

Exact boundary modes in an interacting quantum wire

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The boundary modes of one-dimensional quantum systems can play host to a variety of remarkable phenomena. They can be used to describe the physics of impurities in higher-dimensional systems, such as the ubiquitous Kondo effect, or can support Majorana bound states, which play a crucial role in the realm of quantum computation. In this work we examine the boundary modes in an interacting quantum wire with a proximity-induced pairing term. We solve the system exactly using the Bethe ansatz and show that for certain boundary conditions the spectrum contains bound states localized about either edge. The model is shown to exhibit a first-order phase transition as a function of the interaction strength such that for attractive interactions the ground state has bound states at both ends of the wire, while for repulsive interactions they are absent. In addition we see that the bound-state energy lies within the gap for all values of the interaction strength but undergoes a sharp avoided level crossing for sufficiently strong interaction, thereby preventing its decay. This avoided crossing is shown to occur as a consequence of an exact self-duality which is present in the model.

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I. INTRODUCTION

Distinct equilibrium phases of matter are separated by regions of criticality characterized by diverging length scales and gapless modes. The critical region may lie in parameter space where the distinct phases are attained by tuning an external parameter such as temperature or some other system parameter such as interaction strength [1,2] but also occurs in real space at the interface of different systems. A prominent example of the latter is the existence of gapless modes which lie at the edges of topological materials [3–5]. In one dimension, these edge modes are immobile and form bound states which are localized at the boundaries of the system. Such boundary bound states are of central importance to a number of fields, including quantum computation [6–8], magnetic impurities in higher-dimensional superconductors [9–12], and solitons in one-dimensional organic conductors [13–15].

In this paper we study a model of a one-dimensional (1D), spinful, interacting quantum wire with open boundary conditions. The quantum wire has both density-density interactions and a proximity-induced pairing term. We investigate the effects of different boundary conditions on the system and focus in particular on the existence of boundary bound states, states which decay exponentially away from the end points of the wire. After reformulating the Hamiltonian via a bosonization and refermionization procedure the model is solved exactly using the Bethe ansatz for a subset of the parameters. We find the many-body eigenstates, derive the Bethe ansatz equations, and construct the ground-state and low-lying excitations. We show that for certain boundary conditions, those which break the time-reversal invariance of the bulk, the model supports bound states at the boundaries. These boundary bound states, while being exact eigenstates of the system, do not correspond

to solutions of the Bethe ansatz equations, which marks them as distinct from boundary modes previously studied via the Bethe ansatz [16–23].

When the interactions are absent, these bound states lie within the energy gap at zero energy and provide a fourfold-degenerate ground state. However, when the interactions are present, this degeneracy is lifted. Owing to a redistribution of the interacting Fermi sea the bound-state energy is shifted to nonzero values, leading to a first-order phase transition at zero temperature. In the ground state these bound states are occupied if their energy is pushed below the Fermi level, which occurs for attractive interactions, and are unoccupied otherwise. The bound-state energy remains within the gap for all values of the interaction strength but undergoes a sharp avoided level crossing with the continuum of unbound states for finite interaction strength. This prevents any possible coupling of the bound and unbound states and thereby protects them from decay [24].

II. HAMILTONIAN

We consider the following Hamiltonian describing an interacting 1D quantum wire:

$$\begin{aligned}
 H = & \int_0^L dx \sum_{\sigma=\uparrow,\downarrow} v_F [\psi_{-\sigma}^\dagger i\partial_x \psi_{-\sigma} - \psi_{+\sigma}^\dagger i\partial_x \psi_{+\sigma}] \\
 & + \Delta [\psi_{+\uparrow}^\dagger \psi_{-\downarrow}^\dagger + \psi_{-\downarrow} \psi_{+\uparrow} - \psi_{+\downarrow}^\dagger \psi_{-\uparrow}^\dagger - \psi_{-\uparrow} \psi_{+\downarrow}] \\
 & + g_{\parallel} [\psi_{+\uparrow}^\dagger \psi_{+\uparrow} \psi_{-\uparrow}^\dagger \psi_{-\uparrow} + \psi_{-\downarrow}^\dagger \psi_{-\downarrow} \psi_{+\downarrow}^\dagger \psi_{+\downarrow}] \\
 & + g_{\perp} [\psi_{+\downarrow}^\dagger \psi_{+\downarrow} \psi_{-\uparrow}^\dagger \psi_{-\uparrow} + \psi_{-\downarrow}^\dagger \psi_{-\downarrow} \psi_{+\uparrow}^\dagger \psi_{+\uparrow}]. \quad (1)
 \end{aligned}$$

Here we have two species $\sigma = \uparrow, \downarrow$ of left- (–) and right- (+) moving fermions $\psi_{\pm\sigma}^\dagger, \psi_{\pm\sigma}$ which are restricted to the segment $x \in [0, L]$, and we have taken $\hbar = 1$ [25–27]. The first line is the kinetic energy of the fermions, while the second

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is the pairing term which has a sign difference for pairs about different Fermi points. Pairing of this form occurs in p_x -wave triplet superconductors [28,29], which may be induced via proximity [7,8,30,31] and leads to a bare energy gap of 2Δ . The final lines describe density-density interactions between fermions with parallel or opposite spins, the g_{\parallel} and g_{\perp} terms, respectively. Along with this we specify the boundary condition at $x = 0, L$ which changes the chirality of the particles but can be chosen to either conserve or flip the spin of the particle or some more complicated combination thereof. The first of these is the most natural choice in a quantum wire [32].

We shall see below that the spin-conserving choice leads to the spectrum containing boundary bound states; however, the time-reversal-invariant, spin-flipping boundary condition does not. These boundary bound states are invariant under a \mathbb{Z}_2 , combined particle-hole and chirality transformation $\psi_{\pm,\sigma}^{\dagger} \leftrightarrow -\psi_{\mp,\sigma}$. This anticommutes with the noninteracting part of the Hamiltonian and so pins the bound states to zero energy when $g_{\parallel} = g_{\perp} = 0$. In the interacting case, however, we show below that this transformation is generalized to $H(\delta) \leftrightarrow -H(-\delta)$, where δ is the two-particle phase shift, and so the bound state may no longer lie at zero energy.

III. BOSONIZATION

Our aim is to provide an exact solution of the Hamiltonian for a particular choice of g_{\perp}, g_{\parallel} , which will be achieved by employing the Bethe ansatz method. The exact solution will then allow us to study the boundary bound states of the model. In present form, however, (1) is not amenable to this due to the apparent lack of particle number conservation caused by the pairing term. To bring it to a more suitable form we first bosonize the system, perform a duality transformation, and then refermionize. The outcome of this series of steps is that we will have a Hamiltonian in which the pairing term is replaced with a mass-type term instead. Effectively, this will be equivalent to a particle-hole transformation for one of the chiral branches.

We introduce the bosonic fields $\psi_{\pm,\sigma}^{\dagger} = \sqrt{D}e^{i[\mp\phi_{\sigma} - \theta_{\sigma}]}$, where $D = N/L$ is the average density [33]. Forming symmetric and antisymmetric combinations $\phi_{\pm} = [\phi_{\uparrow} \pm \phi_{\downarrow}]/\sqrt{2}$ and $\theta_{\pm} = [\theta_{\uparrow} \pm \theta_{\downarrow}]/\sqrt{2}$, which govern the charge (+) and spin (-) degrees of freedom, our Hamiltonian becomes

$$H = \sum_{a=\pm} \frac{v_a}{2\pi} \int_0^L dx \frac{1}{K_a} [\partial_x \phi_a(x)]^2 + K_a [\partial_x \theta_a(x)]^2 - 4\Delta D \sin[\sqrt{2}\phi_-] \sin[\sqrt{2}\theta_+], \quad (2)$$

where v_{\pm} is the speed of sound and K_{\pm} is the Luttinger parameter of the charge and spin components [25–27]. The relation between the fermionic parameters g_{\perp}, g_{\parallel} and the bosonic parameters K_{\pm} must be determined by comparing physical observables computed in both models and is nonuniversal except at weak coupling, wherein $K_{\pm} \approx 1 - (g_{\parallel} \pm g_{\perp})/2\pi v_F$.

Next, we make a duality transformation on the symmetric fields $\phi_+ \leftrightarrow \theta_+$, whereupon we get the following:

$$H = \frac{v_-}{2\pi} \int_0^L dx \frac{1}{K_-} [\partial_x \phi_-(x)]^2 + K_- [\partial_x \theta_-(x)]^2 + \frac{v_+}{2\pi} \int_0^L dx K_+ [\partial_x \phi_+(x)]^2 + \frac{1}{K_+} [\partial_x \theta_+(x)]^2 - 4\Delta D \int_0^L dx \sin[\sqrt{2}\phi_-] \sin[\sqrt{2}\phi_+], \quad (3)$$

which is a variant of the double sine-Gordon model (DSG) [34,35]. The scaling dimension of the pairing term is $\varkappa = K_-/2 + 1/2K_+$, and it is known that for $\varkappa = 1$ the DSG model is integrable [36] and enjoys a dual fermionic description [37–39]. We restrict ourselves to this case and define the new fermions $\mathcal{R}_{1,2}^{\dagger} = \sqrt{D}e^{i[-\phi_{\uparrow, \downarrow} - \theta_{\uparrow, \downarrow}]}$ and $\mathcal{L}_{1,2}^{\dagger} = \sqrt{D}e^{i[-\phi_{\downarrow, \uparrow} - \theta_{\downarrow, \uparrow}]}$, in terms of which the Hamiltonian can be written as

$$\mathcal{H} = \int_0^L dx \sum_{\xi=1,2} v_F [\mathcal{L}_{\xi}^{\dagger} i \partial_x \mathcal{L}_{\xi} - \mathcal{R}_{\xi}^{\dagger} i \partial_x \mathcal{R}_{\xi}] + \Delta [\mathcal{R}_1^{\dagger} \mathcal{L}_1 + \mathcal{L}_1^{\dagger} \mathcal{R}_1 - \mathcal{R}_2^{\dagger} \mathcal{L}_2 - \mathcal{L}_2^{\dagger} \mathcal{R}_2] - 2g [\mathcal{R}_1^{\dagger} \mathcal{R}_1 \mathcal{L}_2^{\dagger} \mathcal{L}_2 + \mathcal{R}_2^{\dagger} \mathcal{R}_2 \mathcal{L}_1^{\dagger} \mathcal{L}_1]. \quad (4)$$

Our new Hamiltonian \mathcal{H} describes two new species of right-moving, $\mathcal{R}_{\xi}^{\dagger}, \mathcal{R}_{\xi}$, and left-moving, $\mathcal{L}_{\xi}^{\dagger}, \mathcal{L}_{\xi}$, fermions which interact via density-density interaction and have a mass term with Δ and $-\Delta$. Along our chosen manifold of $K_- + 1/K_+ = 2$ there is only a single free parameter encoding the interactions in the wire which in \mathcal{H} is given by g . The relationship between g and K_{\pm} can be determined at this stage only at weak coupling $1/K_+ - K_- \approx 2g/\pi v_F$. The full relationship will be discussed further below; however, we will refer to $g > 0$ as the repulsive regime, $g < 0$ as the attractive regime, and $g = 0$ as the noninteracting model, with $K_+ = K_- = 1$.

As mentioned before this should be accompanied by boundary conditions at $x = 0, L$. In terms of the new fermions the spin-conserving boundary condition mixes the two species,

$$\mathcal{R}_{1,2}^{\dagger}(0) = -\mathcal{L}_{2,1}^{\dagger}(0), \quad (5)$$

$$\mathcal{R}_{1,2}^{\dagger}(L) = -\mathcal{L}_{2,1}^{\dagger}(L). \quad (6)$$

This will allow for boundary bound states to appear in the spectrum. The alternative choice which does conserve the species is given by

$$\mathcal{R}_{1,2}^{\dagger}(0) = -\mathcal{L}_{1,2}^{\dagger}(0), \quad (7)$$

$$\mathcal{R}_{1,2}^{\dagger}(L) = -\mathcal{L}_{1,2}^{\dagger}(L) \quad (8)$$

and does not allow for boundary bound states to form. These boundary conditions are introduced as a point of comparison to the more natural and nontrivial case of (5) and (6); however, it is worthwhile to note that it may be possible to engineer such boundary conditions through application of

appropriate boundary fields or perhaps coupling to magnetic impurities [40]. In both cases the minus sign accounts for the π phase shift a particle acquires after scattering from a hard wall [32].

IV. BOUNDARY BOUND STATES

We are now in a position to examine the system using the Bethe ansatz, first for the spin-conserving boundary condition (5). We begin by considering the single-particle eigenstates and introduce the notation $\Psi_\xi^\dagger(x, \theta) = e^{i\Delta \sinh(\theta)x/v_F} [e^{\theta/2} \mathcal{R}_\xi^\dagger(x) + \eta e^{-\theta/2} \mathcal{L}_\xi^\dagger(x)]$, where $\eta = (-1)^{\xi-1}$ for $\xi = 1, 2$. In terms of this we can express the single-particle eigenstates as

$$|\epsilon(\theta)\rangle = \int_0^L dx \sum_{\xi=1}^2 [A_+^\xi \Psi_\xi^\dagger(x, \theta) + A_-^\xi \Psi_\xi^\dagger(x, -\theta)] |0\rangle. \quad (9)$$

Acting on this with the Hamiltonian, we find that this has energy $\epsilon(\theta) = \Delta \cosh(\theta)$ and satisfies the boundary condition at $x = 0$ provided $\vec{A}_+ = K_L(\theta) \vec{A}_-$, where

$$K_L(\theta) = \frac{-1}{\cosh(\theta)} \begin{pmatrix} 1 & -\sinh(\theta) \\ \sinh(\theta) & 1 \end{pmatrix} \quad (10)$$

and $\vec{A}_\pm = (A_\pm^1, A_\pm^2)^T$. This also satisfies the boundary condition at $x = L$ if $e^{-2i\Delta \sinh(\theta)L/v_F} \vec{A}_- = K_R(\theta) \vec{A}_+$, where $K_R(\theta) = K_L^{-1}(\theta) = K_L(-\theta)$. Combining these two, we get $e^{-2i\Delta \sinh(\theta)L/v_F} \vec{A}_- = K_R(\theta) K_L(\theta) \vec{A}_-$, which is the boundary condition of free fermions. The single-particle rapidities therefore are quantized according to

$$e^{-2i\Delta \sinh(\theta)L/v_F} = 1. \quad (11)$$

We may interpret this equation in the following fashion: The left-hand side is the total phase shift accrued from the plane wave in (9) by a particle which travels a distance $2L$ from one side of the system to the other and then back to its original position. The right-hand side provides the additional phase shift the particle acquires from scattering off of both boundaries. In this instance the contributions from both boundaries cancel each other. In the interacting case considered below, the right-hand side will be significantly modified to account for the scattering between particles.

Solutions of this equation constitute single-particle scattering states of the model and have a twofold degeneracy corresponding to the eigenvectors $\vec{A}_- = (1, 0)^T$ or $(0, 1)^T$. Note that θ and $-\theta$ correspond to the same state, while at $\theta = 0$ the wave function vanishes. We therefore restrict ourselves to the real part of the rapidity being positive, $\text{Re}(\theta) > 0$, while the imaginary part may be zero or π , with the latter choice giving negative-energy particles.

We may also construct zero-energy boundary bound states of the model. Taking $\theta = i\pi/2$ and $A_-^\xi = 0$ in the above expression for an eigenstate, we have a state which decays as $e^{-\Delta x/v_F}$ and satisfies the boundary conditions at both $x = 0, L$, provided $A_+^2 = -iA_+^1$. Explicitly, this is

$$\int_0^L dx e^{-\Delta x/v_F} \{[\mathcal{R}_1^\dagger(x) - \mathcal{L}_2^\dagger(x)] + i[\mathcal{R}_2^\dagger(x) - \mathcal{L}_1^\dagger(x)]\} |0\rangle.$$

From this we can see that the bound state is invariant under the previously mentioned \mathbb{Z}_2 transformation, $\mathcal{R}_{1,2}^\dagger(x) \leftrightarrow -\mathcal{L}_{2,1}^\dagger(x)$, which preserves the boundary conditions (5) and (6). The same transformation performed on the unbound state, (9), results in a change in sign of the energy. The coherence length of the bound state is given by $\xi = v_F/\Delta$.

A similar zero-energy bound state localized on the right-hand boundary can also be constructed by taking $\theta = -i\pi/2$, instead giving a state which decays as $e^{-\Delta|L-x|/v_F}$. Both bound states occur at the poles of the boundary S matrices, K_L and K_R , but, importantly, are not solutions of the quantization condition (11). If, instead, we choose the boundary conditions (7) and (8), we have that $K_L = K_R = \mathbb{1}$. Evidently, this has no poles and does not support bound states, but nevertheless, the spectrum is also determined by (11).

V. NONINTERACTING MODEL

Before proceeding to the fully interacting model, it is instructive to construct the ground state and excitations of the free model which follows a similar methodology. The N -particle eigenstates when $g = 0$ are merely products over the single-particle states, (9), with rapidities θ_j , $j = 1, \dots, N$. The energy of this state is the sum over single-particle energies $\sum_j \epsilon(\theta_j)$. In the thermodynamic limit, $N, L \rightarrow \infty$, this sum can be changed to an integral $\sum_j \rightarrow L \int_0^\Lambda d\theta \rho_0(\theta)$, where Λ is a cutoff imposed on the rapidities and $\rho_0(\theta)$ is the distribution of rapidities in the state. This distribution is defined in the standard way as [41–44]

$$\rho_0(\theta_j) = \frac{n_{j+1} - n_j}{L(\theta_{j+1} - \theta_j)} \quad (12)$$

where n_j are the integer quantum numbers of the state. They arise from taking the logarithm of (11) such that $n_j = \Delta \sinh(\theta_j)L/v_F$. Note that n_j may be positive or negative depending on the imaginary part of θ_j but must all be distinct and nonzero in order to have a nonvanishing wave function.

The ground state is constructed by taking the values $n_j = -j$, so that it consists of negative-energy particles with no holes. Using this along with (12), we find that the ground-state distribution in the thermodynamic limit is

$$\rho_0(\theta) = \frac{\Delta}{\pi v_F} \cosh(\theta) - \frac{\delta(\theta)}{L}. \quad (13)$$

Here we have subtracted off a δ function so that the distribution is defined for $\theta \geq 0$ and the hole at $\theta = 0$ is accounted for. The cutoff is then fixed by using $D = \int_0^\Lambda d\theta \rho_0(\theta)$, where $D = N/L$ is the density. From this we have that $\Lambda = \ln(2\pi v_F D'/\Delta)$, with $D' = D + 1/L$. The ground-state energy density is then simply given by

$$\epsilon_0 = - \int_0^\Lambda d\theta \rho_0(\theta) \Delta \cosh \theta \quad (14)$$

$$= - \frac{\pi \hbar v_F}{2} D'^2 - \frac{\Delta^2}{2\pi} \ln \left(\frac{2\pi v_F D'}{\Delta} \right) + \frac{\Delta}{L}. \quad (15)$$

In the noninteracting model the ground state (and all other states) enjoys a large degeneracy coming from the amplitude of the wave function which takes the form $[\otimes_{j=1}^M (0, 1)^T] \otimes$

$[\otimes_{j=1}^{N-M} (1, 0)^T]$ for $M \leq N/2$. This degeneracy coming from the decoupling of the species is completely lifted in the interacting case.

The excitations above this ground state consist of either removing a negative-energy particle at, say, $\theta = \theta_h + i\pi$, from the ground state or adding a positive-energy particle on top of this at $\theta = \theta_p$. In the former case we modify ground-state quantum numbers so that one of the integers, n_j , is missing. The distribution is then modified to include this hole, $\rho_0(\theta) \rightarrow \rho_0(\theta) - \delta(\theta - \theta_h)/L$. For either, the energy increase is $\Delta \cosh(\theta_{h,p})$, and the particle number is changed by $\delta N = \pm 1$. Particle-hole excitations, i.e., a state with both types of excitations, leave the particle number unchanged and have a minimum energy of 2Δ , which is the energy gap of the noninteracting system.

On top of this state we may add either one or two bound states with no change in the energy, meaning that the ground state has a further fourfold degeneracy. Unlike the typical degeneracy associated with a free model discussed above, the addition of bound states changes the total fermion number to $N_{\text{total}} = N + n_B$, with n_B being the number of bound states in the system. Consequently, the total fermion parity, defined as $\mathcal{P} = (-1)^{N+n_B}$, may be changed by their inclusion.

In the interacting model we will see that by adding particles or holes to the ground state the distribution is shifted. This leads to a change in the dispersion relation of the excitations as well as the energy gap. The same is true when bound states are added to the system; the ground-state distribution is shifted, and their associated degeneracy is lifted.

VI. MANY-BODY EIGENSTATES

In the interacting model the many-particle eigenstates can be constructed in the standard Bethe ansatz fashion [42,44]. The N -particle scattering eigenstate of energy $E = \sum_{j=1}^N \epsilon(\theta_j)$ is given by

$$|\vec{\epsilon}\rangle = \sum_{\vec{\xi}, \vec{\sigma}, Q} \int_0^L dx A_{\vec{\sigma}}^{\vec{\xi}}[Q] \Theta(x_Q) \prod_{j=1}^N \Psi_{\xi_j}^{\dagger}(x_j, \sigma_j \theta_j) |0\rangle, \quad (16)$$

where $\Theta(x_Q)$ are Heaviside functions which are nonzero only for a particular ordering of particles, e.g., $x_1 < x_2 < \dots < x_N$. The orderings of particles are labeled by Q , which are elements of the symmetric group of N objects \mathcal{S}_N . We sum over all such orderings as well as combinations $\vec{\sigma} = (\sigma_1, \dots, \sigma_N)$, with $\sigma_j = \pm$, and $\vec{\xi} = (\xi_1, \dots, \xi_N)$, with $\xi_j = 1, 2$. The coefficients $A_{\vec{\sigma}}^{\vec{\xi}}[Q]$ are the amplitudes for one specific choice of $Q, \vec{\sigma}$, and $\vec{\xi}$ and are related to each other by products of the boundary S matrices $K_{L,R}$ [see the text above (10) for the analogous condition in the noninteracting case] and two particle S matrices S_{ij} . These two-particle S matrices act on the internal space of the i th and j th particles and are determined to be

$$S_{ij}(\theta_i - \theta_j) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{\sinh[\theta_i - \theta_j]}{\sinh[\theta_i - \theta_j - i\delta]} & \frac{\sinh[-i\delta]}{\sinh[\theta_i - \theta_j - i\delta]} & 0 \\ 0 & \frac{\sinh[-i\delta]}{\sinh[\theta_i - \theta_j - i\delta]} & \frac{\sinh[\theta_i - \theta_j]}{\sinh[\theta_i - \theta_j - i\delta]} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (17)$$

where $\delta = 2 \arctan(g/2v_F)$ is the two-particle phase shift. In deriving this relationship between the phase shift δ and the interaction strength we have chosen a specific regularization of the δ function interaction in the model. The functional form of $\delta(g)$ depends upon this and is therefore not universal except at small g , where $\delta \approx g/v_F$ [45], with positive and negative δ corresponding to the repulsive and attractive regimes, respectively. However, the relationship between δ and K_{\pm} is universal and is given by [39,46]

$$K_- = 1 - \frac{\delta}{\pi}, \quad K_+ = \frac{1}{1 + \delta/\pi}, \quad (18)$$

where we are restricted to $\delta \in [-\pi, \pi]$.

As in the noninteracting case, the particle rapidities are quantized by applying the boundary conditions at $x = 0, L$. This leads to an eigenvalue problem, similar to (11), to determine θ_j ,

$$e^{-2i\Delta \sinh(\theta_j)L/v_F} A_-[\mathbb{1}] = Z_j(\theta_j) A_-[\mathbb{1}], \quad (19)$$

with

$$\begin{aligned} Z_j(\theta_j) &= S_{jj-1}(-\theta_j - \theta_{j-1}) \cdots S_{j1}(-\theta_j - \theta_1) K_R(\theta_j) \\ &\quad \times S_{j1}(\theta_j - \theta_1) \cdots S_{jN}(\theta_j - \theta_N) K_L(\theta_j) \\ &\quad \times S_{jN}(-\theta_j - \theta_N) \cdots S_{jj+1}(-\theta_j - \theta_{j+1}) \end{aligned} \quad (20)$$

and where $A_-[\mathbb{1}]$ is the amplitude for the configuration $x_j < x_k$ for $j < k$ and $\sigma_j = -1 \forall j$. This can be interpreted in the same way as the noninteracting model. The eigenvalues of the object $Z_j(\theta_j)$ are the total phase shift acquired by the particle as it traverses the system, scattering off all other particles and both boundaries as it does so. In the noninteracting limit two-particle S matrices become identities, and we recover $Z_j(\theta_j) = K_R(\theta_j) K_L(\theta_j) = \mathbb{1}$.

Before discussing the solution of this eigenvalue equation we examine the case where bound states are present also. In the same manner as (16) we may also construct many-particle eigenstates which include either or both bound states at the edges of the system. Adding these on top of the previously constructed N -particle eigenstate, we have

$$|\vec{\epsilon}\rangle_B = \sum'_{\vec{\xi}, \vec{\sigma}, Q} \int_0^L dx A_{\vec{\sigma}}^{\vec{\xi}}[Q] \Theta(x_Q) \prod_{j=0}^{N+1} \Psi_{\xi_j}^{\dagger}(x_j, \sigma_j \theta_j) |0\rangle, \quad (21)$$

where x_0, x_{N+1} are the coordinates for the bound states at the left and right boundaries and the sum over orderings now extends to elements of \mathcal{S}_{N+2} because there are $N + 2$ particles in total. In addition, the primed sum indicates that we sum over all possible flavor combinations but we restrict ourselves to $\sigma_0 = \sigma_{N+1} = +$ and $\theta_0 = -\theta_{N+1} = i\pi/2$. Note that the coherence length of the bound state remains unchanged in the presence of interactions $\xi = v_F/\Delta$, as is the case for Majorana bound states [47,48].

The energy of this eigenstate, being the sum of single-particle energies, has the same form as that in which there are no bound states, $E = \sum_{j=1}^N \epsilon(\theta_j)$. However, θ_j are coupled together, and their allowed values are shifted by the presence of the bound states. In particular when there are bound states at both of the edges, the boundary conditions impose Eqs. (19) and (20) but with the boundary matrices replaced with $K_{L,R} \rightarrow$

$K_{L,R}^B$, where

$$\begin{aligned} K_R^B(\theta_j) &= S_{N+1}(-\theta_j + i\pi/2)K_R(\theta_j)S_{N+1}(\theta_j + i\pi/2), \\ K_L^B(\theta_j) &= S_{0j}(\theta_j - i\pi/2)K_L(\theta_j)S_{0j}(-\theta_j - i\pi/2). \end{aligned} \quad (22)$$

Alternatively, one may consider a bound state at only one of the boundaries by replacing only one of $K_{L,R}$.

VII. BETHE ANSATZ EQUATIONS

The spectrum of our model can be determined by obtaining the eigenvalues of the operator $Z_j(\theta_j) \forall j$. This can be solved by means of the off-diagonal Bethe ansatz method, and in fact, it maps directly onto the solution of the inhomogeneous XXZ model with certain open boundary conditions [22]. To make use of this solution and simplify the calculation somewhat we modify the right-hand boundary so that it is given by $K'_R(\theta) = K_R(\theta - i\delta)$ [49]. This reduces to the previous case in the noninteracting limit and also generalizes the relationship between the two boundaries to $K_R(\theta) = K_L(-\theta + i\delta)$, which is known as boundary crossing invariance [20]. With this modification we find that the particle rapidities θ_j are quantized according to

$$e^{-2i\Delta \sinh(\theta_j)L/v_F} = \prod_{\sigma=\pm} \prod_{\alpha=1}^M \frac{\sinh[\theta_j - \sigma\mu_\alpha + i\delta/2]}{\sinh[\theta_j - \sigma\mu_\alpha - i\delta/2]}, \quad (23)$$

where the parameters μ_α are known as Bethe parameters which describe the flavor degrees of freedom. They are determined by the following equations:

$$\begin{aligned} &\left[\frac{\cosh^2[\mu_j + i\delta/2]}{\cosh^2[\mu_j - i\delta/2]} \right]^{2-n_B} \prod_{\sigma=\pm} \prod_{\beta \neq \alpha}^M \frac{\sinh[\mu_\alpha + \sigma\mu_\beta + i\delta]}{\sinh[\mu_\alpha + \sigma\mu_\beta - i\delta]} \\ &= \prod_{\sigma=\pm} \prod_{k=1}^N \frac{\sinh[\mu_\alpha + \sigma\theta_k + i\delta/2]}{\sinh[\mu_\alpha + \sigma\theta_k - i\delta/2]}, \end{aligned} \quad (24)$$

where, as before, $M \leq N/2$ is an integer. We consider only positive values of θ_j, μ_α , and furthermore, all rapidities and Bethe parameters must be distinct, $\theta_j \neq \theta_k, \mu_\alpha \neq \mu_\beta$, and nonzero; otherwise, the corresponding wave function vanishes [42,50]. The set of equations given in (23) and (24) is the Bethe ansatz equations.

The first term on the left-hand side of (24) is the combined phase shift a particle accumulates after scattering off both boundaries and any bound states which are attached to them. If we were to consider the alternative boundary condition given by (7) and (8), which does not mix the flavors, this term would be absent. Interestingly, this has the same effect on the Bethe parameters and therefore spectrum as the presence of both bound states, i.e., $n_B = 2$. The next term on the left-hand side is due to the interaction with other particles within the bulk of the system. These terms vanish upon taking $\delta = 0$, whereupon we recover (11).

The Bethe equations also reduce to (11) when $\delta = \pm\pi$, indicating that there is a self-duality in the theory, i.e., a mapping from the model to itself at a different value of the interaction strength [51]. To investigate this further, note that the Bethe equations are invariant under the combined transformation $\delta \rightarrow -\delta$ along with $\theta_j \rightarrow \theta_j + i\pi$; however,

this changes the sign of the energy, $\sum_j \epsilon(\theta_j) \rightarrow -\sum_j \epsilon(\theta_j)$. Thus, the spectrum is inverted under a change in sign of the interaction strength. This is a manifestation of the particle-hole transformation of our original model. Furthermore, it can be checked that the replacement $\delta \rightarrow \pi - |\delta|$ along with a redefinition $\mu_\alpha \rightarrow \mu + i\pi/2$ has the same effect on the Bethe equations as taking $\delta \rightarrow -\delta$. Combining these two maps therefore leaves the spectrum invariant and allows us to restrict our analysis to $\delta \in [0, \pi/2]$ with results outside this region found using the above transformations.

VIII. GROUND STATE

The structure of the Bethe equations is similar to those appearing in the solutions of a number of other models [37,39,46], and the present analysis follows similar lines using the methodology presented for the noninteracting case.

When $0 \leq \delta \leq \frac{\pi}{2}$, the ground state consists of all θ_j lying on the $i\pi$ line and $M = N/2$. Using this in (23) and (24) and then taking their logarithm, we have

$$\begin{aligned} \frac{\Delta}{\pi v_F} \sinh(\theta_j)L &= n_j - \sum_{\sigma=\pm} \sum_{\alpha=1}^{N/2} \phi_1(\theta_j - \sigma\mu_\alpha), \\ \sum_{\substack{j=1 \\ \sigma=\pm}}^N \phi_1(\mu_\alpha - \sigma\theta_j) &= I_j + \sum_{\substack{\beta=1 \\ \sigma=\pm}}^{N/2} \phi_2(\mu_\alpha - \sigma\mu_\beta) + g(\mu_\alpha). \end{aligned} \quad (25)$$

Here n_j and I_j are integers which are the quantum numbers of the interacting system, and $\phi_n(x, y) = \frac{i}{2\pi} \ln \left[\frac{\sinh(x+i\pi\delta/2)}{\sinh(x-i\pi\delta/2)} \right]$, $g(\mu) = i \frac{2-n_B}{\pi} \ln \left[\frac{\cosh[\mu_j+i\delta/2]}{\cosh[\mu_j-i\delta/2]} \right]$. In the thermodynamic limit we may describe the ground state via the rapidity distribution $\rho(\theta)$, defined by (12) and the analogous distribution for the Bethe parameters $\nu(\mu)$, which is defined similarly. In the thermodynamic limit, Eqs. (25) become a set of coupled integral equations,

$$\begin{aligned} \frac{\Delta}{\pi v_F} \cosh(\theta) - \frac{\delta(\theta)}{L} &= \rho(\theta) - \int d\mu \phi'_1(\theta - \mu)\nu(\mu), \\ \int d\theta \phi'_1(\mu - \theta)\rho(\theta) - \frac{\delta(\mu)}{L} &= \nu(\mu) + \int d\zeta \phi'_2(\mu - \zeta)\nu(\zeta) - \frac{\phi'_2(2\mu)}{L} - \frac{g'(\mu)}{L}, \end{aligned} \quad (26)$$

where the δ functions are included to account for the holes at $\theta = \mu = 0$. These equations may be solved via Fourier transform with the result

$$\rho(\theta) = \frac{2\Delta}{\pi v_F} \cosh(\theta) + \rho_{\text{bdry}}(\theta) + \rho_B(\theta), \quad (27)$$

$$\nu(\mu) = \frac{\Delta \cosh(\mu)}{\pi v_F \cos(\delta/2)} + \nu_{\text{bdry}}(\mu) + \nu_B(\mu). \quad (28)$$

The first terms in the above expressions correspond to the bulk contribution; note that the rapidity distribution is modified in the interacting case compared to (13). The next terms arise

due to the presence of the boundary; they are distinguished from the bulk by being of order $1/L$ and are independent of the number of bound states. The last terms are those which are attributable to the bound states and are proportional to n_B/L . The total energy density of the state is determined solely by the rapidity distribution via $\varepsilon_g = -\int d\theta \rho(\theta)\Delta \cosh(\theta)$, giving

$$\varepsilon_g = \varepsilon_0 + \frac{\Delta}{L} \left[\frac{1}{2 \cos(\delta/2)} - \sqrt{2} \cos(\delta/2) \right] + \frac{n_B - 2}{L} \varepsilon_B.$$

The first term here is the bulk energy density which is given by (15) modulo a δ -dependent shift in D' [52] which vanishes in the thermodynamic limit; the remaining terms are due to the boundary conditions and bound states, with ε_B being the energy per bound state.

Before discussing this bound-state contribution to the energy we shall comment on the excitations of the model. The lowest-lying excitations come in two forms, the first of which are similar to the noninteracting case. They can be created by placing the hole in the rapidity distribution at $\theta = \theta_h + i\pi$ or adding a positive-energy particle at $\theta = \theta_p$; in either case the energy is given by $\varepsilon_1(\theta_{h,p}) = 2\Delta \cosh(\theta_{h,p})$. The factor of 2 present here compared to the noninteracting case can be traced to the overall factor of 2 in (27). A particle-hole excitation of this type has a minimum energy of 4Δ , which is twice that of the noninteracting model. The second type of excitation involves placing a hole in the distribution of Bethe roots at, say, $\mu = \theta_h$. In this case the energy is given by $\varepsilon_2(\theta_h) = \frac{\Delta \cosh(\theta_h)}{\cos(\delta/2)}$. As a result the gap in the interacting system is increased to $2\Delta_g$, where

$$\Delta_g = \frac{\Delta}{\cos(\delta/2)}. \quad (29)$$

The bound-state contribution to the rapidity distribution is used to determine the bound-state energy via $\varepsilon_B = -L \int d\theta \rho_B(\theta)\Delta \cosh(\theta)/n_B$, where

$$\rho_B(\theta) = -\frac{n_B}{L} \int \frac{d\omega}{2\pi} \frac{e^{-i\omega\theta} \sinh[\pi\omega/2] \sinh[\delta\omega/2]}{\sinh[(\pi-\delta)\omega/2] \sinh[(\pi+\delta)\omega/2]},$$

from which we have that the energy per bound state for $0 \leq \delta \leq \pi/2$ is given by $\varepsilon_B = \Delta_g \tan[\delta/2] = \Delta_g \sqrt{(\Delta_g/\Delta)^2 - 1}$. We can then combine this with the various symmetries of the Bethe equations discussed above and reconstruct the bound-state energy for all values of δ to be

$$\varepsilon_B = \begin{cases} \Delta_g \tan(\delta/2) & 0 \leq |\delta| \leq \frac{\pi}{2}, \\ \Delta_g \cot(\delta/2) & \frac{\pi}{2} \leq |\delta| \leq \pi. \end{cases} \quad (30)$$

We see that the bound-state energy is pushed below the Fermi level for $\delta < 0$ and above it for $\delta > 0$, indicating that there is a first-order phase transition at $\delta = 0$. For attractive interactions the ground state consists of a filled Fermi sea with bound states at both ends. Similar transitions are known to occur when magnetic impurities are present in superconductors [9–12, 53–57]. Therein, Shiba or Andreev bound states form at the impurity. In such cases the transition is accompanied by a change in the fermion parity of the ground

state. In the present case this does not occur as bound states will be present at both ends of the wire, leaving \mathcal{P} invariant.

For $|\delta| \leq \pi/2$, $|\varepsilon_B|$ increases, and at $\delta = \pm\pi/2$ it touches the continuum of states in the conduction or valence bands. Upon further increasing $|\delta|$, ε_B undergoes a sharp change in behavior, turning away from the bands and again approaching the Fermi level. Recall that there are holes at $\theta = 0$, and so the bound state does not become degenerate with any scattering state. This sharp avoided level crossing is a consequence of the self-duality of the model, i.e., the invariance of the spectrum under the combined transformations, $\delta \rightarrow -\delta$ and then $\delta \rightarrow \pi - |\delta|$, with the avoided crossing occurring at the special point $\delta = \pm\pi/2$, which corresponds to $\xi \Delta_g/v_F = \sqrt{2}$. As a result the bound states cannot couple to scattering states and are protected from decay. Therefore, in contrast to noninteracting systems where boundary modes are protected by symmetry, in the interacting model they are protected by self-duality.

The bound-state energy reaches the Fermi level once again at the strongly interacting points $\delta = \pm\pi$, indicating that the symmetry of the noninteracting model is restored. This can be seen also in the bosonic language. At the points $\delta = \pi$ the spin Luttinger parameter vanishes, $K_- = 0$, while at $\delta = -\pi$ we have $1/K_+ = 0$. In either case the fields ϕ_{\pm} decouple from each other with only one being gapped. In these cases the bosonic model, (3), can be mapped to a quadratic model of spinless fermions [47]. Therein, the bound states lie at the Fermi level, in agreement with (30) derived using self-duality.

IX. CONCLUSIONS

In this paper we have studied the boundary bound states of a one-dimensional, spinful quantum wire. The wire Hamiltonian has a proximity-induced p_x -wave triplet pairing and density-density interactions. We have solved this system exactly using the Bethe ansatz for a range of parameters and constructed the ground state and excitations of the model. It was shown that for a choice of boundary conditions which breaks time-reversal symmetry, the system can support bound states localized at both ends. The bound-state energy lies at the Fermi level, within the energy gap, when interactions are absent but is shifted when interactions are present. For attractive interactions the bound-state energy is pushed below the Fermi level, while in the repulsive case it is pushed up. This causes a first-order phase transition to occur at zero temperature. Unlike similar transitions in superconductor-impurity systems, this is not accompanied by a change in fermion parity.

The bound-state energy is seen to approach the gap Δ_g as the interaction strength $|\delta|$ is increased but undergoes a sharp avoided level crossing at $\delta = \pm\pi/2$, thus preventing the bound state from entering the continuum of scattering states and decaying. This is a consequence of the self-duality of the model which relates the spectra of the model at different values of the interaction strength.

In the noninteracting case the bound states lead to a Lorentzian, zero-bias peak in the conductance through the edge [29]. When interactions are present, this peak will be shifted owing to the nonzero energy of the bound states but

shall remain in the gap. In addition the Lorentzian shape of the peak is maintained in the presence of interactions owing to the fact that pairing term has scaling dimension 1 irrespective of the value of δ [37,39]. For a more general form of the interaction, which may break the integrability of the model, one can expect that the scaling dimension becomes a function of δ , leading to an energy gap which has a power

law dependence on Δ as well as a power law decay of the conductance away from the peak [25–27].

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