Quantum phase transition induced by topological frustration

Vanja Marić1,2, Salvatore Marco Giampaolo1 & Fabio Franchini1

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.
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. Toward the middle of the last century, 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 from zero to a non-vanishing value, signal the onset of the corresponding phases of many-body systems obeying classical mechanics. Intuition has been challenged. Thus in a concrete example of 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. 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, which have no equivalent in the classical regime, as well as nematic ones, represent instances in which violation of the same symmetry is associated with different (typically non-local) and non-equivalent order parameters, 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 features, such as boundary conditions, are deemed negligible (at least in the thermodynamic limit).

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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 four-fold 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, we can evaluate all the quantities that we need with an almost completely analytical approach. The Hamiltonian describing this system reads

$$H = \sum_{j=1}^{N} \cos \phi \sigma^x_j \sigma^x_{j+1} + \sin \phi \sigma^y_j \sigma^y_{j+1},$$

where $\sigma^\alpha_j$, 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 $\sigma^\alpha_j \equiv \sigma^\alpha_{j-N}$. The angle $\phi \in (-\pi/2, \pi/2)$ 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. (1) commutes with the parity operators $\{\Pi^a \equiv \sum_{j=1}^{N} \sigma^a_j, \Pi^b \}$, i.e., $[H, \Pi^a] = [H, \Pi^b] = 0, \forall a$. At the same time, we are assuming odd $N$, different parity operators satisfy $[\Pi^a, \Pi^b] = 2\delta_{ab} \phi$, hence implying that each eigenstate is at least two-fold degenerate: if $|\psi\rangle$ is an eigenstate of both $H$ and $\Pi^a$, then $\Pi^b |\psi\rangle$, that differs from $\Pi^b |\psi\rangle$ 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

**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$^{13,20,21}$. 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.
macroscopic value, without resorting to the usual approach making use of the cluster decomposition.

Using the standard techniques\textsuperscript{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

$$H = \frac{1 + \Gamma^-}{2} H^+ + \frac{1 - \Gamma^+}{2} H^- - \frac{1 - \Pi^z}{2},$$

(2)

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

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

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

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

(3)

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

The eigenstates of $H$ are constructed by populating the vacuum states $|0\rangle$ 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 $\phi \in (-\frac{\pi}{2}, \frac{\pi}{2})$, 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 $a_0^\dagger |0\rangle$ 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 $a_0^\dagger |0\rangle$ 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: $2\phi \in \Gamma^-$ and $2\phi' \in \Gamma^+$, 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 $\pi$ 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

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

(4)

where the superposition parameters satisfy the normalization constraint $\sum |u_k|^2 = 1$, $|\pm p\rangle = a_{k,\rho}^\dagger |0\rangle$ are states in the odd $\pi$-parity sector and $|\pm p\rangle = \Pi^+ |\pm p\rangle = a_{k,\rho}^\dagger a_{\rho,\lambda}^\dagger |0\rangle$ 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 $E_\phi$, whose first derivative exhibits a discontinuity

$$\frac{dE_\phi}{d\phi} |_{\phi = 0^-} - \frac{dE_\phi}{d\phi} |_{\phi = 0^+} = 2(1 + \cos \frac{\pi}{N}),$$

(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\textsuperscript{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 $\phi \in (\frac{\pi}{2}, \frac{3\pi}{2})$ and $\phi \in (0, \frac{\pi}{2})$ belong to the same AFM phase, have the same degree of ground-state degeneracy, and exhibit the same physical properties\textsuperscript{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:

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

(6)

where $\theta$ 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

$$\langle \sigma_i^\gamma \rangle_{\vec{g}} = \left\langle \left\langle \sigma_i^\gamma \right\rangle \right\rangle = \left\langle \left\langle \sigma_i^\gamma \right\rangle \right\rangle,$$

(7)

where $f_a \equiv \left\langle \left\langle \sigma_i^\gamma \sigma_j^\delta \right\rangle \right\rangle$. The two-phase factors, whose explicit dependence on the arbitrary phase $\theta$ 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 $\langle p| \sigma_i^\gamma \sigma_j^\delta |p'\rangle$ 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
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 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

$$\lim_{N \to \infty} |\langle p | \sigma^x_0 | p \rangle| = \frac{2}{\pi} (1 - \tan^2 \phi)^{\frac{1}{2}}.$$

### 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 $\pi(1 \pm \phi)$. 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 sides of the free energy derivative at two sides of the transition characterizes also first-order wetting transitions, 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.

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 phases are resilient to geometrical frustration. Depending on the nature of the defects, but that ultimately the incommensurate AFM order can survive under very general conditions.

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

$$T^a a^T = a^T_{j+1}, \quad a = x, y, z,$$

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 $P_i$, i.e., $T = e^{ip_i}$. Among the eigenstates of $P$, we have the ground-state vectors $| \mp p \rangle$ and $| \pm p \rangle$ with relative eigenvalues equal to $p$ and $\pi \mp p \equiv p \mp \pi$. 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 $a_{\pm} a_{\pm}^\dagger |\pm0\rangle$ with the states $\Pi^\dagger|\pm\rangle$.

We can exploit the properties of the operator $T$ to determine, for each odd $N$, the spatial dependence of the magnetizations $\langle \sigma_i^a \rangle$ along $x$ and $y$ in the ground state $|\psi\rangle = |\sigma_i^a \rangle$, with $a = x, y$, defined in Eq. (6). In fact, taking into account that $|p\rangle$ and $|\pm p\rangle$ live in different $z$-parity sectors, we have that the magnetization along a direction orthogonal to $z$ on the state $|\psi\rangle$ is given by

$$\langle \sigma_i^a \rangle_z = \langle \sigma_i^a |\sigma_j^a \rangle = \frac{1}{2} e^{i\phi} (|p|\langle p|\sigma_i^a \rangle + e^{-i\phi}\langle p'|\sigma_i^a \rangle).$$

The magnetization is determined by the spin operator matrix elements $\langle \sigma_i^a |\sigma_j^a \rangle$, that can all be related to the ones at the site $j = N$. In fact, considering Eq. (9) we obtain

$$\langle p |\sigma_i^a |\sigma_j^a \rangle = e^{-i\phi} \langle |p| |\sigma_i^a |\sigma_j^a \rangle.$$
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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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Correspondence and requests for materials should be addressed to F.F.

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