Staircase to higher-order topological phase transitions

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We find a series of topological phase transitions of increasing order, beyond the more standard second-order phase transition in a one-dimensional topological superconductor. The jumps in the order of the transitions depend on the range of the pairing interaction, which is parametrized by an algebraic decay with exponent α. Remarkably, in the limit $\alpha = 1$ the order of the topological transition becomes infinite. We compute the critical exponents for the series of higher-order transitions in exact form and find that they fulfill the hyperscaling relation. We also study the critical behaviour at the boundary of the system and discuss potential experimental platforms of magnetic atoms in superconductors.

1. Introduction.— Quantum phase transitions (QPTs) are one of the cornerstones in modern condensed matter physics [1, 2]. These are phase transitions where the variation of a physical parameter (coupling constant) drives a transition from one state of matter with a certain order (phase) to another one with different physical properties. These transitions stem from the quantum fluctuations in the energy spectrum of the system, due to the Heisenberg uncertainty principle. Ideally, they may occur in the absence of thermal fluctuations, at zero temperature. Famous examples of QPTs comprise the superfluid to Mott-insulator transition [3, 4], the insulator to superconductor transition in cuprates [5], metal-insulator transitions in disordered two-dimensional (2D) electron gases [6], etc.

Standard QPTs fit into the Landau theory of phase transitions [7], where different phases can be discriminated by the symmetry of an order parameter. Remarkably, there also exist non-standard phase transitions in topological systems [8]. They go beyond the standard classification of quantum phases, since they can neither be described by a local order parameter nor by the breaking of a symmetry at the phase-transition point. On the contrary, they are characterized by a global order parameter, which is a topological invariant of the system [9–14].

A general criterion to classify phase transitions was put forward initially by Ehrenfest, who associated the degree (order) of the phase transition to the lowest derivative of the free energy that is discontinuous at the transition point [15]. Later on, phase transitions were identified that fell outside the Ehrenfest classification, like the logarithmic singularity in the specific heat of the Onsager solution to the Ising model in 2D [16]. This led to a simplified binary classification of phase transitions into first-order and continuous phase transitions [1, 2]. Though the Ehrenfest criterion is not fully general, it can still be adapted [17, 18] to define the order of the phase transition when non-analyticities in the free energy are encountered. This will be the case for the series of topological phase transitions found in our work.

Examples of higher-order phase transitions do not abound. One instance is found in the large-N approximation of lattice QCD in 2D, that happens to be of third order [19]. Another example appears in the exact solution of the 2D Ising model coupled to quantum gravity, where the transition is also third order [20]. Recently, also a phase transition of infinite order was found in a long-range spin model [21].

When it comes to topological phases of matter [22], only a few examples of first- [23, 24], second- [24, 25], third- [24, 26, 27] and fourth-order [24] topological phase transitions have been found and, to the best of our knowledge, never higher than that. Therefore, the question of whether higher-order topological phase transitions can appear in symmetry-protected topological systems, and of whether the bulk and boundary may behave differently, remains open.

We focus our study on a 1D model of topological superconductors exemplified by the Kitaev chain [25]. An interesting extension of this model includes hopping and pairing interactions that are long range [28]. The study of the topological phases of this long-range Kitaev chain (LRKC) has revealed a very rich structure, including the existence of topological massive Dirac edge states when the pairing is long-range enough [29]. When the model is 2D, the propagating Majorana modes get enhanced by long-range hopping and pairing [30]. This opens new perspectives for their experimental realization.

In this paper, we show that the LRKC displays a staircase of higher-order topological phase transitions as we vary the long-range decaying exponent α of the pairing interaction. Remarkably, when $\alpha \to 1$ the order of the phase transition becomes infinite. By considering the ground-state energy, we determine the order of the phase transition, the corresponding critical exponents and check that they satisfy the hyperscaling relation. Moreover, using correlation functions of the bulk and boundary combined with a thermodynamic approach [24, 27], we also analyse the critical behaviour at the boundary, where a transition from a system with Majorana Zero Modes (MZMs) to non-local massive Dirac fermions occurs. Remarkably, in the LRKC the bulk and

boundary topological phase transition decouple, and the universality found in Ref. [24], where the phase transitions in the bulk was always one order higher than at the edges, no longer holds.

2. The Model.— The Hamiltonian of the LRKC [28, 29] with N sites reads

$$\hat{H} = -\mu \sum_{j=1}^{N} \left(c_j^\dagger c_j - \frac{1}{2} \right) - t \sum_{j=1}^{N-1} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) +$$
$$+ \Delta \sum_{j \neq l} \frac{1}{|j-l|^\alpha} \left(c_j c_l + c_l^\dagger c_j^\dagger \right), \qquad (1)$$

where c_j ($c_j^\dagger$) is the fermionic annihilation (creation) operator for site j, μ the chemical potential, t the hopping parameter, Δ the pairing amplitude and α the parameter characterising the range of the interaction. Long-range hopping terms can be also considered, but they do not provide novel topological phases [29]. Thus, we may consider purely short-range hopping without loss of generality. The spectrum of the LRKC with periodic boundary conditions is given by [28, 29]

$$E_k = \pm\sqrt{\epsilon_k^2 + 4\Delta^2 f_\alpha^2(k)}, \quad f_\alpha(k) = \sum_{l=1}^{N-1} \frac{\sin(kl)}{|l|^\alpha}, \quad (2)$$

where $\epsilon_k = -\mu - 2t\cos(k)$. For $\alpha \to \infty$, this model has a well-defined limit to the short-range Kitaev chain (SRKC) [25], which is known to display a topological phase for $|\mu/t| < 2$, characterized by the presence of Majorana zero modes (MZMs) at the edges. For $|\mu/t| > 2$, a trivial phase is found instead.

The LRKC exhibits even more exotic behaviour than its short-range counterpart [28, 29, 31]. The long-range terms give rise to the function $f_\alpha(k)$ defined in Eq. (2), which is discontinuous at $k = 0$ for $\alpha < 1$, while its derivative is discontinuous for $\alpha < 2$. Therefore, the physics of the model drastically depends on α.

For $\alpha > 2$, the LRKC behaves similarly to the SRKC, i.e. there are MZMs in the topological phase. For $\alpha < 1$, the physics in the topological phase changes drastically, in that the two Majorana modes at the edge merge into a non-local Dirac fermion that acquires mass provided that $\mu/t < 2$. Finally, for $1 < \alpha < 2$, the topological phase diagram becomes more intricate, and the winding number becomes ill-defined, as discussed in Ref. [29]. The critical behaviour at $\mu/t = -2$ in the bulk changes with α, while the one at $\mu/t = 2$ remains the same. Contrarily to the bulk, the boundary of the LRKC behaves still in the same way as the SRKC for $3/2 < \alpha < 2$. However, for $\alpha < 3/2$ one finds, in addition to the MZMs for $|\mu/t| < 2$, non-local massive edge states for $\mu/t < -2$ [29, 35]. A disorder analysis of the sector $1 < \alpha < 2$ (see "The Edge States for $\alpha < 3/2$" in the Sup. Mat. [35]) shows the robustness of these massive edge states to static disorder.

In order to understand the nature of the topological phase transitions at $\mu/t = \pm 2$ within the different topological sectors, we investigate their thermodynamic properties using correlation functions. As it turns out, the order of the phase transition at $\mu/t = 2$ does not change with α, but we find extraordinary behaviour for the order of the phase transition at $\mu/t = -2$, in the form of a staircase of higher-order topological phase transitions towards $\alpha \to 1$. Before we show these results, let us first introduce our method.

3. Thermodynamic Analysis.— To classify the phase transitions of the LRKC, we use an adapted Ehrenfest classification [15, 17, 18], in which one considers the grand potential Ω and assigns the order of the phase transition according to the derivative for which the grand potential has a divergence or a discontinuity. The grand potential can subsequently be decomposed into a bulk term $N\omega_1$, which scales linearly with the system size, and a residual term ω_0, which contains the finite-size and boundary effects, i.e. $\Omega = N\omega_1 + \omega_0$. To obtain these contributions, we consider the derivative of the grand potential Ω w.r.t. μ, such that we can relate it directly to the correlation functions

$$\frac{\partial \Omega}{\partial \mu} = \frac{\partial}{\partial \mu} \left(-\frac{1}{\beta} \log \mathrm{Tr}\left[e^{-\beta\hat{H}} \right] \right) = \left\langle \frac{\partial \hat{H}}{\partial \mu} \right\rangle, \quad (3)$$

where $\langle \hat{A} \rangle := \mathrm{Tr}[\hat{A} e^{-\beta\hat{H}}]/\mathrm{Tr}[e^{-\beta\hat{H}}]$. This thermodynamic analysis is especially well-suited for symmetry-protected topological systems both at zero [27] and finite temperatures [24, 32]. To explicitly find ω_1 and ω_0, we consider an infinitely long and periodic chain at zero temperature with grand-potential density

$$\omega = \frac{\Omega_p}{N} = -\int_{-\pi}^{\pi} \mathrm{d}k\, E_k,$$

where p stands for periodic. This integral is bounded because the spectrum is finite for $\alpha > 1$, and diverges at most as $1/k^{1-\alpha}$ for $\alpha < 1$. Hence, ω is finite for all α and does not depend on the system size in this limit. Similarly, the on-site correlation function $\langle c_r^\dagger c_r \rangle$ does not depend on the system size when N is large enough. Thus, we may add and subtract $\partial \Omega_p / \partial \mu$ to Eq. (3), to find

$$\frac{\partial \Omega}{\partial \mu} = \frac{\partial \Omega_p}{\partial \mu} + \left(\frac{\partial \Omega}{\partial \mu} - \frac{\partial \Omega_p}{\partial \mu} \right). \quad (4)$$

Using Eqs. (1), (3), and (4), we then obtain

$$\frac{\partial \Omega}{\partial \mu} = N\langle c_r^\dagger c_r \rangle + \sum_j \left(\langle c_j^\dagger c_j \rangle - \langle c_r^\dagger c_r \rangle \right),$$

where $\langle c_r^\dagger c_r \rangle$ are the on-site correlation functions for the infinitely long periodic chain and $\langle c_j^\dagger c_j \rangle$ are calculated for the finite chain. Hence, we can read off

$$\frac{\partial \omega_1}{\partial \mu} = \langle c_r^\dagger c_r \rangle, \quad (5)$$

$$\frac{\partial \omega_0}{\partial \mu} = \sum_j \left(\langle c_j^\dagger c_j \rangle - \langle c_r^\dagger c_r \rangle \right) := \sum_j \Lambda(j). \quad (6)$$
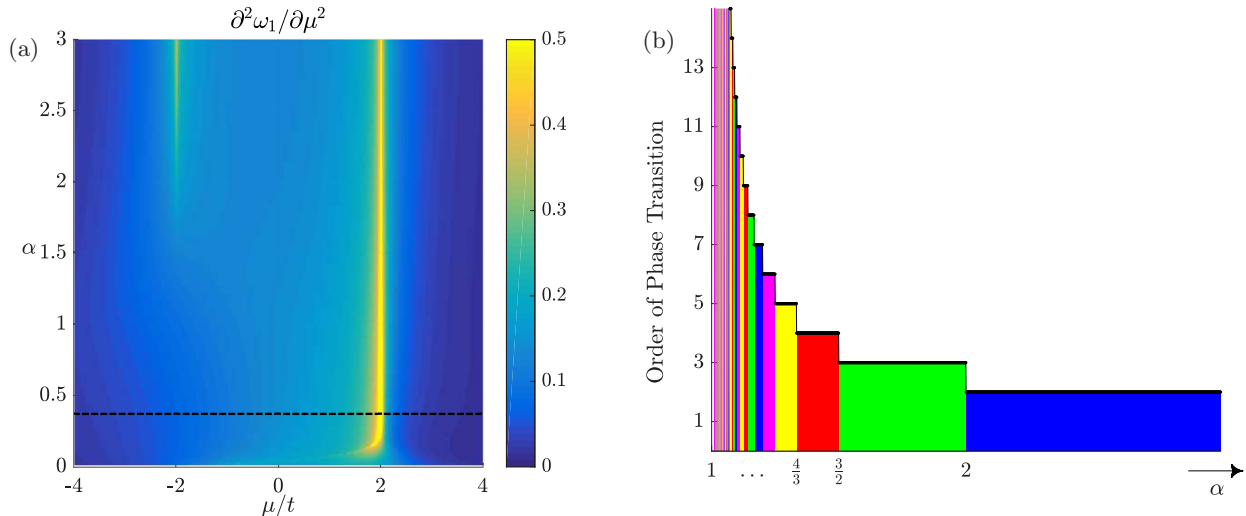
FIG. 1. (a) Second derivative of the bulk thermodynamic potential, obtained from Eq. (5) for the LRKC in the μ/t-α plane. The dashed line indicates the value of α below which our numerical results are not accurate anymore. (b) Staircase of higher-order topological phase transition at $\mu/t = -2$, indicating how the order of the transition increases as one approaches $\alpha = 1$.

The extensive bulk term $\partial\omega_1/\partial\mu$ is simply given by the on-site correlation functions for the infinitely long periodic chain and the residual term $\partial\omega_0/\partial\mu$ is the sum of the difference $\Lambda(j)$ between the on-site correlation functions in the periodic and in the finite chain. As a consequence, the residual contribution ω_0 contains all the subleading terms in N, and therefore includes $\log(N)$, constant, and $1/N$ terms, to name just a few. For large system sizes, one can only consider the log and the constant term and neglect all other subleading contributions.

For the SRKC, it suffices to only consider the constant term [24, 27]. This leads to a first-order phase transition at the boundaries [24], which is due to the appearance/disappearance of the Majorana edge states. The second-order phase transition in the bulk is due to a gap closing at the critical points $\mu/t = \pm 2$. Let us now focus on the LRKC, where higher-order topological phase transitions will arise.

4. Higher-Order Bulk Phase Transitions.— We analyse the zero-temperature behaviour of the bulk grand-potential density defined in Eq. (5) as a function of the long-range exponent α and the chemical potential μ. Although we concentrate here on the zero-temperature behaviour, the method itself is generic and could be applied to finite temperatures. The results are shown in Fig. 1. There is a second-order phase transition at $\mu/t = 2$ separating the topological and trivial phases for every value of α [see Fig. 1(a)], precisely as it is the case for the SRKC. Note the behaviour below the dashed line around $\alpha \approx 0.3$ near $\mu/t = 2$, where the transition line makes a turn and does not go all the way towards $\alpha = 0$. This is merely an artifact due to numerical limitations, since the correlations become too long-ranged, and one needs very large system sizes to suppress this effect.

On the other hand, for $\mu/t = -2$ the behaviour of the phase transition changes drastically, depending on the value of α, and further analytical calculations are needed. Since the non-analytical behaviour of the bulk term in the grand-potential density ω_1 is given by the $k = 0$ mode, we make the separation $\omega_1 = F + G$, where F is the integral around $k = 0$, containing all the non-analyticities, and G is the integral over the remaining part of the Brillouin zone. In this way, we can consider only F to describe the non-analytical part of ω_1, i.e. the information about the order of the phase transition. To calculate F, one can expand the spectrum E_k in Eq. (2) around $k = 0$ and integrate it for $k \in (0, \varepsilon)$, where ε is sufficiently small for the expansion in k to be valid. From this expansion, we can also extract the critical exponent $\tilde{\alpha}$ defined by $\Omega \propto m^{2-\tilde{\alpha}}$, the dynamical exponent z defined by $E_k(m = 0) \propto k^z$ and the critical exponent ν defined by $E_{k=0}(m) \propto m^{z\nu}$ [1], where $m = \mu/t + 2$ denotes the distance from the critical point. The leading term for $\alpha > 2$ (valid also for the SRKC) casts the form

$$F(m, \alpha > 2) := \int_0^\varepsilon dk \sqrt{m^2 + k^2} \propto m^2 \log|m|.$$

This function is divergent in its second derivative at $m = 0$ for all $\alpha > 2$, hence we find a second-order phase transition. For $1 < \alpha < 2$, the leading term is given by

$$F(m, 1 < \alpha < 2) \approx \int_0^\varepsilon dk \sqrt{m^2 + k^{2(\alpha-1)}} \tag{7}$$

$$\propto \Gamma\left(-\frac{\alpha}{2(\alpha-1)}\right)\Gamma\left(\frac{2\alpha-1}{2(\alpha-1)}\right)|m|^{\frac{\alpha}{\alpha-1}},$$

where the last line is not defined if one of the gamma functions diverge, which happens when $\alpha = n/(n-1)$

where $n \in \mathbb{N}$. For $\alpha = 2n/(2n-1)$, one finds, instead of Eq. (7), the relation $F \propto m^n \log(|m|)$, which is divergent in its n-th derivative at $m = 0$. For $\alpha = (2n-1)/(2n-2)$, there will be a discontinuity in the $2n-1$-th derivative at $m = 0$, because in that case $F \propto |m|^{2n-1}$. Hence, for any $\alpha = n/(n-1)$, we find a n-th order phase transition. If α is in between these values, then the power of $|m|$ in Eq. (7) is a non-integer value, meaning that one can differentiate it until its power is negative and it becomes divergent at $|m| = 0$. For example, if $3/2 < \alpha < 2/1$ the exponent of $|m|$ lies between 2 and 3, which means that the third derivative is divergent at $m = 0$. For $4/3 < \alpha < 3/2$, the exponent of $|m|$ lies between 3 and 4, which means that the fourth derivative is divergent, and so forth.

Therefore, we find a staircase behaviour such that the order of the topological phase transition increases stepwise at the points $\alpha = n/(n-1)$ upon lowering α from $\alpha = 2$ to $\alpha = 1$ [see Fig. 1(b)]. This implies that by tuning the exponent α we may address qualitatively different thermodynamic behaviour by inducing higher-order topological phase transitions.

In addition, the critical exponents that follow from this analysis read $\tilde{\alpha} = (\alpha - 2)/(\alpha - 1)$, $z = \alpha - 1$ and $\nu = 1/(\alpha - 1)$. This is consistent with the hyperscaling relation $2 - \tilde{\alpha} = \nu(d + z)$, where d denotes the dimensionality of the model ($d = 1$ in our case) [33, 34].

A remarkable effect occurs in the limit $\alpha = 1$, as the topological phase transition becomes of infinite order. Instead, for $\alpha < 1$, there is no longer a phase transition at $\mu/t = -2$ because the long-range pairing causes the whole chain to be correlated, thus gapping the edge mode everywhere. This can also be clarified from Eq. (7), where the integrand can be expanded as $\sqrt{m^2 + k^{2(\alpha-1)}} = k^{-(1-\alpha)} + k^{1-\alpha}m^2/2 + \mathcal{O}(k^{1-\alpha}(k^{2(1-\alpha)}m^2)^2)$, such that $F(m, \alpha < 1)$ exhibits no non-analyticities. Thus, $\alpha = 1$ constitute a critical-end point in the $\alpha - \mu/t$ quantum phase diagram. This behaviour is consistent with the Dirac Sector found in Ref. [29].

5. *Boundary Phase Transition.*— The separation between the bulk and residual contribution to the grand potential allows us to investigate the behaviour of both independently. Using Eq. (6), we calculate numerically $\partial\omega_0/\partial\mu$ in the $\alpha - \mu/t$ plane and find the result given in Fig. 2 (a) for $N = 200$. Below the dashed line, the results are not accurate due to numerical limitations, as was the case for the bulk. Along the line $\mu/t = 2$, there is a clear indication of a first-order phase transition for all values of α (dark-blue line). However, for $\mu/t = -2$ there is only a clear indication of a first-order phase transition down to $\alpha = 3/2$ (bright-yellow line), below which the boundaries of the phase transition blur out. The reason for this is that for short-range models, when the system is large enough (although finite), the features characterizing the phase transition are so sharp, that one can confidently draw conclusions that would - strictly speaking - only hold for infinite systems. However, when the model becomes long-range, this is no longer the case (see the
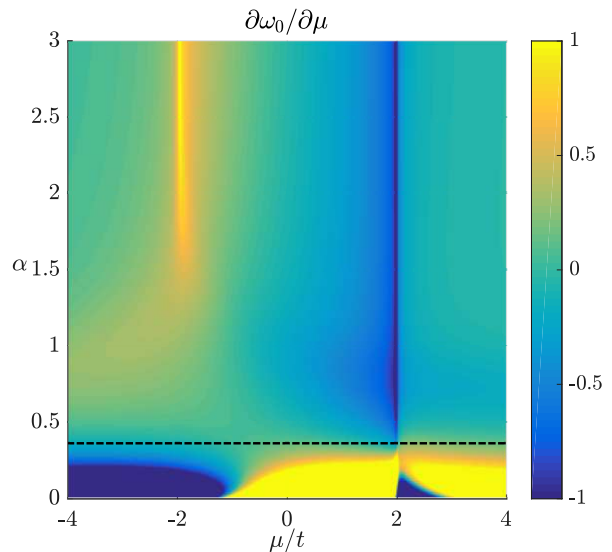

FIG. 2. First derivative of the boundary thermodynamic potential as a function of μ/t, given by Eq. (6). The dashed line indicates the value of α below which our numerical results are not accurate anymore. Although the topological phase transition at $\mu/t = 2$ remains of first order in the entire regime of α, in the thermodynamic limit the phase transition at $\mu/t = -2$ terminates at a quantum critical point located at $\alpha = 1$. However, numerical limitations prevent us from going below $\alpha = 3/2$.

end-to-end correlations analysis in the Sup. Mat. [35]).

6. *Conclusions and Outlook.*— We discovered a staircase of higher-order topological phase transitions in a long-range Kitaev chain. We have shown that the order of the topological phase transition increases step-wise with the long-range decaying exponent α of the pairing interaction. In the limit $\alpha = 1$, we remarkably found an infinite-order phase transition. By separating the bulk from the residual contribution in the grand potential and performing a thermodynamic analysis, we have established not only the order of the topological phase transitions, but also the corresponding critical exponents and checked that they satisfy the hyperscaling relation. Moreover, we have also studied the critical behaviour at the boundary, where there is a transition from a topological phase with MZMs to another topological phase with non-local massive Dirac edge modes [29].

For the long-range Kitaev chain, the correlation functions decay algebraically at long distances, and exponentially at short distances [28, 31]. Hence, the system is critical, and the correlation length can no longer be straightforwardly defined [31]. Although the algebraic term in the correlation functions (which gives the quasi-long-range order) is present for all α, it becomes important around the region where the winding number becomes ill-defined. Therefore, both the criticality and the ill-defined winding number arise due to the relevance of long-range effects at small α. We would like to empha-

sise that our results do not depend on the definition of the correlation length in any way, nor on the correlation length itself, in contrast to scaling theories, where the scaling of the correlation length is used to determine the critical exponents. This is one of the main advantages of our approach, which allows us to describe even critical systems.

We determine the critical exponents by analysing the behaviour of the grand-potential density at the critical point, and characterise thus the topological phase transition. Although the results are applied here at zero temperature, the formalism is generic and may also be used at finite temperatures [24]. In this case, one should be able to connect the central charge c obtained from the entanglement entropy [28] to the central charge found from the heat capacity C_V at very small temperatures, since $C_V \propto cT$ within a first order expansion in T [36]. This would allow for an independent verification of the anomalous behaviour of the central charge at $\mu/t = -2$ predicted in Ref. [28].

Spin and fermionic topological systems with long-range interactions have recently attracted much attention [28–31, 37–48]. In particular, our long-range model is motivated by current experiments of 1D arrays of magnetic atoms deposited on top of conventional s-wave superconductor substrates [49–51]. These arrays of magnetic impurities form subgap states known as Shiba states [52–54]. The particular wavefunction of these states have power-law tails that lead to hopping and pairing amplitudes that decay algebraically with the distance. For 3D superconducting substrates (for instance lead as in Ref. [49] and [51]) the decay goes as $1/r$, whereas for 2D substrates (for example 2D transition metals dichalcogenides) the decay goes as $1/\sqrt{r}$. This long-range behaviour of Shiba impurities has already been observed in recent experiments [55]. Apart from the power-law decay, there is an exponential factor that depends on the coherence length of the superconductor. However, when the length of the chain is small with respect to this coherence length [56], the dominant decay is algebraic, and p-wave Hamiltonians with intrinsic long-range pairing are induced [56–60]. A possible way to tune the decaying exponents, such that the hopping and pairing amplitudes decay differently could be achieved through Floquet driving fields as proposed in Ref. [61]. Thus, the staircase of higher-order topological phase transitions, found in our paper, could be experimentally detected.

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