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Quantum phase transition induced by topological frustration

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In quantum many-body systems with local interactions, the effects of boundary conditions are considered to be negligible, at least for sufficiently large systems. Here we show an example of the opposite. We consider a spin chain with two competing interactions, set on a ring with an odd number of sites. When only the dominant interaction is antiferromagnetic, and thus induces topological frustration, the standard antiferromagnetic order (expressed by the magnetization) is destroyed. When also the second interaction turns from ferro to antiferro, an antiferromagnetic order characterized by a site-dependent magnetization which varies in space with an incommensurate pattern, emerges. This modulation results from a ground state degeneracy, which allows to break the translational invariance. The transition between the two cases is signaled by a discontinuity in the first derivative of the ground state energy and represents a quantum phase transition induced by a special choice of boundary conditions.

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Modern physics follows a reductionist approach, in that it tries to explain a great variety of phenomena through a 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], which 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. Thus in[14] 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. In this line of research, particular attention was devoted to analyzing one-dimensional translational-invariant antiferromagnetic (AFM) spin models with frustrated boundary conditions (FBC), i.e, periodic boundary conditions in rings with an odd number of sites N. For purely classical systems (Ising chains), FBC 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 excitations in touch with the lowest energy state(s)[15–18] in a phase that, without frustration, would otherwise be gapped. In particular, while without frustration, the ground state of these models can be mapped exactly into the vacuum of a free fermionic system, the effect of FBC is to add a single excitation over this vacuum[19]. The naive expectation is that, as the chain length is increased, the contributions from this single quasi-particle get diluted up to becoming irrelevant in the thermodynamic limit. But this is not what was observed in[20] where, in the presence of FBC, a short-range dominant AFM interaction competes with a ferromagnetic one. Indeed, the single-particle excitation brings $1/N$ corrections to the fundamental Majorana correlation functions, but these contributions can add up in the physical observables, due to the peculiar strongly correlated nature of the system. For instance, the two-point function, whose connected component is usually separated in the long-distance limit to extract the spontaneous magnetization, acquires a multiplicative algebraic correction that suppresses it toward zero at distances scaling like the system size[15,20,21]. The vanishing of the spontaneous magnetization and the replacement of the standard AFM local order with a mesoscopic ferromagnetic one was also established through the direct evaluation of the one-point function in refs. [20,21].

In the present work, we focus on the transition that occurs when also the second interaction becomes AFM. This transition is characterized, even at finite size, by a level crossing associated with a discontinuity in the first derivative of the free energy at zero temperature (i.e., the ground-state energy). In the phase where both interactions are AFM, the ground state becomes fourfold degenerate and this increased degeneracy allows for the existence of a different magnetic order. This order is characterized by a staggered magnetization as in the standard AFM case, but with a modulation that makes its amplitude slowly varying in space. The results are surprising not only because of the order we find, but also because the quantum phase transition, signaled by the discontinuity, does not exist with other boundary conditions (BC), such as open (OBC) or periodic (PBC) boundary conditions with an even number of sites N., For this reason, we term it "Boundary-conditions-induced Quantum Phase Transition" (BCI QPT).

Results

Level crossing. We illustrate our results by discussing the XY chain at zero field in FBC. Even if this phenomenology is not limited to this model, it is useful to focus on it, because exploiting the well-known Jordan–Wigner transformation[22] we can evaluate all the quantities that we need with an almost completely analytical approach. The Hamiltonian describing this system reads

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

where σ_j^α, 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 $\sigma_j^\alpha \equiv \sigma_{j+N}^\alpha$. The angle $\phi \in (-\frac{\pi}{4}, \frac{\pi}{4})$ 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 ϕ, the Hamiltonian in Eq. (1) commutes with the parity operators $(\Pi^\alpha \equiv \otimes_{i=1}^N \sigma_i^\alpha)$, i.e., $[H, \Pi^\alpha] = 0$, $\forall\alpha$. At the same time, since we are considering odd N, different parity operators satisfy $\{\Pi^\alpha, \Pi^\beta\} = 2\delta_{\alpha,\beta}$, hence implying that each eigenstate is at least two-fold degenerate: if $|\psi\rangle$ is an eigenstate of both H and Π^z, then $\Pi^x|\psi\rangle$, that differs from $\Pi^y|\psi\rangle$ by a global phase factor, is also an eigenstate of H with the same energy but opposite z-parity. These symmetries are important because they imply an exact ground-state degeneracy even in finite chains and thus the possibility to select states with a definite magnetization within the ground-state manifold (for more details about the symmetries of the model see Supplementary Note 1). Furthermore, using the techniques introduced in ref. [20], it is possible to directly evaluate the magnetization of these states: having it as a function of the number of sites of the chain, we can take the thermodynamic limit and thus recover directly its macroscopic value, without resorting to the usual approach making use of the cluster decomposition.

Using the standard techniques[23], that consist of the Jordan–Wigner transformation and a Fourier transform followed by a Bogoliubov rotation (more details in Supplementary Note 2), the Hamiltonian can be reduced to

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

Here a_q ($a_q^{\dagger}$) is the annihilation (creation) fermionic operator with momentum q. The Hilbert space has been divided into two sectors of different z-parity Π^z. Accordingly, the momenta run over two disjoint sets, corresponding to the two sector: $\Gamma^- = \{2\pi k/N\}$ and $\Gamma^+ = \{2\pi(k+\frac{1}{2})/N\}$ with k ranging over all integers from 0 to $N-1$. The dispersion relation reads

$$\begin{aligned} \epsilon(q) &= 2|\cos\phi\, e^{\imath 2q} + \sin\phi|,\ q \neq 0, \pi\,, \\ \epsilon(0) &= -\epsilon(\pi) = 2(\cos\phi + \sin\phi)\ , \end{aligned} \tag{3}$$

where we note that only $\epsilon(0)$, $\epsilon(\pi)$ can become negative.

The eigenstates of H are constructed by populating the vacuum states $|0^{\pm}\rangle$ in the two sectors and by taking care of the parity constraints. The effect of frustration is that the lowest energy states are not admissible due to the parity requirement. For instance, from Eq. (3) we see that, assuming $\phi \in (-\frac{\pi}{4}, \frac{\pi}{4})$, 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 $a_\pi^{\dagger}|0^+\rangle$ 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 $a_\pi^{\dagger}|0^+\rangle$ considering the minimal excitation coherent with the parity constraint.

While for $\phi < 0$, there is a unique state in each parity sector that minimizes the energy while respecting the parity constraint (and these states both have zero momentum), for $\phi > 0$ the dispersion relation in Eq. (3) becomes a double well and thus develops two minima: $\pm p \in \Gamma^-$ and $\pm p' \in \Gamma^+$, approximately at $\pi/2$ (for their precise values and more details, see "Methods" section). Thus, for $\phi > 0$ the ground-state manifold becomes 4-fold degenerate, with states of opposite parity and momenta. This degeneracy has a solid geometrical origin, 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 π momentum (Supplementary Note 4). Thus, every other state must come in degenerate doublets of opposite momentum/chirality. In accordance to this picture, a generic element in the four-dimensional ground-state subspace can be written as

$$|g\rangle = u_1|p\rangle + u_2|-p\rangle + u_3|p'\rangle + u_4|-p'\rangle\,, \tag{4}$$

where the superposition parameters satisfy the normalization constraint $\sum_i |u_i|^2 = 1$, $|\pm p\rangle = a^{\dagger}_{\pm p}|0^-\rangle$ are states in the odd z-parity sector and $|\pm p'\rangle = \Pi^x|\mp p\rangle = a^{\dagger}_{\pm p'}a^{\dagger}_{\pi}|0^+\rangle$ are the states in the even sector (for the second equality, that holds up to a phase factor, see "Methods" section).

Hence, independently from N, once FBC 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

$$\frac{dE_g}{d\phi}\Big|_{\phi\to 0^-} - \frac{dE_g}{d\phi}\Big|_{\phi\to 0^+} = 2\left(1 + \cos\frac{\pi}{N}\right), \tag{5}$$

which goes to a non-zero 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[4].

However, such a transition is present only when FBC 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[24,25]. Hence, it is the introduction of the FBC that induces the presence of a quantum phase transition at $\phi = 0$.

The magnetization. Having detected a phase transition, we need to identify the two phases separated by it. In ref. [20], it was proved that the two-fold degenerate ground state for $\phi < 0$ is characterized by a ferromagnetic mesoscopic order: for any finite odd N, the chain exhibits non-vanishing, site-independent, ferromagnetic magnetizations along with 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, this phase can also show a different magnetic order, that is forbidden for $\phi < 0$. However, from all the possible orders that can be realized, we can, for sure, discard the standard staggerization that characterizes the AFM order in the absence of FBC. 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 the magnetization let us consider a ground-state vector that is not an eigenstate of the translation operator:

$$|\tilde{g}\rangle = \frac{1}{\sqrt{2}}\left(|p\rangle + e^{\imath\theta}|p'\rangle\right)\,, \tag{6}$$

where θ is a free phase. We compute the expectation value of spin operators in this state. Having broken translational invariance, we can expect the magnetization to develop a site dependence, which can be found by exploiting the translation and the mirror symmetry (see "Methods" section), giving

$$\langle\sigma_j^{\alpha}\rangle_{\tilde{g}} = (-1)^j \cos\left[\pi\frac{j}{N} + \lambda(\alpha,\theta,N)\right] f_{\alpha}\,, \tag{7}$$

where $f_\alpha \equiv |\langle p|\sigma_N^{\alpha}|p'\rangle|$. The two-phase factors, whose explicit dependence on the arbitrary phase θ is given in Supplementary Note 5, are related as $\lambda(y,\theta,N) - \lambda(x,\theta,N) = \pi/2$, which corresponds to a shift by half of the whole ring between the x and y magnetization profiles. The obtained spatial dependence, depicted in Figs. 1 and 2, 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 over-imposed to the staggerization.

While the simple argument just presented explains how and why the magnetizations along x and y acquire a nontrivial spatial dependence, we still have to determine how their magnitudes scale with N. The magnitudes depend on the spin operator matrix elements $\langle p|\sigma_N^{\alpha}|p'\rangle$ and their evaluation is explained in "Methods".

As we can see from Fig. 3, 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

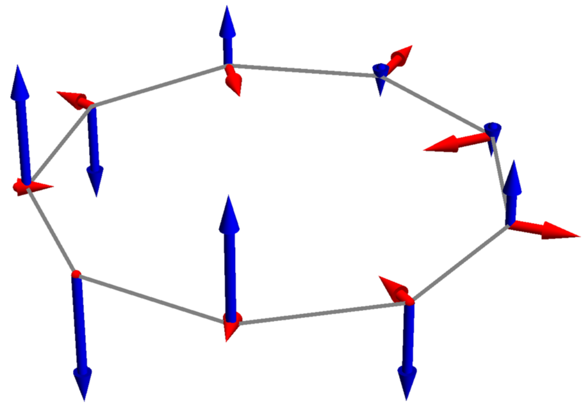

Fig. 1 Three-dimensional representation of the site-dependent magnetization. Site-dependent magnetizations along x (blue darker arrows) and y (red lighter arrows) for each spin of a lattice with $N = 9$ sites. The magnetizations are obtained setting $\phi = \frac{\pi}{8}$ and recovering the maximum amplitudes $f_x \simeq 0.613$ and $f_y \simeq 0.329$, see discussion around Eq. (7).

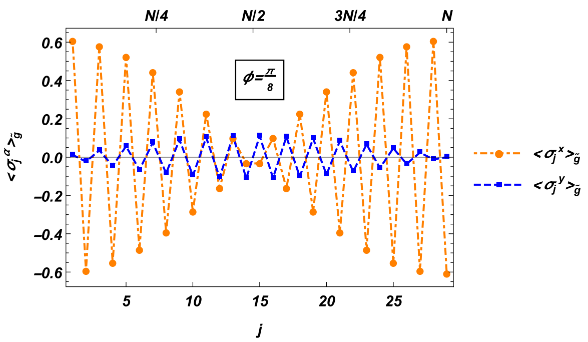

Fig. 2 Site-dependent magnetization. Plot of the site-dependent magnetizations along x (orange points) and y (blue ones) for each spin of a lattice with $N = 29$ sites. The magnetizations are obtained setting $\phi = \frac{\pi}{8}$. The dashed lines are a guide to the eye to show the almost staggered order, while the modulation in space is given by Eq. (7).

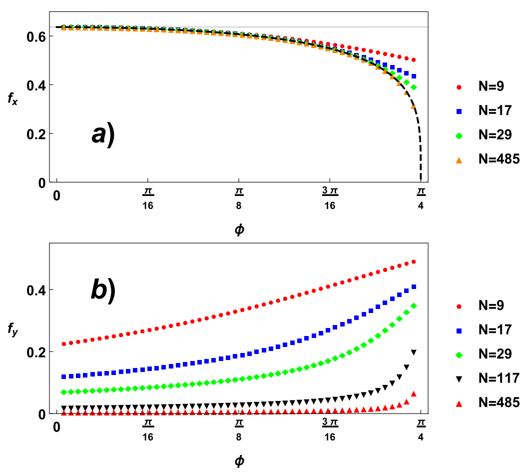

Fig. 3 Matrix elements that determine the magnetization. Behavior of matrix elements f_x (**a**) and f_y (**b**) as function of the Hamiltonian parameter ϕ for different sizes of the system N. The magnetizations are site-dependent, as given by the formula $\langle\sigma_j^\alpha\rangle_{\tilde{g}} = (-1)^j \cos\left[\pi\frac{j}{N} + \lambda(\alpha,\theta,N)\right] f_\alpha$ for $\alpha = x, y$, where λ is a phase factor that depends on additional details of the ground state. The matrix elements f_x and f_y thus determine the maximal value the magnetization can achieve over the ring.

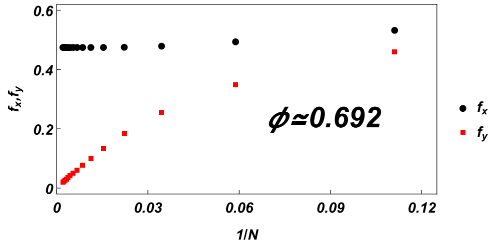

Fig. 4 Difference in the scaling of the two matrix elements. Dependence of the two $f_\alpha = |\langle p|\sigma_N^\alpha|p'\rangle|$ on the inverse of the size of the system $1/N$ for $\phi \simeq 0.692$. The black points represent the values obtained for f_x while the red squares stand for f_y.

parameter $\phi > 0$, the latter, for large enough systems, is proportional to $1/N$ (see also Fig. 4) 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 $\phi \to 0^+$ and diverging N, f_x goes to $2/\pi$ (see Supplementary Note 7 for details). Moreover, numerical analysis has also shown that in the whole region $\phi \in (0, \pi/4)$ we have

$$\lim_{N\to\infty} |\langle p|\sigma_N^x|p'\rangle| = \frac{2}{\pi}(1-\tan^2\phi)^{\frac{1}{4}}. \tag{8}$$

Discussion

Summarizing, we have proved how, in the presence of FBC, the Hamiltonian in Eq. (1) shows a quantum phase transition for $\phi = 0$. Such transition is absent both for OBC 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.

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 mesoscopic ferromagnetism, whose magnitude decays to zero with the system size[20] or through an approximate staggerization, so that the phase difference between neighboring spins is $\pi\left(1 \pm \frac{1}{N}\right)$. For large systems, these $1/N$ corrections induced by frustration are indeed negligible at short distances. However, they become 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 ref. [20], in which we already proved that FBC can affect local order. While in ref. [20] AFM was destroyed by FBC and replaced with a mesoscopic ferromagnetic order, here we encounter an AFM order, which spontaneously breaks translational invariance, is modulated in an incommensurate way and does not vanish in the thermodynamic limit. Most of all, the transition between these two orders is signaled by a discontinuity in the derivative of the free energy, indicating a first-order quantum phase transition.

The phase transition we have found resembles several well-known phenomena of quantum complex systems, without being completely included in any of them. A finite-difference of the values of the free energy derivative at two sides of the transition characterizes also first-order wetting transitions[26–28], which are associated with the existence of a border. On the other hand, in our system, we cannot individuate any border, since the chain under analysis is perfectly invariant under spatial translations. Delocalized boundary transitions have already been reported and are called "interfacial wetting", but they differ from the phenomenology we discussed here, as they refer to multi-kink states connecting two different orders (prescribed at the boundary) separated by a third intermediate state[29].

The transition we have found, and the incommensurate AFM order might also be explored experimentally. To observe them, one could, for example, measure the magnetization at different positions in the ring. In the phase exhibiting incommensurate AFM order, the measurements will yield different values at different positions, while in the other phase, exhibiting mesoscopic ferromagnetic order the values are going to be the same. One could also examine the maximum value of the magnetization over the ring. In the incommensurate AFM phase, this value is finite, while in the other it goes to zero in the thermodynamic limit. The maximum of the magnetization over the ring thus exhibits a jump at the transition point.

The strong dependence of the macroscopic behavior on boundary conditions that we have found seemingly contradicts one of the tenants 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[30–35], 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 fact, while in the ferromagnetic phases of the model the ground-state degeneracy in the thermodynamic limit is independent of boundary conditions, in the parameter region exhibiting incommensurate AFM order the degeneracy is doubled with FBC, thus clearly depending on the (real space) topology of the system. But, there is a second more subtle connection. Indeed, while magnetic phases show symmetry-breaking order parameters, topological phases are characterized by the expectation value of a non-local string operator that does not violate the bulk symmetry of the system. In our system, as we have shown before, the value of the local magnetization is associated with the expectation value of the operator $\sigma_N^x\Pi^x = \bigotimes_{j=1}^{N-1}\sigma_j^x$, which is a string operator that does not break the parity symmetries of the model. However, while geometrical frustration induces some topological effects in the XY chain, interestingly, we have found evidence that suggests that topological phases are resilient to geometrical frustration[36].

A natural question that emerges is how robust is the observed phenomenology to defects, that destroy the translational symmetry of the model. In fact, a common expectation is that such defect would pin the domain wall and restore the unfrustrated physics in the bulk. This question has been addressed in ref. [37], where it has been shown that a complex picture emerges depending on the nature of the defects, but that ultimately the incommensurate AFM order can survive under very general conditions. Thus, the physics we have discussed in this work is not only a remarkable point of principle but also a physically measurable phenomenon.

Methods

Ground-state degeneracy. We have two different pictures depending on the sign of ϕ. 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 Π^z are $|g_0^-\rangle = a_0^\dagger|0^-\rangle$ and $|g_0^+\rangle = \Pi^x|g_0^-\rangle = |0^+\rangle$, where the last equality holds up to a phase factor. On the contrary, when ϕ becomes positive, the energy in Eq. (3) admits, for each z-parity sector, two local minima at opposite momenta, $\pm p \in \Gamma^-$ and $\pm p' \in \Gamma^+$, where $p = \frac{\pi}{2}\left(1 - \frac{1}{N}\right)$ for a system size N satisfying $N\mathrm{mod}4 = 1$, $p = \frac{\pi}{2}\left(1 + \frac{1}{N}\right)$ for $N\mathrm{mod}4 = 3$ and $p' = \pi - p$.

Spatial dependence of the magnetization. To study the spatial dependence of the magnetization, it is useful to introduce the unitary lattice translation operator T, whose action shifts all the spins by one position in the lattice as

$$T^\dagger \sigma_j^\alpha T = \sigma_{j+1}^\alpha, \quad \alpha = x, y, z, \tag{9}$$

and which commutes with the system's Hamiltonian in Eq. (1), i.e., $[H, T] = 0$. The operator T admits, as a generator, the momentum operator P, i.e., $T = e^{\imath P}$. 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 $\pi \pm p' = \mp p$. A detailed definition of the operator and a proof of these properties is given in Supplementary Note 3. The latter equality allows identifying the ground states $a_{\pm p'}^\dagger a_\pi^\dagger |0^+\rangle$ with the states $\Pi^x|\mp p\rangle$.

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 in Eq. (6). 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

$$\langle\sigma_j^\alpha\rangle_{\tilde{g}} \;=\; \langle\tilde{g}|\sigma_j^\alpha|\tilde{g}\rangle \;=\; \frac{1}{2}\left(e^{\imath\theta}\langle p|\sigma_j^\alpha|p'\rangle \;+ e^{-\imath\theta}\langle p'|\sigma_j^\alpha|p\rangle\right). \tag{10}$$

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 $j = N$. In fact, considering Eq. (9) we obtain

$$\langle p|\sigma_j^\alpha|p'\rangle = e^{-\imath 2pj}\langle p|\sigma_N^\alpha|p'\rangle\,. \tag{11}$$

The advantage of this representation is that the matrix element $\langle p|\sigma_N^\alpha|p'\rangle$ is a real number for $\alpha = x$, and a purely imaginary one for $\alpha = y$, making it simple to express the magnetization. Let us illustrate the computation of the x magnetization, while the details for the y magnetization can be found in Supplementary Note 5. The special role of site N is singled out by the choice made in the construction of the states through the Jordan–Wigner transformation. To prove that the matrix element is real it is useful to introduce the unitary and hermitian, mirror operator with respect to site N, denoted as M_N, that makes the mirroring

$$M_N \sigma_j^\alpha M_N = \sigma_{-j}^\alpha, \quad \alpha = x, y, z, \tag{12}$$

and, in particular, leaves the Nth site unchanged. The operator satisfies $M_N|\pm p\rangle = |\mp p\rangle$, while the reflections with respect to other sites would introduce additional phase factors. A detailed definition of the mirror operators and discussion of their properties is given in Supplementary Note 4. Exploiting the properties of M_N, we have then

$$\langle p|\sigma_N^x\Pi^x|-p\rangle = \langle -p|\sigma_N^x\Pi^x|p\rangle = \left(\langle p|\sigma_N^x\Pi^x|-p\rangle\right)^*, \tag{13}$$

so $\langle p|\sigma_N^x|p'\rangle$ is real. Evaluating $\langle p|\sigma_N^x|p'\rangle$ using the methods of the next paragraph, we can see that the quantity is actually positive, and therefore equal to its magnitude f_x. Then from Eqs. (10) and (11) we get the spatial dependence of the magnetization

$$\left\langle\sigma_j^x\right\rangle_{\tilde{g}} = \cos(2pj - \theta)\langle p|\sigma_N^x|p'\rangle. \tag{14}$$

Inserting the exact value of the momentum, we get Eq. (7) for $\alpha = x$, where the exact value of $\lambda(x, \theta, N)$ is given in Supplementary Note 5.

Scaling of the magnetization with *N*. The magnetization is determined by the matrix elements $f_\alpha = |\langle p|\sigma_N^\alpha|p'\rangle|$. To evaluate them, we exploit the trick introduced in ref. [20] and used to compute the magnetization.

Within the ground-state manifold, we define the vectors

$$|g_\pm\rangle \equiv \frac{1}{\sqrt{2}}(|p\rangle \pm |-p\rangle), \tag{15}$$

and, further using the, already introduced, properties of the mirror operator M_N (see Supplementary Note 6 for details), we get

$$\langle p|\sigma_N^\alpha|p'\rangle \;=\; \frac{1}{2}\left(\;\langle g_+|\sigma_N^\alpha\Pi^x|g_+\rangle \;-\; \langle g_-|\sigma_N^\alpha\Pi^x|g_-\rangle\;\right). \tag{16}$$

In this way, we represent a notoriously hard one-point function in terms of standard expectation values of products of an even number of spin operators $\sigma_N^\alpha\Pi^x$, which can be expressed as a product of an even number (parity preserving) of fermionic operators. Using Wick's theorem, the expectation values can then be expressed as determinants and evaluated numerically efficiently (Supplementary Note 6).

Moreover, in the limit $\phi \to 0^+$, the matrix elements can also be evaluated analytically using a perturbative approach (Supplementary Note 7).

Data availability

Data sharing not applicable to this article as no data sets were generated or analyzed during the current study.

Code availability

The numerical computations performed to reach the results of the present work have been achieved using the software Mathematica and the code is provided in the Supplementary Code file which accompanies the paper.

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Author contributions

All authors conceived and discussed the work collectively and have written and edited different parts of the manuscript. V.M. did most of the analytical computations, while S.M.G. was charged with the majority of the numerical computations and the final creation of the figures. F.F. contributed in both processes.

Competing interests

The authors declare no competing interests.

Additional information

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