} \frac{1}{\Delta(\varepsilon_n)}, \qquad \Delta(\varepsilon_n) = \varepsilon_n^2 + \Gamma \left(\sqrt{\varepsilon_n^2 + m^2} - m \right). \tag{91}$$

At $T \to 0$ the sum in (91) transforms to the integral

$$\chi_0(0) = \frac{4}{\pi} \int_0^\infty \frac{\mathrm{d}\varepsilon}{\Delta(\varepsilon)}. \tag{92}$$

For an isolated spin ($\Gamma = 0$) $\Delta(\varepsilon) = \varepsilon^2$ and the integral in (92) diverges at the lower limit, implying that the Matsubara sum in (91) cannot be replaced by the integral (92). Doing the Matsubara sum leads to the standard Curie law:

$$\chi_0(T) = 4T \sum_{\varepsilon_n} \frac{1}{\varepsilon_n^2} = \frac{8}{\pi^2 T} \sum_{n \geq 0} \frac{1}{(2n+1)^2} = \frac{1}{T}. \tag{93}$$

In spite of its simplicity, this result is quite noteworthy. It indicates that, for a boundary impurity spin in a QIC, the response of the system to the local transverse magnetic field h_0 will follow a singular Curie behavior

$$\chi_0(T \to 0) = \frac{C}{T}, \quad 0 < C < 1, \tag{94}$$

only if $\Delta(\varepsilon) \sim \varepsilon^2$ as $\varepsilon \to 0$. If, on the other hand, $\Delta(\varepsilon) \to \text{const} \neq 0$ as $\varepsilon \to 0$, the local boundary response will be non-singular, and the limit $\lim_{T \to 0} \chi_0(T)$ will be finite. In such a situation, the ground state of the impurity spin is non-degenerate. The arguments we will give below unambiguously indicate that, irrespective of the magnitude of the ratio $\Gamma/|m|$, the non-singular behavior of $\chi_0(T)$ in the limit $T \to 0$ is entirely due to the presence of the boundary zero Majorana mode in the bulk spectrum of the QIC at $m < 0$.

The contribution of the boundary MZM can be singled out by representing $\Delta(\varepsilon_n)$ as follows:

$$\Delta(\varepsilon_n) = \varepsilon_n^2 + \Gamma \left(\sqrt{\varepsilon_n^2 + m^2} - |m| \right) + 2\Gamma |m| \theta(-m). \tag{95}$$

Consider now the region of small frequencies, $|\varepsilon_n| \ll |m|$ (which automatically implies that $T \ll |m|$) in which case

$$\Delta(\varepsilon_n) \simeq \left(1 + \frac{\Gamma}{2|m|}\right)\varepsilon_n^2 + 2\Gamma|m|\theta(-m). \tag{96}$$

It then follows from (96) that in the disordered phase ($m > 0$), when the second term in the r.h.s. of (96) is absent, $\Delta(\varepsilon_n) \sim \varepsilon_n^2$ and the susceptibility maintains its singular Curie form (94) with the renormalized Curie constant:

$$C = \mu_{\text{eff}}^2 = \frac{2m}{\Gamma + 2m}. \tag{97}$$

Obviously, the results of Eqs. (94) and (97) are contributed by the low-frequency ($\omega^2 < m^2$) part of the impurity spectral weight $A(\omega)$, while the contribution of the high-frequency continuum ($\omega^2 > m^2$) represents a relatively small correction.

On the other hand, in the ordered (topological) phase ($m < 0$) $\Delta(\varepsilon_n) \to 2\Gamma|m| \neq 0$ as $\varepsilon_n \to 0$. So, the presence of the boundary MZM in the spectrum at $m < 0$ is the ultimate reason *why* the local response of the topologically ordered phase is non-singular. This reflects the fact that, in the thermodynamic limit, coupling locally to a boundary degree of freedom does not allow to switch the topological sector, or the sector of spontaneously broken symmetry. Thus the linear response remains non-singular even at points where there is a spectral degeneracy between the different sectors.

However, this argument does not always imply that the finite value of χ_0 in the topologically ordered phase will be contributed by the region of small ε where the expansion (96) is valid. Such an approximation is valid in the limit of strong localization, $|m| \gg \Gamma$. The sum over ε_n will then mostly be contributed by frequencies $|\varepsilon| \sim \sqrt{\Gamma|m|} \ll |m|$. In this case we can approximate $\Delta(\varepsilon)$ by the expression

$$\Delta(\varepsilon) \simeq \left(1 + \frac{\Gamma}{2|m|}\right)\varepsilon^2 + 2\Gamma|m| \simeq \varepsilon^2 + 2\Gamma|m|, \tag{98}$$

and estimate $\chi_0(0)$

$$\chi_0(T=0) = \frac{4}{\pi}\int_0^{\varepsilon_{\max}} \frac{d\varepsilon}{\varepsilon_n^2 + 2\Gamma|m|} = \frac{2}{\sqrt{2\Gamma|m|}}, \quad m < 0. \tag{99}$$

As follows from the structure of the impurity spectral weight $A(\omega)$, in the strong localization limit the quantity $\omega_0 = \sqrt{2\Gamma|m|}$ represents a characteristic energy scale of a subgap bound state of the impurity Majorana β_1 and the boundary zero mode γ_0. The contribution of the high-frequency continuum to $\chi_0(0)$ is subdominant.

In the strong hybridization limit, $\Gamma \gg |m|$, the situation is different. Let us first estimate the contribution of small frequencies, $\varepsilon^2 \ll m^2$. From (98) we have

$$\Delta(\varepsilon) \simeq \frac{\Gamma}{2|m|}(\varepsilon^2 + 4m^2). \tag{100}$$

The contribution of the region $\varepsilon^2 < m^2$ to $\chi_0(0)$ in (92) is easily estimated:

$$\chi_<(0) = \frac{8|m|}{\pi\Gamma}\int_0^{\sim|m|} \frac{d\varepsilon}{\varepsilon^2 + 4m^2} \simeq \frac{4}{\pi\Gamma}. \tag{101}$$

At this point we should recall that at temperatures $T < |m| \ll \Gamma$ the high-frequency continuum of local states provides a logarithmically enhanced contribution to the susceptibility

$$\chi_>(0) \simeq \frac{4}{\pi\Gamma}\ln\frac{\Gamma}{|m|}, \tag{102}$$

the mass gap $|m|$ serving as the infrared cutoff of the logarithm. Since within the logarithmic accuracy, a large logarithm $\ln(\Gamma/|m|)$ is admitted to have a relatively small correction $\sim O(1)$, in the strong hybridization limit $\chi_>(0)$ logarithmically dominates $\chi_<(0)$. However, the most important fact here is that, contrary to the situation in the disordered phase, $\chi_<(T=0)$ is *finite* at $m<0$. This is due to the presence of the boundary MZM, as is clearly seen from formulae (100), (101).

Thus, the role of the boundary MZM in the topological phase is clear. Hybridization with the bulk MZM suppresses the low-frequency part of the fluctuation spectrum of the impurity spin and renders the local response non-singular, as illustrated in Table 1. Therefore, the non-singular zero-temperature limit of the local response function χ_0 of an impurity at the edge of a chain serves as an indication of the existence of a boundary Majorana zero mode in the topologically ordered phase.

7. Impurity in the bulk of a quantum Ising chain

In this section we consider a zero-field impurity in the *bulk (rather than the edge)* of a non-critical QIC. As we have shown in Section 5.1, this model reduces to a problem of two semi-infinite QICs coupled to the impurity spin at the boundary. We will assume that the chains $a=1,2$ are identical ($v_1=v_2, m_1=m_2$) but characterized by independent nonzero hybridization constants Γ_1 and Γ_2. At $\Gamma_1=\Gamma_2$ the model is equivalent to a spinless, semi-infinite Peierls insulator (PI) chain with a boundary fermionic d-level, as we show in Appendix D. In the PI model, χ_0 also describes the local compressibility at the impurity site. The role of the mass m is played by the difference between the alternating hopping amplitudes of the Peierls chain, $t_\pm = t\pm\Delta$. For a positive Δ the first two sites next to the impurity form a more strongly coupled dimer, and the corresponding massive phase of the PI is non-topological. In the opposite case, $\Delta<0$, the ground state of the PI is topologically degenerate and supports boundary zero modes.

We might as well consider an impurity located at a domain wall separating the ordered ($x>0$) and disordered ($x<0$) phases of a QIC. For topological reasons, to understand the low-energy sector, we can formally take the limit $m\to+\infty$ at $x\to-\infty$. Thus, in the low-energy limit, this case reduces to the already considered problem of a single semi-infinite QIC in the ordered phase ($m<0$) with a boundary impurity.

For a bulk classical spin the local susceptibility can be calculated for arbitrary Γ_1 and Γ_2 using the general formula (C.15) for $G(\varepsilon_n, h_0)$ and the rules of analytic continuation (53). Since at $h_0=0$ the impurity Majorana fermions β_1 and β_2 are decoupled, the resulting model represents a direct sum of two semi-infinite KM chains (28) (see Fig. 5). Accordingly, the spectral weight of the impurity center in such a model is given by

$$A(\omega)=A_1(\omega)+A_2(\omega)-\delta(\omega)=\frac{1}{2}\left[A_{f1}(\omega)+A_{f2}(\omega)\right],\quad (h_0=0), \tag{103}$$

where $A_a(\omega)=(1/2)\left[\delta(\omega)+\frac{1}{2}A_{fa}(\omega)\right]$ are the spectral weights of isolated semi-infinite QICs labeled by $a=1,2$. However, for $h_0\neq 0$ the additive structure of $A(\omega)$, given by (103), is no more valid.

Using the definition (103) and formulae (57), (58), at $h_0=0$ we obtain

$$m>0:\ A(\omega)=\frac{1}{2}(Z_1+Z_2)\delta(\omega)+\theta(\omega^2-m^2)\frac{1}{2\pi}\sum_{a=1,2}\frac{\Gamma_a\sqrt{\omega^2-m^2}}{|\omega|(\omega^2+2\Gamma_a m+\Gamma_a^2)}; \tag{104}$$

$$\begin{aligned}m<0:\ A(\omega)&=\frac{1}{2}\sum_{a=1,2}\theta(|m|-\Gamma_a)\left(\frac{|m|-\Gamma_a}{2|m|-\Gamma_a}\right)[\delta(\omega-\omega_a)+\delta(\omega+\omega_a)]\\&\quad+\theta(\omega^2-m^2)\frac{1}{2\pi}\sum_{a=1,2}\frac{\Gamma_a\sqrt{\omega^2-m^2}}{|\omega|(\omega^2-2\Gamma_a|m|+\Gamma_a^2)},\end{aligned} \tag{105}$$

where

$$Z_a=\frac{2m}{2m+\Gamma_a},\quad (m>0),$$
$$\omega_a=\sqrt{\Gamma_a(2|m|-\Gamma_a)}<|m|\quad (m<0).$$

7.1. Topologically disordered phase, $m > 0$

In the disordered phase ($m > 0$), the low-frequency part of the local spectral weight $A(\omega; h_0 = 0)$ is contributed by the $\delta(\omega)$ singularity in the r.h.s. of (104). The local susceptibility follows the Curie law $\chi_< = \mu_{\rm eff}^2/T$. The effective magnetic moment of the impurity

$$\mu_{\rm eff} = \sqrt{Z_1 Z_2} \tag{106}$$

interpolates between the values $\mu_{\rm eff} = \sqrt{Z_1}$ at $\Gamma_2 = 0$ (single semi-infinite QIC) and $\mu_{\rm eff} = Z_1$ at $\Gamma_2 = \Gamma_1$ (equivalent to the PI chain). At $\Gamma_1, \Gamma_2 \neq 0$, on approaching the criticality ($m \to 0$) the Curie constant scales as

$$C = \mu_{\rm eff}^2 \sim \frac{m^2}{\Gamma_1 \Gamma_2}. \tag{107}$$

It thus approaches zero much faster than in the case of a single chain with a boundary impurity ($\Gamma_2 = 0$), where C scales as $C \sim m$.

The contribution of the high-frequency part of the spectral weight to the local susceptibility is given by

$$\chi_> = \frac{4}{\pi} \int_m^\infty d\omega \, \frac{\sqrt{\omega^2 - m^2}}{\omega^2} \tanh\left(\frac{\omega}{2T}\right) \frac{\Gamma_1(\omega^2 + \Gamma_2 m) + \Gamma_2(\omega^2 + \Gamma_1 m)}{(\omega^2 + \Omega_1^2)(\omega^2 + \Omega_2^2)}, \tag{108}$$

where $\Omega_a^2 = \Gamma_a(2m + \Gamma_a)$. As for a single QIC, in the strong localization limit, $|m| \gg \Gamma_{1,2}$, $\chi_>$ in (108) leads to small corrections to the low-frequency contribution to $\chi_<$.

The frequency region $\omega^2 > m^2$ becomes important when the impurity state is strongly hybridized with at least one of the two chains. To analyze such cases, it is convenient to transform $\chi_>$ in (108) to an equivalent form

$$\chi_> = \frac{\Gamma_1 \chi_>^{(1)} - \Gamma_2 \chi_>^{(2)}}{\Gamma_1 - \Gamma_2}, \tag{109}$$

where $\chi_>^a$ ($a = 1, 2$) are the high-frequency contributions to the susceptibilities of isolated QICs, Eqs. (69), already discussed in Section 6 B.

Suppose that $\Gamma_1 \gg \Gamma_2$. We consider first the case $\Gamma_2 \ll m \ll \Gamma_1$. It describes a situation when the impurity Majorana fermion β_1 is strongly hybridized with the bulk excitations of the first chain, whereas the fermion β_2 is strongly localized. So, the impurity MZM β_2 can be approximately regarded as completely decoupled from both chains. It follows from (70), at $\Gamma_2 \ll m \ll \Gamma_1$ $\chi_>^{(2)} \simeq \Gamma_2/m^2$. Then, as one expects, up to small relative corrections $\sim \Gamma_2/\Gamma_1$ and $(\Gamma_2/m)^2$, the total susceptibility χ_0 coincides with $\chi_0^{(1)}$, i.e. the local susceptibility of an isolated semi-infinite first chain ($a = 1$) in the strong hybridization regime.

Consider now the case when both chains are in the strong hybridization regime, $m \ll \Gamma_1, \Gamma_2$. In the temperature range $m \lesssim T \ll \Gamma_1, \Gamma_2$, using the logarithmic asymptotics (72) for $\chi_>^{(1,2)}$, we arrive at a temperature independent susceptibility (a "local-Fermi-liquid" regime):

$$\chi_0 \simeq \chi_> = \frac{4}{\pi(\Gamma_1 - \Gamma_2)} \ln \frac{\Gamma_1}{\Gamma_2}. \tag{110}$$

For two chains coupled symmetrically to the impurity, $\Gamma_1 = \Gamma_2 \equiv \Gamma$, the result (110) becomes $\chi_0 = 4/\pi\Gamma$. According to (107), at $m \ll \Gamma$ the effective Curie asymptotics (contained in $\chi_<$) is $(m/\Gamma)^2/T$. Comparing this to (110) we find that

$$\chi_0 \simeq \frac{4}{\pi\Gamma}, \quad \text{if } \frac{m^2}{\Gamma} \ll T \ll m, \tag{111}$$

$$\chi_0 \simeq \left(\frac{2m}{\Gamma}\right)^2 \frac{1}{T}, \quad \text{if } T \ll \frac{m^2}{\Gamma}. \tag{112}$$

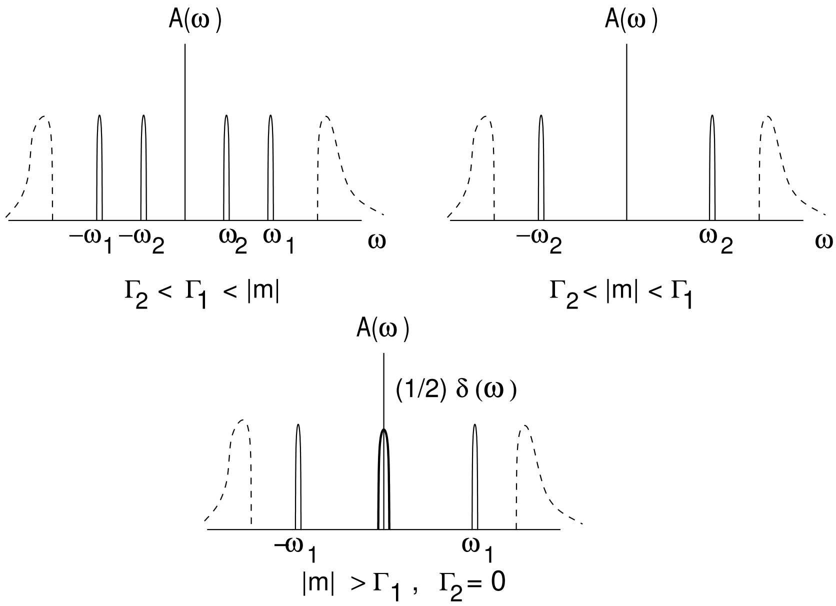


Fig. 8. The spectral weight of an impurity spin coupled to two quantum Ising chains in the absence of a local field ($h_0 = 0$).

Thus, also in the channel-symmetric case (or equivalently, in a PI chain), there exists a re-entrant crossover between two Curie regimes, $\chi_0 = 1/T$ at $T \gg \Gamma$ and $\chi_0 = (2m/\Gamma)^2/T$ at $T \ll m^2/\Gamma$, separated by a temperature independent susceptibility plateau (111).

7.2. Topologically ordered phase, $m < 0$

In the ordered phase ($m < 0$), the spectral weight $A(\omega; h_0 = 0)$ at $\omega^2 < m^2$ is given by the first term in the r.h.s. of (105). The subgap peaks shown in Fig. 8 describe bound states between the impurity Majorana fermions β_1, β_2 and the MZMs of the bulk spectra of the corresponding chains. Depending on the relation between the parameters m and $\Gamma_1 \neq \Gamma_2$, there may be 0, 2 or 4 peaks. In the limit of a single semi-infinite chain ($\Gamma_2 \to 0$, $\Gamma_1 \neq 0$), the two peaks at $\omega = \pm\omega_2$ merge to produce a central peak $(1/2)\delta(\omega)$ representing the contribution of the decoupled β_2-fermion. The corresponding contribution to the zero-temperature local susceptibility is finite:

$$\chi_<(0) = 4\frac{K_1 - K_2}{\Gamma_1 - \Gamma_2}, \qquad K_a = \theta(|m| - \Gamma_a)\left(\frac{\Gamma_a}{\omega_a}\right)\left(\frac{|m| - \Gamma_a}{2|m| - \Gamma_a}\right).$$

In particular, in the strong localization limit ($|m| \gg \Gamma_{1,2}$)

$$\chi_<(0) = \sqrt{\frac{2}{|m|}}\frac{1}{\sqrt{\Gamma_1} + \sqrt{\Gamma_2}}. \tag{113}$$

In the symmetric case $\Gamma_1 = \Gamma_2$ this transforms to

$$\chi_<(0) = \frac{1}{\sqrt{2|m|\Gamma}}. \tag{114}$$

Like for a single semi-infinite QIC with a boundary impurity, the zero-temperature local susceptibility is finite, but its value in the presence of two attached chains is twice smaller than the single-chain value (81) of χ_0. It may be interesting to generalize this result to junctions of $n > 2$ semi-infinite chains.

At $m < 0$ the high-frequency part of the local susceptibility is given by

$$\chi_> = \frac{4}{\pi}\int_{|m|}^{\infty} d\omega \, \frac{\sqrt{\omega^2 - m^2}}{\omega^2} \tanh\left(\frac{\omega}{2T}\right) \frac{\Gamma_1(\omega^2 - \Gamma_2|m|) + \Gamma_2(\omega^2 - \Gamma_1|m|)}{\left(\omega^2 - \Gamma_1(2|m| - \Gamma_1)\right)\left(\omega^2 - \Gamma_2(2|m| - \Gamma_2)\right)}. \tag{115}$$

This expression can again be rewritten as in Eq. (109). Using that formula, one easily checks that, in the strong localization limit, $|m| \gg \Gamma_1, \Gamma_2$, the high frequency corrections to $\chi_<$ in (113) are small, and thus $\chi_0(0) \simeq \chi_<(0)$. In the strong hybridization regime, $|m| \ll \Gamma_1, \Gamma_2$, the local susceptibility χ_0 coincides with $\chi_>$. As follows from our discussion in Section 6 B3 there the 2-channel Kondo asymptotics of single-chain susceptibilities $\chi_>^{(1,2)}$ are insensitive to the sign of m ($|m|$ only serves as a low-energy cutoff of the logarithms). We thus conclude that in the absence of a singular low-temperature Curie susceptibility at $m < 0$, χ_0 becomes temperature independent at $T \ll \min(\Gamma_1, \Gamma_2)$ and is given by (110).

Thus, for symmetrically coupled chains (the case of PI), the susceptibility $\chi_0(T)$ approaches the constant value (114) at any $T \ll |m|$ if $|m| \gg \Gamma$, or the constant value (111) at any $T \ll \Gamma$ if $|m| \ll \Gamma$.

7.3. Comparing the local response: boundary impurity versus impurity in the bulk

The Kondo-like multiplicative logarithmic renormalization of $\chi_>$ in (102) is a feature specific to a single semi-infinite QIC. This renormalization emerges in the strong hybridization limit, $|m| \ll \Gamma$, where it is contributed by the broad continuum of high-frequency states ($\omega^2 \gg m^2$) forming the “tail” of the spectral weight $A(\omega)$. In this frequency region (and in the leading order in $|m/\omega| \ll 1$) $A(\omega)$ does not depend on the mass m and coincides with that for a critical QIC. According to formulae (69) or (82), the local susceptibility and at $T, |m| \ll \Gamma$ displays a logarithmic asymptotics (84), as in the closely related 2-channel Kondo problem.

As we have seen in this section, for an impurity in the bulk symmetrically coupled to two equivalent chains (which maps to a model of an impurity coupled to a semi-infinite PI chain) the logarithm disappears and $\chi(0) = 4/\pi\Gamma$. This difference stems from the fact that in the topologically massive phases of the two chains the impurity spin interacts with both boundary MZMs. This suppresses the singularity of the critical low-frequency Green’s functions more strongly than in the case of a single chain attached to the impurity.

The logarithmic asymptotics (64) of the edge susceptibility of a semi-infinite QIC occurs not only at criticality but also in the quantum critical window at finite m, $|m| < T \ll \Gamma$. The logarithmic multiplicative renormalization of the local susceptibility is an *unambiguous indication* of the existence of a boundary MZM at the impurity site. This is seen at the edge of a QIC, but not at the edge of a PI chain, which only hosts fermionic boundary zero modes.

8. Relation to the 1D p-wave superconductor model

In this section we make contact with the Kitaev’s model of a 1D p-wave superconductor [5] described by the Hamiltonian (1). The pairing amplitude Δ is chosen to be real and positive. There exists a particle–hole transformation, $a_n \to (-1)^n a_n^\dagger$, that changes the sign of μ but keeps the rest of the Hamiltonian (1) invariant. Therefore one can always assume that $\mu \geq 0$. In this region, there exists a critical point $\mu = t$ which separates two gapped phases: the topologically trivial phase at $\mu > t$ and the topologically non-trivial phase [5,2] at $\mu < t$.

Comparing (5) and (1) one sees that the 1DPS model exactly maps onto the QIC at $\Delta = t$. However, universal scaling properties of the two models coincide in the general case provided that one concentrates on the vicinity of the critical point. Indeed, setting $\mu = t + m$ and introducing the Majorana lattice operators ζ_n and η_n (see Section 5.1), we first rewrite the Hamiltonian (1) in the form

$$H = \frac{it}{4}\sum_n (\eta_n\zeta_{n+1} + \eta_{n+1}\zeta_n - 2\eta_n\zeta_n) + \frac{i\Delta}{4}\sum_n (\eta_n\zeta_{n+1} - \eta_{n+1}\zeta_n) - \frac{im}{2}\sum_n \eta_n\zeta_n. \quad (116)$$

Assuming then that $|m| \ll t$, and passing to the continuum limit according to the rule (29), we find that the first term on the r.h.s. of (116) represents a surface term while the remaining part of H transforms to a Hamiltonian of a massive Majorana fermion given by

$$H_M = \int \mathrm{d}x\, \mathcal{H}_M(x), \quad \mathcal{H}_M(x) = iv\eta(x)\partial_x\zeta(x) - im\eta(x)\zeta(x), \quad (117)$$

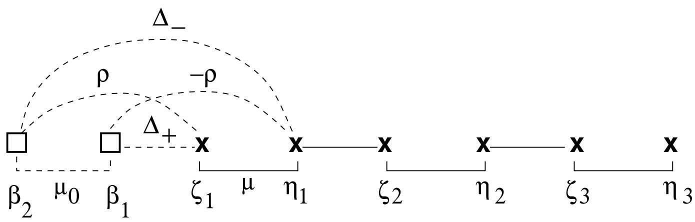


Fig. 9. Boundary impurity in the Kitaev–Majorana chain for a 1DPS model.

where $v = \Delta a_0$. From this equivalence it follows that close to the Ising criticality the ordered ($m < 0$) and disordered ($m > 0$) phases of the QIC adequately describe the topological and non-topological phases of the 1DPS. It can be readily seen that in the vicinity of the second Ising critical point, $\mu = -t + m$ ($|m| \ll t$) the emerging continuum model still has the Majorana structure (117) but with m replaced by $-m$. So in this case the nomenclature of the ordered and disordered phases according to the sign of the mass m is inverted. This is in agreement with the known fact [5,2] that the phase located within the interval $-t < \mu < t$ is topological, whereas the phases occurring at $\mu > t$ and $\mu < -t$ are non-topological.

Now we can construct a model of a 1DPS on a semi-axis $x > 0$ with an impurity at the open end. Using the spin-fermion equivalence (40), we associate the isolated impurity with a local d-fermion level,

$$H_0 = -\mu_0(d^\dagger d - 1/2) = -ih_0\beta_1\beta_2,$$

where $h_0 = \mu_0/2$. Accordingly, the local spin susceptibility of the semi-infinite QIC, χ_0, becomes proportional to the boundary charge susceptibility (local "compressibility") of the 1DPS, κ_0:

$$\chi_0 = 4\kappa_0, \qquad \kappa_0 = \frac{\partial n_d}{\partial \mu_0},$$

where n_d is the mean occupancy of the d level. The bulk of the system is described by the Majorana Hamiltonian (117). However, in a 1DPS, in addition to the standard single-particle tunneling between the impurity site and the superconductor (t_0), the hybridization term may also contain a local pairing contribution (Δ_0):

$$\begin{aligned} H' &= \frac{t_0}{2}d^\dagger a_1 + \frac{\Delta_0}{2}d^\dagger a_1^\dagger + \text{h.c.} \\ &= i\left(\Delta_+\beta_1\zeta_1 + \Delta_-\beta_2\eta_1\right) + i\rho\left(\beta_2\zeta_1 - \beta_1\eta_1\right), \end{aligned} \tag{118}$$

where

$$\Delta_\pm = \frac{1}{2}\Re e\Delta_0 \pm \frac{t_0}{4}, \qquad \rho = \frac{1}{2}\Im m\Delta_0. \tag{119}$$

While by a global gauge transformation of the fermion operators a_n it is possible to make in Eq. (1) the pairing amplitude Δ real, the phases of the global (Δ) and local (Δ_0) amplitudes do not generally coincide. This is why the hybridization term in (118) is characterized by three real parameters.

The first term in (118) has the same structure as that already considered in Section 5.1. To clarify the role of new boundary terms in the Hamiltonian, it is instructive to consider a toy KM model which involves two impurity Majorana sites (β_1 and β_2) and two more sites at the open boundary of the chain (ζ_1 and η_1)—see Fig. 9. The Hamiltonian of the model is given by

$$H_4 = -\frac{i\mu_0}{2}\beta_1\beta_2 - \frac{i\mu}{2}\eta_1\zeta_1 + i\Delta_+\beta_1\zeta_1 + i\Delta_-\beta_2\eta_1 + i\rho\left(\beta_2\zeta_1 - \beta_1\eta_1\right). \tag{120}$$

The spectrum of H_4 has a $E \to -E$ symmetry and consists of two pairs of levels, $\pm E_1$ and $\pm E_2$, where

$$E_1 = \frac{1}{2}\left(\sqrt{\Omega_+} + \sqrt{\Omega_-}\right), \qquad E_2 = \frac{1}{2}\left(\sqrt{\Omega_+} - \sqrt{\Omega_-}\right), \tag{121}$$

$$\Omega_+ = \left(\frac{\mu+\mu_0}{2}\right)^2 + (\Delta_+ + \Delta_-)^2 + 4\rho^2, \qquad \Omega_- = \left(\frac{\mu-\mu_0}{2}\right)^2 + (\Delta_+ - \Delta_-)^2. \tag{122}$$

Assuming that $\Omega_\pm \neq 0$, it is possible to fine-tune μ_0 to satisfy the condition $\Omega_+ = \Omega_-$, in which case the levels $\pm E_2$ become degenerate at the value $E = 0$. This condition translates to

$$\mu_0 = -\frac{4(\Delta_+\Delta_- + \rho^2)}{\mu}. \tag{123}$$

The model (120) is expected to yield a satisfactory description of the boundary degrees of freedom in the topologically disordered phase of the 1DPS. In that case it predicts the degeneracy of the occupied and unoccupied impurity states at the specific value (123) of μ_0. At that value of μ_0 the local charge at the impurity site, $n_d(T = 0; \mu_0)$, should display a discontinuity entirely analogous to the zero-temperature jump of the impurity magnetization in the disordered phase of the QIC (see Section 6.2.2). However, the extra Δ_- and ρ-terms in (120) break the local particle–hole symmetry ($\beta_2 \to -\beta_2$) and thereby generate a non-zero intrinsic local field at the impurity site. Therefore, the impurity occupancy $n_d^\pm$ right before and after the jump will in general not be situated symmetrically around 1/2, but be shifted by a finite amount. In the topologically ordered phase, it is still possible to tune the impurity degrees of freedom to bring about an exact degeneracy between the ground and the first excited states (which are anyway already exponentially close in energy). However, now they differ in their topological sector and thus are not connected by a local perturbation. This suppresses the singularity in the local compressibility.

The above expectations are confirmed by calculations similar to those done in Section 5. As before, the boundary condition for the bulk modes is (32). In the continuum limit $\zeta_1 \to \sqrt{2a_0}\zeta(a_0)$, $\eta_1 \to \sqrt{2a_0}\eta(a_0)$. The boundary values of the fields, $\zeta(a_0)$ and $\eta(a_0)$, can be expanded in powers of $a_0 \to 0$. Keeping the leading terms of these expansions and using the normal mode expansion (B.14) one finds the explicit expressions for $\zeta(0)$ and $\eta'(0)$ and thus derives the total Hamiltonian in terms of quasiparticle operators

$$\begin{aligned} H &= H_0 + H' \\ &= -ih_0\beta_1\beta_2 - \frac{i}{2}\sum_{k>0}\varepsilon_k b_k f_k - i\lambda_0\beta_1\gamma_0 - i\tilde{\lambda}_0\beta_2\gamma_0 \\ &\quad - i\sqrt{\frac{2}{N}}\sum_{k>0}\lambda_k\beta_1 b_k - i\sqrt{\frac{2}{N}}\sum_{k>0}\tilde{\lambda}_k\beta_2 b_k + i\sqrt{\frac{2}{N}}\sum_{k>0}\delta_k\beta_2 f_k \\ &\quad - i\sqrt{\frac{2}{N}}\sum_{k>0}\tilde{\delta}_k\beta_1 f_k, \end{aligned} \tag{124}$$

with the coupling constants

$$\begin{aligned} &\lambda_0 = 2\Delta_+\sqrt{\frac{|m|a_0}{v}}\theta(-m), \qquad \tilde{\lambda}_0 = 2\rho\sqrt{\frac{|m|a_0}{v}}\theta(-m), \\ &\lambda_k = \Delta_+\frac{kv}{\varepsilon_k}, \qquad \tilde{\lambda}_k = \rho\frac{kv}{\varepsilon_k}, \qquad \delta_k = \left(\frac{\Delta_- a_0}{v}\right)kv, \qquad \tilde{\delta}_k = \left(\frac{\rho a_0}{v}\right)kv. \end{aligned} \tag{125}$$

Notice that, due to the boundary pairing described by the complex amplitude Δ_0, both impurity Majorana fermions, β_1 and β_2, hybridize with the boundary zero mode γ_0, as well as with the gapped continuum states of the bulk spectrum.

The Greens' functions (GF) of the model (124) can be easily calculated. Since the parameter v/a_0 represents an ultraviolet cutoff of the theory, small terms of the order $\varepsilon_n a_0/v$ and $|m|a_0/v$ can be systematically dropped. Skipping the details, here we only outline the main results. From the structure of the resulting Matsubara GFs $D_{jk}(\varepsilon_n)$ $(j, k) = 1, 2$, one can read off that the only effect of finite ρ,

Δ_- is to additively renormalize the boundary "magnetic field" h_0 or, equivalently, the d-level local potential μ_0,

$$h_0 \rightarrow \tilde{h}_0 = h_0 + \frac{4a_0}{v}\left(\Delta_+\Delta_- + \rho^2\right). \tag{126}$$

This could have been anticipated qualitatively from Fig. 9: non-zero values of the couplings Δ_- and ρ break the local particle–hole symmetry ($\beta_2 \rightarrow -\beta_2$) present at $\mu_0 = 0$ and thus contribute to an effective pairing of the Majorana fermions β_1 and β_2 with an amplitude $\sim \Delta_+\Delta_- a_0/v,\ \rho^2 a_0/v$. Therefore, the point of the double degeneracy of the spectrum, i.e., the condition for the boundary impurity degree of freedom to be classical (that is, conserved by the dynamics), is $\tilde{h}_0 = 0$ rather than $h_0 = \mu_0 = 0$.

Using the obtained GFs $D_{jk}(\varepsilon_n)$ and the general formula (50) for the static local susceptibility, we find that at the degeneracy point $\tilde{h}_0 = 0$ the local charge susceptibility of the 1DPS is still given by formula (92), where the width of the d-level is given by $\Gamma = 4(a_0/v)(\Delta_+^2 + \rho^2)$. With this modification and the redefinition of the spectral degeneracy point ($\tilde{h}_0 = 0$) the results of the preceding sections fully apply to the 1DPS model.

9. Summary and conclusions

The central result of this paper is summarized in Table 1: The local equilibrium response of an edge or bulk impurity site distinguishes the non-topological and topological phases of the bulk chains, respectively. In the non-topological phase (or, in the disordered phase of the Ising chain), the impurity can be tuned by the local transverse field or the chemical potential through a degeneracy point, where the energy of a localized boundary mode crosses zero and thus changes occupation in the ground state. At $T = 0$ this change is seen as a discontinuity of the transverse magnetization (in the QIC) or the charge (PI, 1DPS) at the impurity site. For the Ising chain and the PI the degeneracy point is dictated by symmetry to be at $h_0 = \epsilon_d = 0$, while in a 1DPS one needs to tune the impurity potential μ_0 to find the degeneracy point. At finite temperatures, being at the degeneracy point implies a Curie-type divergence of the corresponding susceptibility as $T \rightarrow 0$. The coefficient of the Curie law tends to zero upon approaching the topological phase transition. On the topologically (or magnetically) ordered side instead, we find that it is impossible to find discontinuous response at the impurity site at $T = 0$, and there is no Curie-like divergence of the susceptibility. In the case of the Ising chain this is simple to understand as the symmetry broken ground state exerts a longitudinal field on the impurity site, which keeps the transverse susceptibility finite despite the occurrence of an exact spectral degeneracy at $h_0 = 0$. However, it is less obvious to reach the analogous statement for the PI and 1DPS models, in which the constituent physical degrees of freedom are spinless fermions and no symmetry is spontaneously broken. A unified understanding is possible after a JW transform of the QIC. Then the topological phase of all three models is characterized by boundary zero modes on the semi-infinite bulk chains. Their coupling with the impurity levels forbids any localized boundary mode to cross zero energy, as a consequence of the level repulsion from the rigid zero mode which cannot be moved by modifying local parameters. This avoids the occurrence of any degeneracy not associated with the zero mode itself. This fact can also be understood as a consequence of the topological protection of the ordered phase against local perturbations: A discontinuity in the local response at $T = 0$ would require to switch the parity. Even though at specific values of the parameters h_0, ϵ_d a global spectral degeneracy is encountered (such as at $h_0 = \epsilon_d = 0$ for the cases of QIC and PI), this is not reflected in the local susceptibility, because the relevant matrix element connects states of opposite parity. In the topological phase those are exponentially suppressed in the system size.

The smoothness of the local charge response is easily understood in the case of a PI, upon analyzing the two phases as the impurity potential ϵ_d is tuned from $+\infty$ to $-\infty$. In the non-topological phase, when the degeneracy point is crossed at $\epsilon_d = 0$, an extra charge enters the system and fills a level which is localized close to the impurity. The sudden presence (at $T = 0$) of the new charge is seen as a discontinuity in the charge response function $n_d(\epsilon_d)$. On the topological side, however, a slow decrease of ϵ_d does not allow an extra charge to enter at the impurity site. Indeed, at large positive ϵ_d, the level concentrated on the first site of the PI chain is occupied, having a negative energy $\approx -t_0^2/\epsilon_d$, where t_0 is the tunneling between the impurity and the PI. As ϵ_d is reduced, that boundary state hybridizes with the impurity site, pushing the energy down to $-t_0$. Meanwhile, the occupancy of the impurity smoothly increases, reaching $n_d = 1/2$ at $\epsilon_d = 0$. As ϵ_d becomes more negative the occupied boundary mode shifts more and more weight onto the impurity site. Note that this level is always occupied, while its weight on the impurity site increases smoothly. Nevertheless, for an even PI chain it follows from particle–hole symmetry that at $\epsilon_d = 0$ there must be an exact zero mode, also in the topological phase: Indeed, it corresponds to the level localized at the opposite boundary of the PI chain. Its energy changes sign at $\epsilon_d = 0$, even though it always remains exponentially close to zero. The occupation of that boundary mode freely fluctuates at any finite temperature, while at strictly $T = 0$ it undergoes a sharp jump at $\epsilon_d = 0$. However, neither of these are visible at the impurity site sitting at the other end of the chain.

As usual, the distinction between the topological and the non-topological phase is sharp only at $T = 0$, while at finite T a quantum critical window ranging roughly from $-m$ to m smears out the transition between the respective behaviors. Right at criticality, an impurity at the end of a semi-infinite quantum Ising chain realizes the physics of a two-channel Kondo problem, with a logarithmically diverging local susceptibility [14]. This reflects the fact that one of the two Majoranas that form the impurity spin completely decouples from the rest of the system. In contrast, an impurity embedded in the bulk of a critical chain shows only a saturating susceptibility.

We propose to use the difference between the local response in the two phases as an indirect experimental probe for the presence or absence of topologically protected boundary zero modes. We expect very similar thermodynamic signatures in the local response of impurities coupled to the edge of large insulators in higher dimensions: in its trivial gapped phase the proximity of such a system will not hinder the discontinuous response of a nearby impurity site [24]. However, in the topological phase hybridization with the gapless edge modes is expected to smoothen out the local response. A closely analogous effect is indeed well-known form coupling quantum dots to gapless Fermi liquids [25]. The case of a 1d topological wire is a special case though, in the sense that it does not possess a continuum of edge modes. Finally, we expect that this phenomenology is robust to interactions, which are currently being discussed in the literature [26–28], as long as they do not induce a phase transition and gap the edge. Numerical studies similar to those of Ref. [22] might help to obtain a quantitative characterization of interaction effects.

It is worthwhile to compare the equilibrium features in the local response discussed here with probes of Majorana zero modes in transport. The latter focus on the zero-bias anomaly detected in the differential conductance as current is passed *through* the wire. Thereby charge enters at one end of the wire and exits at the opposite end. In this *transport* set-up the zero mode is constantly populated and emptied. In contrast, the *thermodynamics* of the zero mode is essentially blind to the application of local potentials, as it never shifts from zero energy. However, as discussed above, the zero mode has a non-trivial effect on the local spectrum at the impurity, in that it repels the available levels from zero energy. This effect can be probed by transport measurements which use the end of the wire, or an impurity coupled to it, as a quantum point contact between source and drain contacts on either side of the wire. In such a geometry one does not expect the zero mode to contribute to transport directly, not even at zero bias, but to show up in its indirect effects on the levels available for transmission. An analysis of these effects is left for future work.

The results obtained in this paper may be relevant to the studies of topological effects in junctions and/or quasi-one-dimensional arrays of quantum spin chains and 1D p-wave superconductors. However, in this article, we have mostly considered impurities at the end of a semi-infinite chain, or impurities in the bulk of a single chain. Only occasionally we commented on junctions of more than two semi-infinite chains at an impurity site, e.g. when predicting the critical behavior (26) of the Curie weight. Our explicit construction of a quasi-local spin operator for junctions of quantum Ising chains suggests that also this case can be solved exactly. It would thus be interesting to investigate potentially non-trivial traces of exchange statistics when comparing the susceptibility of classical spins at junctions of QICs with the analogous response in junctions of 1DPS wires. This question is of particular interest, given that such junctions are experimentally relevant elements in any braiding set-up.

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Appendix A. Impurity in a critical QIC. Comparison to the two-channel Kondo problem

Consider the model (31) and set $m_1 = m_2 = 0$, $v_1 = v_2$. Passing to new Majorana fields $\xi_{a;R,L}(x)$, defined in (33), and using the identification $\xi^a_L(-x) = -\xi^a_R(x)$, one arrives at a model of two chiral (right-moving) Majorana fields on the axis $-L < x < L$, coupled to different impurity Majorana fermions:

$$H = -ih_0\beta_1\beta_2 - 2i\sqrt{a_0}\sum_{a=1,2}\tilde{J}_a\beta_a\xi^a_R(0) - \frac{iv}{2}\sum_{a=1,2}\int_{-L}^{L}\mathrm{d}x\,\xi^a_R(x)\partial_x\xi^a_R(x). \tag{A.1}$$

Introducing a single chiral complex field $\psi(x) = [\xi^1_R(x) + i\xi^2_R(x)]/\sqrt{2}$ and recombining the two impurity Majorana operators β_1 and β_2 into a local complex fermionic degree of freedom, $d^\dagger = (\beta_2 + i\beta_1)/2$, we rewrite the Hamiltonian (A.1) as follows:

$$\begin{aligned} H &= \varepsilon_d(d^\dagger d - 1/2) - iv\int_{-L}^{L}\mathrm{d}x\,\psi^\dagger(x)\partial_x\psi(x) \\ &\quad + \sqrt{2a_0}\Big\{(\tilde{J}_1+\tilde{J}_2)\left[\psi^\dagger(0)d + d^\dagger\psi(0)\right] + (\tilde{J}_1-\tilde{J}_2)\left[\psi(0)d + d^\dagger\psi^\dagger(0)\right]\Big\}. \end{aligned} \tag{A.2}$$

The two-channel Kondo problem describes two kinds of chiral (right-moving) electrons, each carrying spin $s = 1/2$, which couple to the impurity spin via two channel-dependent, coupling constants. Bosonizing an XXZ version of this model and then refermionizing, it is possible for specially chosen values of the strength of the couplings that do not flip the impurity spin (at the so-called Toulouse point) to map the original Kondo Hamiltonian to a channel anisotropic version of the resonant-level model [14,18]. This model has the structure of the Hamiltonian (A.2) in which $\tilde{J}_1 = \alpha(g_1+g_2)$, $\tilde{J}_2 = \alpha(g_1-g_2)$, where $g_{1,2}$ are the coupling constants of spin-flip processes associated with the two channels, and α is a constant.

So, for a critical QIC with an impurity in the bulk, the channel-symmetric Majorana version of the resonant-level model emerges either at $\tilde{J}_2 = 0$ or $\tilde{J}_1 = 0$. These are the cases when the impurity spin couples either to the right semi-axis or to left semi-axis only. In other words, only a semi-infinite QIC with a boundary impurity spin exhibits the Majorana resonant-level behavior typical for the channel-symmetric two-channel Kondo problem. All cases with $\tilde{J}_1 \neq \tilde{J}_2$ map to channel-asymmetric two-channel Kondo problems. In the special case when the impurity couples to its right and left nearest-neighbor spins symmetrically ($\tilde{J}_1 = \pm\tilde{J}_2$), the mapping is to a standard, one-channel resonant-level model.

Appendix B. Diagonalization of the massive Majorana model on a semi-axis

Consider the Hamiltonian of a massive Majorana fermion:

$$H_M = \frac{1}{2}\int_0^L \mathrm{d}x\,\xi^T(x)\hat{h}(x)\xi(x), \tag{B.1}$$

$$\xi(x) = \begin{pmatrix}\xi_R(x)\\ \xi_L(x)\end{pmatrix}, \qquad \hat{h}(x) = -iv\partial_x\hat{\sigma}_3 + m\hat{\sigma}_2. \tag{B.2}$$

Diagonalization of this model is standard (see e.g. Ref. [29]). We are looking for solutions of the Dirac equation on an interval $0 < x < L$, assuming that $L \to \infty$:

$$\hat{h}(x)\chi_\varepsilon(x) = \varepsilon\chi_\varepsilon(x), \quad \chi_\varepsilon(x) = \begin{pmatrix}u_\varepsilon(x)\\ v_\varepsilon(x)\end{pmatrix}. \tag{B.3}$$

The boundary condition

$$u_\varepsilon(0) = -v_\varepsilon(0) \tag{B.4}$$

follows from (35). From the property $\hat{h}^*(x) = -\hat{h}(x)$ it follows that $\chi^*_\varepsilon(x) = \chi_{-\varepsilon}(x)$. Therefore the spectrum consists of $(\varepsilon, -\varepsilon)$ pairs and, possibly, a zero-energy mode ($\varepsilon = 0$). This leads to the following normal-mode expansion of the Majorana field $\xi(x)$:

$$\xi(x) = \gamma_0\chi_0(x) + \sum_{\varepsilon>0}\left[\gamma_\varepsilon\chi_\varepsilon(x) + \gamma^\dagger_\varepsilon\chi^*_\varepsilon(x)\right] = \xi^\dagger(x). \tag{B.5}$$

Here $\gamma^\dagger_0 = \gamma_0$ is a Majorana operator describing the localized zero mode with a normalizable wave function $\chi_0(x)$, and $\gamma_\varepsilon,\ \gamma^\dagger_\varepsilon$ are standard second-quantized fermionic operators describing the states within the continuous part of the spectrum and satisfying the standard algebra

$$\{\gamma_\varepsilon, \gamma^\dagger_{\varepsilon'}\} = \delta_{\varepsilon\varepsilon'}, \qquad \{\gamma_\varepsilon, \gamma_0\} = 0, \qquad \{\gamma_0, \gamma_0\} = 2\gamma_0^2 = 1. \tag{B.6}$$

Notice that in (B.5) the summation in the second term goes over states of positive energy only. Substituting the expansion (B.5) into (B.1) we arrive at the diagonalized Hamiltonian

$$H = \sum_{\varepsilon>0}\varepsilon\hat{\gamma}_\varepsilon\hat{\gamma}_\varepsilon, \qquad [H, \gamma_0] = 0, \tag{B.7}$$

which is valid if the eigenvectors belonging to the continuous part of the spectrum satisfy the orthonormalization conditions

$$\begin{aligned}
&\int_0^L \mathrm{d}x\ \left[u^*_\varepsilon(x)u_{\varepsilon'}(x) + v^*_\varepsilon(x)v_{\varepsilon'}(x)\right] = \delta_{\varepsilon\varepsilon'},\\
&\int_0^L \mathrm{d}x\ [u_\varepsilon(x)u_{\varepsilon'}(x) + v_\varepsilon(x)v_{\varepsilon'}(x)] = 0.
\end{aligned} \tag{B.8}$$

The algebra (34) of the Majorana fields implies the completeness relations:

$$u_0(x)u_0(x') + \sum_{\varepsilon>0}\left[u_\varepsilon(x)u^*_\varepsilon(x') + \text{c.c.}\right] = \delta(x-x'), \tag{B.9}$$

$$v_0(x)v_0(x') + \sum_{\varepsilon>0}\left[v_\varepsilon(x)v^*_\varepsilon(x') + \text{c.c.}\right] = \delta(x-x'), \tag{B.10}$$

$$u_0(x)v_0(x') + \sum_{\varepsilon>0}\left[u_\varepsilon(x)v^*_\varepsilon(x') + \text{c.c.}\right] = 0. \tag{B.11}$$

The solution of the Dirac equation (B.3) has the following form. The normalizable zero-energy solution only exists for $m < 0$:

$$\begin{aligned}
\chi_0(x) &= \begin{pmatrix}1\\-1\end{pmatrix}\phi_0(x),\\
\phi_0(x) &= \sqrt{\frac{|m|}{v}}\,\theta(-m)\exp\left(-|m|x/v\right),\\
\langle\chi_0|\chi_0\rangle &= \int_0^\infty \mathrm{d}x\ \left[u_0^2(x) + v_0^2(x)\right] = 1.
\end{aligned} \tag{B.12}$$

This is an indication of the topological nature of the ordered ($m < 0$) massive phase of the QIC. There also exists a continuum of extended states with energies $\varepsilon^2 \geq m^2$. The latter are parametrized by the quantum numbers $k_j = \pi j/L > 0$ ($j = 1, 2, \ldots, N = L/a_0$):

$$\chi_k(x) \equiv \begin{bmatrix}u_k(x)\\v_k(x)\end{bmatrix} = \begin{bmatrix}W_k(x)\\-W^*_k(x)\end{bmatrix}, \quad \varepsilon_k = \sqrt{k^2v^2 + m^2},$$

$$W_k(x) = \frac{1}{\sqrt{2L}}\left[\cos(kx - \theta_k) + i \sin kx\right], \quad k > 0. \tag{B.13}$$

The phase shift θ_k is defined through the relation $\tan\theta_k = m/kv$. Using (B.12) and (B.13) one can easily verify the relations (B.8)–(B.11). The expansion (B.5) takes its final form

$$\xi(x) = \gamma_0 \chi_0(x) + \sum_{k>0}\left[\gamma_k \chi_k(x) + \gamma_k^\dagger \chi_k^*(x)\right], \tag{B.14}$$

and the diagonalized Hamiltonian becomes

$$H = \sum_{k>0} \varepsilon_k \hat{\gamma}_k^\dagger \hat{\gamma}_k + \text{const.} \tag{B.15}$$

Appendix C. Majorana Green's functions for the impurity

Here we derive the d-fermion GF $G(\varepsilon_n)$ in the most general case described by the Hamiltonian (39). $G(\varepsilon_n)$ can be expressed in terms of the impurity Majorana GFs $D_{jk}(\varepsilon_n)$:

$$G(\varepsilon_n) = \frac{1}{4}\left[D_{11}(\varepsilon_n) + D_{22}(\varepsilon_n) + 2iD_{21}(\varepsilon_n)\right], \tag{C.1}$$

where

$$D_{jk}(\varepsilon_n) = -\int_0^{1/T} d\tau\, e^{i\varepsilon_n\tau}\langle T_\tau \beta_j(\tau)\beta_k\rangle. \tag{C.2}$$

Using the equations of motion for the Heisenberg operators $\beta_j(\tau)$ we obtain a set of equations for the GFs:

$$i\varepsilon_n D_{11}(\varepsilon_n) = 2 - 2ih_0 D_{21}(\varepsilon_n) - 2i\lambda_{10}L_1(\varepsilon_n) - 2i\sqrt{2/N}\sum_{k>0}\lambda_{1k}B_{1k}(\varepsilon_n); \tag{C.3}$$

$$i\varepsilon_n D_{21}(\varepsilon_n) = 2ih_0 D_{11}(\varepsilon_n) - 2i\lambda_{20}L_2(\varepsilon_n) - 2i\sqrt{2/N}\sum_{k>0}\lambda_{2k}B_{2k}(\varepsilon_n); \tag{C.4}$$

$$i\varepsilon_n\, L_a(\varepsilon_n) = i\lambda_{a0}D_{a1}(\varepsilon_n); \tag{C.5}$$

$$i\varepsilon_n B_{ak}(\varepsilon_n) = -i\varepsilon_{ak}F_{ak}(\varepsilon_n) + 2i\sqrt{2/N}\lambda_{ak}D_{a1}(\varepsilon_n); \tag{C.6}$$

$$i\varepsilon_n F_{ak}(\varepsilon_n) = i\varepsilon_{ak}B_{ak}(\varepsilon_n). \tag{C.7}$$

In the above formulae the following notations have been used:

$$L_a(\varepsilon_n) = -\int_0^{1/T} d\tau\, e^{i\varepsilon_n\tau}\langle T_\tau \gamma_{a0}(\tau)\beta_1(0)\rangle,$$

$$B_{ak}(\varepsilon_n) = -\int_0^{1/T} d\tau\, e^{i\varepsilon_n\tau}\langle T_\tau b_{ak}(\tau)\beta_1(0)\rangle,$$

$$F_{ak}(\varepsilon_n) = -\int_0^{1/T} d\tau\, e^{i\varepsilon_n\tau}\langle T_\tau f_{ak}(\tau)\beta_1(0)\rangle, \quad (a = 1, 2).$$

From Eqs. (C.3)–(C.7) one obtains a closed set of equations for the Majorana GFs $D_{jk}(\varepsilon_n)$:

$$\Omega_1(\varepsilon_n)D_{11}(\varepsilon_n) = 2 - 2ih_0 D_{21}(\varepsilon_n),$$
$$\Omega_2(\varepsilon_n)D_{21}(\varepsilon_n) = 2ih_0 D_{11}(\varepsilon_n),$$

where

$$\Omega_a(\varepsilon_n) = i\varepsilon_n - \frac{2\lambda_{a0}^2}{i\varepsilon_n} + i\varepsilon_n \frac{8}{N}\sum_{k>0}\frac{\lambda_{ak}^2}{\varepsilon_n^2 + \varepsilon_{1k}^2}.$$

The sums over $k > 0$ are easily evaluated:

$$\frac{1}{N}\sum_{k>0}\frac{\lambda_{ak}^2}{\varepsilon_n^2+\varepsilon_{ak}^2} = \frac{\tilde{J}_a^2 a_0}{\pi}\int_0^\infty \mathrm{d}k\,\frac{k^2 v_a^2}{\varepsilon_{ak}^2(\varepsilon_{ak}^2+\varepsilon_n^2)} = \left(\frac{\tilde{J}_a^2 a_0}{2v_a}\right)\frac{\sqrt{\varepsilon_n^2+m_a^2}-|m_a|}{\varepsilon_n^2}. \tag{C.8}$$

Denoting

$$\Gamma_a = \frac{4\tilde{J}_a^2 a_0}{v_a}, \tag{C.9}$$

$$\Delta_a(\varepsilon_n) = \varepsilon_n^2 + \Gamma_a\left(\sqrt{\varepsilon_n^2+m_a^2}-m_a\right), \tag{C.10}$$

we arrive at the final expressions for the impurity Majorana GFs,

$$D_{11}(\varepsilon_n) = -\frac{2i\varepsilon_n\Delta_2(\varepsilon_n)}{\Delta_1(\varepsilon_n)\Delta_2(\varepsilon_n)+4h_0^2\varepsilon_n^2}, \tag{C.11}$$

$$D_{21}(\varepsilon_n) = -\frac{4ih_0\varepsilon_n^2}{\Delta_1(\varepsilon_n)\Delta_2(\varepsilon_n)+4h_0^2\varepsilon_n^2}. \tag{C.12}$$

By symmetry, the remaining GFs are

$$D_{22}(\varepsilon_n) = -\frac{2i\varepsilon_n\Delta_1(\varepsilon_n)}{\Delta_1(\varepsilon_n)\Delta_2(\varepsilon_n)+4h_0^2\varepsilon_n^2}, \tag{C.13}$$

$$D_{12}(\varepsilon_n) = -D_{21}(\varepsilon_n). \tag{C.14}$$

According to (C.1), the local GF of the complex fermion, $G(\varepsilon_n)$, is given by

$$G(\varepsilon_n) = -\frac{1}{2}\frac{i\varepsilon_n[\Delta_1(\varepsilon_n)+\Delta_2(\varepsilon_n)+4ih_0\varepsilon_n]}{\Delta_1(\varepsilon_n)\Delta_2(\varepsilon_n)+4h_0^2\varepsilon_n^2}. \tag{C.15}$$

In particular, at $\Gamma_2 = 0$,

$$G(\varepsilon_n) = \frac{1}{2i\varepsilon_n}\left[1-\frac{(i\varepsilon_n-2h_0)^2}{\Delta_1(\varepsilon_n)+4h_0^2}\right]. \tag{C.16}$$

At $h_0 = 0$ the expressions of all impurity GFs simplify:

$$D_{aa}(\varepsilon) = \frac{2i\varepsilon_n}{\Delta_a(\varepsilon_n)}, \qquad D_{12}(\varepsilon_n) = D_{21}(\varepsilon_n) = 0, \tag{C.17}$$

$$G(\varepsilon_n) = \frac{1}{4}[D_{11}(\varepsilon_n)+D_{22}(\varepsilon_n)] = -\frac{i\varepsilon_n}{2}\left[\frac{1}{\Delta_1(\varepsilon_n)}+\frac{1}{\Delta_2(\varepsilon_n)}\right]. \tag{C.18}$$

When both Majorana chains (channels) are identical ($v_1 = v_2 \equiv v,\ m_1 = m_2 \equiv m$) and the hybridization constants also coincide ($\Gamma_1 = \Gamma_2 \equiv \Gamma$), we get:

$$G(\varepsilon_n) = -\frac{i\varepsilon_n}{\Delta(\varepsilon_n)-2ih_0\varepsilon_n} = \frac{i\varepsilon_n}{i\varepsilon_n(i\varepsilon_n+2h_0)-\Gamma(\sqrt{\varepsilon_n^2+m^2}-m)}. \tag{C.19}$$

Under the replacements $2h_0 \to -\varepsilon_d$ $G(\varepsilon_n)$ in (C.19) coincides with the GF of the impurity d-fermion in a slightly non-critical semi-infinite PI chain (see Appendix D).

Appendix D. Relation to Peierls insulator

In this Appendix we consider the two-chain massive Majorana model (36) in the case when all its parameters referring to different chains coincide:

$$\tilde{J}_a = \tilde{J}, \qquad v_a = v, \qquad m_a = m \quad (a = 1, 2).$$

In this case the model acquires an extra O(2)-symmetry related to global rotations of the Majorana vector $\boldsymbol{\xi} = (\xi_1, \xi_2)$. Therefore it is natural to reformulate the problem in terms of a complex Dirac field,

$$\psi_\nu(x) = \frac{\xi_{1\nu}(x) + i\xi_{2\nu}(x)}{\sqrt{2}}, \tag{D.1}$$

$\nu = R, L$ being the fermion chirality index. Passing simultaneously from the pair of boundary Majorana operators (β_1, β_2) to the second quantized operators of the complex d-fermion, $d^\dagger = (\beta_2 + i\beta_1)/2$, we transform the Hamiltonian (36) to a semi-infinite model of a *massive*, U(1)-symmetric resonant-level model:

$$\begin{aligned} H &= \varepsilon_d(d^\dagger d - 1/2) - 2\sqrt{2a_0}\,\tilde{J}\left[d^\dagger \psi_R(0) + \psi_R^\dagger(0) d\right] \\ &\quad + \int_0^L \mathrm{d}x \left[i v_F \left(\psi_L^\dagger(x)\partial_x\psi_L(x) - \psi_R^\dagger(x)\partial_x\psi_R(x)\right) - im\left[\psi_R^\dagger(x)\psi_L(x) - \psi_L^\dagger(x)\psi_R(x)\right]\right]. \end{aligned} \tag{D.2}$$

Here $\varepsilon_d = -2h_0$, and the fermionic field satisfies the boundary condition $\psi_R(0) = -\psi_L(0)$.

It is well-known that the Lorentz-invariant Dirac model (D.2) emerges in the continuum description of a spinless version of a Peierls insulator at half filling (the so-called polyacetylene model) [30,31]. In a broken-symmetry, spontaneously dimerized state the fermionic part of the PI Hamiltonian is a tight-binding model with alternating nearest-neighbor hopping amplitudes:

$$H_{\mathrm{PI}} = -\sum_{n\geq 1} t_{n,n+1}\left(c_n^\dagger c_{n+1} + \text{h.c.}\right), \quad t_{n,n+1} = t - (-1)^n \Delta. \tag{D.3}$$

At $|\Delta| \ll t$ a continuum limit can be taken in (D.3),

$$c_n \to \sqrt{a_0}\left[i^n \psi_R(x) + (-i)^n \psi_L(x)\right], \quad (k_F = \pi/2a_0),$$

yielding the bulk term in (D.2) with $v_F = 2ta_0$ and $m = 2\Delta$. The ground state of the Hamiltonian (D.3) is dimerized. Accordingly, there are two massive phases, $\Delta = \pm\Delta_0$, separated by a gapless metallic state ($\Delta = 0$). The two phases with the same $|\Delta|$ have identical bulk spectra. Their topological difference [21] shows up in the boundary conditions at the edges of a finite chain. Repeating the Kitaev's argument and turning to special cases $\Delta = \pm t$ (with $t > 0$) one finds a topologically degenerate ground state with two boundary zero modes at $\Delta < 0$ and a nondegenerate ground state at $\Delta > 0$. These zero modes are bound states of a massive complex fermion, each state carrying a fractional fermion number (charge) $q_F = 1/2$ [31,32].

The Green's function of the impurity d-fermion for the PI, $G(\varepsilon_n)$, is given in Appendix C, Eq. (C.19). Passing to the retarded GF $\mathcal{G}(\omega + i\delta)$ we can calculate the spectral weight $A_f(\omega)$ of the d-electron states. The result is given by Eqs. (57) and (58).

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