The Frustration of being Odd: Can Boundary Conditions induce a Quantum Phase Transition?

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The answer to the question in the title is clearly “No”, but we report on something very similar to that, namely a “Boundary-less Wetting Transitions” (BWT). We consider the effect of frustrated boundary condition (FBC) on generic local spin-1/2 chains in zero field, specifically, we apply periodic boundary conditions on chains with an odd number of sites. In a previous work, we already proved that when only one antiferromagnetic interaction dominates over ferromagnetic ones, in the thermodynamic limit local order (expressed by the spontaneous magnetization) is destroyed.

Here, we show that with two competing AFM interactions a new type of order can emerge, with a magnetization profile that varies in space with an incommensurate pattern. This modulation is the result of a ground state degeneracy which leads to a breaking of translational invariance. The transition between the two cases is signaled by an intensive discontinuity in the first derivative of the ground state energy: this is thus not a standard first-order QPT, but rather looks like a boundary QPT, in a system without boundaries, but with FBC.

Modern physics follows a reductionist approach, in that it tries to explain a great variety of phenomena through the minimal amount of variables and concepts. Thus, a successful theory should apply to a number as large as possible of situations and provide a predictive framework, depending on a number of variables as small as possible, within which one can describe the physical systems of interest. On the other hand, further discoveries tend to enrich the phenomenology making more complicated, for the existing theories, to continue to predict accurately all the situations, sometimes to the point of exposing the need for new categories altogether.

Landau’s theory of phases is a perfect example of such an evolution [1]. Toward the middle of the last century [2], all the different phases of many-body systems obeying classical mechanics were classified in terms of local order parameters that, turning from zero to a non-vanishing value, signal the onset of the corresponding order. Each order parameter is uniquely associated with a particular kind of order, which in turn can be traced back to a specific local symmetry that is violated in that phase [3]. Hence symmetries play a key role in Landau’s theory, while other features, such as boundary conditions, are deemed negligible (at least in the thermodynamic limit).

Because of its success, Landau’s theory has been borrowed at first without modifications in the quantum regime [4]. Nonetheless, after a few years, it has become clear that the richness of quantum many-body systems goes beyond the standard Landau paradigm. Indeed, topologically ordered phases [5] [6], that have no equivalent in the classical regime, as well as nematic ones [7], represent instances in which violation of the same symmetry is associated with different (typically non-local) and non-equivalent order parameters [8] [10], depending on the model under analysis. This implied that Landau’s theory had to be extended to incorporate more general concepts of order, which include the non-local effects that come along with the quantum regime and have no classical counterpart.

In more recent years, even boundary conditions, which are expected to be irrelevant for the onset of a classical ordered phase in the thermodynamic limit, have been shown to play a role when paired with quantum interactions. Intuitively, one supposes that the contributions of boundary terms, that increase slowly with the size of the system with respect to the bulk ones, can be neglected when the dimension of the system diverges [11] [13]. Recently, this intuition has been challenged with hard, mathematical proofs. Indeed, it was proven that finite-size data is not always sufficient to determine whether a system is gapless or gapped in the thermodynamic limit, even in translational invariant systems [14] [15]. Furthermore, a concrete example of a boundary-driven quantum phase transition was provided, showing that, by tuning the coupling between the edges of an open chain, the system can visit different phases [16]. In this line of research, particular attention was devoted to analyzing one-dimensional translational-invariant antiferromagnetic (AFM) spin models in frustrated boundary conditions (FBCs), i.e. periodic boundary conditions in rings with an odd number of sites N. For purely classical systems (Ising chains), FBCs produce 2N degenerate lowest energy states, characterized by one domain wall defect in one of the two Neel orders. Quantum effects split this degeneracy, producing, in the thermodynamic limit, a Galilean band of gapless excitation in touch with the lowest energy state(s) [17] [20] in a phase that, without frustration, would otherwise be gapped. The so-obtained ground state can indeed be characterized as a one-particle excitation moving in a strongly correlated background state [21]. Even if a single particle excitation does not appear to be very relevant when the size of the system diverges, in [22] we showed that it is sufficient to destroy
the AFM local order and to replace it with a mesoscopic ferromagnetic order.

The results in [22] were obtained considering a system in which a dominant AFM coupling in just one direction competes with ferromagnetic ones in the orthogonal axes. On the contrary, here we focus on the analysis of the transition that occurs when also a second interaction becomes AFM. Indeed, we find a discontinuity in the first derivative of the free energy at zero temperature (i.e., the ground state energy) associated with a doubling of the ground state degeneracy, even at finite sizes. This picture is coherent with a first-order phase transition. This is surprising since this discontinuity does not exist with other boundary conditions (BC), such as open (OBC) or periodic (PBC) boundary conditions with an even $N$. Moreover, the discontinuity in the first derivative of the free energy does not diverge and remains finite in the thermodynamic limit, in contrast with traditional first-order transitions. Hence, what we observe is akin to a “Boundary-less Wetting Transitions” (BWT).

In the new phase, the increased degeneracy of the ground state allows for the existence of a new magnetic order. In this case the magnetization is (almost) staggered as in the standard antiferromagnetic case, but with a modulation that makes its amplitude slowly varying in space. From a physical point of view, the presence of the modulation superimposed to the standard magnetization can be easily understood. Indeed, since perfect staggered order is not sustainable with FBC, the system has only two options: a) either to implement a mesoscopic ferromagnetic order as in the case discussed in [22], or b) to realize an almost staggered order with momentum $\pi - \pi/N$. In the latter case, while the new order cannot be distinguished from the usual one for neighboring sites, it becomes manifest over the whole chain, producing the modulation we are going to discuss in the following.

We illustrate our results discussing the XY chain at zero field in FBC. Even if this phenomenon is not limited to this model, it is useful to focus on it, because exploiting the well–known Jordan–Wigner transformation [20] we can evaluate all the quantities that we need with an almost completely analytical approach. The Hamiltonian describing this system reads

$$H = \sum_{j=1}^{N} \cos \phi \, \sigma_{j}^{x} \sigma_{j+1}^{x} + \sin \phi \, \sigma_{j}^{y} \sigma_{j+1}^{y},$$

where $\sigma_{j}^{\alpha}$, with $\alpha = x, y, z$, are Pauli matrices and $N$ is the number of spins in the lattice. Having assumed frustrated boundary conditions, we have that $N = 2M + 1$ is odd and $\sigma_{j}^{\alpha} = \sigma_{j+N}^{\alpha}$. The angle $\phi \in (-\pi, \pi)$ tunes the relative weight of the two interactions, as well as the sign of the smaller one. Hence, while the role of the dominant term is always played by the AFM interaction along the $x$-direction, we have that the second Ising–like interaction switches from FM to AFM at $\phi = 0$.

Regardless of the value of $\phi$, the Hamiltonian in eq. (14) commutes with the parity operators ($\Pi^{\pm} = \otimes_{j=1}^{N} \sigma_{j}^{z}$), i.e. $[H, \Pi^{\pm}] = 0$, $\forall \alpha$. At the same time, since we are considering odd $N$, different parity operators satisfy the conditions (14) and (15) for the odd number of sites $N$, hence implying that each eigenstate is at least two-fold degenerate: if $|\psi\rangle$ is an eigenstate of both $H$ and $\Pi^{\pm}$, then $\Pi^{\pm} |\psi\rangle$, that differs from $\Pi^{\mp} |\psi\rangle$ by a global phase factor, is also an eigenstate of $H$ with the same energy but opposite $z$-parity.

Mapping spins into spinless fermions, the model can be analytically diagonalized [26]. Indeed, by means of a Fourier transform, followed by a Bogoliubov rotation, the Hamiltonian can be reduced to [27]

$$H^{\pm} = \sum_{q \in \Gamma^{\pm}} \epsilon(q) \left( \begin{array}{c} a_{q}^\dagger a_{q} - \frac{1}{2} \\ \end{array} \right).$$

Here $a_{q} (a_{q}^\dagger)$ is the annihilation (creation) fermionic operator with momentum $q$. The momenta run over two disjoint sets, corresponding to the two different sectors of $z$-parity: $\Gamma^{-} = \{ 2\pi k/N \}$ and $\Gamma^{+} = \{ 2\pi (k + \frac{1}{2})/N \}$ with $k \in [0, N-1]$. The dispersion relation reads

$$\epsilon(q) = 2 |\cos \phi \, e^{i2q} + \sin \phi|, \quad q \neq 0, \pi,$$

$$\epsilon(0) = -\epsilon(\pi) = 2 (\cos \phi + \sin \phi),$$

The eigenstates of $H$ are constructed by populating the vacuum states $|0^{\pm}\rangle$, taking care of the parity requirements. From eq. (3) we see that, assuming $\phi \in (-\pi, \pi)$, the single negative energy mode is $\epsilon(\pi)$, which lives in the even sector ($\pi \in \Gamma^{+}$). Therefore the lowest energy states are, respectively, $|0^{-}\rangle$ in the odd sector and $a_{q}^\dagger |0^{+}\rangle$ in the even one. But, since both of them violate the parity constraint of the relative sector, they cannot represent physical states. Hence, the physical ground states must be recovered from $|0^{-}\rangle$ and $a_{q}^\dagger |0^{+}\rangle$ considering the minimal excitation coherent with the parity constraint.

We have two different pictures depending on the sign of $\phi$. For $\phi < 0$ the excitation energy, given by eq. (3), admits two equivalent local minima, one for each parity, i.e. $q = 0 \in \Gamma^{-}$ and $q = \pi \in \Gamma^{+}$. Consequently, the ground state is two-fold degenerate, and the two ground states that are also eigenstates of $\Pi^{\pm}$ are $|g_{0}^{-}\rangle = a_{0}^\dagger |0^{-}\rangle$ and $|g_{0}^{+}\rangle = |0^{+}\rangle = \Pi^{x} |g_{0}^{-}\rangle$, where the last equality holds up to a phase factor. On the contrary, when $\phi$ becomes positive, the energy in eq. (3) admits, for each $z$-parity sector, two local minima at opposite momenta, $\pm p \in \Gamma^{-}$ and $\pm p' \in \Gamma^{+}$. For a system size $N$ satisfying $N \mod 4 = 1$, $p$ and $p'$ are respectively equal to $p = \frac{\pi}{2} \left( 1 - \frac{1}{N} \right)$ and $p' = \frac{\pi}{2} \left( 1 + \frac{1}{N} \right)$. On the other hand, for $N \mod 4 = 3$, we
have $p = \frac{x}{2} (1 + \frac{1}{N})$ and $p' = \frac{x}{2} (1 - \frac{1}{N})$. Thus, for $\phi < 0$ the ground state manifold becomes 4-fold degenerate, with states of opposite parity and momenta. The latter degeneracy has a deep geometrical meaning, which goes beyond the exact solution to which the XY is amenable, and has to do with the fact that, with FBC, the lattice translation operator does not commute with the mirror (or chiral) symmetry, except than for states with $0$ or $\pi$ momentum. Thus, every other state must come in degenerate doublets of opposite momentum/chirality, regardless of the interactions [28]. Accordingly with this picture, a generic element in the four-dimensional ground state subspace can be written as

$$|g\rangle = u_1 |p\rangle + u_2 |-p\rangle + u_3 |p'\rangle + u_4 |-p'\rangle ,$$

(4)

where the superposition parameters satisfy the normalization constraint $\sum_i |u_i|^2 = 1$ and $|\pm p\rangle$ ($|\pm p'\rangle$) are states in the odd (even) $z$-parity sector equal to $|\pm p\rangle = a_{\frac{x}{2}p}^\dagger |0\rangle$ ($|\pm p'\rangle = a_{\frac{x}{2}p'}^\dagger |0\rangle$).

Hence, independently from $N$, once FBC conditions are imposed, the system presents a level crossing at the point $\phi = 0$, where the Hamiltonian reduces to the classical AFM Ising. The presence of the level crossing is reflected on the behavior of the ground state energy $E_g$, whose first derivative exhibits a discontinuity

$$\frac{dE_g}{d\phi} \bigg|_{\phi \to 0^-} - \frac{dE_g}{d\phi} \bigg|_{\phi \to 0^+} = 2 \left(1 + \cos \frac{\pi}{N}\right) ,$$

(5)

which goes to a nonzero finite value in the thermodynamic limit. The presence of both a discontinuity in the first derivative of the ground state energy, and a different degree of degeneracy even at finite sizes, is coherent with a first-order quantum phase transition [11].

However, such a transition is present only when FBCs are considered. Indeed, without frustration, hence considering either OPC or PBC conditions in a system with even $N$, the two regions $\phi \in (-\frac{\pi}{4}, 0)$ and $\phi \in (0, \frac{\pi}{4})$ belong to the same AFM phase, have the same degree of ground-state degeneracy, and exhibit the same physical properties [29][30]. Hence it is the introduction of the FBC that induces the presence of a quantum phase transition at $\phi = 0$.

Differently from what happens in standard first-order transitions, in the present case, the discontinuity in the first derivative does not diverge with the size of the system. This peculiar behavior of the ground state energy makes this transition very similar to a family of boundary phase transitions known as wetting transition [23][25], which are due to the existence of a border, interpreted as a defect. However, in our system, we cannot individuate any border, since the chain under analysis is perfectly invariant under spatial translation. Therefore we can call this a “Boundary-less Wetting Transition” (BWT).

Having detected a novel phase transition, we need to identify the two phases separated by it. In [22] it was proved that the two-fold degenerate ground state for $\phi < 0$ is characterized by a ferromagnetic mesoscopic order: for any odd $N$, the chain exhibits nonvanishing, site-independent, ferromagnetic magnetizations along any spin directions. These magnetizations scale proportionally to the inverse of the system size and, consequently, vanish in the thermodynamic limit. For suitable choices of the ground state, this mesoscopic magnetic order is present also for $\phi > 0$, but, taking into account that now the ground state degeneracy is doubled, the new phase can also show a novel magnetic order that was forbidden for $\phi < 0$. However, from all the possible orders we can, for sure, discard the standard staggerization that characterizes the AFM order in the absence of FBCs. In fact, for odd $N$, it is not possible to align the spins perfectly antiferromagnetically, while still satisfying PBC. In a classical system, the chain develops a ferromagnetic defect (a domain wall) at some point, but quantum-mechanically this defect gets delocalized and its effect is not negligible in the thermodynamic limit as one would naively think.

To study such a spatial dependence, it is useful to introduce the unitary lattice translation operator $T$, whose action shifts all the spins by one position in the lattice as

$$T^\dagger \sigma_j^\alpha T = \sigma_j^\alpha_{j+1} , \quad \alpha = x, y, z$$

(6)

and which commutes with the system’s Hamiltonian in eq. (14), i.e. $[H, T] = 0$. The operator $T$ admits, as a generator, the momentum operator $P$, i.e. $T = e^{iPT}$. Among the eigenstates of $P$, we have the ground state vectors $|\pm p\rangle$ and $|\pm p'\rangle$ with relative eigenvalues equal to $\pm p$ and $\pm(\pi + p') = \mp p$. The latter equality allows to identify the ground states $a_{\frac{x}{2}p}^\dagger a_{\frac{x}{2}p'}^\dagger |0\rangle$ with the states $|\pm p\rangle$.

We can exploit the properties of the operator $T$ to determine, for each odd $N$, the spatial dependence of the magnetizations along $x$ and $y$ in the ground state $|\tilde{g}\rangle$ ($\langle \sigma_j^\alpha \rangle_{\tilde{g}}$ with $\alpha = x, y$) defined as

$$|\tilde{g}\rangle = \frac{1}{\sqrt{2}} \left( |p\rangle + e^{i\theta} |p'\rangle \right) ,$$

(7)

where $\theta$ is a free phase. In fact, taking into account that $|p\rangle$ and $|p'\rangle$ live in two different $z$-parity sectors, we have that the magnetization along a direction orthogonal to $z$ on the state $|\tilde{g}\rangle$ is given by

$$\langle \sigma_j^\alpha \rangle_{\tilde{g}} = \langle \tilde{g} | \sigma_j^\alpha | \tilde{g} \rangle = \frac{1}{2} (e^{i\theta} \langle p | \sigma_j^\alpha | p' \rangle + e^{-i\theta} \langle p' | \sigma_j^\alpha | p \rangle) .$$

(8)

The magnetization is determined by the spin operator matrix elements $\langle p | \sigma_j^\alpha | p' \rangle$, that can all be related to the ones at the site $j = \tilde{N}$. In fact, considering eq. (28) we obtain

$$\langle p | \sigma_j^\alpha | p' \rangle = e^{i(\pi + p' - p)j} \langle p | \sigma_N^\alpha | p' \rangle .$$

(9)
The advantage of this representation is that the matrix element $\langle p | \sigma_N^x | p' \rangle$ is a real number for $\alpha = x$, and a purely imaginary one for $\alpha = y$. This role is singled out for the site $N$ by the choice made in the construction of the states through the Jordan-Wigner transformation. In particular, the mirror symmetry $M_N$ with respect to the $N$-th site maps $M_N | \pm p \rangle = \mp p \rangle$, while the reflections with respect to other sites introduce additional phase factors. (Further details can be found in supplementary materials). In this way we recover the spatial dependence of the magnetizations as

$$
(\sigma_j^y)_{\alpha} = (-1)^{N/2} \cos \left[ \frac{\pi}{N} j + \lambda(\alpha, \theta, N) \right] f_\alpha ,
$$

where $f_\alpha \equiv |\langle p | \sigma_N^x | p' \rangle|$ and the two phase factors, whose explicit form is given in the supplementary materials, are related as $\lambda(y, \theta, N) - \lambda(x, \theta, N) = \pi/2$, which corresponds to a shift by half of the ring of the $x$ and $y$ magnetization profiles. Notice that, while translational invariance was broken by Jordan-Wigner transformation, through the phase $\theta$ the magnetization profiles can be shifted in space. The spatial dependence so obtained, which is depicted in Fig. 1, thus breaks lattice translational symmetry, not to a reduced symmetry as in the case of the staggerization that characterizes the standard AFM order, but completely, since we have an incommensurate modulation that depends on the system size, imposed to the staggerization.

While the simple argument just presented explains how and why the magnetizations along $x$ and $y$ acquire a non-trivial spatial dependence, we still have to determine how their magnitudes scale with $N$. To do so, we can exploit the trick introduced in [22], to develop an algorithm which provides the matrix elements $f_\alpha = |\langle p | \sigma_N^x | p' \rangle|$ for generic sizes. Within the ground state manifold, we define the vectors

$$
|g_\pm\rangle = \frac{1}{\sqrt{2}}(|p\rangle \pm |-p\rangle) ,
$$

and, further using the properties of the mirror operator $M_N$ (see supplementary material), we have

$$
|g_+\rangle = \frac{1}{2} \left( |g_+\rangle |\sigma_N^x \Pi^x |g_+\rangle - |g_-\rangle |\sigma_N^x \Pi^x |g_-\rangle \right) .
$$

In this way, we represent a notoriously hard one point function in terms of a standard expectation values of a product of an even number of spin operators $\sigma_N^x \Pi^x$, which can be expressed as a product of an even number of fermionic operators.

As we can see from Fig. 2 we have two different behaviors for the magnetizations along $x$ and $y$. While for the former we can see that it admits a finite non zero limit, which is a function of the parameter $\phi > 0$, the latter, for large enough systems, is proportional to $1/N$ (see also Fig. 3) and vanishes in the thermodynamic limit. Hence, differently from the one along the $y$ spin direction, the “incommensurate antiferromagnetic order” along $x$ survives also in the thermodynamic limit. By exploiting perturbative analysis around the classical point $\phi = 0$ it is possible to show that, for $\phi \rightarrow 0^+$ and diverging $N$, $f_x$ goes to $2/\pi$ (see supplementary materials for details). Moreover, numerical analysis also shown that in the whole region $\phi \in (0, \pi/4)$ we have

$$
\lim_{N \rightarrow \infty} |\langle p | \sigma_N^x | p' \rangle| = \frac{2}{\pi} (1 - \tan^2 \phi) \frac{2}{\pi} .
$$
Summarizing, we have proved how, in the presence of FBCs, the Hamiltonian in eq. (14) shows a quantum phase transition for $\phi = 0$. Such transition is absent both for OBCs and for systems with PBC made of an even number of spins. This quantum phase transition separates two different gapless, non-relativistic phases that, even at a finite size, are characterized by different values of ground-states degeneracy: one shows a two-fold degenerate ground-state, while in the second we have a four-fold degenerate one. This difference, together with the fact that the first derivative of the ground-state energy shows a discontinuity in correspondence with the change of degeneracy, supports the idea that there is a first-order transition. However, differently from the standard first-order transitions, the discontinuity in the first derivative of the ground-state energy remains finite also in the thermodynamic limit, as in 2D wetting transitions. But, in contrast with the systems that usually exhibit a wetting transition, in our system of interest, there are no boundaries or fixed defects around which to nucleate a surface tension: hence we can talk about “boundary-less wetting transition”.

The two phases display the two ways in which the system can adjust to the conflict between the local AFM interaction and the global FBC: either by displaying a mesoscopic ferromagnetism, whose magnitude decays to zero with the system size [22], or through an approximate staggerization, so that the phase difference between neighboring spins is $\pi \left( 1 \pm \frac{1}{\Delta} \right)$. For large systems, these $1/N$ corrections induced by frustration are indeed negligible at short distances. However, they becomes relevant when fractions of the whole chain are considered. Crucially, the latter order spontaneously breaks translational invariance and remains finite in the thermodynamic limit. Let us remark once more that, with different boundary conditions, all these effects are not present.

The results presented in this work are much more than an extension of [22], in which we already proved that FBC can affect local order. While in [22] AFM was destroyed by FBC and replaced with a mesoscopic ferromagnetic order, here we encounter a new type of AFM order, which spontaneously breaks translational invariance and is modulated in an incommensurate way. Most of all, the transition between these two orders is signaled by a discontinuity akin to a boundary phase transition, but in absence of a physical boundary. Such a strong dependence on boundary conditions seemingly contradicts one of the tenant of Landau Theory and we cannot offer at the moment a unifying picture that would reconcile our results with the general theory. Indeed, FBC are special, as the kind of spin chains we consider are the building blocks of every frustrated system, which are known to present peculiar properties. We can also speculate that FBC induce a topological effect that puts the system outside the range of validity of Landau’s theory.

In this work, we focused on the XY chain to best show these peculiar results. Moreover, in the Supplementary Material which accompanies this manuscript, we show that all these outcomes can also be derived using perturbation theory around the classical point, thus providing an even clearer physical picture. In our next works [28, 31] we will extend the analysis to interacting systems and to chains with defects. Preliminary results show the resilience of the phenomenology we presented to these modifications, thus establishing the physics we just discussed not only as a remarkable point of principle but also as a physically measurable phenomenon.

**ACKNOWLEDGMENTS**

We thank Giuseppe Mussardo, Rosario Fazio, and Marcello Dalmonte for useful discussions and suggestions. We acknowledge support from the European Regional Development Fund – the Competitiveness and Cohesion Operational Programme (KK.01.1.06 – RBI TWIN SIN) and from the Croatian Science Foundation (HrZZ) Projects No. IP–2016–6–3347 and IP–2019–4–3321. SMG and FF also acknowledge support from the QuantixLXie Center of Excellence, a project co–financed by the Croatian Government and European Union through the European Regional Development Fund – the Competitiveness and Cohesion.
Supplementary Materials

The model and its symmetries

The XY chain studied in the letter is given by the Hamiltonian

$$H = \sum_{j=1}^{N} \left( \cos \phi \sigma_j^x \sigma_{j+1}^x + \sin \phi \sigma_j^y \sigma_{j+1}^y \right), \quad (14)$$

where $\sigma_j^\alpha$, with $\alpha = x, y, z$, are Pauli operators acting on the $j$-th spin, $N$ is the number lattice sites and we assume frustrated boundary conditions (FBC), given by periodic boundary conditions $\sigma_j^\alpha = \sigma_{j+N}^\alpha$ and an odd number of lattice sites. In these supplementary materials we will focus on the region $\phi \in (0, \pi/4)$, where both of the two interactions are antiferromagnetic. We also compare the results obtained for this region with the one analyzed in Ref. [22], which, keeping $\phi \in (-\pi/4, 0)$, describes the situation where one dominant, antiferromagnetic coupling appears together with a ferromagnetic smaller one.

Since the model in eq. (14) does not include an external magnetic field, the Hamiltonian commutes with all three parity operators $\Pi^\alpha \equiv \bigotimes_{j=1}^{N} \sigma_j^\alpha$, $\alpha = x, y, z$, i.e. $[H, \Pi^\alpha] = 0$, $\forall \alpha$. However, assuming FBC and hence setting the number of sites to be an odd number, different parity operators anticommute, satisfying $\{\Pi^\alpha, \Pi^\beta\} = 2\delta_{\alpha,\beta}$. The fact that the different parity operators anticommute has an immediate relevant consequence: each eigenstate is at least two-fold degenerate. To explain this point, let us assume that $|\varphi\rangle$ is simultaneously an eigenstate of $H$ and one of the three parity operators, for instance $\Pi^x$. Then, the image of $|\varphi\rangle$ under the action of one of the other parity operators, for example $\Pi^y |\varphi\rangle$, is still an eigenstate of both $H$ and $\Pi^x$. But while $|\varphi\rangle$ and $\Pi^z |\varphi\rangle$ have the same energy, they have different $z$ parity. As a consequence, for each eigenstate of the Hamiltonian in the even sector of one of the parities ($\Pi^\alpha = 1$), there will be a second eigenstate of the Hamiltonian, with the same energy but living in the odd sector ($\Pi^\alpha = -1$). Hence each eigenvalue of the Hamiltonian is, at least, two-fold degenerate.

However, other symmetry properties of the Hamiltonian will prove to be of extreme relevance in the following. At first, due to periodic boundary conditions, the model exhibits exact translational symmetry, which is expressed in the commutation of the Hamiltonian with the lattice translation operator $T$. Finally, the model also exhibits mirror symmetry with respect to any lattice site. Namely, for any lattice site $k$ the Hamiltonian in eq. (14) is invariant under the mirror image with respect to it, achieved by the transformation $j \rightarrow 2k - j$ on spins, associated to the action of the mirror operator $M_k$.

Exact solution

As it is well-known, the model in eq. (14) can be diagonalized exactly, using standard techniques of mapping spins to fermions [21]. The Jordan-Wigner transformation defines the fermionic operators as

$$c_j = \left( \bigotimes_{l=1}^{j-1} \sigma_l^z \right) \otimes \sigma_j^+, \quad c_j^\dagger = \left( \bigotimes_{l=1}^{j-1} \sigma_l^z \right) \otimes \sigma_j^-,$$ \quad (15)

where $\sigma_j^\pm = (\sigma_j^x \pm \text{i}\sigma_j^y)/2$ are spin raising and lowering operators. In this notation, not explicitly mentioning a lattice site in the tensor product corresponds to making a tensor product with an identity operator on that site. In terms of Jordan-Wigner fermionic operators, the Hamiltonian in eq. (14) reads as

$$H = \sum_{j=1}^{N-1} \left[ (\sin \phi - \cos \phi) c_j c_{j+1} - (\cos \phi + \sin \phi) c_j c_{j+1}^\dagger + \text{h.c.} \right] - \Pi^z \left[ (\sin \phi - \cos \phi) c_N c_1 - (\cos \phi + \sin \phi) c_N c_1^\dagger + \text{h.c.} \right].$$ \quad (16)

Due to the presence of the parity operator along $z$, the Hamiltonian given by eq. (16) is not in a quadratic form, but becomes quadratic in each of the two parity sector of $\Pi^z$, i.e.

$$H = \frac{1 + \Pi^z}{2} H + \frac{1 + \Pi^z}{2} H - \frac{1 - \Pi^z}{2} H - \frac{1 - \Pi^z}{2},$$ \quad (17)
where both $H^+$ and $H^-$ are quadratic. Being quadratic, they can be brought to a form of free fermions, which is done conveniently in two steps. First, $H^\pm$ are written in terms of the Fourier transformed Jordan-Wigner fermions,

$$b_q = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_j e^{-i \omega_j}, \quad b_q^\dagger = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_j e^{i \omega_j},$$

for $q \in \Gamma^\pm$, where the two sets of quasi-momenta are given by $\Gamma^- = \{2\pi k/N\}$ and $\Gamma^+ = \{2\pi (k + \frac{1}{2})/N\}$ with $k$ running on all integers between 0 and $N - 1$. Then a Bogoliubov rotation

$$a_q = \cos \theta_q b_q + i \sin \theta_q b_q^\dagger, \quad q \neq 0, \pi$$

$$a_q = b_q, \quad q = 0, \pi$$

with a momentum-dependent Bogoliubov angle given by

$$\theta_q = \arctan \frac{|\sin \phi + \cos \phi e^{i \omega q}| - (\sin \phi + \cos \phi) \cos q}{(\cos \phi - \sin \phi) \sin q}$$

is used to bring them to a form of free fermions. We end up with

$$H^\pm = \sum_{q \in \Gamma^\pm} \varepsilon(q) \left(a_q^\dagger a_q - \frac{1}{2}\right),$$

where the dispersion law is given by

$$\varepsilon(q) = 2|\sin \phi + \cos \phi e^{i \omega q}|, \quad q \neq 0, \pi,$$

$$\varepsilon(0) = -\varepsilon(\pi) = 2(\sin \phi + \cos \phi).$$

The eigenstates of $H$ are formed by populating the vacuum states $|0^\pm\rangle$ of Bogoliubov fermions $a_q$, $q \in \Gamma^\pm$, and by taking care of the parity requirements in $[17]$. The parity-dependent vacuum states are given by

$$|0^\pm\rangle = \prod_{0 < q < \pi, q \in \Gamma^\pm} (\cos \theta_q - i \sin \theta_q b_q^\dagger b_q^\dagger) |0\rangle,$$

where $|0\rangle \equiv \bigotimes_{j=1}^{N} |1\rangle_j$ is the vacuum for Jordan-Wigner fermions, satisfying the relation $c_j |0\rangle = 0 \forall j$. As it is easy to see from eq. (22), the vacuum states $|0^+\rangle$ and $|0^-\rangle$ by construction have even $\Pi^z$ parity. Since each excitation $a_q^\dagger$ changes the parity of the state it follows that the eigenstates of $H$ belonging to $\Pi^z = -1$ sector are of the form $a_{q_1}^\dagger a_{q_2}^\dagger ... a_{q_m}^\dagger |0^-\rangle$ with $q_i \in \Gamma^-$ and $m$ odd, while $\Pi^z = +1$ sector eigenstates are of the same form but with $q_i \in \Gamma^+$, $m$ even and the vacuum $|0^+\rangle$ used.

On the other hand, as we have discussed in the previous section of these supplementary materials, from an eigenstate of one parity of $\Pi^z$ we can, by applying $\Pi^z$, obtain a second eigenstate, with the same energy, but different $\Pi^z$ parity. This implies that to each aforementioned odd parity state, for instance, there is a corresponding even parity state $\Pi^z a_{q_1}^\dagger a_{q_2}^\dagger ... a_{q_m}^\dagger |0^-\rangle$ with the same energy.

In accordance with these facts, and keeping in mind that, as we can see from eq. (22), in the range of $\phi$ of our interest there is no momenta in the odd sector with a negative energy, the ground states in the odd parity sector of $\Pi_z$ are constructed by exciting the lowest energy modes $q \in \Gamma^-$ and have the form $a_{q_1}^\dagger |0^-\rangle$. To each such state is associated an equivalent ground state in the even sector of the form $\Pi^z a_{q_1}^\dagger |0^-\rangle$. Similarly, the lowest lying excited states are obtained by exciting the other single modes. Therefore, the ground state is part of a band of $2N$ state, in which the energy gap between the states is, due to the spectrum of the form eq. (22), closing algebraically with the system size. The closing of the gap is a phenomenology analogous to Refs. [17, 21, 22], and is an aspect of geometrical frustration in general.

In the region $\phi \in (-\pi/4, 0)$, studied in Ref. [22], the energy in eq. (22) for the momenta in the odd sector is minimized by $q = 0$. So the ground state manifold is two-fold degenerate, spanned by the states $a_{q_1}^\dagger |0^-\rangle$ and $\Pi^z a_{q_1}^\dagger |0^-\rangle$. On the other hand, for $\phi \in (0, \pi/4)$ the energy would be minimized assuming $q = \pm \pi/2$. However, for any finite system with odd $N$ the momenta $q = \pm \pi/2$ are not allowed. As a consequence the modes in the odd sector with the lowest energy, that we denote as $\pm p \in \Gamma^-$, are given by

$$p = \begin{cases} \pi 2 \left(1 - \frac{1}{N}\right), & N \text{ mod } 4 = 1 \\ \pi 2 \left(1 + \frac{1}{N}\right), & N \text{ mod } 4 = 3 \end{cases}$$
Hence the two states $|\pm p\rangle = a_{\pm p}^\dagger |0\rangle$ represent the two ground states in the odd parity sector. The ground state manifold is, therefore, four-fold degenerate and a generic ground state can be written as a superposition

$$|g\rangle = u_1 |p\rangle + u_2 |-p\rangle + u_3 \Pi^- |p\rangle + u_4 \Pi^+ |p\rangle ,$$

where we have assumed that the normalization condition $\sum |u|^2 = 1$ is satisfied.

### The Translation Operator

The lattice translation operator $T$ is a linear operator that shifts cyclically all the spins in the lattice by one site. To define it, we choose a basis of the space and specify its action on the basis. One basis of the Hilbert space of $N$ spins are the states

$$|\psi\rangle = \bigotimes_{k=1}^N (\sigma_k^-)^{n_k} |\uparrow_k\rangle ,$$

where $n_1, n_2, ..., n_N \in \{0,1\}$. The translation operator $T$ can then be defined by

$$T |\psi\rangle = \bigotimes_{k=1}^N (\sigma_k^-)^{n_k+1} |\uparrow_k\rangle ,$$

where we make the identification $n_{N+1} \equiv n_1$. From eq. (27) it follows immediately that, for each state $|\psi\rangle$, we have that $\langle \psi | T^\dagger T |\psi\rangle = 1$. Hence the translation operator is unitary, i.e. $T^\dagger T = 1$ and the adjoint $T^\dagger$ plays the role of the translation operator in the other direction. Moreover, applying the $T$ operator $N$ times translates the spins by the whole lattice and results in recovering the initial state, implying the idempotence of order $N$ of $T$, i.e. $T^N = 1$. As a consequence, the only possible eigenvalues of the translation operator are the $N$-th roots of unity, given by $e^{i\theta}, q \in \Gamma^-.$

On the other hand, moving from the spin states to the operators, it is easy to see that the translation operator shifts the Pauli operators as

$$T^\dagger \sigma^\alpha_j T = \sigma^\alpha_{j+1}, \quad \alpha = x,y,z ,$$

where $\sigma^\alpha_{N+1} = \sigma^\alpha_1$, and, consequently it commutes with both the Hamiltonian in eq. (14) ($[T,H] = 0$) and the parity operator $\Pi$ ($[T,\Pi^\alpha] = 0$ for $\alpha = x,y,z$).

The fact that the Hamiltonian and the translation operator commute implies that they admit a complete set of common eigenstates. In the following we prove that such a complete set is made by the eigenstates introduced in the previous section. Let us start by proving the following theorem.

**Theorem 1.** The states $b_{q_1}^\dagger b_{q_2}^\dagger ... b_{q_m}^\dagger |0\rangle$, with $m$ odd and $\{q_k\} \subset \Gamma^-$, are eigenstates of $T$ with eigenvalue equal to $e^{i\sum_{k=1}^m q_k}$.

**Proof.** We write $\prod_{k=1}^m b_{q_k}^\dagger$ to indicate the ordered product of fermionic operators $b_{q_1}^\dagger b_{q_2}^\dagger ... b_{q_m}^\dagger$. From the defining properties of $T$ we know how it acts on spin states and how it transforms the spin operators. Hence to study its action on the fermionic states $(\prod_{k=1}^m b_{q_k}^\dagger) |0\rangle$ it is convenient to write them in terms of spin states. This can be done in two steps. At first, using the eq. (18), we can write our state in terms of the Jordan-Wigner fermions, obtaining

$$\left( \prod_{k=1}^m b_{q_k}^\dagger \right) |0\rangle = \frac{1}{N^{m/2}} \sum_{j_1,..,j_m=1}^N e^{\frac{i}{2} \sum_{k=1}^m q_k j_k} \prod_{k=1}^m \left( c_{j_k}^\dagger \right) |0\rangle .$$

Being the $c_{j_k}^\dagger$ operators fermionic, only the terms with all different $j_k$ survive. The second step is to invert the Jordan-Wigner mapping to bring back the fermionic states to spin ones. To do this step we first sort the fermionic operators, after which it’s easy to invert the Jordan-Wigner transformation. To provide an example we have

$$c_1^\dagger c_2^\dagger c_3^\dagger |0\rangle = -c_1^\dagger c_2^\dagger c_4^\dagger |0\rangle = -\sigma_1^- (\sigma_1^\dagger \sigma_2^- (\sigma_1^\dagger \sigma_2^- \sigma_3^-) \sigma_4^- \bigotimes_{k=1}^N |\uparrow_k\rangle) = -\sigma_1^- \sigma_2^- \sigma_4^- \bigotimes_{k=1}^N |\uparrow_k\rangle .$$

(30)
More generally we can write

$$
\bigotimes_{k=1}^{m} \left( c_{jk}^\dagger \right) |0\rangle = S[\{j_k\}] \bigotimes_{k=1}^{m} (\sigma_{jk}^-) \bigotimes_{k'=1}^{N} |\uparrow_{k'}\rangle ,
$$

where $S[\{j_k\}]$ is the sign of the permutation that brings the tuple $\{j_k\}$ to normal order. Hence, the states can be re-written in terms of spin operators as

$$
\left( \prod_{k=1}^{m} b_{q_k}^j \right) |0\rangle = \frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S[\{j_k\}] e^{i \sum_{k=1}^{m} q_k j_k} \bigotimes_{k=1}^{m} (\sigma_{jk}^-) \bigotimes_{k'=1}^{N} |\uparrow_{k'}\rangle .
$$

Having the representation of the state in terms of spins, it is easy to see what is the result of the application of $T$. Using its discussed properties and taking into account that $T$ leaves the state $\bigotimes_{k'=1}^{N} |\uparrow_{k'}\rangle$ unchanged we recover

$$
T \left( \prod_{k=1}^{m} b_{q_k}^j \right) |0\rangle = \frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S[\{j_k\}] e^{i \sum_{k=1}^{m} q_k j_k} \bigotimes_{k=1}^{m} (\sigma_{jk}^-) \bigotimes_{k'=1}^{N} |\uparrow_{k'}\rangle ,
$$

Now we have two different cases. If none of the elements in $\{j_k\}$ is equal to 1, then none of the elements in $\{j_k - 1\}$ is equal to zero, and trivially $S[\{j_k\}] = S[\{j_k - 1\}]$. On the contrary if one element of $\{j_k\}$ is equal to 1, then $j_k - 1$ becomes 0. However, the number $m$ of the elements in $\{j_k\}$ is odd. Hence to move an element from the first to the last place requires an even number $m - 1$ of permutations and hence the sign of the permutation $S[\{j_k\}] = S[\{j_k - 1\}]$ remains the same if we replace $j_k - 1 = 0$ with $N$. From this and the fact that, since $\{q_k\} \subset \Gamma^-$, the exponential $e^{i q_k (j_k - 1)}$ remains the same if we replace $j_k - 1 = 0$ with $N$, it follows that we can write

$$
T \left( \prod_{k=1}^{m} b_{q_k}^j \right) |0\rangle = \frac{e^{i \sum_{k=1}^{m} q_k}}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S[\{j_k - 1\}] e^{i \sum_{k=1}^{m} q_k (j_k - 1)} \bigotimes_{k=1}^{m} (\sigma_{jk-1}^-) \bigotimes_{k'=1}^{N} |\uparrow_{k'}\rangle ,
$$

where, if for some $k$ we have $j_k - 1 = 0$, we can identify it with $j_k - 1 = N$. Because of this identification it’s easy to write each term in the sum in terms of fermions:

$$
T \left( \prod_{k=1}^{m} b_{q_k}^j \right) |0\rangle = \frac{e^{i \sum_{k=1}^{m} q_k}}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} e^{i \sum_{k=1}^{m} q_k j_k} \prod_{k=1}^{m} \left( c_{jk}^\dagger \right) |0\rangle .
$$

In [34] we can, again on the basis of the identification of 0 with $N$, rename the indices to get

$$
T \left( \prod_{k=1}^{m} b_{q_k}^j \right) |0\rangle = \frac{e^{i \sum_{k=1}^{m} q_k}}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} e^{i \sum_{k=1}^{m} q_k j_k} \prod_{k=1}^{m} \left( c_{jk}^\dagger \right) |0\rangle = \exp \left( i \sum_{k=1}^{m} q_k \right) \left( \prod_{k=1}^{m} b_{q_k}^j \right) |0\rangle ,
$$

which proves Theorem [1] \[\square\]

From Theorem [1] it follows immediately, by taking into account the definition of the Bogoliubov particles in eq. [19], the definition of the Bogoliubov vacua in eq. [23], and the linearity of the translation operator, that also the states $\left( \prod_{k=1}^{m} a_{q_k}^j \right) |0\rangle$ are eigenstates of $T$ with eigenvalues equal to $\exp \left( i \sum_{k=1}^{m} q_k \right)$.

**The Mirror Operator**

As we have seen in the first section of these supplementary materials, the Hamiltonian is invariant under the mirror transformation with respect to a generic site $k$ that changes spin operators defined on the site $j$ to ones defined on the site $2k - j$. Note that, with the odd number $N$ of sites we work with, in a circular geometry, the line of mirror reflection crosses a site and a bond. Hence, only site $k$ remains unchanged by the mirror action.
As we have done for translations, the mirror transformation can also be expressed by the action of a suitable operator. The mirror operator $M_k$, that makes the mirror transformation of the states with respect to the $k$-th site, is defined by its action on the spin basis states $|\psi\rangle$, defined in eq. (26), as

$$M_k |\psi\rangle = M_k \bigotimes_{j=1}^N (\sigma_j^-)^{n_j} |\uparrow_j\rangle = \bigotimes_{j=1}^N (\sigma_j^-)^{n_{2k-j}} |\uparrow_j\rangle,$$

where, as always, $n_{j+N} = n_j$. From eq. (36) it follows immediately that, for each state $|\psi\rangle$, we have that $\langle \psi | M_k^\dagger M_k |\psi\rangle = 1$. Hence, as the translation operator, also $M_k$ is unitary, i.e. $M_k^\dagger M_k = 1$. Moreover, applying the mirror operator two times results in recovering the initial state, hence implying the idempotence of order 2 of $M_k$, i.e. $M_k^2 = 1$. This implies that $M_k$ is also Hermitian, i.e. $M_k^\dagger = M_k$, and that the only possible eigenvalues of $M_k$ are ±1. Moreover, different mirror operators are related by translations,

$$T^\dagger M_k T = M_{k+1}$$

(37)

From this relation it is also clear that the mirror operators do not commute with the translation operator ($[M_k, T] \neq 0$).

Since each of the mirror operators commutes with the Hamiltonian, the Hamiltonian shares a common basis with each one of them. The following theorem gives the relation between the eigenstates we have constructed and the mirror operators. Essentially, the mirror operators change the sign of the momenta of the excitations, up to a possible phase factor, depending on $k$. Since different mirror operators are related by eq. (37) we focus on the one with $k = N$ for which the phase factor is absent.

**Theorem 2.** The mirror operator $M_N$ acts on the eigenstates of the model $a_1^\dagger a_2^\dagger ... a_m^\dagger |0^\gamma\rangle$, with $m$ an odd number and $q_1, q_2, ..., q_m \in \Gamma^-$, as

$$M_N a_1^\dagger a_2^\dagger ... a_m^\dagger |0\rangle = a_1^- a_2^- ... a_m^- |0\rangle$$

(38)

The theorem is proven in a similar way as Theorem 1 and we omit the details. The other mirror operators $M_k$, with $k \neq N$, would introduce an additional phase factor by acting on the aforementioned eigenstates. The phase factor depends on the momentum of the state and can be reconstructed from eq. (37). The $N$-th site being special here is a consequence of its special position in the Jordan-Wigner transformation, which implicitly enters in the definition of the states we work on. In the proof of Theorem 2 the $N$-th site is special because for $k = N$ the exponentials of the type $e^{i\gamma}$ can be replaced by $e^{-i\gamma(2k-j)}$, while for other $k$ a compensating factor has to be introduced.

Since we construct the even parity states from the odd parity ones by applying $\Pi^\gamma$, for our purposes it is sufficient to notice that mirroring does not change the parity and so the mirror operator commutes with the parity operators, i.e. $[M_N, \Pi^\gamma] = 0$, $\alpha = x, y, z$. Note that, as a consequence of Theorem 2, only states with total momentum satisfying $\exp \{ i \sum_{j=1}^m q_j \} = \pm 1$ can simultaneously be eigenstates of $T$ and $M_N$.

**The Spatial Dependence of the Magnetization**

As we have proved in the section about the exact solution of the model, in the region $\phi \in (0, \pi/4)$ the ground state manifold is four fold degenerate. Hence a large variety of possible ground states with different magnetic properties can be selected. Among them, the ground states at the center of the manuscript to which this supplementary material is attached are of the form

$$|\tilde{g}\rangle = \frac{1}{\sqrt{2}} \left( |p\rangle + e^{i\theta} \Pi^\gamma |\bar{p}\rangle \right),$$

(39)

where $\theta$ is a free phase. For such state the magnetization in the $\gamma$ direction, with $\gamma = x, y$, shows the peculiar incommensurate antiferromagnetic order that we discussed in the main paper and that we will elaborate on in the following. By definition, the magnetization in the $\gamma$ direction is equal to

$$\langle \sigma_j^- \rangle_{\tilde{g}} = \frac{1}{2} \left( e^{i\theta} \langle p | \sigma_j^\gamma \Pi^\gamma |\bar{p}\rangle + \text{c.c.} \right).$$

(40)

The magnetization is thus determined by the quantities $\langle p | \sigma_j^\gamma \Pi^\gamma |\bar{p}\rangle$, which are matrix elements of the spin string operators $\sigma_j^\gamma$ between the ground states vectors $|p\rangle$ and $\Pi^\gamma |\bar{p}\rangle$. The matrix elements at any site $j$ can be related to
the ones at site $N$, using the translation operator. Using the relation $\sigma_k^\gamma = (T^\dagger)^k \sigma_N^\gamma (T)^k$ and knowing the eigenvalues of $T$ we get

$$\langle p | \sigma_j^\gamma \Pi^\gamma | -p \rangle = e^{-ipj} \langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle .$$  \hspace{1cm} (41)

The advantage of expressing the quantity $\langle p | \sigma_j^\gamma \Pi^\gamma | -p \rangle$ in terms of the one at site $j = N$ is that this last one is real for $\gamma = x$ and purely imaginary for $\gamma = y$, as we will now show. The reason why the $N$-th site is special is because the Jordan-Wigner transformation, which implicitly enters into the definition of the states, breaks the invariance under spatial translation by identifying a first (and a last) spin in the ring.

To show that the quantity $\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle$ is real we resort to the mirror operator, which relates the states with opposite momentum as $M_N |p\rangle = | -p\rangle$, according to Theorem 2. Using this relation and taking into account that $M_N$ is hermitian we get

$$\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle = (-p) M_N \sigma_N^\gamma \Pi^\gamma M_N |p\rangle .$$  \hspace{1cm} (42)

But, as we have said, $\Pi^\gamma$ commutes with the mirror operator, which together with the property $M_N \sigma_N^\gamma M_N = \sigma_N^\gamma$ gives

$$\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle = (-p) \sigma_N^\gamma \Pi^\gamma |p\rangle = (\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle)^* ,$$  \hspace{1cm} (43)

where the last equality holds because the operator $\sigma_N^\gamma \Pi^\gamma$ is hermitian. Hence $\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle$ is equal to its conjugate and therefore real. To show that $\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle$ is purely imaginary we can use the same method together with the property that $\sigma_N^\gamma \Pi^\gamma$ is antihermitian, or we can use the relation

$$\Pi^\gamma = (-i)^N \Pi^y \Pi^x$$  \hspace{1cm} (44)

and the eigenstate property $\Pi^\gamma |\pm p\rangle = - |\pm p\rangle$, which give

$$\langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle = -(-i)^N \langle p | \sigma_N^\gamma \Pi^y | -p \rangle .$$  \hspace{1cm} (45)

The quantity $\langle p | \sigma_N^\gamma \Pi^y | -p \rangle$ is real, by the same argument which shows that $\langle p | \sigma_N^\gamma \Pi^x | -p \rangle$ is real and The factor in front, due to oddity of $N$, makes the whole quantity imaginary.

Taking these properties into account, we get the following spatial dependence for the magnetizations

$$\langle \sigma_j^\gamma \rangle_{\tilde{g}} = \cos(2pj - \theta) \langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle ,$$  \hspace{1cm} (46)

$$\langle \sigma_j^y \rangle_{\tilde{g}} = \cos(2pj - \theta + \frac{N}{2} + \pi) \langle p | \sigma_N^y \Pi^y | -p \rangle .$$  \hspace{1cm} (47)

Inserting the exact value of the momentum $\frac{\pi}{2N}$, which is equal to $p = \frac{\pi}{2} + (-1)^{\frac{N+1}{2}} \frac{\pi}{2N}$, we get finally the dependence of the magnetizations on the position in the ring,

$$\langle \sigma_j^\gamma \rangle_{\tilde{g}} = (-1)^j \cos \left[ \frac{\pi j}{N} + \lambda(\gamma, \theta, N) \right] \langle p | \sigma_N^\gamma \Pi^\gamma | -p \rangle ,$$  \hspace{1cm} (48)

where

$$\lambda(\gamma, \theta, N) \equiv \begin{cases} 
(-1)^{\frac{N+1}{2}} \theta, & \gamma = x, \\
(-1)^{\frac{N-1}{2}} \theta + \frac{\pi}{2}, & \gamma = y .
\end{cases}$$  \hspace{1cm} (49)

The magnetization is antiferromagnetic, i.e. staggered, but its magnitude is modulated. Since the number of sites is odd, it is not possible to have every bond aligned antiferromagnetically, but there is necessarily at least a one ferromagnetic one. The magnetization is modulated in such a way to achieve the minimal absolute value at the ferromagnetic bond, thus minimizing the energy. The position of this ferromagnetic bond is determined by the phase $\theta$. The position of the ferromagnetic bond of the magnetization in the $x$ direction is shifted by half of the ring with the respect to the ferromagnetic bond of the magnetization in the $y$ direction.
Explicit evaluation of the magnetizations on the \(N\)-th site

We can evaluate the magnetization on the \(N\)-th spin of the lattice exploiting a method similar to the one we developed in Ref. [22]. It consists on expressing the matrix elements \(\langle p | \sigma_N^z \Pi^x | -p \rangle\) in terms of expectation values of \(\sigma_N^z \Pi^x\) in a definite \(\Pi^x\) parity state, using the representation of \(\sigma_N^z \Pi^x\) in terms of Majorana fermions

\[
A_j = \left( \bigotimes_{l=1}^{j-1} \sigma_l^z \right) \otimes \sigma_j^z, \quad B_j = \left( \bigotimes_{l=1}^{j-1} \sigma_l^z \right) \otimes \sigma_j^y,
\]

using Wick theorem to express the expectation values as a determinant, and finally evaluating the determinant.

We express \(\langle p | \sigma_N^z \Pi^x | -p \rangle\) in terms of expectation values of \(\sigma_N^z \Pi^x\) on ground states living in the odd parity sector of \(\Pi^x\). A general ground state belonging to the odd parity sector of \(\Pi^x\) can be written as in eq. (25) setting \(u_3 = u_4 = 0\),

\[
| u_1, u_2 \rangle \equiv | u_1 \rangle + | -u_2 \rangle
\]

It is immediate to see that

\[
\langle \sigma_j^z \Pi^x \rangle_{u_1 = \frac{i}{u_2}} = \frac{1}{2} \left( \langle \sigma_j^z \Pi^x \rangle_{u_1 = \frac{i}{u_2}} - \langle \sigma_j^z \Pi^x \rangle_{u_1 = -\frac{i}{u_2}} \right) = \langle p | \sigma_j^z \Pi^x | -p \rangle + \langle -p | \sigma_j^z \Pi^x | p \rangle
\]

Using the properties of the mirror operator, in the previous section we have shown that \(\langle p | \sigma_N^z \Pi^x | -p \rangle = \langle -p | \sigma_N^y \Pi^x | p \rangle\), while in an analogous way we have also \(\langle p | \sigma_N^z \Pi^x | -p \rangle = \langle -p | \sigma_N^y \Pi^x | p \rangle\). Using these relations we get, finally,

\[
\langle p | \sigma_N^y \Pi^x | -p \rangle = \frac{1}{2} \left( \langle \sigma_N^z \Pi^x \rangle_{u_1 = \frac{i}{u_2}} - \langle \sigma_N^z \Pi^x \rangle_{u_1 = -\frac{i}{u_2}} \right).
\]

Now, \(\sigma_N^z \Pi^x\) and \(\sigma_N^y \Pi^x\), being products of spin operators, can be expressed in terms of Majorana fermions, as

\[
\sigma_N^z \Pi^x = (-1)^{\frac{N-1}{2}} \prod_{l=1}^{\frac{N-1}{2}} (-iA_B 2B_{2l-1}), \quad \sigma_N^y \Pi^x = -i(-1)^{\frac{N-1}{2}} \left( \prod_{l=1}^{\frac{N-1}{2}} (-iA_B 2B_{2l-1}) \right) (-iA_N B_N).
\]

The expectation values of these operators in a definite \(z\) parity ground state can be expressed as a Pfaffian of the matrix of two-point correlators, using Wick theorem. It is crucial that the state has a definite parity in order for the expectation values of single fermionic operators to vanish, as required by Wick theorem to be applied. We find the two-point correlators of Majorana fermions to be given by

\[
(A_j A_l)_{u_1, u_2} = \langle B_j B_l \rangle_{u_1, u_2} = \delta_{jl} - \frac{2}{N} (|u_1|^2 - |u_2|^2) \sin \left[ p(j - l) \right],
\]

\[
-i \langle A_j B_l \rangle_{u_1, u_2} = \frac{1}{N} \sum_{q \in \Gamma} e^{2i\theta_q} e^{-ip(j - l)} - \frac{2}{N} \cos \left[ p(j - l) - 2\theta_p \right] - \frac{2}{N} \left( u_1 u_2 e^{-ip(j + l)} + \text{c.c.} \right)
\]

where the Bogoliubov angle \(\theta_q\) is defined in eq. (20). The Bogoliubov angle also satisfies

\[
e^{2i\theta_q} = e^{\theta} \frac{\cos \phi + \sin \phi e^{-2i\phi}}{\cos \phi + \sin \phi e^{-2i\phi}},
\]

which should be used in (56) for the mode \(q = 0\), for which (20) is undefined.

As a matter of fact, in the evaluation of the matrix elements we encounter only states of the type \(|u_1| = |u_2| = 1/\sqrt{2}\), for which the correlators \((55)\) vanish for \(j \neq l\). This allows us to use the standard approach \(29\) on the basis of Wick theorem to express the expectation value of \((54)\) as a determinant. For \(\langle \sigma_N^y \Pi^x \rangle_{u_1, u_2}\) we have that

\[
\langle \sigma_N^y \Pi^x \rangle_{u_1, u_2} = -i(-1)^{\frac{N-1}{2}} \det C,
\]

with the \((N + 1)/2 \times (N + 1)/2\) correlation matrix \(C\) given by

\[
C = \begin{bmatrix}
F(2, 1) & F(2, 3) & F(2, 5) & \cdots & F(2, N - 2) & F(2, N) \\
F(4, 1) & F(4, 3) & F(4, 5) & \cdots & F(4, N - 2) & F(4, N) \\
& \vdots & \vdots & \ddots & \vdots & \vdots \\
F(N - 1, 1) & F(N - 1, 3) & F(N - 1, 5) & \cdots & F(N - 1, N - 2) & F(N - 1, N) \\
F(N, 1) & F(N, 3) & F(N, 5) & \cdots & F(N, N - 2) & F(N, N)
\end{bmatrix},
\]
Knowing that the eigenstates of the model in the limit \(\phi \to 0^+\) are superpositions of kinks

\[ |j\rangle = \cdots, 1, -1, 1, -1, 1, \ldots \),

with the ferromagnetic bond \(\sigma_j^x = \sigma_{j+1}^x = 1\) between sites \(j\) and \(j+1\), and antiferromagnetic bonds between all other adjacent sites. The kink state \(\Pi^z |j\rangle\), with all spins reversed, has the ferromagnetic bond \(\sigma_j^x = \sigma_{j+1}^x = -1\) and all the other bonds antiferromagnetic. The parity of the states \(|j\rangle\) is \(\Pi^z = (-1)^{(N-1)/2}\), while \(\Pi^z |j\rangle\) have, of course, the opposite parity. The higher energy states are separated by a finite gap and can be neglected in perturbation theory.

Increasing \(\phi\) from zero to a small non-zero value the exact degeneracy between the kink states splits. The ground states, and the corresponding energies, are found by diagonalizing the perturbation \(\sin \phi \sum_j \sigma_j^x \sigma_{j+1}^y\) in the basis of kink states. This has already been done in [22] and details can be found there. It has been found that the ground states of the model in the limit \(\phi \to 0\) are superpositions of kinks

\[ |s_q\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{iqj} |j\rangle \]  

and \(\Pi^z |s_q\rangle\), for \(q \in \Gamma^-\). The corresponding energies are

\[ E(q) = -(N - 2) \cos \phi + 2 \sin \phi \cos(2q) \]  

It’s easy to see that for \(\phi < 0\) the energy is minimized by \(q = 0\), while for \(\phi > 0\) it is by \(q = p\), where \(p\) is given by [24], as in the exact solution. Evaluating the derivative of the ground state energy \(E_g\) we find a discontinuity at \(\phi = 0\),

\[ \left. \frac{dE_q}{d\phi} \right|_{\phi \to 0^-} - \left. \frac{dE_q}{d\phi} \right|_{\phi \to 0^+} = 2 \left( 1 + \cos \frac{\pi}{N} \right) \],

which goes to a constant non-zero value in the thermodynamic limit \(N \to \infty\).

We now turn to the evaluation of the matrix element. We can identify the states from perturbation theory with those from the exact solution, in the limit \(\phi \to 0\), by looking at the eigenstates of various operators. The translation operator shifts the kink as \(T |j\rangle = |j - 1\rangle\), from which it follows that the states \(|s_q\rangle\) are eigenstates of \(T\) with the eigenvalue \(e^{iq}\). The mirror operator acts on the kink states as \(M_N |j\rangle = |-j - 1\rangle\), and therefore on the superpositions as

\[ M_N |s_q\rangle = e^{-iq} |s_{-q}\rangle \].

Knowing that the eigenstates \(|q\rangle\) from the exact solution have parity \(\Pi^z = -1\), are eigenstates of \(T\) with the eigenvalue \(e^{iq}\) and that under mirroring behave as \(M_N |q\rangle = |q\rangle\) we can make the identification

\[ |q\rangle = \frac{1 - \Pi^z}{\sqrt{2}} |s_q\rangle \], \[ |-q\rangle = \frac{1 - \Pi^z}{\sqrt{2}} e^{-iq} |s_{-q}\rangle \].
up to an irrelevant phase factor which is the same for the two states. From the identification we can express the matrix elements as

\[ \langle q | \sigma^x_N \Pi^x | -q \rangle = (-1)^{q-1} e^{-i\phi} \langle s_q | \sigma^x_j | s_{-q} \rangle , \]

where the factor \((-1)^{(N-1)/2}\) stems from the parity of the states \( |s_q\rangle \). Using the definition of the states on the right we get

\[ \langle q | \sigma^x_N \Pi^x | -q \rangle = (-1)^{q-1} \sum_{j=1}^{N} e^{-i2\phi j} \langle j | \sigma^x_N | j \rangle , \]

which can be evaluated using the property of the kink states

\[ \langle j | \sigma^x_N | j \rangle = \left\{ \begin{array}{ll} (-1)^j, & j = 1, 2, \ldots, N - 1 \\ 1, & j = N \end{array} \right. \]

that follows from their definition. We end up with

\[ \langle q | \sigma^x_N \Pi^x | -q \rangle = (-1)^{q-1} \frac{1}{N \cos q} . \]

The matrix element for the ground state momentum \( p = \pi/2 + (-1)^{(N+1)/2}\pi/2N \) becomes

\[ \langle p | \sigma^x_N \Pi^x | -p \rangle = \frac{1}{N \sin \frac{\pi}{2N}} , \]

and in the limit \( \phi \to 0^+ \) determines the maximum value the magnetization achieves over the ring in the ground state \( |\hat{g}\rangle \). For large \( N \) it becomes

\[ \langle p | \sigma^x_N \Pi^x | -p \rangle = \frac{2}{\pi} + \frac{\pi}{12N^2} + O(N^{-4}) , \]

which approaches quadratically the value \( 2/\pi \approx 0.64 \) in the thermodynamic limit.

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