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► **To cite this version:**

Philippe Lecheminant, Edmond Orignac. Magnetization and dimerization profiles of the cut two-leg spin ladder. *Physical Review B*, 2002, 65, pp.174406. <10.1103/PhysRevB.65.174406>. <hal-00007701>

**HAL Id: hal-00007701**

**<https://hal.science/hal-00007701v1>**

Submitted on 26 Jan 2026

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# Magnetization and dimerization profiles of the cut two-leg spin ladder

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The physical properties of the edge states of the cut two-leg spin ladder are investigated by means of the bosonization approach. By carefully treating boundary conditions, we derive the existence of spin-1/2 edge states in the spin ladder with a ferromagnetic rung exchange and for the open spin-1 Heisenberg chain. In contrast, such states are absent in the antiferromagnetic rung coupling case. The approach, based on a mapping onto decoupled semi-infinite off-critical Ising models, allows us to compute several physical quantities of interest. In particular, we determine the magnetization and dimerization profiles of the cut two-leg spin ladder and of the open biquadratic spin-1 chain in the vicinity of the  $SU(2)_2$  WZNW critical point.

PACS numbers: 75.10.Jm 75.30.Hx 75.50.Ee 71.10.Pm

## I. INTRODUCTION

The influence of impurities and imperfections on the behavior of low-dimensional strongly correlated systems has attracted considerable attention in recent years. The introduction of static non-magnetic impurities, like Zn or Li, at the location of the magnetic ions is a sensitive probe of the correlations that develop in these magnetic systems. A particularly striking example is the observation of fractional spin-1/2 edge states in the Haldane gap<sup>1</sup> spin-1 compound NENP cut by non-magnetic impurities.<sup>2</sup> These spin-1/2 degrees of freedom are associated with static staggered moments close to the chain ends which are revealed unambiguously in the NMR profile of the Mg-doped  $Y_2BaNiO_5$ .<sup>3</sup> This effect can be viewed as a local restoration of antiferromagnetism by impurities. In fact, a transition to an antiferromagnetic state induced by the local moments has been observed recently in the Haldane gap compound  $PbNi_2V_2O_8$ .<sup>4</sup> Such a local enhancement of antiferromagnetism induced by non-magnetic impurities is a rather general phenomenon in gapful quasi-one dimensional systems.<sup>5</sup> The spin ladder material  $SrCu_2O_3$  lightly doped with Zn impurities exhibits a Curie-like behavior at low temperature which has been explained by the unpaired free spins in the vicinity of the impurity.<sup>6</sup> Further, it has been shown by NMR measurements that a staggered magnetization is induced along the leg by very small (0.25%) concentrations of impurities.<sup>7,8</sup> At low temperature, the induced moments get frozen, leading to Néel order.<sup>6,8,9</sup> Similar effects have been observed in the ladder compound  $Cu_2(C_5H_{12}N_2)_2Cl_4$  doped with Zn impurities<sup>10</sup> and in the spin-Peierls gap material  $CuGeO_3$ .<sup>11</sup>

A simple explanation of the existence of free spin-1/2 moments at the ends of a broken spin-1 chain can be obtained from the Valence Bond Solid (VBS) model<sup>12</sup> where each  $S=1$  spin is viewed as two  $S=1/2$  spins in the symmetric triplet state. In this model, the singlet ground state of a chain with periodic boundary is described by two valence bonds originating from each site to form singlets with adjacent neighbors. If the chain is broken (i.e. open boundary conditions are considered), unpaired bonds are left at each end of the chain resulting in two free  $S=1/2$  objects at the boundaries and a fourfold ground state degeneracy. This VBS picture provides a good and intuitive description of the ground state of the spin-1 chain. In particular, the exact diagonalization<sup>13</sup> of finite open samples with even number of sites has shown that the ground state is a singlet and the existence of an exponentially low-lying triplet state in the Haldane gap. This leads to a fourfold ground state degeneracy in the thermodynamic limit. Such degeneracy can also be interpreted as the consequence of a spontaneously broken hidden  $Z_2 \times Z_2$  symmetry<sup>14</sup> associated with the formation of the Haldane gap. A string order parameter has been introduced to reveal this hidden symmetry.<sup>15,16</sup> More generally, it is expected within the VBS and non-linear sigma model approaches that the integer spin- $S$  Heisenberg chain has spin- $S/2$  chain-end excitations.<sup>17</sup>

The physical properties of the  $S=1/2$  chain-boundary excitations in the open spin-1 chain have been investigated in details in a quantum Monte Carlo (QMC) study<sup>18</sup> and by means of the density-matrix renormalization group (DMRG) approach.<sup>19,20,21,22,23</sup> Recently, the magnetization profiles at finite temperatures and fields have been determined using continuous time QMC techniques to reconstruct the experimentally measured NMR spectrum of the Mg-doped  $Y_2BaNiO_5$ .<sup>24</sup> The properties of the edge states of a more general model, the bilinear biquadratic spin-1 Heisenberg

chain, defined by the Hamiltonian:

$$\mathcal{H} = J \sum_i [\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \beta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \quad (1)$$

have also been considered.<sup>25</sup> For  $\beta = 1/3$ , (the so-called AKLT point) the VBS state turns out to be the exact ground state of the bilinear-biquadratic model.<sup>12</sup> For  $\beta = -1$ , the Hamiltonian (1) has a critical point separating the Haldane phase ( $-1 < \beta < 1$ ) from a dimerized phase ( $\beta < -1$ ). At this ( $\beta = -1$ ) critical point, the model is integrable<sup>26</sup> and belongs to the  $SU(2)_2$  Wess-Zumino-Novikov-Witten (WZNW) universality class.<sup>27</sup> The authors of Ref. 25 have established that the edge states are present through the whole Haldane phase and disappear as soon as the  $\beta = -1$  critical point is reached.

In this paper, we shall investigate the physical properties of the  $S=1/2$  chain-end excitations of the semi-infinite (or cut) two-leg spin ladder and of the open spin-1 chain by means of the bosonization method.<sup>28</sup> In the strong ferromagnetic rung limit, this two-leg ladder model is equivalent to the open spin-1 Heisenberg chain with the two spins on the rung forming an effective  $S=1$  local moment. Since this strong coupling limit is smoothly connected to the weak coupling one,<sup>29,30,31</sup> the approach provides a simple way to extract the low-energy properties of the open spin-1 chain. In this respect, it gives an alternative derivation of the existence of the spin-1/2 edge states predicted by the VBS theory<sup>12</sup> and the Schwinger-boson mean-field analysis.<sup>17</sup> Furthermore, we shall be able to calculate explicitly the physical properties of the open spin-1 chain such as the magnetization profile or the NMR relaxation rate. To this end, the mapping<sup>32</sup> of the low-energy Hamiltonian of a weakly coupled two-leg ladder onto off-critical two-dimensional Ising models will be exploited to derive the chain-boundary excitations as it has been done in the study of disordered spin-1/2 ladders.<sup>33</sup> By paying a careful attention on the boundary conditions on the fields that occur in the continuum limit, the staggered magnetization profiles of the model can be determined using exact results of semi-infinite one-dimensional quantum Ising model. The results strongly depend on the sign of the interchain coupling and for an antiferromagnetic rung exchange, no magnetic chain-end excitations are found. However, a weak dimerization, induced by the presence of the boundary,<sup>17,21,34</sup> exists for all signs of the interchain interaction and can be computed by this mapping onto semi-infinite Ising models. Finally, the influence of a strong external magnetic field fixing the spins at the edge can be investigated by a similar approach.

The rest of the paper is organized as follows. In Section II, the low-energy Hamiltonian of the cut two-leg spin ladder is mapped onto an  $O(3) \times Z_2$  symmetric theory of four massive Majorana fermions with suitable boundary conditions. The nature of the edge states that occur in the problem is then discussed in Section III where the uniform magnetization profile and the NMR relaxation rate are computed for a ferromagnetic interchain interaction. Section IV presents the calculation of the staggered magnetization and dimerization profiles of the model by exploiting the mapping onto semi-infinite off-critical quantum Ising models. The effect of a strong applied magnetic field fixing the spins at the boundary is investigated in Section V. Finally, our concluding remarks are presented in Section VI and the paper is supplied with four Appendices which provide some technical details used in this work.

## II. DERIVATION OF THE EFFECTIVE LOW-ENERGY HAMILTONIAN

In this section, we apply the bosonization approach to the semi-infinite two-leg spin ladder described by the Hamiltonian

$$\mathcal{H} = \sum_{n=0}^{\infty} \left[ J_{\parallel} \sum_{p=1,2} \mathbf{S}_{n,p} \cdot \mathbf{S}_{n+1,p} + J_{\perp} \mathbf{S}_{n,1} \cdot \mathbf{S}_{n,2} \right], \quad (2)$$

where  $\mathbf{S}_{n,p}$  is a spin-1/2 operator at site  $n$  on chain  $p$  ( $p = 1, 2$ ) and we consider an antiferromagnetic inchain interaction  $J_{\parallel} > 0$ . The bosonization method will be applied to the Hamiltonian (2) in the regime  $|J_{\perp}| \ll J_{\parallel}$  and with a suitable redefinition of the effective coupling constants it captures the physical properties of the model for arbitrary  $J_{\perp}$  since there is a continuity between the weak and strong coupling limits in the two-leg spin ladder.<sup>29,30,31</sup> In particular, local  $S=1$  spins are formed in each rung of the ladder in the strong ferromagnetic interchain coupling limit ( $J_{\perp} < 0$ ) so that the approach provides, in turn, a way to investigate the physical properties of the broken spin-1 Heisenberg chain.

### A. Bosonization of the open two-leg spin ladder

Let us first consider the decoupling limit ( $J_{\perp} = 0$ ) where the system reduces to two independent spin-1/2 Heisenberg chains with open boundary conditions. The low-energy properties of the latter model can be still determined by

means of the bosonization method.<sup>35,36,37,38,39,40</sup> As it is described in the Appendix A, starting from the underlying Hubbard model, the bosonized Hamiltonian for the open spin-1/2 Heisenberg chain with index  $p = 1, 2$  reads as follows neglecting the marginally irrelevant term:

$$\mathcal{H}_p^0 = \frac{v}{2\pi} \int_0^\infty dx [(\pi\Pi_p)^2 + (\partial_x \Phi_p)^2], \quad (3)$$

where  $v$  is the spin velocity and  $\Pi_p$  is the momentum operator conjugate to the bosonic field  $\Phi_p$ . The boundary condition on the fields  $\Phi_p$  reads

$$\Phi_p(0) = 0, \quad (4)$$

which corresponds to a Dirichlet boundary condition. In the continuum limit, the effective spin density  $\mathbf{S}_p(x)$  separates into an uniform and staggered parts:

$$\mathbf{S}_p(x) = \mathbf{J}_{pR}(x) + \mathbf{J}_{pL}(x) + (-1)^{x/a} \mathbf{n}_p(x), \quad (5)$$

$a$  being the lattice spacing. As shown in the Appendix A, the bosonized description for the uniform spin density is given by

$$\begin{aligned} J_{pR,L}^z &= -\frac{1}{2\pi\sqrt{2}} \partial_x \Phi_{pR,L} \\ J_{pR}^\dagger &= \frac{e^{i\sqrt{2}\Phi_{pR}}}{2\pi a} \\ J_{pL}^\dagger &= \frac{e^{-i\sqrt{2}\Phi_{pL}}}{2\pi a}, \end{aligned} \quad (6)$$

$\Phi_{pR,L}$  being the chiral components of the bosonic field  $\Phi_p$ :  $\Phi_p = (\Phi_{pR} + \Phi_{pL})/2$ . The staggered part of the spin density (5) can be expressed in terms of  $\Phi_p$  and its dual field  $\Theta_p$ :

$$\mathbf{n}_p = \frac{\lambda}{\pi a} \left[ \cos(\sqrt{2}\Theta_p), -\sin(\sqrt{2}\Theta_p), -\sin(\sqrt{2}\Phi_p) \right], \quad (7)$$

where  $\lambda$  is a constant stemming from the underlying charge degrees of freedom that have been integrated out.

In the weak coupling regime  $|J_\perp| \ll J_\parallel$ , the continuum limit of the Hamiltonian (2) can then be derived using all these results. To this end, we introduce the symmetric and antisymmetric combinations of the bosonic fields:

$$\Phi_{\pm R,L} = \frac{\Phi_{1R,L} \pm \Phi_{2R,L}}{\sqrt{2}}, \quad (8)$$

so that the leading part of the Hamiltonian (2) that imposes the strong coupling behavior of the system decomposes into two commuting parts  $\mathcal{H}_\pm$ :<sup>32,41</sup>

$$\mathcal{H} \simeq \mathcal{H}_+ + \mathcal{H}_- \quad [\mathcal{H}_+, \mathcal{H}_-] = 0, \quad (9)$$

with the following bosonized expressions

$$\begin{aligned} \mathcal{H}_+ &= \frac{v}{2\pi} \int_0^\infty dx [(\pi\Pi_+)^2 + (\partial_x \Phi_+)^2] - \frac{J_\perp \lambda^2}{2\pi^2 a} \int_0^\infty dx \cos 2\Phi_+ \\ \mathcal{H}_- &= \frac{v}{2\pi} \int_0^\infty dx [(\pi\Pi_-)^2 + (\partial_x \Phi_-)^2] + \frac{J_\perp \lambda^2}{2\pi^2 a} \int_0^\infty dx \cos 2\Phi_- + \frac{J_\perp \lambda^2}{\pi^2 a} \int_0^\infty dx \cos 2\Theta_-, \end{aligned} \quad (10)$$

where the boundary conditions on the bosonic fields are of Dirichlet type:

$$\Phi_\pm(0) = 0. \quad (11)$$

In this derivation of the low-energy theory, one should note that we have only taken into account the most relevant perturbation that appears in the continuum limit of the spin ladder. In particular, we have discarded the marginal contribution that stems from the uniform pieces of the spin densities (5). We shall later comment on its main effect when the Hamiltonian (9) will be refermionized.

## B. Refermionization

The next step of the approach is to observe that the scaling dimension of the interacting part in  $\mathcal{H}_\pm$  is equal to one. The bosonic fields are precisely at the free-fermion point where the cosine terms in Eq. (10) can be expressed in terms of massive fermions.<sup>32</sup> To this end, we first introduce the left and right bosonic fields corresponding to  $\Phi_\pm$ :

$$\begin{aligned}\Phi_\pm &= \frac{1}{2}(\Phi_{\pm L} + \Phi_{\pm R}) \\ \Theta_\pm &= \frac{1}{2}(\Phi_{\pm L} - \Phi_{\pm R}).\end{aligned}\quad (12)$$

These chiral fields are no longer independent due to the existence of the boundary condition (11) and one has:

$$\Phi_{\pm R}(0) = -\Phi_{\pm L}(0). \quad (13)$$

The refermionization of the Hamiltonian (10) can then be obtained through the bosonization formula

$$\begin{aligned}\psi_{\pm R} &= \frac{\kappa_\pm e^{-i\Phi_{\pm R}}}{\sqrt{2\pi a}} \\ \psi_{\pm L} &= \frac{\kappa_\pm e^{i\Phi_{\pm L}}}{\sqrt{2\pi a}},\end{aligned}\quad (14)$$

where  $\kappa_\pm$  are Klein factors that obey the anticommutation relation  $\{\kappa_+, \kappa_-\} = 0$  to ensure the anticommutation between the fermion fields with different channel index  $\pm$ . The anticommutation between  $\psi_{\pm R}$  and  $\psi_{\pm L}$  results from  $[\Phi_{\pm R}(x), \Phi_{\pm L}(y)] = -i\pi$  which stems from the Dirichlet boundary condition (11) as described in the Appendix A. The boundary conditions on the fermionic fields can be deduced from Eq. (13)

$$\psi_{\pm R}(0) = \psi_{\pm L}(0). \quad (15)$$

The cosine terms of Eq. (10) can then be refermionized using the identification (14) as well as the commutation relation  $[\Phi_{\pm R}(x), \Phi_{\pm L}(x)] = -i\pi, x > 0$ :

$$\begin{aligned}\cos 2\Phi_\pm &= -i\pi a \left( \psi_{\pm R}^\dagger \psi_{\pm L} - \psi_{\pm L}^\dagger \psi_{\pm R} \right) \\ \cos 2\Theta_\pm &= i\pi a \left( \psi_{\pm R}^\dagger \psi_{\pm L}^\dagger - \psi_{\pm L} \psi_{\pm R} \right).\end{aligned}\quad (16)$$

The Hamiltonians  $\mathcal{H}_\pm$  of Eq. (10) can thus be expressed in terms of the fermion fields

$$\begin{aligned}\mathcal{H}_+ &= -iv \int_0^\infty dx \left( \psi_{+R}^\dagger \partial_x \psi_{+R} - \psi_{+L}^\dagger \partial_x \psi_{+L} \right) + \frac{iJ_\perp \lambda^2}{2\pi} \int_0^\infty dx \left( \psi_{+R}^\dagger \psi_{+L} - \psi_{+L}^\dagger \psi_{+R} \right) \\ \mathcal{H}_- &= -iv \int_0^\infty dx \left( \psi_{-R}^\dagger \partial_x \psi_{-R} - \psi_{-L}^\dagger \partial_x \psi_{-L} \right) - \frac{iJ_\perp \lambda^2}{2\pi} \int_0^\infty dx \left( \psi_{-R}^\dagger \psi_{-L} - \psi_{-L}^\dagger \psi_{-R} \right) \\ &\quad + \frac{iJ_\perp \lambda^2}{\pi} \int_0^\infty dx \left( \psi_{-R}^\dagger \psi_{-L}^\dagger - \psi_{-L} \psi_{-R} \right),\end{aligned}\quad (17)$$

with the boundary conditions (15) for the fermion fields.

At this point, it is convenient to introduce four Majorana (real) fermions from the Dirac ones (14)

$$\begin{aligned}\psi_{+R,L} &= \frac{\xi_{R,L}^2 + i\xi_{R,L}^1}{\sqrt{2}} \\ \psi_{-R,L} &= \frac{\xi_{R,L}^3 + i\xi_{R,L}^0}{\sqrt{2}}.\end{aligned}\quad (18)$$

This identification together with the correspondences (6,14) enable us to derive the refermionization of the uniform part of the spin densities (5)

$$\begin{aligned}I_{R,L}^a &= J_{1R,L}^a + J_{2R,L}^a = -\frac{i}{2} \epsilon^{abc} \xi_{R,L}^b \xi_{R,L}^c \\ K_{R,L}^a &= J_{1R,L}^a - J_{2R,L}^a = i \xi_{R,L}^a \xi_{R,L}^0,\end{aligned}\quad (19)$$

where we have fixed the product  $\kappa_+\kappa_-$  of the Klein factors that appear in Eq. (14) to  $i$  to obtain Eq. (19). In fact, this identification (19) is nothing but the faithful representation of two independent  $SU(2)_1$  Kac-Moody currents  $\mathbf{J}_{pR,L}$ ,  $p = 1, 2$  in terms of four Majorana fermions.<sup>28,42,43</sup>

With the above results, the Hamiltonian (9) can be rewritten with the four Majorana fermions and be separated into two commuting (triplet and singlet) pieces

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_s, \quad (20)$$

with

$$\begin{aligned} \mathcal{H}_t &= -\frac{iv}{2} \int_0^\infty dx \sum_{a=1}^3 (\xi_R^a \partial_x \xi_R^a - \xi_L^a \partial_x \xi_L^a) + \frac{iJ_\perp \lambda^2}{2\pi} \int_0^\infty dx \sum_{a=1}^3 \xi_R^a \xi_L^a \\ \mathcal{H}_s &= -\frac{iv}{2} \int_0^\infty dx (\xi_R^0 \partial_x \xi_R^0 - \xi_L^0 \partial_x \xi_L^0) - \frac{3iJ_\perp \lambda^2}{2\pi} \int_0^\infty dx \xi_R^0 \xi_L^0. \end{aligned} \quad (21)$$

The boundary conditions on the Majorana fermions are obtained from the constraint (15) and the definition (18)

$$\xi_R^a(0) = \xi_L^a(0), \quad a = 0, \dots, 3. \quad (22)$$

Moreover, the marginal interchain perturbation that we have so far neglected can be expressed in terms of the Majorana fermions using the correspondence (19). As shown in Ref. 32, the resulting contribution leads to a velocity anisotropy and a mass-renormalization in the singlet and triplet sectors so that the low-energy Hamiltonian (20) takes now the following form

$$\begin{aligned} \mathcal{H}_t &= -\frac{iv_t}{2} \int_0^\infty dx \sum_{a=1}^3 (\xi_R^a \partial_x \xi_R^a - \xi_L^a \partial_x \xi_L^a) - im_t \int_0^\infty dx \sum_{a=1}^3 \xi_R^a \xi_L^a \\ \mathcal{H}_s &= -\frac{iv_s}{2} \int_0^\infty dx (\xi_R^0 \partial_x \xi_R^0 - \xi_L^0 \partial_x \xi_L^0) - im_s \int_0^\infty dx \xi_R^0 \xi_L^0, \end{aligned} \quad (23)$$

where  $m_t > 0$  and  $m_s < 0$  (respectively  $m_t < 0$  and  $m_s > 0$ ) for a ferromagnetic (respectively antiferromagnetic) interchain coupling and in particular in the weak coupling case  $|J_\perp| \ll J_\parallel$  one has the identification from Eq. (21):  $m_t = -J_\perp \lambda^2 / 2\pi$  and  $m_s = 3J_\perp \lambda^2 / 2\pi$ .

We thus observe that in the low-energy limit the initial Hamiltonian (2) of the cut two-leg spin ladder is mapped onto a model of four free massive Majorana fermions with the boundary conditions (22). In the strong ferromagnetic rung limit  $-J_\perp \gg J_\parallel$ , the singlet excitation described by the Majorana fermion  $\xi_{R,L}^0$  are frozen ( $|m_s| \rightarrow \infty$ ) so that the low-energy properties of the model are governed by the triplet magnetic excitations corresponding to the fields  $\xi_{R,L}^a$ ,  $a = 1, 2, 3$ . In this strong ferromagnetic rung limit, we expect the system to be equivalent to a broken spin-1 chain. Indeed, it was shown by Tsvetik<sup>44</sup> by perturbing around the  $SU(2)_2$  WZNW critical point<sup>26</sup> of the biquadratic spin-1 chain, which is described by three massless Majorana fermions, that the low-energy properties of a gapped spin-1 chain could be obtained from a triplet of massive Majorana fermions. Furthermore, it can be seen easily that the boundary conditions (22) imply that the  $SU(2)_2$  currents obey  $I_R^a(0) = I_L^a(0)$  which means that there is no spin current flowing across the boundary. Therefore, an open biquadratic spin-1 chain is described by a triplet of massive Majorana fermions:

$$\mathcal{H}_t = -\frac{iv_t}{2} \int_0^\infty dx \sum_{a=1}^3 (\xi_R^a \partial_x \xi_R^a - \xi_L^a \partial_x \xi_L^a) - im_t \int_0^\infty dx \sum_{a=1}^3 \xi_R^a \xi_L^a, \quad (24)$$

with the boundary conditions (22) and the Haldane (respectively dimerized) phase is characterized by a positive (respectively negative) triplet mass  $m_t$ .

### III. S=1/2 CHAIN-BOUNDARY EXCITATIONS

In this section, the nature of the edge states of the cut two-leg spin ladder and open spin-1 chain are investigated using the low-energy description (23) of the model in terms of four Majorana fermions with boundary conditions. In particular, physical quantities such as the uniform component of the magnetization profile and the NMR relaxation rate will be computed within this approach. The calculation of the staggered magnetization near the edge will be presented in the next section since it involves quantities that are nonlocal in terms of the Majorana fermions.

### A. Localized Majorana fermion state

The special structure of the low-energy Hamiltonian (23) together with the constraint (22) lead us to consider a single massive Majorana fermion Hamiltonian of the form

$$\mathcal{H}_{\text{toy}} = \frac{1}{2} \int_0^\infty dx \Psi(x)^T (-iv\sigma_3\partial_x + m\sigma_2) \Psi(x), \quad (25)$$

where  $\sigma_i$  are the usual Pauli matrices and  $\Psi(x)$  is a Majorana 2-spinor that writes

$$\Psi(x) = \begin{pmatrix} \xi_R(x) \\ \xi_L(x) \end{pmatrix}, \quad (26)$$

with boundary condition  $\xi_R(0) = \xi_L(0)$ . The Hamiltonian (25) is exactly-solvable being quadratic in terms of the fermions and the resulting eigenvectors read as follows in the Heisenberg representation

$$\Psi(x, t) = \frac{1}{\sqrt{2L}} \sum_{k>0} \left\{ \xi_k \begin{pmatrix} \cos(kx + \theta_k) + i \sin(kx) \\ \cos(kx + \theta_k) - i \sin(kx) \end{pmatrix} e^{-i\epsilon_k t} + H.c. \right\} + \sqrt{\frac{m}{v}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-mx/v} \theta(m) \eta, \quad (27)$$

where  $\xi_k$  is a fermion annihilation operator with  $k = \pi n/L$ ,  $\eta$  is a zero mode Majorana fermion, and  $\theta$  is the Heaviside step function. In Eq. (27),  $\epsilon_k$  denotes the energy dispersion of the model:

$$\epsilon_k = \sqrt{v^2 k^2 + m^2}, \quad (28)$$

and  $\theta_k$  is given by

$$\begin{aligned} \cos \theta_k &= \frac{vk}{\epsilon_k} \\ \sin \theta_k &= \frac{m}{\epsilon_k}. \end{aligned} \quad (29)$$

For a positive mass  $m$ , one observes from the decomposition (27) the existence of an exponentially localized state with zero energy inside the gap. Such localized Majorana fermionic states have already been discussed in several different contexts such as the holon edge state in an attractive one-dimensional electron gas,<sup>37,45</sup> the random mass Majorana fermion model,<sup>33,46,47</sup> and the problem of a magnetic impurity in a superconductor.<sup>48,49</sup> Finally it has been pointed out recently that such bound states may find applications in quantum computation.<sup>50,51</sup>

From this analysis of the toy model (25), we deduce the decomposition of the triplet and singlet Majorana fields in the basis of the eigenvectors of the Hamiltonian (23) subject to the boundary conditions (22). For  $J_\perp < 0$  i.e.  $m_t > 0$  and  $m_s < 0$ , one obtains for the triplet sector  $a = 1, 2, 3$  with obvious notations

$$\begin{pmatrix} \xi_R^a \\ \xi_L^a \end{pmatrix}(x, t) = \frac{1}{\sqrt{2L}} \sum_{k>0} \left\{ \xi_k^a \begin{pmatrix} \cos(kx + \theta_k^a) + i \sin(kx) \\ \cos(kx + \theta_k^a) - i \sin(kx) \end{pmatrix} e^{-i\epsilon_k^a t} + H.c. \right\} + \sqrt{\frac{m_t}{v_t}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-m_t x/v_t} \eta^a, \quad (30)$$

whereas the decomposition for the singlet excitations with  $m_s < 0$  reads

$$\begin{pmatrix} \xi_R^0 \\ \xi_L^0 \end{pmatrix}(x, t) = \frac{1}{\sqrt{2L}} \sum_{k>0} \left\{ \xi_k^0 \begin{pmatrix} \cos(kx + \theta_k^s) + i \sin(kx) \\ \cos(kx + \theta_k^s) - i \sin(kx) \end{pmatrix} e^{-i\epsilon_k^s t} + H.c. \right\}. \quad (31)$$

Therefore, the localized Majorana zero mode state only appears in the triplet sector for a ferromagnetic interchain interaction. The translation of these results to the context of the spin-1 chain is straightforward: we just need to consider only the triplet sector. We find that in the Haldane gap phase ( $m_t > 0$ ) we have localized Majorana fermion modes at the edge, but, in contrast, the dimerized phase ( $m_t < 0$ ) is characterized by the absence of such degrees of freedom. In Ref. 33, it was shown that local zero modes were associated with kinks and antikinks of the mass  $m(x)$ . In the present problem, with a semi-infinite system, the edge can be seen as a mass kink  $m\theta(x)$  and local zero modes should thus be induced irrespective of the sign of  $m$ . However, with the semi-infinite chain, the boundary condition (22) selects only one chiral component. The sign of the mass then determines whether the local mode belongs to the physical chiral component. This is the reason for the difference of physical behavior between positive and negative mass<sup>52</sup>.

## B. The uniform component of the magnetization profile

With all these results, the physical properties of the edge states of the open spin-1 chain can be investigated. We first analyse the smooth part of the magnetization profile of the system. To this end, we consider the uniform part  $\mathbf{M}(x)$  of the total spin density ( $\mathbf{S}_+(x) = \mathbf{S}_1(x) + \mathbf{S}_2(x)$ ) which takes the following form in the continuum limit using Eq. (5):

$$\mathbf{M}(x) = \sum_{a=1}^2 (\mathbf{J}_{aR}(x) + \mathbf{J}_{aL}(x)). \quad (32)$$

With the help of the identification (19), we immediately find that the field  $\mathbf{M}(x)$  is expressed locally in terms of the Majorana fermions that account for the triplet excitations in the system:

$$M^a(x) = -\frac{i}{2} \epsilon^{abc} \xi_R^b(x) \xi_R^c(x) - \frac{i}{2} \epsilon^{abc} \xi_L^b(x) \xi_L^c(x). \quad (33)$$

Using the decomposition (30), we write the uniform density  $\mathbf{M}(x)$  in the basis of the eigenvectors of the Hamiltonian  $\mathcal{H}_t$  (23)

$$\begin{aligned} M^a(x) &= -i\epsilon^{abc} \eta^b \eta^c \frac{m_t}{v_t} e^{-2m_t x/v_t} - \sqrt{\frac{2m_t}{v_t L}} e^{-m_t x/v_t} \sum_{k>0} \epsilon^{abc} \cos(kx + \theta_k^t) (i\xi_k^b \eta^c + H.c.) \\ &\quad - \frac{\epsilon^{abc}}{2L} \sum_{k,q>0} (A(k, q, x) i\xi_k^b \xi_q^{c\dagger} + B(k, q, x) i\xi_k^b \xi_q^c + H.c.), \end{aligned} \quad (34)$$

with

$$\begin{aligned} A(k, q, x) &= \cos(kx + \theta_k^t) \cos(qx + \theta_q^t) + \sin(kx) \sin(qx) \\ B(k, q, x) &= \cos(kx + \theta_k^t) \cos(qx + \theta_q^t) - \sin(kx) \sin(qx). \end{aligned} \quad (35)$$

The total uniform magnetization  $\mathbf{S}_0$  is defined by

$$\mathbf{S}_0 = \int_0^\infty dx \mathbf{M}(x), \quad (36)$$

so that we obtain

$$S_0^a = -\frac{i}{2} \epsilon^{abc} \eta^b \eta^c - 2i\epsilon^{abc} \sum_{k>0} \xi_k^b \xi_k^{c\dagger}. \quad (37)$$

The first term in this equation describes a spin-1/2 moment since it corresponds to the Majorana representation of a spin-1/2 operator.<sup>53</sup> In particular, the result (37) implies that the electron-spin-resonance (ESR) response of the cut two-leg spin ladder with a ferromagnetic interchain coupling decomposes into the bulk response and the response at a chain end. The latter one is identical to the ESR response of an isolated spin-1/2 impurity. Since there is a continuity between the weak and strong coupling limits in this system,<sup>29,30,31</sup> the Majorana approach provides thus an alternative description of the chain-end S=1/2 mode of the open spin-1 Heisenberg chain that has been obtained within the Schwinger bosons formalism.<sup>17</sup>

The uniform part of the magnetization profile of the model can be also read from the decomposition (34). For completeness, we give in the Appendix B an alternative derivation of the z-component of the uniform magnetization profile of the cut two-leg spin ladder without using the Majorana fermions method. We obtain the following result using Eq. (34)

$$\langle M^a(x) \rangle = \frac{2m_t}{v_t} e^{-2m_t x/v_t} \langle -\frac{i}{2} \epsilon^{abc} \eta^b \eta^c \rangle, \quad (38)$$

which can be interpreted as a spin-1/2 chain-boundary excitation localized over a length  $v_t/2m_t$  with an amplitude  $2m_t/v_t$ . This implies that the size of the spin-1/2 edge state diverges while its amplitude vanishes as the  $SU(2)_2$  WZNW critical point of the S=1 biquadratic chain is approached from the Haldane phase, in full agreement with the DMRG analysis of Ref. 25. The Majorana fermion description also implies that the uniform component of the

magnetization profile should not be affected by temperature in the absence of an applied magnetic field. Let us finally mention that if the triplet mass  $m_t$  is negative then the S=1/2 chain-boundary excitations disappear as it can be easily seen from the decomposition (27). We thus conclude that these free S=1/2 end spins are absent in a ladder with an antiferromagnetic interchain exchange  $J_\perp > 0$  as well as in the dimerized phase of the spin-1 biquadratic chain. It is worth noting that the absence of free spin-1/2 moments in the spontaneously dimerized phase of a frustrated spin chain has been shown very recently.<sup>54</sup>

### C. Calculation of the NMR relaxation rate

The NMR relaxation rate  $1/T_1$  of the cut two-leg spin ladder with a ferromagnetic interchain interaction can be computed by means of the Majorana approach described in the previous sections. For the standard two-leg spin ladder, it has been theoretically investigated in Refs. 55,56,57. We shall only consider here the uniform part of the NMR relaxation rate and restrict for simplicity to the contribution that identifies to the  $1/T_1$  of the spin-1 Heisenberg chain in the limit of strong ferromagnetic interchain coupling  $-J_\perp \gg J_\parallel$ .

The general formula giving this NMR relaxation rate reads as follows<sup>55</sup>

$$\frac{1}{T_1(x)} = \frac{T}{\omega} \text{Im} \chi(x, \omega), \quad (39)$$

where  $\omega$  is the nuclear resonance frequency which is the smallest energy scale of the problem:  $\omega \ll T, m_t$ . We introduce the following susceptibility to perform the calculation of the NMR rate  $1/T_1$ :

$$\chi(x, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \mathbf{M}(x, \tau) \cdot \mathbf{M}(x, 0) \rangle, \quad (40)$$

with the analytical continuation  $\chi(x, \omega) = \chi(x, i\omega_n)|_{i\omega_n \rightarrow \omega + i0}$ . Using the decomposition (34) in the basis of the eigenvectors of the Hamiltonian  $\mathcal{H}_t$  (23) that describes the triplet degrees of freedom, the NMR relaxation rate can be expressed as

$$\frac{1}{T_1(x)} = \frac{6T\pi}{\omega L^2} \sum_{k, q > 0} A^2(k, q, x) (n_F(\epsilon_k^t) - n_F(\epsilon_q^t)) \delta(\omega + \epsilon_k^t - \epsilon_q^t), \quad (41)$$

$n_F(\epsilon)$  being the Fermi distribution function. The sum in Eq. (41) can be replaced by an integral through the substitution  $\sum_{k > 0} \rightarrow L \int_0^\infty dk / \pi$  and the NMR relaxation rate simplifies, in the low-temperature limit  $T \ll m_t$ , as

$$\frac{1}{T_1(x)} = \frac{6}{\pi v_t^2} \int_0^\infty dk e^{-\epsilon_k^t/T} \frac{\epsilon_k^t}{\sqrt{k^2 + \frac{2m_t \omega}{v_t^2}}} [\cos^2(kx + \theta_k^t) + \sin^2(kx)], \quad (42)$$

where the frequency  $\omega$  insures the convergence of the integral at  $k = 0$ . Using the energy dispersion (28) of massive Majorana fermions and the identification (29), one finally obtains the expression

$$\begin{aligned} \frac{1}{T_1(x)} = & \frac{6}{\pi v_t^2} \int_0^\infty dk e^{-\epsilon_k^t/T} \frac{\epsilon_k^t}{\sqrt{k^2 + \frac{2m_t \omega}{v_t^2}}} \left[ \frac{(v_t k)^4}{\left((v_t k)^2 + m_t^2\right)^2} - \frac{2m_t v_t k}{m_t^2 + (v_t k)^2} \sin(2kx) \right. \\ & \left. + \frac{m_t^3 v_t k}{\left((v_t k)^2 + m_t^2\right)^2} \sin(4kx) + \frac{2m_t^2}{(v_t k)^2 + m_t^2} (1 - \cos(2kx)) + \frac{m_t^2 \left((v_t k)^2 - m_t^2\right)}{2 \left((v_t k)^2 + m_t^2\right)^2} (1 - \cos(4kx)) \right]. \quad (43) \end{aligned}$$

At the extremity of the chain ( $x = 0$ ), the NMR relaxation rate takes a simple form in the low-temperature limit  $T \ll m_t$

$$\frac{1}{T_1(x=0)} = \frac{6m_t}{\pi v_t^2} \left[ \left( \frac{T}{m_t} - 1 \right) e^{-m_t/T} + \frac{m_t}{T} E_1 \left( \frac{m_t}{T} \right) \right] \sim \left( \frac{T}{m_t} \right)^2 e^{-m_t/T}, \quad (44)$$

$E_1(x)$  being the exponential integral function. Therefore, we conclude that the presence of the boundary leads to a narrowing of NMR line at low temperature compared to the bulk system. In principle, this NMR rate can be measured experimentally<sup>58</sup> by measurements of nuclear magnetization recovery.<sup>59</sup>

Now, we turn to the calculation of the  $x$  dependence of  $1/T_1$ . The sine terms that appear in Eq. (43) can be rewritten as

$$I = -\frac{12m_t}{\pi v_t^2} \int_0^\infty d\theta e^{-m_t \cosh \theta/T} \sin\left(\frac{2m_t x}{v_t} \sinh \theta\right) + \frac{6m_t}{\pi v_t^2} \int_0^\infty d\theta \frac{e^{-m_t \cosh \theta/T}}{\cosh^2 \theta} \sin\left(\frac{4m_t x}{v_t} \sinh \theta\right). \quad (45)$$

In the regime  $T \ll m_t$ , this expression can be approximated as

$$I \simeq \frac{3m_t}{\pi v_t^2} e^{-m_t/T} \sqrt{\frac{2T}{m_t}} \left( \varphi\left(\frac{2x}{\xi_T}\right) - 2\varphi\left(\frac{x}{\xi_T}\right) \right), \quad (46)$$

where the function  $\varphi(y)$  is defined by

$$\varphi(y) = \sum_{n=0}^{\infty} (-1)^n \frac{n!}{(2n+1)!} y^{2n+1}, \quad (47)$$

and  $\xi_T$  is a thermal length which writes

$$\xi_T = \frac{v_t}{\sqrt{8m_t T}}. \quad (48)$$

This length scale diverges when  $T \rightarrow 0$  and plays the role of an effective coherence length for the NMR relaxation rate. Similarly, the cosine terms of Eq. (43) can be rewritten in the low-temperature limit as

$$J \simeq \frac{3m_t}{\pi v_t^2} e^{-m_t/T} \int_0^\infty d\theta \frac{e^{-m_t \theta^2/2T}}{\sqrt{\theta^2 + \frac{2\omega}{m_t}}} \left[ 3 - 4 \cos\left(\frac{2m_t x \theta}{v_t}\right) + \cos\left(\frac{4m_t x \theta}{v_t}\right) \right]. \quad (49)$$

We note that, for  $x \gg a$  i.e. far from the chain end, the low-temperature behavior of the NMR relaxation reads as follows

$$\frac{1}{T_1(x \gg a)} \simeq \frac{9m_t}{\pi v_t^2} e^{-m_t/T} \int_0^\infty \frac{d\theta}{\sqrt{\theta^2 + \frac{2\omega}{m_t}}} e^{-m_t \theta^2/2T}, \quad (50)$$

which corresponds to the bulk behavior of the NMR relaxation rate of the spin-1 Heisenberg chain found in Ref. 60 where the Haldane gap identifies to the triplet mass  $m_t$ .

#### IV. STAGGERED MAGNETIZATION AND DIMERIZATION PROFILES

The staggered magnetization component of a two-leg spin ladder with a defect has been investigated semiclassically in Ref. 61. Such semiclassical approach has the inconvenient of breaking SU(2) rotational symmetry. Nevertheless, it gives useful qualitative indications on the expected magnetization profile. For the open ladder, the boundary condition on the bosonic fields is  $\Phi_\pm(0) = 0$ . In the bulk, a semiclassical minimization of the ground state energy implies  $\langle \Phi_+ \rangle = 0$  ( $J_\perp > 0$ ) and  $\langle \Phi_+ \rangle = \pi/2$  ( $J_\perp < 0$ ). Thus, we expect no staggered magnetization profile in the case of an antiferromagnetic rung coupling, and a profile with exponential decay far from the boundary in the case of a ferromagnetic rung coupling. In this section, we present an approach that has the advantage over the semiclassical method of preserving the full rotational symmetry. As is well known, the low-energy properties of the two-leg spin ladder can be described using four decoupled off-critical two-dimensional Ising models.<sup>32</sup> In particular, this approach allows the calculation of the leading asymptotics of the staggered part of the spin-spin correlation functions which involve non-local operators in terms of the underlying Majorana fermions. In this section, we shall exploit the existence of a similar mapping for the semi-infinite two-leg spin ladder to determine the staggered component of the magnetization profile and the induced dimerization in the system.

##### A. Staggered magnetization

Let us discuss more precisely this mapping onto an effective Ising model. It is well known that a 1D theory of massive Majorana fermions describes the long-distance properties of 1D quantum Ising model.<sup>62,63,64,65</sup> For a recent

detailed review on this correspondence, the reader may consult for instance the chapter 12 of the book Ref. 28. In the case of a semi-infinite system, this mapping remains valid and the boundary conditions on the Ising spins depends on the ones for the Majorana fermions.<sup>66</sup> More specifically, we shall follow here the conventions of Ref. 66 so that if the Majorana fermions  $\xi_{R,L}$  obey the boundary condition

$$\xi_R(0) = \xi_L(0), \quad (51)$$

then the Ising model satisfies to a free boundary condition (i.e. the boundary spin is free to fluctuate and takes the values  $\pm 1$ ). On the other hand, the Ising model experiences a fixed boundary condition (i.e. the boundary spin is fixed to the value  $\sigma(0) = 1$  for instance) when the Majorana fields verify

$$\xi_R(0) = -\xi_L(0). \quad (52)$$

The mass  $m$  of these fermions is a linear measurement of the deviation of the temperature with respect to the critical one:  $m = T_c - T$  as in Ref. 66 such that a positive mass corresponds to the low-temperature phase of the Ising model. The low-energy Hamiltonian (23) of the cut two-leg spin ladder with the boundary conditions (22) on the fermions can thus be viewed as four decoupled off-critical 1D quantum Ising models with free boundary conditions. In particular, the localized Majorana fermionic states with zero energy in the triplet sector found for a ferromagnetic interchain coupling ( $J_\perp < 0$ ) in Section III can be interpreted physically, in the Ising mapping, as a domain wall attached to the boundary which separates two domains of opposite magnetization ( $m_t = T_c - T > 0$ ). In the singlet sector, one has in contrast  $m_s < 0$  so that the corresponding Ising model with free boundary conditions is in its disordered phase. As a consequence, the zero-energy Majorana mode cannot exist in that case as it can be seen from the decomposition (31).

The next step of the approach is to use the exact results<sup>66,67,68</sup> known for the semi-infinite Ising model to determine the staggered part of the magnetization profile of the cut two-leg spin ladder. To this end, the staggered magnetization  $\mathbf{n}_+ = \mathbf{n}_1 + \mathbf{n}_2$  of the total spin density  $\mathbf{S}_+ = \mathbf{S}_1 + \mathbf{S}_2$  is expressed in terms of the order and disorder operators  $\sigma_a, \mu_a$  of the different Ising models using the bosonic description (7) and the bosonization approach for two Ising models<sup>63,64,65</sup>

$$\begin{aligned} n_+^x &\sim \mu_1 \sigma_2 \sigma_3 \mu_0 \\ n_+^y &\sim \sigma_1 \mu_2 \sigma_3 \mu_0 \\ n_+^z &\sim \sigma_1 \sigma_2 \mu_3 \mu_0. \end{aligned} \quad (53)$$

At this point, it is worth discussing on the ground state degeneracy of the semi-infinite two-leg spin ladder with a ferromagnetic interchain coupling. As it was first pointed out by Kennedy,<sup>13</sup> an exponentially low-lying triplet, above the singlet ground state, is found in the Haldane gap for a finite open spin-1 Heisenberg chain. In the thermodynamic limit, the ground state is thus fourfold degenerate. At first sight, it seems difficult to reproduce this result starting from three decoupled semi-infinite quantum Ising models. Indeed, in the strong coupling limit  $-J_\perp \gg J_\parallel$ , the singlet degrees of freedom are frozen and the three Ising models for the triplet sector are all in their ordered phases ( $m_t > 0$  for  $J_\perp < 0$ ) so that  $\langle \sigma_i \rangle \neq 0$  ( $i = 1, 2, 3$ ). In that case, each Ising model has a doubly degenerate ground state which gives thus an eightfold degeneracy. However, it is important to note that there is a redundancy in the Ising description since the triplet Hamiltonian in Eq. (23), the boundary conditions on the Majorana fermions (22), the Ising representation of the staggered magnetization (53) are all invariant under the following transformation

$$\begin{aligned} \xi_{R,L}^i &\rightarrow -\xi_{R,L}^i \\ \mu_i &\rightarrow \mu_i \\ \sigma_i &\rightarrow -\sigma_i, \end{aligned} \quad (54)$$

which leads to a physical fourfold ground state degeneracy as it should be. Let us return to the calculation of the magnetization profile for a ferromagnetic interchain coupling  $J_\perp < 0$  where  $m_t > 0$  and  $m_s < 0$ . The identification (53) shows that the average staggered magnetization goes to zero far from the chain end since  $\langle \mu_{1,2,3} \rangle = 0$  in the case of a positive triplet mass. However, due to the presence of the boundary, a staggered magnetization can appear close to the chain end i.e. when  $x = 0$ . The magnetization profile encodes the cross-over effect on the local magnetization as a function of the distance from the boundary. The magnetization profile of the spin-1 chain is obtained from the one of the ladder with ferromagnetic interchain interaction by taking the limit  $|m_s| \rightarrow \infty$  or equivalently  $\mu_0 \rightarrow 1$ .<sup>32,44</sup>

In this respect, let us first present general results by exploiting the duality transformation on 1D quantum Ising model. This transformation exchanges the order and disorder operators  $\sigma \leftrightarrow \mu$  but also the boundary conditions on Ising spins i.e. free boundary conditions become fixed and vice versa. Therefore, one obtains the following equivalences on the different one-point functions of the model

$$\langle \sigma(T > T_c) \rangle_{\text{free}} = \langle \mu(T < T_c) \rangle_{\text{fixed}} = 0$$

$$\begin{aligned}
\langle \sigma(T > T_c)(x) \rangle_{\text{fixed}} &= \langle \mu(T < T_c)(x) \rangle_{\text{free}} = \sigma_\infty F\left(\frac{mx}{v}\right) \\
\langle \sigma(T < T_c)(x) \rangle_{\text{fixed}} &= \langle \mu(T > T_c)(x) \rangle_{\text{free}} = \sigma_\infty G\left(\frac{mx}{v}\right) \\
\langle \sigma(T < T_c)(x) \rangle_{\text{free}} &= \langle \mu(T > T_c)(x) \rangle_{\text{fixed}} = \sigma_\infty H\left(\frac{mx}{v}\right),
\end{aligned} \tag{55}$$

$v$  being the velocity of the underlying Majorana fermion and  $\sigma_\infty$  is the expectation value of  $\sigma$  (respectively  $\mu$ ) for  $T < T_c$  (respectively  $T > T_c$ ). An estimate of  $\sigma_\infty$  valid for  $m \ll v/a$  is  $\sigma_\infty = 2^{1/12} e^{-1/8} A^{3/2} (|m|a/v)^{1/8}$  where  $A$  is the Glaisher constant.<sup>69</sup> It is indeed obvious that one has  $\langle \sigma(T > T_c) \rangle_{\text{free}} = 0$  for an Ising model with  $T > T_c$  and free boundary conditions. In contrast, one should observe that, even in the disordered phase of the model, a non-zero magnetization  $\langle \sigma(T > T_c) \rangle_{\text{fixed}} \neq 0$  exists for fixed boundary conditions since the Ising spins are polarized at the boundary. In that case, the precise cross-over between the boundary and bulk behaviors is described by the function  $F$ . The staggered part of the magnetization profile of the cut two-leg spin ladder with a ferromagnetic interchain coupling can thus be deduced from the correspondence (53) and the general results (55)

$$\begin{aligned}
\langle n_+^x(x) \rangle &\sim \left(\frac{m_t^3 |m_s| a^4}{v_t^3 v_s}\right)^{1/8} F\left(\frac{m_t x}{v_t}\right) H^2\left(\frac{m_t x}{v_t}\right) G\left(\frac{|m_s| x}{v_s}\right) \\
\langle n_+^y(x) \rangle &\sim \left(\frac{m_t^3 |m_s| a^4}{v_t^3 v_s}\right)^{1/8} F\left(\frac{m_t x}{v_t}\right) H^2\left(\frac{m_t x}{v_t}\right) G\left(\frac{|m_s| x}{v_s}\right) \\
\langle n_+^z(x) \rangle &\sim \left(\frac{m_t^3 |m_s| a^4}{v_t^3 v_s}\right)^{1/8} F\left(\frac{m_t x}{v_t}\right) H^2\left(\frac{m_t x}{v_t}\right) G\left(\frac{|m_s| x}{v_s}\right),
\end{aligned} \tag{56}$$

which exhibits a full rotationally invariant form as it should be. Remarkably, a staggered magnetization appears although there is none for an isolated spin-1/2 Heisenberg chain. The expressions of  $G$  and  $H$  are exactly known and have been determined by Bariev<sup>67</sup> from a lattice description and later by Konik et al.<sup>68</sup> in the continuum case by the form factor approach. As it is shown in the Appendix C using this latter formalism, the function  $F$  can, in fact, be directly expressed in terms of  $G$ :

$$F(x) = e^{-x} G(x). \tag{57}$$

As a consequence, the z-component of the staggered magnetization for instance simplifies as

$$\langle n_+^z(x) \rangle \sim \left(\frac{m_t^3 |m_s| a^4}{v_t^3 v_s}\right)^{1/8} e^{-m_t x/v_t} H^2\left(\frac{m_t x}{v_t}\right) G\left(\frac{m_t x}{v_t}\right) G\left(\frac{|m_s| x}{v_s}\right). \tag{58}$$

In the case of the open spin-1 chain, performing the substitution  $\mu_0 \rightarrow 1$  in Eq. (53), we obtain in a similar way the magnetization profile:

$$\langle n_+^z(x) \rangle \sim \left(\frac{m_t a}{v_t}\right)^{3/8} e^{-m_t x/v_t} H^2\left(\frac{m_t x}{v_t}\right) G\left(\frac{m_t x}{v_t}\right). \tag{59}$$

The functions  $G$  and  $H$  that appear in these equations can be cast into a Fredholm determinant form (see for instance the Appendix C) or expressed in terms of a solution to the Painlevé III differential equation.<sup>67,68</sup> Complete expressions for  $G$  and  $H$  can be found in the Appendix D. For the sake of simplicity, we only need here the asymptotic behaviors of these functions which read as follows in the long-distance limit  $X = mx/v \gg 1$ <sup>67,68</sup>

$$\begin{aligned}
G(X) &\simeq 1 + \frac{1}{16\sqrt{\pi}} \frac{e^{-2X}}{X^{3/2}} \\
H(X) &\simeq 1 - \frac{1}{2\sqrt{\pi}} \frac{e^{-2X}}{X^{1/2}},
\end{aligned} \tag{60}$$

whereas in the short-distance limit  $X = mx/v \ll 1$ , one has the following estimates<sup>67,68</sup>

$$\begin{aligned}
G(X) &\sim X^{-1/8} \\
H(X) &\sim X^{3/8}.
\end{aligned} \tag{61}$$

From these results, we deduce the behavior of the staggered component of the magnetization profile far from the chain end:

$$\langle n_+^z(x) \rangle \sim \left( \frac{m_t^3 |m_s| a^4}{v_t^3 v_s} \right)^{1/8} e^{-m_t x / v_t} = \left( \frac{m_t^3 |m_s| a^4}{v_t^3 v_s} \right)^{1/8} e^{-x / \xi_t}, \quad (62)$$

with a similar behavior for the open spin-1 chain. As expected, the local staggered magnetization decays exponentially with the distance from the boundary with a length scale that depends only on the bulk properties and identifies to the correlation length  $\xi_t = v_t / m_t$  of the model. It is worth noting the absence of any  $x$  prefactor in front of the exponential term in Eq. (62) in the long-distance limit  $x \gg \xi_t$ . This suggests that the staggered magnetization for long chains with open boundary conditions is the relevant quantity to extract a very precise value of the Haldane gap as it has been done by means of the DMRG approach.<sup>19</sup> A similar exponential behavior is also obtained in the semiclassical treatment<sup>61</sup> and in a phenomenological theory of the open spin-1 chain describing the system as a spin-1/2 coupled to one-dimensional massive bosons.<sup>20</sup> Comparing to Eq. (38), we notice that the staggered magnetization has a correlation length  $\xi_t$  whereas the uniform magnetization has a correlation length  $\xi_t / 2$ , in agreement with the phenomenological free boson theory.<sup>20</sup> In contrast to the free boson theory, we find no  $x^{-3/2}$  prefactor in the uniform component of the magnetization. In the short distance limit  $x \ll \xi_t$ , one obtains the following power law behavior from Eq. (61) for the two-leg ladder with a ferromagnetic interchain interaction:

$$\langle n_+^z(x) \rangle \sim \frac{m_t}{v_t} (ax)^{1/2}, \quad (63)$$

whereas, in the case of the spin-1 chain, this power law is modified to:

$$\langle n_+^z(x) \rangle \sim \frac{m_t a}{v_t} \left( \frac{x}{a} \right)^{5/8}. \quad (64)$$

We note that the staggered magnetization profile (59) has a vanishing intensity and a diverging correlation length when the Haldane gap goes to zero, in agreement with the DMRG analysis of Ref. 25. Moreover, our calculation predicts that a staggered magnetization will exist at  $T = 0$  in the  $S_{tot}^z = 0$  sector. This has indeed been observed in a DMRG calculation.<sup>23</sup> At first sight, it seems to contradict the results of QMC simulations.<sup>18</sup> However, these calculations are performed at finite temperature. For the one-dimensional quantum Ising model with free boundary conditions, there is no long range order in  $\langle \sigma \rangle$  at  $T > 0$  due to the thermal nucleation of soliton excitations. Hence, we expect that as soon as the temperature is switched on, the average magnetization in  $S_{tot}^z = 0$  state will vanish in agreement with what is observed in QMC calculations.

The magnetization profile, in the antiferromagnetic interchain coupling case, can be investigated by a similar approach. For  $J_\perp > 0$ , one has now  $m_t < 0$  and  $m_s > 0$  so that the Ising models of the triplet sector are in their disordered phases whereas the Ising model of the singlet sector belongs to its ordered phase. We thus obtain using the results (53,55) that  $\langle \mathbf{n}_+ \rangle = \mathbf{0}$  and similarly it can also be shown that  $\langle \mathbf{n}_- \rangle = \langle \mathbf{n}_1 - \mathbf{n}_2 \rangle = \mathbf{0}$ . Therefore, we conclude on the absence of S=1/2 chain-boundary excitations and of a non-zero magnetization profile for the cut two-leg spin ladder with an antiferromagnetic rung coupling. This result is consistent with the fact that the ground state of this model is always unique whether open or periodic boundary conditions are used. In this respect, the standard two-leg spin ladder with  $J_\perp > 0$ , in contrast to the  $J_\perp < 0$  case, is not equivalent to the Haldane phase characterized by these S=1/2 chain-end excitations eventhough they share similar properties like the presence of a spin gap, and a non-zero string order parameter.<sup>31,70</sup> In fact, it has been recently pointed out that the two systems belong to two topologically distinct classes.<sup>16</sup> In particular, it has been argued that the S=1 spin chain and the two-leg spin ladder with  $J_\perp > 0$  have two different types of string order that are intimately related to the valence bond structure of the ground states. The topological distinction is made by counting the number  $Q_y$  of valence bond's crossing an arbitrary vertical line. In the case of an antiferromagnetic spin ladder,  $Q_y$  is always even whereas it is odd for a system weakly connected to the spin-1 chain. Furthermore, the authors of Ref. 16 have noticed that for open boundary conditions ground states characterized by an odd value of  $Q_y$  have spin-1/2 edge states while these end states disappear when  $Q_y$  is even. This is in full agreement with the results for the cut two-leg spin ladder obtained in this work within the bosonization approach.

### B. Dimerization induced by open boundary condition

The dimerization profile induced by the presence of a boundary can be also computed by this mapping onto semi-infinite Ising models. The dimerization operator in terms of the original lattice spins is defined by

$$\epsilon_{+n} = (-1)^n \sum_{p=1}^2 \mathbf{S}_{n,p} \cdot \mathbf{S}_{n+1,p}. \quad (65)$$

The bosonized description of this operator in the continuum limit reads as follows in terms of the bosonic fields  $\Phi_{\pm}$  of Eq. (8)

$$\epsilon_{+} \sim \cos \Phi_{+} \cos \Phi_{-}. \quad (66)$$

Using the bosonization representation of two Ising models,<sup>63,64,65</sup> this operator can then be expressed in terms of the different Ising disorder operators:

$$\epsilon_{+} \sim \mu_1 \mu_2 \mu_3 \mu_0. \quad (67)$$

In the bulk, the system does not experience any dimerization pattern since the Ising models in the triplet sector are in their ordered phases for  $J_{\perp} < 0$  so that  $\langle \mu_i \rangle = 0$  ( $i = 1, 2, 3$ ). However, as for the existence of a local staggered magnetization, the presence of the boundary induces a non-trivial dimerization in the system<sup>17,21,34</sup> which can be obtained from the results (55):

$$\langle \epsilon_{+}(x) \rangle \sim \left( \frac{m_t^3 |m_s| a^4}{v_t^3 v_s} \right)^{1/8} e^{-3m_t x / v_t} G^3 \left( \frac{m_t x}{v_t} \right) G \left( \frac{|m_s| x}{v_s} \right). \quad (68)$$

Using the asymptotics (60, 61), we deduce the following estimates for the local dimerization

$$\begin{aligned} \langle \epsilon_{+}(x) \rangle &\sim \left( \frac{m_t^3 |m_s| a^4}{v_t^3 v_s} \right)^{1/8} e^{-3x/\xi_t}, \quad x \gg \xi_t \\ \langle \epsilon_{+}(x) \rangle &\sim \left( \frac{x}{a} \right)^{-1/2}, \quad x \ll \xi_t. \end{aligned} \quad (69)$$

Note that the exponent 1/2 is identical to the exponent that would have been obtained in two decoupled gapless spin-1/2 chains by boundary conformal field theory.<sup>35</sup> Physically, this means that the edge is making the system behaves as if it was gapless for distances shorter than the correlation length. In the case of the spin-1 chain, the dimerization operator (67) simplifies to  $\epsilon_{+} \sim \mu_1 \mu_2 \mu_3$  ( $\mu_0 \rightarrow 1$ ) so that we get

$$\langle \epsilon_{+}(x) \rangle \sim \left( \frac{m_t a}{v_t} \right)^{3/8} e^{-3m_t x / v_t} G^3 \left( \frac{m_t x}{v_t} \right). \quad (70)$$

The long-distance limit of this dimerization has a similar form as in Eq. (69) and the short distance behavior is modified to  $\langle \epsilon_{+}(x) \rangle \sim x^{-3/8}$ . Again, this exponent could have been predicted from boundary conformal field theory.<sup>71</sup> We also observe that this exponent has been obtained in the DMRG study of biquadratic spin-1 chain at the  $SU(2)_2$  WZNW critical point.<sup>34</sup>

In the antiferromagnetic interchain coupling case, a similar calculation can be made. The dimerization operator (67) has again a zero ground-state expectation value in the bulk since the Ising model in the singlet sector is in its ordered phase ( $m_s > 0$ ). As seen above, the two-leg spin ladder with an antiferromagnetic rung coupling has no magnetic  $S=1/2$  chain-boundary excitations but a localized Majorana state in the singlet sector still remains as it can be deduced from the decomposition (27) with  $m_s > 0$ . This zero mode manifests itself in the existence of a dimerization profile which is given by

$$\langle \epsilon_{+}(x) \rangle \sim \left( \frac{|m_t|^3 m_s a^4}{v_t^3 v_s} \right)^{1/8} e^{-m_s x / v_t} G^3 \left( \frac{|m_t| x}{v_t} \right) G \left( \frac{m_s x}{v_s} \right), \quad (71)$$

with the following asymptotics ( $\xi_s = v_s / m_s$ )

$$\begin{aligned} \langle \epsilon_{+}(x) \rangle &\sim \left( \frac{|m_t|^3 m_s a^4}{v_t^3 v_s} \right)^{1/8} e^{-x/\xi_s}, \quad x \gg \xi_s \\ \langle \epsilon_{+}(x) \rangle &\sim \left( \frac{x}{a} \right)^{-1/2}, \quad x \ll \xi_s. \end{aligned} \quad (72)$$

In the case of the spontaneously dimerized spin-1 chain, the dimerization profile takes the form

$$\langle \epsilon_+ (x) \rangle \sim \left( \frac{|m_t|a}{v_t} \right)^{3/8} G^3 \left( \frac{|m_t|x}{v_t} \right). \quad (73)$$

Its short distance asymptotics becomes thus:  $\langle \epsilon_+ (x) \rangle \sim x^{-3/8}$ , whereas the long distance one reads as follows using Eq. (60)

$$\langle \epsilon_+ (x) \rangle \simeq \epsilon_\infty \left( 1 + \frac{3\xi_t^{3/2}}{16\sqrt{\pi}} \frac{e^{-2x/\xi_t}}{x^{3/2}} \right), \quad (74)$$

$\epsilon_\infty$  being the non-zero bulk dimerization.

## V. EFFECT OF A STRONG EXTERNAL BOUNDARY MAGNETIC FIELD

The effect of a strong applied magnetic field which fixes the spins at the boundary can be investigated using the Ising representation described in the previous section. To this end, let us first recall the effect of a transverse edge magnetic field in the semi-infinite XXZ spin-1/2 Heisenberg chain.<sup>72</sup> It has been found that the system, along the entire XXZ critical line, renormalizes to the infinite field fixed point where the spin at the edge is polarized. In the bosonization language, one has an example of a  $c=1$  boundary flow between the Dirichlet and Neumann boundary conditions. At the SU(2) invariant point, the edge field is exactly marginal and a line of fixed point occurs between the Dirichlet and Neumann limiting cases.<sup>72,73</sup> In the following, we shall only consider the physical situation where the spin at the edge is fully polarized or fixed so that it corresponds to the infinite field fixed point or Neumann boundary condition on the bosonic field  $\Phi_p$  associated to the spin-1/2 chain with index  $p = 1, 2$ :

$$\partial_x \Phi_p (0, t) = 0 \quad \forall t, \quad (75)$$

or equivalently it can be interpreted as a Dirichlet boundary condition on the dual field  $\Theta_p$ :

$$\Theta_p (0, t) = 0 \quad \forall t. \quad (76)$$

The value of the constant in this expression stems from the fact that a magnetic field along the x-axis is considered in the following. The actual direction of the applied field is not important since the model is SU(2) invariant. The chiral fields  $\Phi_{\pm R, L}$ , defined by Eq. (8), are no longer independent due to the boundary condition (76) and satisfy now

$$\Phi_{\pm L} (0) = \Phi_{\pm R} (0), \quad (77)$$

from which we deduce the following analytic continuation ( $x \geq 0$ )

$$\Phi_{\pm L} (x, t) = \Phi_{\pm R} (-x, t). \quad (78)$$

The change of boundary conditions in comparison to the Dirichlet case (13) in zero field has several consequences. First of all, the commutator between the left and right bosonic fields is modified due to the folding condition (78):  $[\Phi_{\pm R}(x), \Phi_{\pm L}(y)] = +i\pi$ . As a consequence, the low-energy Hamiltonian of the model for a ferromagnetic interchain coupling  $J_\perp < 0$  is still given by Eq. (23) but with a negative triplet mass  $m_t = J_\perp \lambda^2 / 2\pi < 0$  and a positive singlet mass  $m_s = -3J_\perp \lambda^2 / 2\pi > 0$ . Moreover, the boundary conditions on the Majorana fermions have also changed in the Neumann case (77). They can be deduced as in Section II from the identifications (14, 18) so that we obtain the following boundary conditions

$$\begin{aligned} \xi_L^1 (0) &= -\xi_R^1 (0) \\ \xi_L^2 (0) &= \xi_R^2 (0) \\ \xi_L^3 (0) &= \xi_R^3 (0) \\ \xi_L^0 (0) &= -\xi_R^0 (0). \end{aligned} \quad (79)$$

One can interpret these results in light of the Ising description presented in the previous section. The Ising models in the triplet sector with index 2, 3 (respectively 1) have free (respectively fixed) boundary conditions and belong to their disordered phases ( $m_t < 0$ ). The Ising model that accounts for the singlet excitations has fixed boundary conditions and is in its ordered phase ( $m_s > 0$ ). The S=1/2 chain-boundary excitations of the open spin-1 chain have

thus disappeared in the presence of a strong applied edge magnetic field. It remains only a single localized Majorana fermionic state  $\xi^1$  with zero energy that describes fluctuations in the  $S^x = 0$  triplet subspace which is unaffected by the applied magnetic field along the x-direction. The Ising representations of the staggered magnetization (53) and the dimerization operator (67) have to be modified slightly due to the change of sign of the commutator between the left and right components of the bosonic fields  $\Phi_{\pm}$  and they are now given by

$$\begin{aligned} n_+^x &\sim \sigma_1 \mu_2 \mu_3 \sigma_0 \\ n_+^y &\sim \mu_1 \sigma_2 \mu_3 \sigma_0 \\ n_+^z &\sim \mu_1 \mu_2 \sigma_3 \sigma_0 \\ \epsilon_+ &\sim \sigma_1 \sigma_2 \sigma_3 \sigma_0. \end{aligned} \quad (80)$$

From these results and the identification (55), we thus deduce the staggered magnetization and dimerization profiles of the two-leg spin ladder with a ferromagnetic interchain coupling in a strong applied magnetic field along the x-axis:

$$\langle n_+^x(x) \rangle \sim e^{-|m_t|x/v_t} G^3 \left( \frac{|m_t|x}{v_t} \right) G \left( \frac{m_s x}{v_s} \right), \quad (81)$$

whereas  $\langle n_+^y \rangle = \langle n_+^z \rangle = \langle \epsilon_+ \rangle = 0$ . The asymptotics of the non-zero staggered magnetization can be extracted from Eqs. (60, 61)

$$\begin{aligned} \langle n_+^x(x) \rangle &\sim e^{-x/\xi_t}, \quad x \gg \xi_t \\ \langle n_+^x(x) \rangle &\sim x^{-1/2}, \quad x \ll \xi_t. \end{aligned} \quad (82)$$

The short distance exponent is identical to the one predicted from boundary conformal field theory in a gapless spin-1/2 chain with a strong magnetic field at the boundary.<sup>72</sup> The same result (82) also holds in the case of the spin-1 chain, albeit with a different short distance behavior  $\langle n_+^x(x) \rangle \sim x^{-3/8}$  which can be obtained from boundary conformal field theory. We conclude that the staggered magnetization in a strong applied field decays in the same way as in Eq. (62) far from the boundary but is enhanced in the vicinity of the chain end in comparison to the behavior (63) in zero field. These results are in agreement with QMC simulations of the spin-1 Heisenberg chain with free and fixed boundary conditions.<sup>18</sup>

A similar calculation can be made in the case of an antiferromagnetic interchain interaction. The only difference is that we must make the following substitution  $T - T_c \rightarrow T_c - T$ . For a strong applied field along the x-direction, we get now

$$\langle n_+^x(x) \rangle \sim e^{-2m_t x/v_t - |m_s|x/v_s} G^3 \left( \frac{m_t x}{v_t} \right) G \left( \frac{|m_s|x}{v_s} \right), \quad (83)$$

and  $\langle n_+^y \rangle = \langle n_+^z \rangle = 0$ . However, there is now a non-zero staggered relative magnetization  $\langle \mathbf{n}_- = \mathbf{n}_1 - \mathbf{n}_2 \rangle$  in the  $J_{\perp} > 0$  case which can be determined using the Ising representation of this operator:

$$\begin{aligned} n_-^x &\sim \mu_1 \sigma_2 \sigma_3 \mu_0 \\ n_-^y &\sim \sigma_1 \mu_2 \sigma_3 \mu_0 \\ n_-^z &\sim \sigma_1 \sigma_2 \mu_3 \mu_0, \end{aligned} \quad (84)$$

so that

$$\langle n_-^{y,z}(x) \rangle \sim e^{-m_t x/v_t} G^2 \left( \frac{m_t x}{v_t} \right) H \left( \frac{m_t x}{v_t} \right) H \left( \frac{|m_s|x}{v_s} \right), \quad (85)$$

and  $\langle n_-^x \rangle = 0$ . Finally, the dimerization profile in the  $J_{\perp} > 0$  case reads as follows

$$\langle \epsilon_+(x) \rangle \sim e^{-|m_s|x/v_s} G \left( \frac{m_t x}{v_t} \right) H^2 \left( \frac{m_t x}{v_t} \right) G \left( \frac{|m_s|x}{v_s} \right), \quad (86)$$

so that we obtain the following asymptotics respectively in the long and short distance limits

$$\begin{aligned} \langle \epsilon_+(x) \rangle &\sim e^{-x/\xi_s} \\ \langle \epsilon_+(x) \rangle &\sim x^{1/2}. \end{aligned} \quad (87)$$

We close this section by discussing the case of the spontaneously dimerized spin-1 chain. The Ising representations of staggered and dimerization fields are now given by Eq. (80) with  $\sigma_0 \rightarrow 1$ . The staggered magnetization and dimerization profiles are

$$\begin{aligned}\langle n_+^x(x) \rangle &\sim e^{-2x/\xi_t} G^3 \left( \frac{x}{\xi_t} \right) \\ \langle \epsilon_+(x) \rangle &\sim G \left( \frac{x}{\xi_t} \right) H^2 \left( \frac{x}{\xi_t} \right).\end{aligned}\quad (88)$$

In the short distance limit, we obtain the following power law behaviors

$$\begin{aligned}\langle n_+^x(x) \rangle &\sim x^{-3/8} \\ \langle \epsilon_+(x) \rangle &\sim x^{5/8},\end{aligned}\quad (89)$$

whereas for long distances we have

$$\begin{aligned}\langle n_+^x(x) \rangle &\sim e^{-2x/\xi_t} \\ \langle \epsilon_+(x) \rangle &\simeq \epsilon_\infty \left( 1 - \frac{\xi_t^{1/2}}{\sqrt{\pi}} \frac{e^{-2x/\xi_t}}{x^{1/2}} \right).\end{aligned}\quad (90)$$

Therefore, we observe that the dimerization reaches here its bulk expectation value from below in contrast to the free boundary case (74).

## VI. CONCLUDING REMARKS

In this paper, we have investigated the nature of the chain-boundary excitations of the cut two-leg spin ladder and the open spin-1 chain by means of the bosonization method. The crucial point of the analysis is the mapping<sup>32,44</sup> of the low-energy Hamiltonian of these systems onto free massive Majorana fermions (or equivalently decoupled non-critical quantum Ising models) with suitable boundary conditions. In particular, the exact results<sup>66,67,68</sup> of the semi-infinite one-dimensional quantum Ising model allow the determination of the low-energy properties of the cut two-leg spin ladder such as, for instance, the magnetization and dimerization profiles. For a ferromagnetic rung coupling ( $J_\perp < 0$ ), the system is characterized by the presence of fractional spin-1/2 edge states which, in the limit  $J_\perp/J_\parallel \rightarrow -\infty$ , identify to the well known S=1/2 chain-end degrees of freedom of the open spin-1 chain. In this respect, the approach, presented in this paper, provides an alternative derivation of the existence of these edge states first predicted theoretically within the VBS model<sup>12</sup> and the Schwinger boson mean-field analysis.<sup>17</sup> In the case of an antiferromagnetic interchain interaction  $J_\perp > 0$ , no S=1/2 chain-end excitations are found but a non-magnetic localized Majorana fermion zero mode is still present and leads to the formation of a non-zero dimerization profile in the system.

The magnetization and dimerization profiles, derived in this paper, should be confronted to numerical simulations of the cut two-leg spin ladder or the open biquadratic spin-1 chain in the vicinity of the  $SU(2)_2$  WZNW critical point. Due to the semi-infinite geometry considered here, our results would best be compared with DMRG calculations of a finite spin-1 chain with a spin-1/2 attached to one of the extremities to cancel one of the edge states.<sup>19,23</sup> At this point, it is worth noting that all the calculations were done at zero temperature. Our results could in principle be extended to finite temperature using the thermal form factor techniques derived for the one-dimensional quantum Ising model.<sup>74</sup> Unfortunately, it is not an easy task within this formalism to obtain explicit expressions for  $\langle \sigma(x) \rangle$  for fixed boundary conditions. This makes difficult any direct comparison to QMC simulations.<sup>18,24</sup> However, one can argue by finite size scaling arguments that the correlation functions should not be strongly affected by a finite temperature as long as  $m \gg T$ . This can be checked by an explicit computation of the two-point correlation function.<sup>75</sup> We also stress that at finite temperature and for free boundary conditions, one has  $\langle \sigma(x) \rangle = 0$  in the quantum Ising model. This implies the absence of any staggered magnetization profile in the  $S = 0$  state and also of a non-zero string order parameter at finite temperature in agreement with the QMC simulations.<sup>18</sup>

Regarding perspectives, the approach, presented in this work, could be applied to other one-dimensional gapful systems. The effects of an uniaxial single-ion anisotropy  $D_z \sum_i (S_i^z)^2$  on the magnetic properties of the open spin-1 chain can be investigated. Since the different species of Majorana fermions do not interact, we expect that spin-1/2 edge states excitations should still be observed, in agreement with the QMC results.<sup>76</sup> The calculation of magnetization profiles with our method should not pose any difficulty. The approach could also be generalized to study the effect of a weak bond or magnetic impurities in a spin-1 chain<sup>77</sup> as it will be discussed in a separate publication. Another

interesting situation is the nature of the edge states of two open spin-1/2 Heisenberg chains coupled by a biquadratic interchain interaction.<sup>78</sup> Due to the extended O(4) symmetry of the model, we expect to find two spin-1/2 excitations at the edge of the system. A more challenging problem is the generalization of our approach to  $S \geq 3/2$  Heisenberg chains. According to Ref. 17, it is expected that edge states with fractionalized spin  $S'$  exist in the spin-S chain with  $S' = S/2$  (respectively  $S' = (S - 1/2)/2$ ) for integer (respectively half-odd-integer) spins. This conjecture, based on the large-N limit of SU(N) quantum antiferromagnets and strong-coupling expansion, has been verified by a DMRG analysis for  $S = 3/2, 2$ .<sup>21</sup> A generalization of the approach presented here in the S=1 case is to describe spin-S Heisenberg chain as perturbed  $SU(2)_{2S} = U(1) \otimes Z_{2S}$  WZNW models.<sup>27,79</sup> For  $S$  half-odd integer, only the parafermion sector  $Z_{2S}$  is gapped. We should thus expect the edge spin excitations to be generated by the bound states of the massive  $Z_{2S}$  theory on the half-line. For  $S$  integer, edge excitations should be induced by the boundary bound states of the perturbed WZNW model. A similar problematic should also be considered for the related problem of  $n$ -leg spin-1/2 ladders. Finally, an interesting question would be the study of interactions between edge states in chains of finite length<sup>22</sup> using the Majorana fermions description.

### Acknowledgments

The authors would like to thank T. Jolicoeur, D. Allen, P. Azaria, M. Bocquet, A. A. Nersesyan, M. Saito, and Y. Suzumura for valuable discussions. E. O. thanks Nagoya University for kind hospitality and support during his stay at the Physics Department where this project was initiated.

## APPENDIX A: BOSONIZATION APPROACH OF THE OPEN S=1/2 HEISENBERG CHAIN

In this appendix, we describe the bosonization approach of the spin-1/2 Heisenberg chain with open boundary conditions.<sup>35,36,38,40</sup> This enables us to fix the conventions that will be used in this paper and also to discuss some subtleties related to the presence of open boundary conditions. To this end, we consider the repulsive Hubbard model at half-filling with open boundary conditions described by the Hamiltonian

$$\mathcal{H}_U = -t \sum_{i=1}^{N-1} \left( c_{i\sigma}^\dagger c_{i+1\sigma} + H.c. \right) + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow}, \quad (\text{A1})$$

where  $c_{i\sigma}$  is the electronic annihilation operator of spin index  $\sigma = \uparrow, \downarrow$  at site  $i$  ( $1 \leq i \leq N$ ) and  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  stands for the occupation number of electron with spin index  $\sigma$ . The summation over repeated greek symbols is assumed in the following and the hopping term  $t$  is positive. In this model, it is well known that a charge gap  $m_c$  exists for any positive value of the interaction  $U$  and in the low-energy limit ( $E \ll m_c$ ) only the spin excitations remain and describe the universal scaling properties of the spin-1/2 Heisenberg chain. In this way, we shall derive the continuous description of the spin density of the S=1/2 Heisenberg chain with open boundary conditions starting from the electronic model (A1). An alternative approach as described in Refs. 35,38,40 is to consider the spin-1/2 XXZ Heisenberg chain with open boundary conditions and the use of the Jordan-Wigner transformation. Since in this work we shall only consider SU(2) invariant interactions, it is more appropriate to start from the Hubbard model (A1). The open boundary conditions are taken into account by introducing two fictitious sites 0 and  $N + 1$  in Eq. (A1) and by imposing vanishing boundary conditions on the fermion operators:  $c_0 = c_{N+1} = 0$ .<sup>35,37</sup> The low-energy properties of the model can then be determined by applying the bosonization method<sup>28</sup> with suitable boundary conditions on the bosonic fields.<sup>35,36,37,39</sup>

### 1. Non-interacting case

In the low-energy limit, the continuum version of the non-interacting part of the Hamiltonian (A1) can be derived by expressing the lattice fermions  $c_{n\sigma}$  in terms of left and right moving spinful fermionic fields  $\Psi_{L,R\sigma}(x)$ :

$$\frac{c_{n\sigma}}{\sqrt{a}} \sim i^{x/a} \Psi_{R\sigma}(x) + (-i)^{x/a} \Psi_{L\sigma}(x), \quad (\text{A2})$$

with  $x = na$ ,  $a$  being the lattice spacing. The resulting boundary conditions on the fermionic fields of Eq. (A2) are thus

$$\begin{aligned} \Psi_{L\sigma}(0) &= -\Psi_{R\sigma}(0) \\ \Psi_{L\sigma}(L) &= -(-1)^{L/a} \Psi_{R\sigma}(L), \end{aligned} \quad (\text{A3})$$

with  $L = (N + 1)a$ . The left and right excitations are no longer independent due to the presence of these boundaries.

The next step of the approach is the introduction of right and left moving bosonic fields  $\Phi_{R,L\sigma}$  through

$$\begin{aligned}\Psi_{R\sigma} &= \frac{\kappa_\sigma e^{i\pi\tau_\sigma/4}}{\sqrt{2\pi a}} e^{-i\Phi_{R\sigma}} \\ \Psi_{L\sigma} &= \frac{\kappa_\sigma e^{i\pi\tau_\sigma/4}}{\sqrt{2\pi a}} e^{i\Phi_{L\sigma}},\end{aligned}\tag{A4}$$

where  $\kappa_\sigma$  are Klein factors that obey the anticommutation relations  $\{\kappa_\sigma, \kappa_{\sigma'}\} = \delta_{\sigma,\sigma'}$  to ensure the anticommutation between the fermion fields of different spin index. In Eq. (A4), we have also introduced some phase factors with  $\tau_\uparrow = 1$  and  $\tau_\downarrow = -1$  for later convenience. The boundary conditions on the chiral bosonic fields are then obtained from Eq. (A3):

$$\begin{aligned}\Phi_{L\sigma}(0) &= -\Phi_{R\sigma}(0) + \pi \\ \Phi_{L\sigma}(L) &= -\Phi_{R\sigma}(L) + \pi \left(\frac{L}{a} - 1\right) + 2q_\sigma\pi,\end{aligned}\tag{A5}$$

$q_\sigma$  being an integer. In our conventions, the total bosonic field  $\Phi_\sigma$  with spin index  $\sigma$  and its dual  $\Theta_\sigma$  are related to the chiral components  $\Phi_{R,L\sigma}$  through

$$\begin{aligned}\Phi_\sigma &= \frac{1}{2}(\Phi_{R\sigma} + \Phi_{L\sigma}) \\ \Theta_\sigma &= \frac{1}{2}(\Phi_{L\sigma} - \Phi_{R\sigma}),\end{aligned}\tag{A6}$$

so that Eq. (A5) imposes Dirichlet boundary conditions on the bosonic field:

$$\begin{aligned}\Phi_\sigma(0) &= \frac{\pi}{2} \\ \Phi_\sigma(L) &= \frac{\pi}{2} \left(\frac{L}{a} - 1\right) + q_\sigma\pi.\end{aligned}\tag{A7}$$

The low-energy dynamics of the non-interacting Hamiltonian  $\mathcal{H}_0$  of the original model (A1) is thus described by two independent free massless boson Hamiltonian with the boundary conditions (A7):

$$\mathcal{H}_0 = \frac{v_F}{2\pi} \sum_{\sigma=\uparrow,\downarrow} \int_0^L dx \left( (\partial_x \Phi_\sigma)^2 + (\pi \Pi_\sigma)^2 \right),\tag{A8}$$

$v_F$  being the Fermi velocity and  $\Pi_\sigma$  is the momentum operator conjugate to  $\Phi_\sigma$ . The mode decomposition of the bosonic field  $\Phi_\sigma$  compatible with these boundary conditions reads as follows

$$\Phi_\sigma(x, t) = \frac{\pi}{2} + \left( \frac{\pi}{2} \left( \frac{L}{a} - 2 \right) + \sqrt{\pi} \tilde{\pi}_{0\sigma} \right) \frac{x}{L} + \sum_{n=1}^{\infty} \frac{\sin(k_n x)}{\sqrt{n}} (\alpha_{n\sigma} e^{-ik_n v_F t} + H.c.),\tag{A9}$$

where  $k_n = n\pi/L$ ,  $\alpha_{n\sigma}$  is the boson annihilation operator obeying  $[\alpha_{n\sigma}, \alpha_{m\sigma'}^\dagger] = \delta_{n,m} \delta_{\sigma,\sigma'}$  and the zero mode operator  $\tilde{\pi}_{0\sigma}$  has a discrete spectrum  $\sqrt{\pi}q_\sigma$ . The mode decomposition of the momentum operator  $\Pi_\sigma = \partial_t \Phi_\sigma / \pi v_F$  conjugate to the bosonic field can thus be deduced from Eq. (A9)

$$\Pi_\sigma(x, t) = \sum_{n=1}^{\infty} \frac{i\sqrt{n}}{L} \sin(k_n x) (-\alpha_{n\sigma} e^{-ik_n v_F t} + \alpha_{n\sigma}^\dagger e^{ik_n v_F t}).\tag{A10}$$

In particular, one can check that the mode decompositions (A9, A10) satisfy the canonical commutation relation:

$$[\Phi_\sigma(x, t), \Pi_{\sigma'}(y, t)] = i\delta_{\sigma,\sigma'} \delta_L(x - y),\tag{A11}$$

$\delta_L(x - y)$  being the delta function at finite size:  $\delta_L(x) = \sum_n e^{ik_n x} / 2L$ . The dual field  $\Theta_\sigma$  satisfies  $\partial_x \Theta_\sigma = \pi \Pi_\sigma$  and  $\partial_t \Theta_\sigma = v_F \partial_x \Phi_\sigma$  so that one obtains the following mode expansion:

$$\Theta_\sigma(x, t) = \sqrt{\pi} \tilde{\phi}_{0\sigma} + \left( \frac{\pi}{2} \left( \frac{L}{a} - 2 \right) + \sqrt{\pi} \tilde{\pi}_{0\sigma} \right) \frac{v_F t}{L} + i \sum_{n=1}^{\infty} \frac{\cos(k_n x)}{\sqrt{n}} (\alpha_{n\sigma} e^{-ik_n v_F t} - \alpha_{n\sigma}^\dagger e^{ik_n v_F t}),\tag{A12}$$

where the zero mode coordinate  $\tilde{\phi}_{0\sigma}$  is conjugate to  $\tilde{\pi}_{0\sigma}$ :  $[\tilde{\phi}_{0\sigma}, \tilde{\pi}_{0\sigma'}] = i\delta_{\sigma,\sigma'}$  and it is not fixed by the boundary conditions (A7). Finally, the mode decompositions of the chiral bosonic fields  $\Phi_{R,L\sigma}$  can be determined by the identification (A6):

$$\begin{aligned}\Phi_{L\sigma} &= \frac{\pi}{2} + \left( \frac{\pi}{2} \left( \frac{L}{a} - 2 \right) + \sqrt{\pi} \tilde{\pi}_{0\sigma} \right) \frac{x + v_F t}{L} + \sqrt{\pi} \tilde{\phi}_{0\sigma} + \sum_{n=1}^{\infty} \frac{i}{\sqrt{n}} \left( \alpha_{n\sigma} e^{-ik_n(x+v_F t)} - \alpha_{n\sigma}^\dagger e^{ik_n(x+v_F t)} \right) \\ \Phi_{R\sigma} &= \frac{\pi}{2} + \left( \frac{\pi}{2} \left( \frac{L}{a} - 2 \right) + \sqrt{\pi} \tilde{\pi}_{0\sigma} \right) \frac{x - v_F t}{L} - \sqrt{\pi} \tilde{\phi}_{0\sigma} - \sum_{n=1}^{\infty} \frac{i}{\sqrt{n}} \left( \alpha_{n\sigma} e^{ik_n(x-v_F t)} - \alpha_{n\sigma}^\dagger e^{-ik_n(x-v_F t)} \right)\end{aligned}\quad (\text{A13})$$

In addition, one can show that these chiral fields satisfy the following commutation relations when  $L \gg a$

$$\begin{aligned}[\Phi_{L\sigma}(x, t), \Phi_{L\sigma'}(y, t)] &= -i\pi\delta_{\sigma,\sigma'} \text{sgn}(x - y) \\ [\Phi_{R\sigma}(x, t), \Phi_{R\sigma'}(y, t)] &= i\pi\delta_{\sigma,\sigma'} \text{sgn}(x - y) \\ [\Phi_{R\sigma}(x, t), \Phi_{L\sigma'}(y, t)] &= 0 \quad \text{if } x = y = 0 \\ &= -2i\pi\delta_{\sigma,\sigma'} \text{ if } x = y = L \\ &= -i\pi\delta_{\sigma,\sigma'} \text{ if } 0 < x, y < L,\end{aligned}\quad (\text{A14})$$

$\text{sgn}(x)$  being the sign function.

## 2. Effective spin density

The next step of the approach is the introduction of the bosonic fields that describe the charge and spin degrees of freedom:

$$\begin{aligned}\Phi_{cR,L} &= \frac{\Phi_{R,L\uparrow} + \Phi_{R,L\downarrow}}{\sqrt{2}} \\ \Phi_{sR,L} &= \frac{\Phi_{R,L\uparrow} - \Phi_{R,L\downarrow}}{\sqrt{2}}.\end{aligned}\quad (\text{A15})$$

This basis as well as the commutation relations (A14) allow us to express the Hamiltonian (A8) in terms of two commuting gapless spin and charge contributions:

$$\mathcal{H}_0 = \frac{v_F}{2\pi} \int_0^L dx \left( (\partial_x \Phi_c)^2 + (\pi \Pi_c)^2 \right) + \frac{v_F}{2\pi} \int_0^L dx \left( (\partial_x \Phi_s)^2 + (\pi \Pi_s)^2 \right).\quad (\text{A16})$$

As well known, a weak Hubbard interaction preserves this famous spin-charge separation and opens at half-filling a mass gap  $m_c$  for the charge degrees of freedom. In the spin sector, the effect of the interaction is exhausted by a renormalization of the spin velocity and by the existence of a marginal irrelevant contribution in the Hamiltonian. In particular, the interaction does not renormalize the bosonic field  $\Phi_s$  since it is protected by the underlying SU(2) symmetry of the model. Neglecting the logarithmic corrections introduced by the marginal irrelevant term, the low-energy ( $E \ll m_c$ ) Hamiltonian that describes the universal properties of the S=1/2 Heisenberg chain is simply

$$\mathcal{H}_s = \frac{v_s}{2\pi} \int_0^L dx \left( (\partial_x \Phi_s)^2 + (\pi \Pi_s)^2 \right),\quad (\text{A17})$$

$v_s$  being the velocity of the spin collective mode. The boundary conditions of the bosonic field  $\Phi_s$  can be obtained from Eqs. (A7, A15):

$$\begin{aligned}\Phi_s(0) &= 0 \\ \Phi_s(L) &= \frac{q\pi}{\sqrt{2}},\end{aligned}\quad (\text{A18})$$

$q$  being an integer. Similarly, the mode decompositions of the chiral bosonic fields  $\Phi_{sR,L}$  read as follows with help of Eq. (A13)

$$\begin{aligned}\Phi_{sL}(x, t) &= \sqrt{\pi} \tilde{\pi}_{0s} \frac{x + v_s t}{L} + \sqrt{\pi} \tilde{\phi}_{0s} + \sum_{n=1}^{\infty} \frac{i}{\sqrt{n}} \left( \alpha_{ns} e^{-ik_n(x+v_s t)} - \alpha_{ns}^\dagger e^{ik_n(x+v_s t)} \right) \\ \Phi_{sR}(x, t) &= \sqrt{\pi} \tilde{\pi}_{0s} \frac{x - v_s t}{L} - \sqrt{\pi} \tilde{\phi}_{0s} - \sum_{n=1}^{\infty} \frac{i}{\sqrt{n}} \left( \alpha_{ns} e^{ik_n(x-v_s t)} - \alpha_{ns}^\dagger e^{-ik_n(x-v_s t)} \right),\end{aligned}\quad (\text{A19})$$

with  $[\tilde{\phi}_{0s}, \tilde{\pi}_{0s}] = i$  and  $[\alpha_{ns}, \alpha_{ms}^\dagger] = \delta_{n,m}$ . Moreover, we deduce from Eq. (A14) that these fields obey the commutation relations

$$\begin{aligned} [\Phi_{sL}(x, t), \Phi_{sL}(y, t)] &= -i\pi \text{sgn}(x - y) \\ [\Phi_{sR}(x, t), \Phi_{sR}(y, t)] &= i\pi \text{sgn}(x - y) \\ [\Phi_{sR}(x, t), \Phi_{sL}(y, t)] &= 0 \quad \text{if } x = y = 0 \\ &= -2i\pi \quad \text{if } x = y = L \\ &= -i\pi \quad \text{if } 0 < x, y < L. \end{aligned} \quad (\text{A20})$$

At this point, it is important to note that the last commutator in Eq. (A20) has the opposite sign of the prescription made in Refs. 28,32. The actual value of its sign stems from the fact that we are considering open boundary conditions in the lattice system which identify to the Dirichlet boundary conditions (A18) on the bosonic field  $\Phi_s$ . In fact, one can derive the value of the commutator  $[\Phi_{sR}, \Phi_{sL}]$  by a different method. The boundary condition at  $x = 0$  on the chiral bosonic spin fields is

$$\Phi_{sL}(0, t) = -\Phi_{sR}(0, t) \quad \forall t. \quad (\text{A21})$$

Since  $\Phi_{sL}(x, t) = \Phi_{sL}(x + v_s t)$  and  $\Phi_{sR}(x, t) = \Phi_{sR}(v_s t - x)$ , one thus obtains the folding condition ( $x \geq 0$ ):

$$\Phi_{sL}(x, t) = -\Phi_{sR}(-x, t), \quad (\text{A22})$$

which is satisfied by the mode decompositions (A19). Moreover, the commutator  $[\Phi_{sR}(x, t), \Phi_{sR}(y, t)]$  is fixed by the requirement that  $\Phi_s$  and  $\Pi_s$  are canonical conjugate operators so that by using the folding condition (A22) we deduce:

$$\begin{aligned} [\Phi_{sR}(x, t), \Phi_{sL}(y, t)] &= -[\Phi_{sR}(x, t), \Phi_{sR}(-y, t)] \\ &= -i\pi \text{sgn}(x + y) = -i\pi. \end{aligned} \quad (\text{A23})$$

It turns out that the sign of this commutator is important for the investigation of the S=1/2 chain-boundary excitations of the open two-leg spin ladder as described in Sections II and III of this work.

With all these results at hands, it is straightforward to derive the continuum description of the spin density starting from the lattice spin operator  $\mathbf{S}_i$ :

$$S_i^a = \frac{1}{2} c_{i\alpha}^\dagger \sigma_{\alpha\beta}^a c_{i\beta}, \quad (\text{A24})$$

$\sigma^a (a = x, y, z)$  being the Pauli matrices. Using the decomposition (A2), the spin density separates into a uniform and staggered parts in the continuum limit:

$$\mathbf{S}(x) = \mathbf{J}_{sR}(x) + \mathbf{J}_{sL}(x) + (-1)^{x/a} \mathbf{n}_s(x), \quad (\text{A25})$$

with the identification

$$\begin{aligned} J_{sR,L}^a &= \frac{1}{2} \Psi_{R,L\alpha}^\dagger \sigma_{\alpha\beta}^a \Psi_{R,L\beta} \\ n_s^a &= \frac{1}{2} \left( \Psi_{L\alpha}^\dagger \sigma_{\alpha\beta}^a \Psi_{R\beta} + \Psi_{R\alpha}^\dagger \sigma_{\alpha\beta}^a \Psi_{L\beta} \right). \end{aligned} \quad (\text{A26})$$

The bosonized description of the spin density can then be obtained with help of the bosonization formula (A4), the commutation relations (A14), and the canonical transformation (A15). The resulting expressions for the uniform part read as follows

$$\begin{aligned} J_{sL}^z &= -\frac{1}{2\pi\sqrt{2}} \partial_x \Phi_{sL} \\ J_{sR}^z &= -\frac{1}{2\pi\sqrt{2}} \partial_x \Phi_{sR} \\ J_{sR}^\dagger &= -\frac{i\kappa_\uparrow \kappa_\downarrow}{2\pi a} e^{i\sqrt{2}\Phi_{sR}} \\ J_{sL}^\dagger &= -\frac{i\kappa_\uparrow \kappa_\downarrow}{2\pi a} e^{-i\sqrt{2}\Phi_{sL}}, \end{aligned} \quad (\text{A27})$$

whereas the staggered part is given by

$$\begin{aligned} n_s^x &= -\frac{\lambda i \kappa_\uparrow \kappa_\downarrow}{\pi a} \cos(\sqrt{2} \Theta_s) \\ n_s^y &= \frac{\lambda i \kappa_\uparrow \kappa_\downarrow}{\pi a} \sin(\sqrt{2} \Theta_s) \\ n_s^z &= -\frac{\lambda}{\pi a} \sin(\sqrt{2} \Phi_s), \end{aligned} \quad (\text{A28})$$

$\lambda$  being a constant stemming from the charge degrees of freedom that have been integrated out in the low-energy regime  $E \ll m_c$ . The product  $\kappa_\uparrow \kappa_\downarrow$  has no dynamic and in this work we use the prescription  $\kappa_\uparrow \kappa_\downarrow = i$  for simplicity. Finally, as it can be checked from the correspondence (A27), the left-moving contribution of the uniform part of the spin density (A25) obeys the following operator product expansion (with a similar result for the right-moving term)

$$J_{sL}^a(z) J_{sL}^b(w) \sim \frac{\delta_{a,b}}{8\pi^2(z-w)^2} + \frac{i\epsilon^{abc} J_{sL}^c(w)}{2\pi(z-w)}, \quad (\text{A29})$$

with  $z = v_s \tau + ix$ . The uniform left spin density  $\mathbf{J}_{sL}$  identifies to the  $SU(2)_1$  Kac-Moody currents which are the generators of the conformal field theory associated to the criticality of the spin-1/2 Heisenberg chain (see for instance the book<sup>28</sup> for a review).

## APPENDIX B: ALTERNATIVE DERIVATION OF THE UNIFORM MAGNETIZATION PROFILE

In this Appendix, we derive the  $z$ -component of the uniform magnetization profile of the cut two-leg spin ladder with a ferromagnetic rung coupling without using the Majorana fermion formalism. To this end, we return to the complex fermion Hamiltonian  $\mathcal{H}_+$  (17) with  $J_\perp < 0$ . The  $z$ -part of the total magnetization density is given by:  $M^z =: \psi_{+R}^\dagger \psi_{+R} + \psi_{+L}^\dagger \psi_{+L} ::$ . Using the boundary condition (15) and the Hamiltonian (17) with  $m = -J_\perp/2\pi > 0$ , we obtain the following mode decomposition for the fermionic fields  $\psi_{+R,L}$ :

$$\begin{aligned} \psi_{+R}(x) &= \sqrt{\frac{m}{v}} e^{-mx/v} a_0 + \frac{1}{\sqrt{2L}} \sum_k (f(k, x) a_{k,+} + f^*(k, x) a_{k,-}) \\ \psi_{+L}(x) &= \sqrt{\frac{m}{v}} e^{-mx/v} a_0 + \frac{1}{\sqrt{2L}} \sum_k (f^*(k, x) a_{k,+} + f(k, x) a_{k,-}), \end{aligned} \quad (\text{B1})$$

$$(\text{B2})$$

where  $f(k, x) = \cos(kx + \theta_k) + i \sin(kx)$ ,  $\theta_k$  being defined by Eq. (29). The Hamiltonian  $\mathcal{H}_+$  (17) can be expressed in terms of the  $a_{k,\pm}$  fermionic modes

$$\mathcal{H}_+ = \sum_k \epsilon(k) (a_{k,+}^\dagger a_{k,+} - a_{k,-}^\dagger a_{k,-}), \quad (\text{B3})$$

with the energy dispersion  $\epsilon(k) = \sqrt{v^2 k^2 + m^2}$ . The uniform magnetization profile along the  $z$ -axis is then given by

$$\langle M^z(x) \rangle = \frac{1}{L} \sum_{k>0} [\cos^2(kx + \theta_k) + \sin^2(kx) - 1] (\langle a_{k,-}^\dagger a_{k,-} + a_{k,+}^\dagger a_{k,+} \rangle) + \frac{2m}{v} e^{-2mx/v} \langle a_0^\dagger a_0 \rangle. \quad (\text{B4})$$

Using the expressions (29), noting that  $n_F(\epsilon(k)) + n_F(-\epsilon(k)) = 1$  and  $\sum_{k>0} \rightarrow L \int_0^\infty dk/\pi$  in the large  $L$  limit, the uniform magnetization simplifies as

$$\begin{aligned} \langle M^z(x) \rangle &= \frac{2m}{v} e^{-2mx/v} \langle a_0^\dagger a_0 \rangle \\ &\quad - \int_0^\infty \frac{dk}{\pi} \left[ \frac{m^2}{(vk)^2 + m^2} \cos(2kx) + \frac{m v k}{(vk)^2 + m^2} \sin(2kx) \right]. \end{aligned} \quad (\text{B5})$$

Performing the integrals, we finally find the following result

$$\langle M^z(x) \rangle = \frac{2m}{v} e^{-2mx/v} [\langle a_0^\dagger a_0 \rangle - 1/2]. \quad (\text{B6})$$

This profile is identical to the one obtained by the Majorana fermions calculation (38).

If we apply a uniform magnetic field along the  $z$ -axis, the Hamiltonian  $\mathcal{H}_+$  (B3) is modified as follows

$$\mathcal{H}_+ = \sum_{k,r=\pm} (r\epsilon(k) - h) : a_{k,r}^\dagger a_{k,r} : - h(a_0^\dagger a_0 - 1/2), \quad (\text{B7})$$

whereas the Hamiltonian  $\mathcal{H}_-$  in Eq. (9) is not affected by the magnetic field. The resulting free energy per unit length is then given by

$$f_s = -\frac{1}{\beta} \int_0^\infty \frac{dk}{\pi} \sum_{r=\pm} \ln(1 + e^{-\beta(\epsilon(k)-rh)}) - \frac{1}{\beta} \ln(2 \cosh(\beta h/2)) = f_s^{\text{bulk}} + f_s^{\text{edge}}. \quad (\text{B8})$$

From  $f_s^{\text{bulk}}$ , we recover the usual susceptibility and specific heat of the spin-1 chain. We see that  $f_s^{\text{edge}}$  is the free energy of an isolated spin-1/2. Thus, for  $h \ll \beta$  and  $h \ll m$ , the thermodynamic properties of the system are identical to those of an isolated spin-1/2. This result is in agreement with the QMC simulations of long chains<sup>18</sup> and DMRG calculations of effective interaction of edge states in long chains<sup>22</sup>.

### APPENDIX C: CALCULATION OF THE FUNCTION $F(x)$

In this Appendix, we compute the one-point function of the disorder operator in the low-temperature phase of the semi-infinite one-dimensional quantum Ising model with free boundary conditions. To this end, the form factor approach to correlation functions<sup>80</sup> will be used as in Ref. 68 for the calculation of the magnetization one-point function.

Let us first recall some results on the form factors of the bulk quantum Ising model.<sup>81,82</sup> The excited states of this model are created by acting on the ground state with fermion creation operators  $A^\dagger$ :

$$|\theta_1 \dots \theta_n\rangle = A^\dagger(\theta_1) \dots A^\dagger(\theta_n)|0\rangle, \quad (\text{C1})$$

where the  $\theta_i$ 's are the usual rapidity variables parametrizing momentum and energy as  $p(\theta_i) = m \sinh \theta_i$ ,  $e(\theta_i) = m \cosh \theta_i$ ,  $m$  being the fermion's mass ( $m > 0$  for  $T < T_c$ ) and its velocity has been set to unity here for simplicity. The creation  $A^\dagger$  and annihilation  $A$  operators satisfy the fermionic anticommutation relation normalized as follows

$$\{A(\theta_1), A^\dagger(\theta_2)\} = 2\pi\delta(\theta_1 - \theta_2). \quad (\text{C2})$$

For  $T < T_c$ , the form factors of the order operator  $\sigma$  are:

$$\langle 0|\sigma(0)|\theta_1 \dots \theta_{2n}\rangle = i^n \prod_{1 \leq i < j \leq 2n} \tanh\left(\frac{\theta_i - \theta_j}{2}\right), \quad (\text{C3})$$

whereas the form factors with an odd number of rapidities are zero. They are normalized such that the conformal limit of the spin-spin correlation function is

$$\langle \sigma(r) \sigma(0) \rangle = \frac{\mathcal{F}^2}{r^{1/4}}, \quad (\text{C4})$$

with  $r = \sqrt{x^2 + \tau^2}$  and  $\mathcal{F} = 2^{-1/12} e^{1/8} A^{-3/2} m^{-1/8}$ ,  $A$  being the Glaisher constant. In the low-temperature phase, the form factors of the disorder operator are given by

$$\langle 0|\mu(0)|\theta_1 \dots \theta_{2n+1}\rangle = i^n \prod_{1 \leq i < j \leq 2n+1} \tanh\left(\frac{\theta_i - \theta_j}{2}\right), \quad (\text{C5})$$

and those with an even number of rapidities are zero. For  $T > T_c$ , the roles of  $\sigma$  and  $\mu$  are interchanged.

With these results, one can extend the method of Ref. 68 to calculate the one-point function of the disorder operator in the low-temperature phase of the semi-infinite Ising model with free boundary conditions. The free boundary condition on the Majorana fermions ( $\xi_L(0) = \xi_R(0)$ ) is interpreted as a boundary state  $|B\rangle$  which encodes all informations about the boundary condition.<sup>66</sup> In this approach, the Hilbert space of the theory is the same as in the bulk so that the one-point function can be extracted through

$$\langle \mu(x) \rangle = \sum_n \langle 0|\mu(0)|n\rangle \langle n|B\rangle e^{-xE_n}, \quad (\text{C6})$$

$|n\rangle$  being a complete set of states of the bulk Hilbert space. The boundary state corresponding to the Ising model at  $T < T_c$  on the half line with free boundary conditions is<sup>66</sup>

$$|B\rangle = (1 + A^\dagger(0)) \exp \left[ \int_0^\infty \frac{d\theta}{2\pi} \hat{R}(\theta) A^\dagger(-\theta) A^\dagger(\theta) \right] |0\rangle, \quad (\text{C7})$$

with  $\hat{R}(\theta) = -i \coth(\theta/2)$ . This boundary state contains a zero-momentum one-particle state which corresponds to a domain wall, attached to the boundary, that separates two domains of opposite magnetization ( $T < T_c$ ). Such term contributes to the expectation value (C6) while it does not enter the calculation of the one-point function of the order operator. Expanding the exponential in Eq. (C7), we get the following expression using the fact that the form factors of  $\mu$  are non-zero only for an odd number of rapidities:

$$\langle \mu(x) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\infty \frac{d\theta_1}{2\pi} \dots \int_0^\infty \frac{d\theta_n}{2\pi} \langle 0 | \mu(0) | 0; -\theta_1, \theta_1; \dots; -\theta_n, \theta_n \rangle \hat{R}(\theta_1) \dots \hat{R}(\theta_n) e^{-mx[1+2\cosh(\theta_1)+\dots+2\cosh(\theta_n)]}, \quad (\text{C8})$$

from which we deduce the identity

$$\langle \mu(x) \rangle = e^{-mx} A(mx). \quad (\text{C9})$$

The next step of the approach is to use the form factor of  $\mu$  (C5) to derive an expression for  $A(mx)$ . First of all, one has

$$\langle 0 | \mu(0) | 0; \theta_1, -\theta_1; \dots; \theta_n, -\theta_n \rangle = i^n \prod_{i=1}^n \tanh^2 \frac{\theta_i}{2} \tanh \theta_i \prod_{i < j} \tanh^2 \left( \frac{\theta_i - \theta_j}{2} \right) \tanh^2 \left( \frac{\theta_i + \theta_j}{2} \right), \quad (\text{C10})$$

so that, using the expression of  $\hat{R}(\theta)$ , we obtain:

$$A(mx) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\infty \frac{d\theta_1}{2\pi} \dots \int_0^\infty \frac{d\theta_n}{2\pi} \left( \prod_{i=1}^n \tanh \frac{\theta_i}{2} \tanh \theta_i \right) \det W(\theta_i, \theta_j) e^{-2mx \sum_{k=1}^n \cosh(\theta_k)}, \quad (\text{C11})$$

with

$$W(\theta_i, \theta_j) = \frac{2\sqrt{\cosh \theta_i \cosh \theta_j}}{\cosh \theta_i + \cosh \theta_j}. \quad (\text{C12})$$

Following Ref. 68, we introduce the quantity

$$V(\theta_i, \theta_j, mx) = \frac{\sqrt{\cosh \theta_i - 1} \sqrt{\cosh \theta_j - 1}}{\cosh \theta_i + \cosh \theta_j} e^{-mx(\cosh \theta_i + \cosh \theta_j)}. \quad (\text{C13})$$

The function  $A(mx)$  can then be expressed as a Fredholm determinant:

$$\begin{aligned} A(mx) &= \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} \frac{d\theta_1}{2\pi} \dots \int_{-\infty}^{\infty} \frac{d\theta_n}{2\pi} \det V(\theta_i, \theta_j, mx) \\ &= \text{Det} \left( 1 + \frac{V}{2\pi} \right). \end{aligned} \quad (\text{C14})$$

Using the results obtained in Ref. 68,  $A(mx)$ , given by Eq. (C14), coincides with the Fredholm determinant representation of the one-point function of the Ising magnetization for  $T < T_c$  with fixed boundary conditions i.e.  $G(mx)$  in our notations (see in particular Eq. (55)). Therefore, from Eq. (C9), we finally deduce the following relation:

$$F(mx) = e^{-mx} G(mx). \quad (\text{C15})$$

#### APPENDIX D: EXPRESSION OF THE FUNCTIONS $G(x)$ AND $H(x)$ IN TERMS OF SOLUTIONS OF THE PAINLÉVÉ III EQUATION

According to Bariev,<sup>67</sup> the functions  $G$  and  $H$ , describing the cross-over effect on the local magnetization of the semi-infinite Ising model at  $T < T_c$  with free and fixed boundary conditions, can be expressed in terms of a solution  $\eta(\theta)$  of the Painlevé III differential equation. This latter equation reads as follows

$$\frac{1}{\eta} \frac{d^2 \eta}{d\theta^2} = \left( \frac{1}{\eta} \frac{d\eta}{d\theta} \right)^2 - \frac{1}{\theta \eta} \frac{d\eta}{d\theta} + \eta^2 - \frac{1}{\eta^2}. \quad (\text{D1})$$

The boundary conditions on  $\eta$  are:

$$\begin{aligned}\eta(\theta) &\sim -\theta \left[ \ln \frac{\theta}{4} + \gamma_E \right] (\theta \rightarrow 0) \\ \eta(\theta) &\sim 1 - \frac{K_0(2\theta)}{2\pi} (\theta \rightarrow \infty),\end{aligned}\tag{D2}$$

$\gamma_E$  being the Euler's constant. The functions  $G$  and  $H$  that are the building blocs of the staggered magnetization and dimerization profiles are related to the solution  $\eta(\theta)$  by

$$\begin{aligned}G(y) &= \eta^{-1/4}(y) \exp \left[ \int_y^\infty d\theta \left\{ \frac{\theta}{8} \eta^{-2}(\theta) \left( (1 - \eta^2(\theta))^2 - \left( \frac{d\eta}{d\theta} \right)^2 \right) - \frac{1}{2} (1 - \eta(\theta)) \right\} \right] \\ H(y) &= \eta^{1/4}(y) \exp \left[ \int_y^\infty d\theta \left\{ \frac{\theta}{8} \eta^{-2}(\theta) \left( (1 - \eta^2(\theta))^2 - \left( \frac{d\eta}{d\theta} \right)^2 \right) - \frac{1}{2} (\eta^{-1}(\theta) - 1) \right\} \right].\end{aligned}\tag{D3}$$

There is an interesting connection between the Painlevé III differential equation and the two-dimensional sinh-Gordon equation. Indeed, the relation is obtained by considering  $\eta(\theta) = e^{-\chi(\theta)}$  so that the differential equation (D1) takes the form

$$\frac{d^2\chi}{d\theta^2} + \frac{1}{\theta} \frac{d\chi}{d\theta} = 2 \sinh 2\chi.\tag{D4}$$

The functions  $G$  and  $H$  in Eq. (D3) can then be expressed in terms of  $\chi$

$$\begin{aligned}G(y) &= e^{\chi(y)/4} \exp \left[ \int_y^\infty d\theta \left\{ \frac{\theta}{8} \left[ 4 \sinh^2 \chi - \left( \frac{d\chi}{d\theta} \right)^2 \right] - \frac{1}{2} (1 - e^{-\chi(\theta)}) \right\} \right] \\ H(y) &= e^{-\chi(y)/4} \exp \left[ \int_y^\infty d\theta \left\{ \frac{\theta}{8} \left[ 4 \sinh^2 \chi - \left( \frac{d\chi}{d\theta} \right)^2 \right] - \frac{1}{2} (e^{\chi(\theta)} - 1) \right\} \right].\end{aligned}\tag{D5}$$

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