Exact full counting statistics for the staggered magnetization and the domain walls in the XY spin chain

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We calculate exactly cumulant generating functions (full counting statistics) for the transverse, staggered magnetization, and the domain walls at zero temperature for a finite interval of the XY spin chain. In particular, we also derive a universal interpolation formula in the scaling limit for the full counting statistics of the transverse magnetization and the domain walls which is based on the solution of a Painlevé V equation. By further determining subleading corrections in a large interval asymptotics, we are able to test the applicability of conformal field theory predictions at criticality. As a by-product, we also obtain exact results for the probability of formation of ferromagnetic and antiferromagnetic domains in both the σ^z and σ^x basis in the ground state. The analysis hinges upon asymptotic expansions of block Toeplitz determinants, for which we formulate and check numerically a different conjecture.

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I. INTRODUCTION

In probability theory [1], full counting statistics are generating functions for the cumulants of a random variable. After the recent groundbreaking advances with cold atom experiments [2–5], their calculation has become of increasing relevance in one-dimensional quantum many-body systems. For such models, indeed, exact derivations, which are otherwise not possible, can be performed by relying on mathematical tools borrowed from the asymptotics of block Toeplitz determinants [6], random matrices [7], or field theory and integrability [8,9]. The characterization of quantum fluctuations in one dimension beyond the first few cumulants is nowadays a recurrent theme of research both in [10–20] and out of equilibrium [21–30]. Analytical calculations have been also performed for non-translation-invariant systems such as Fermi gases in a trap [31].

Through their Fourier transforms, full counting statistics allow accessing the probability distribution of a set of quantum measurements, whose outcomes are inherently random. In a real system at equilibrium, local observables are measurable on a finite interval of length L. The theoretical analysis is then focused on the estimation of the asymptotics for large L of their cumulant generating functions. In the large-L limit, full counting statistics depend crucially on the conserved quantities of the whole quantum system and might include universal contributions at a quantum phase transition [32]. These features are inherited by the correlation functions. Moreover, similarly to entanglement entropies [33–36], they can distinguish among different universality classes of quantum critical behavior at equilibrium [32] and far from it [37].

This paper is then devoted to a detailed study of the full counting statistics in the XY spin chain at zero temperature, complementing the existing literature on the subject [10,13,14,38]. The XY spin chain is a paradigmatic model of statistical mechanics [39]. Its phase diagram contains a quantum critical point with \mathbb{Z}_2 symmetry and a critical line where such a discrete group is enhanced to a global U(1) symmetry, which preserves the total magnetization. It is therefore an ideal test bed to scrutinize universality conjectures and understand how symmetries can suppress quantum fluctuations.

In particular, by exploiting the asymptotic expansions for large sizes of block Toeplitz determinants, we will calculate analytically generating functions for the transverse and staggered magnetization and the domain walls. Whenever possible, comments will be made about the existence of universal terms and their comparison with field theory predictions. We will also obtain a universal formula in the scaling limit for the full counting statistics of the transverse magnetization and the domain walls by solving a Painlevé V equation [40,41]. The latter result applies to any system close to a quantum critical point within the Ising universality class. Finally, in the large-coupling limit, cumulant generating functions are proportional to the expectation value of the projector onto a given spin configuration. The best known example is the so-called emptiness formation probability introduced in a Bethe ansatz context by Ref. [42]. Our approach is also suitable to determine analytically the variants thereof, such as the formation probabilities considered in Refs. [43,44]. In particular, we calculate exactly the probability of formation of ferromagnetic and antiferromagnetic domains in both the σ^z and σ^x basis in the ground state.

The summary of this paper is as follows: In Sec. II, we will review how generating functions can be obtained from the subsystem reduced density matrix, and in Secs. III-V the formalism will be applied to the transverse, staggered magnetization, and the domain walls, respectively. We conclude in Sec. VI. Most of the technical details for the interested reader are relegated to a series of Appendixes.

II. REDUCED DENSITY MATRIX AND FULL COUNTING STATISTICS

General formalism. We start by recalling [15] how the full counting statistics (FCS) of fermionic quadratic forms on an interval A of the real line can be calculated from the knowledge of the reduced density matrix. Consider then a free fermionic Hamiltonian,

$$H = \sum_{l,m=1}^{N} c_{l}^{\dagger} P_{lm} c_{m} + \frac{1}{2} \sum_{l,m=1}^{N} (c_{l}^{\dagger} Q_{lm} c_{m}^{\dagger} + \text{H.c.}), \quad (1)$$

where the matrix P is real and symmetric while Q is real and antisymmetric; the operators c_l and c_l^{\dagger} are fermionic annihilation and creation operators and satisfy $\{c_l^{\dagger}, c_m\} = \delta_{lm}$. The state $|\Omega\rangle$ is defined by $c_l|\Omega\rangle = 0$, l = 1, ..., N. Following Lieb, Schultz, and Mattis [39], it is convenient to introduce Majorana fermions

$$a_l = c_l^{\dagger} + c_l, \quad b_l = c_l^{\dagger} - c_l,$$
 (2)

which obey

$${a_l, b_m} = 0, \quad {a_l, a_m} = -{b_l, b_m} = 2\delta_{lm}.$$
 (3)

Suppose now that the correlation matrix $(G_{ba})_{lm} \equiv$ $\langle \Psi | b_l a_m | \Psi \rangle$ is known for a certain quantum state $| \Psi \rangle$. The reduced density matrix ρ_A of an interval A of length L is then defined implicitly by

$$(G_{ba})_{lm} = \text{Tr}[\rho_A b_l a_m]. \tag{4}$$

The matrix elements of ρ_A could be obtained from those of G_{ba} [45], however, for our analytical calculations it is more useful to represent ρ_A on the basis of fermionic coherent states. These are eigenstates of the fermionic annihilation operators c_i with eigenvalue ξ_i defined as $|\xi\rangle = e^{-\sum_l \xi_l c_l^{\dagger}} |\Omega\rangle$, where $\xi^T = (\xi_1, \dots, \xi_L)$ is an L-dimensional vector of Grassmann numbers. Analogously, we define $\langle \eta | = \langle \Omega | e^{\sum_{l} \eta_{l}^{*} c_{l}}$ as the dual coherent state. There is no obvious way to extract the matrix elements of the reduced density matrix in the coherent state basis. However, taking a pragmatic approach, one can postulate an expression for ρ_A that reproduces the correlation matrix G_{ba} through Eq. (4). Such an expression is [46]

$$\langle \eta | \rho_A | \xi \rangle = K e^{-\frac{1}{2}(\eta^* - \xi)F(\eta^* + \xi)}, \quad F = \frac{G_{ba} + 1}{G_{ba} - 1},$$
 (5)

with an obvious notation for the matrix inverse. Notice that Eq. (5) can be valid only if $(G_{aa})_{lm} \equiv \langle \Psi | a_l a_m | \Psi \rangle = 0$ and $(G_{bb})_{lm} \equiv \langle \Psi | b_l b_m | \Psi \rangle = 0$. The normalization K is obtained requiring $\text{Tr}[\rho_A] = 1$, yielding $K = \det[\frac{1}{2}(1 - G_{ba})]$. Given Eq. (5), the validity of Eq. (4) can then be checked by standard manipulations with coherent state integrals. See for instance Appendix A in Ref. [47] for a neat presentation of the relevant formulas that will not be repeated here.

The coherent state representation of the reduced density matrix can then be exploited to obtain determinant representations for the FCS of fermionic quadratic forms. Let us consider an operator \mathfrak{O} with finite support in the interval A

$$\mathfrak{O} = \sum_{l,m \in A} c_l^{\dagger} M_{lm} c_m + \frac{1}{2} \sum_{l,m \in A} (c_l^{\dagger} N_{lm} c_m^{\dagger} + \text{H.c.}) - \frac{1}{2} \text{Tr}[M],$$
(6)

its FCS for a quantum state $|\Psi\rangle$ is

$$\chi_{\mathfrak{O}}(\lambda) = \langle \Psi | e^{\lambda \mathfrak{O}} | \Psi \rangle, \tag{7}$$

with $\lambda \in \mathbb{R}$. When the support of \mathfrak{O} is the interval A, we can also obtain χ_{Ω} as

$$\chi_{\mathfrak{O}}(\lambda) = \text{Tr}[\rho_A e^{\lambda \mathfrak{O}}].$$
 (8)

To derive an explicit expression for the FCS, first one recasts the exponential in Eq. (7) in normal ordered form [48]

$$e^{\lambda \mathfrak{O}} = e^{-\frac{1}{2} \text{Tr} \, Y} e^{\frac{1}{2} c_l^{\dagger} X_{lm} c_m^{\dagger}} e^{c_l^{\dagger} Y_{lm} c_m} e^{\frac{1}{2} c_l Z_{lm} c_m}, \tag{9}$$

with suitable matrices X, Y, Z that will be specified later. For our purposes, it turns out that $X = -X^T = -Z$ and $Y = Y^T$. After inserting Eq. (9) into Eq. (8), the trace can be expanded in the coherent state basis, and its calculation boils down to the evaluation of Gaussian Grassmann integrals. It is then not difficult to show [15]

$$\chi_{\mathfrak{D}}(\lambda) = \frac{1}{\sqrt{\det e^{Y}}} \det \left[\frac{1 - G_{ba}}{2} + \frac{1 + G_{ba}}{2} (-X + e^{Y}) \right],$$
(10)

which is our final expression for the FCS. Finally, the matrices X, Y are obtained as follows: Given Eq. (6), let

$$T = e^{\lambda \begin{bmatrix} M & N \\ -N & -M \end{bmatrix}} \equiv \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}, \tag{11}$$

then [48] $X = T_{12}T_{22}^{-1}$ and $e^{-Y} = T_{22}^{T}$. The XY spin chain. The final formula in Eq. (10) is useful to calculate the ground state FCS in the XY spin chain. The latter is defined by the Hamiltonian [39]

$$H_{XY} = -\sum_{l=1}^{N} \left[\left(\frac{1+\gamma}{2} \right) \sigma_{l}^{x} \sigma_{l+1}^{x} + \left(\frac{1-\gamma}{2} \right) \sigma_{l}^{y} \sigma_{l+1}^{y} + h \sigma_{l}^{z} \right], \tag{12}$$

where $\gamma > 0$ is the anisotropy, h is called the transverse field, and σ_l^{α} are Pauli matrices. In short we will refer to the eigenvalues of σ_i^z as the *transverse* spins, while those of σ_i^x will be dubbed the longitudinal spins. In the thermodynamic limit $N \to \infty$ and for $h = \pm 1$, $\gamma \neq 0$, the XY chain has a quantum phase transition, belonging to the Ising universality class [49,50] whose order parameter is the longitudinal magnetization $\mathfrak{M}_x = \sum_l \sigma_l^x$. When $\gamma = 0$ and |h| < 1 instead, it is also critical but its large distance fluctuations are described by a two-dimensional Euclidean free bosonic action compactified

Equation (12) can be mapped to a fermionic quadratic form of the type introduced in Eq. (1) by a Jordan-Wigner transformation. Our conventions for the Jordan-Wigner mapping are the following,

$$c_l^{\dagger} = \left(\prod_{i=1}^{l-1} \sigma_j^z\right) \sigma_l^+,\tag{13}$$

$$\sigma_l^z = 2c_l^{\dagger}c_l - 1. \tag{14}$$

Even if the formalism outlined in this section allows us to keep track of the finite-N and finite-temperature effects, we will only consider the thermodynamic limit at zero temperature from now on. The ground state correlation matrix G_{ba} in the thermodynamic limit is then [39]

$$(G_{ba})_{lm} = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi(l-m)} e^{i\theta(\phi)}, \tag{15}$$

where we have introduced the shorthand notation

$$e^{i\theta(\phi)} \equiv \frac{h - \cos\phi - i\gamma\sin\phi}{\sqrt{(h - \cos\phi)^2 + \gamma^2\sin^2\phi}}.$$
 (16)

III. EXAMPLE I: THE TRANSVERSE MAGNETIZATION

We start by analyzing the ground state FCS of the transverse magnetization. The results in Secs. III A and III B were already obtained (for $\gamma=1$) by Refs. [10,32,38] but we rederive and integrate them to introduce some notations. The determination of the FCS in the scaling limit given in Sec. III C is instead different. The focus will be on the calculation of the asymptotic behavior of the FCS when the length of the interval A, denoted by L, is large.

A. Full counting statistics

The transverse magnetization is the operator $\mathfrak{M}_z = \sum_{j \in A} \sigma_j^z$, which, according to Eqs. (6) and (13), leads to M = 2I, N = 0, and therefore X = 0 and $e^Y = e^{2\lambda}I$. From the determinant representation in Eq. (10), one obtains the FCS,

$$\chi_{\mathfrak{M}_{z}}(\lambda) = \det[\cosh \lambda I + \sinh \lambda G_{ba}].$$
 (17)

The $L \times L$ matrix inside the determinant is a Toeplitz matrix. One can estimate the large-L behavior of its determinant analytically by exploiting known—and sometimes less known—theorems or conjectures, which are collected in Appendix A. In particular, the key quantity for the asymptotic analysis is the so-called symbol of the Toeplitz matrix, which for Eq. (17) reads

$$g_{\mathfrak{M}_{c}}(\phi) = \cosh \lambda + \sinh \lambda e^{i\theta(\phi)},$$
 (18)

where $\theta(\phi)$ was defined in Eq. (16). The large-L limit of the FCS is then obtained by studying, for real values of λ , the zeros and jump discontinuities of Eq. (18) in the interval $\phi \in [0, 2\pi]$.

Away from criticality (when $|h| \neq 1$), the symbol is free of zeros and jump discontinuities, therefore the Szegő theorem [51] holds and for $L \gg 1$,

$$\ln \chi_{\mathfrak{M}_{z}}(\lambda) = L \left[\int_{0}^{2\pi} \frac{d\phi}{2\pi} \ln[g_{\mathfrak{M}_{z}}(\phi)] \right] + O(1). \tag{19}$$

The O(1) term can be estimated numerically [see Eq. (A1)].

Along the critical lines $h=\pm 1$ instead, the argument of the function $g_{\mathfrak{M}_{\epsilon}}(\phi)$ is discontinuous at $\phi=0$ and $\phi=\pi$, respectively. As first noticed in Ref. [52], jump discontinuities in the symbol are responsible for the divergence of the O(1) term in Eq. (19) and the appearance of subleading logarithmic corrections. Explicitly, one finds the asymptotic expansion for the critical FCS,

$$\ln \chi_{\mathfrak{M}_{z}}(\lambda) = L \left[\int_{0}^{2\pi} \frac{d\phi}{2\pi} \ln[g_{\mathfrak{M}_{z}}(\phi)] \right] - \beta^{2}(\lambda) \ln L + O(1), \tag{20}$$

with $\beta(\lambda) = \frac{1}{\pi} \arctan \tanh(\lambda)$ and the O(1) term is given in Eq. (A4).

Universal terms in the critical FCS. At criticality and in the limit $\lambda \to \pm \infty$, the $O(\ln L)$ term in the asymptotic expansion of the FCS was argued to be universal [32]. Its prefactor, which is γ independent, can be computed by relying only on (boundary) conformal field theory (CFT) techniques, following the crucial assumption that the spin configuration in region A renormalizes at large distances to a conformal invariant boundary condition (bc) [53].

In the limit $\lambda \to \infty$, the operator $e^{\lambda \mathfrak{M}_z}$ is proportional to the projector onto a configuration of L consecutive spins aligned in the positive z direction. Reference [32] conjectured that the latter renormalizes to a free boundary condition for the longitudinal spins. In such a case, field theory predicts that $\beta^2(\infty) = c/8$, where c = 1/2 is the central charge of the CFT associated with the quantum critical point of the XY spin chain for $\gamma \neq 0$. As anticipated in Sec. II, critical fluctuations are encoded into the action of a free massless Majorana fermion.

The same holds in the $\lambda \to -\infty$ limit, when the FCS is proportional to the emptiness formation probability (EFP) for the transverse magnetization [38]. In this case, a configuration of L consecutive spins aligned in the negative z direction flows toward a linear combination of fixed boundary conditions for the longitudinal spins [44]. Within a field theoretical framework, however, the coefficient of the logarithmic term in Eq. (20), does not depend on the boundary conditions—albeit conformal—and is always -c/8 = -1/16.

In the limit $|\lambda| \to \infty$, Ref. [32] conjectured further the existence at criticality of a semiuniversal $O(\ln L/L)$ term in the expansion of Eq. (20). Such a subleading correction is produced by an irrelevant deformation of the CFT action localized on the interval A and its explicit form for h = 1 is [32]

$$\frac{c\xi_{\text{free}}(\gamma)}{8\pi} \frac{\ln L}{L}, \text{ if } A \text{ flows to a free bc,}$$
 (21)

$$\frac{\xi_{\text{fixed}}(\gamma)}{8\pi} \frac{\ln L}{L} (c - 16h_{\text{bcc}}), \text{ if } A \text{ flows to a fixed bc.}$$
 (22)

For $\gamma > 0$, in Eqs. (21) and (22), c = 1/2 and $h_{bcc} = 1/16$ is the dimension of the free-fixed boundary condition changing operator (bcc). The positive quantity $\xi_{free/fixed}(\gamma)$ is the so-called extrapolation length and in principle it depends on the boundary conditions to which the longitudinal spins renormalize. Reference [32] argued through numerical lattice calculations that $\xi_{free}(\gamma) = \xi_{fixed}(\gamma) = \frac{1}{2\gamma}$ and verified the validity of Eqs. (21) and (22) by a nonrigorous—but numerically backed—asymptotic analysis [see also Eq. (A6)].

In particular, the $O(\ln L/L)$ contribution to the expansion of the Toeplitz determinant in Eq. (20) is [32]

$$\operatorname{sgn}(h) \frac{\tanh(2\lambda)\arctan^{2}[\tanh(\lambda)]}{2\pi^{3}\gamma} L^{-1}\ln L. \tag{23}$$

As anticipated, for $\lambda \to \pm \infty$, Eq. (23) is fully consistent with the CFT predictions, provided the identification of the extrapolation length proposed in Ref. [32]. In Secs. IV and V, we will repeat the calculation of the subleading $O(\ln L/L)$ corrections to the FCS for the staggered magnetization and the domain walls to further test the validity of Eqs. (21) and (22).

B. The probability distribution at criticality

The probability distribution for the transverse magnetization is

$$P_{\mathfrak{M}_z}(M) = \langle \delta(\mathfrak{M}_z - M) \rangle. \tag{24}$$

Taking for simplicity L even and exploiting $\chi_{\mathfrak{M}_z}(i\lambda) = \chi_{\mathfrak{M}_z}(i\lambda + \pi)$, it turns out that Eq. (24) can be rewritten as

$$P_{\mathfrak{M}_z}(M) = \mathcal{P}_z(M) \sum_{s \in \mathbb{Z}} \delta(s - M/2). \tag{25}$$

The function $\mathcal{P}_z(M)$ is the Fourier transform of the FCS analytically continued to imaginary values of λ , that is,

$$\mathcal{P}_{z}(M) \equiv \int_{0}^{\pi} \frac{d\lambda}{2\pi} e^{-iM\lambda} \chi_{\mathfrak{M}_{z}}(i\lambda). \tag{26}$$

It can be calculated exactly in the large-L limit and turns out to be a Gaussian (see Appendix B). The Gaussian behavior of the probability distribution of the transverse magnetization has been first observed in Ref. [54], when the subsystem A coincides with the full chain. A quick derivation is the following. The exponential decay of the critical FCS in Eq. (20) implies that all the cumulants of the transverse magnetization are O(L). In particular, let us define

$$\mu \equiv \lim_{L \to \infty} \frac{\langle \mathfrak{M}_z \rangle}{L}, \quad \sigma^2 \equiv \lim_{L \to \infty} \frac{\langle (\mathfrak{M}_z - \langle \mathfrak{M}_z \rangle)^2 \rangle}{L}, \quad (27)$$

then the rescaled random variable

$$m_z \equiv \lim_{L \to \infty} \frac{\mathfrak{M}_z - \mu L}{\sqrt{\sigma^2 L}}$$
 (28)

is Gaussian with zero mean and unit variance, since all its cumulants of order larger than two are zero. The same conclusion can be obtained more formally from a saddle-point analysis [10] of Eq. (25), which is discussed in Appendix B. One finds for large L,

$$\mathcal{P}_{z}(M) = \frac{e^{-\frac{(M-\mu L)^{2}}{2\sigma^{2}L}}}{\sqrt{2\pi\sigma^{2}L}} \left[1 + B\cos\frac{\pi(L-M)}{2}L^{-\frac{1}{4}} \right], \quad (29)$$

valid for L, M even and B is a constant. We observe then that the Shannon entropy of the probability distribution of the transverse magnetization scales as $O(\ln L)$ for large enough L. The values of the parameters μ , σ^2 , and B can be explicitly determined from Eq. (20) and one has

$$\mu = \frac{2\ln(\gamma + \sqrt{\gamma^2 - 1})}{\pi\sqrt{\gamma^2 - 1}}, \quad \sigma^2 = \frac{2\gamma}{\gamma + 1}.$$
 (30)

The coefficient B is the exponential of the O(1) term in the expansion (20) evaluated at $\lambda = i\pi/2$, which can be determined from Eq. (A4). For arbitrary γ , B has an involved expression, but it is particularly simple when $\gamma = 1$: $B = 2^{1/12}e^{1/4}\mathfrak{A}^{-3}$, where \mathfrak{A} is the Glaisher constant [10].

C. Interpolation formula in the scaling limit and Painlevé V equation

Let us consider preliminarily the Ising spin chain, i.e., $\gamma = 1$. By defining $z = e^{i\phi}$, we can rewrite the symbol in Eq. (18) as

$$\tilde{g}_{\mathfrak{M}_z}(z) = \cosh \lambda + \sinh \lambda \frac{h - z}{\sqrt{(h - z)(h - z^{-1})}}.$$
 (31)

Equation (31) shows explicitly that for h > 1 (h < 1) the branch cuts of the symbol can be chosen along the segments (0, 1/h), (h, ∞) [(0, h), $(1/h, \infty)$]. When $|h| \to 1$, and approaching the critical point, the branch points merge at z = 1 on the unit circle, generating a discontinuity in the imaginary part of $\tilde{g}_{\mathfrak{M}_z}$. This is associated with the Fisher-Hartwig exponent $\beta(\lambda)$, which was discussed below Eq. (20). The emergence of a Fisher-Hartwig singularity in the scaling limit $|h| \to 1$ is described by a Painlevé V equation [55]. By introducing the scaling variable $x = 2L|\ln|h|$, one has for $L \to \infty$ and $h \to 1^{\pm}$,

$$\ln \chi_{\mathfrak{M}_z}(\lambda; x) = L \int_0^{2\pi} \frac{d\phi}{2\pi} \ln[g_{\mathfrak{M}_z}(\phi)] - \beta(\lambda)^2 \ln x + \ln \tau_V(x) + O(1), \quad (32)$$

where O(1) denotes finite terms in the $L \to \infty$ limit given in Appendix C and $\tau_V(x)$ is the τ function of the Painlevé V equation [56],

$$(x\zeta'')^2 = [\zeta - x\zeta' + 2(\zeta')^2]^2 - 4(\zeta')^2[\zeta' + \beta(\lambda)][\zeta' - \beta(\lambda)],$$
(33)

namely $\zeta(x) = x \frac{d \ln \tau_V(x)}{dx} - \beta(\lambda)^2$. The function τ_V is constructed in such a way that for $x \to 0$, at short distances, $\ln \chi_{\mathfrak{M}_z}(\lambda; x)$ coincides with Eq. (20), while for $x \to \infty$, at large distances, $\ln \chi_{\mathfrak{M}_z}(\lambda; x)$ is given by the Szegő theorem in Eq. (19). Following the ideas introduced in Refs. [40,41], to which we refer for any additional details, it is possible to write down an explicit power series expansion about x = 0 of the function τ_V . The latter could be also extended to $\gamma \neq 0$, provided [41] one considers the scaling variable $x = 2L \ln |h|/\gamma$; the first few terms of such an expansion are

$$\begin{aligned}
&\text{In } \tau_V(x) \\
&= -\beta^2 [\ln(x) - s_0 - 1] x \\
&- \beta^4 \left[\frac{1}{2} (\ln x)^2 - (s_0 + 1) \ln(x) + \frac{s_0^2}{2} + s_0 \right] \\
&+ \frac{5}{4} - \frac{1}{4\beta^2} x^2 + O[x^3 (\ln x)^3],
\end{aligned} (34)$$

where $s_0 = -\psi(1 + \beta(\lambda)) - \psi(1 - \beta(\lambda)) + 3\psi(1) + 1$, and $\psi(z)$ is the digamma function. The expansion of τ_V until order $O(x^4)$ can be also straightforwardly obtained from Ref. [41]. For $x \to \infty$, $\ln \tau_V(x)$ must behave as

$$\ln \tau_V(x) \sim \beta^2(\lambda) \ln(x) - \ln[G(1 + \beta(\lambda))G(1 - \beta(\lambda))], \tag{35}$$

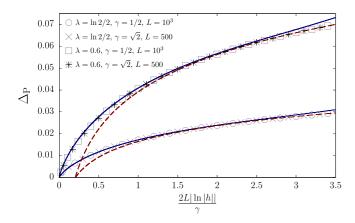


FIG. 1. Numerical check of the interpolation formula of Eq. (32) between the noncritical and the critical regimes of the FCS of the transverse magnetization $\chi_{\mathfrak{M}_z}(\lambda)$. We represent Δ_P , defined in Eq. (C2), as a function of $x=2L|\ln|h||/\gamma$, for different fixed values of γ and L, and varying h. The dots have been calculated numerically using Eq. (17) for $\chi_{\mathfrak{M}_z}(\lambda)$. As we explain in Appendix C, $\Delta_P \sim \ln \tau_V(x)$ for large L. The solid curves represent the expansion (34) around x=0 up to order $O(x^4)$ of $\ln \tau_V(x)$. The dashed curves correspond to the asymptotic behavior (35) for large x of this τ function.

where G(z) is the Barnes double gamma function, in order to recover the asymptotics (19) outside the critical lines; see also Appendix C.

In physical terms, Eqs. (32) and (34) provide a complete interpolation formula for the FCS of the transverse magnetization in the scaling limit $\xi \gg 1$, where $\xi = \frac{\gamma}{|h-1|}$ is the XY chain correlation length. In the limit $|h| \to 1$ the scaling variable x is the ratio $2L/\xi$; the regime of small x ($\xi \gg L$) describes the fluctuation of the transverse magnetization at the quantum phase transition, while in the regime of large x ($\xi \ll L$) the chain is off critical. The validity of Eq. (32) can be checked numerically, as described in the caption of Fig. 1.

It is an interesting question to understand whether the subleading corrections discussed in the previous section [cf. Eqs. (21) and (22)] are also encapsulated in the expansion of the τ function in Eq. (34).

D. The case $\gamma = 0$

At $\gamma = 0$, the XY spin chain after a Jordan-Wigner transformation reduces to a model of spinless fermions hopping on a one-dimensional lattice, that is, up to a constant,

$$H_{XY}|_{\gamma=0} = \frac{1}{2} \sum_{l=1}^{N} (c_l^{\dagger} c_{l+1} + \text{H.c.}) - h \sum_{l=1}^{N} c_l^{\dagger} c_l.$$
 (36)

By further assuming $0 \le h < 1$, let us define $k_F \equiv \arccos h$, with $0 < k_F \le \pi/2$. The ground state of Eq. (36) is then a Fermi sea, where all the single-particle states with momenta $\phi \in [k_F, 2\pi - k_F]$ are filled. The average transverse magnetization per site is $\lim_{N\to\infty} N^{-1}\langle \mathfrak{M}_z \rangle = 2\rho - 1$, with $\rho = 1 - \frac{k_F}{\pi}$, the average ground state fermion density. In spin language, the model in Eq. (36) is also dubbed the XX chain and corresponds to the zero anisotropy limit of the XXZ spin chain [8].

The FCS of the transverse magnetization at $\gamma=0$ can be determined directly by studying the $\gamma \to 0$ limit of the symbol in Eq. (18). The resulting function is piecewise constant, with two jump discontinuities at $\phi=\{k_F, 2\pi-k_F\}$. An immediate application of Eq. (A3) leads to [13]

$$\ln \chi_{\mathfrak{M}_{z}}(\lambda)|_{\gamma=0} = (2\rho - 1)\lambda L + \frac{2\lambda^{2}}{\pi^{2}} \ln L + O(1), \quad (37)$$

valid for large L. By calculating the Fourier transform of the analytic continuation to imaginary λ ($\lambda \rightarrow i\lambda$) of the FCS in Eq. (37), one obtains the probability distribution of the transverse magnetization at $\gamma = 0$. For $L \gg 1$, this is a Gaussian, with the mean centered at $\mu = L(2\rho - 1)$ and variance $\sigma^2 =$ $4 \ln L/\pi^2$. The Shannon entropy of the transverse magnetization at $\gamma = 0$ scales then as $O(\ln \ln L)$. Its sublogarithmic behavior (cf. Sec. III B) is a consequence of the conservation of the *total* transverse magnetization $\lim_{N\to\infty}\sum_{l=1}^N\sigma_l^z$: When the interval A is big, large fluctuations of the transverse magnetization are severely suppressed. Furthermore, the limits $\lambda \to \pm \infty$ and $L \to \infty$ cannot be interchanged at $\gamma = 0$, and (see Refs. [38,57]) the EFP of the transverse magnetization is, for $L \gg 1$, $O(e^{-L^2})$, contrary to what happens at $\gamma \neq 0$ where it decays exponentially (cf. Sec. III A). The Gaussian decay can also be interpreted as an arctic phenomenon (see, e.g., Refs. [32,58]): Taking imaginary time, one can argue that, if the transverse magnetization is conserved, the ferromagnetic string generates an area of order L^2 in which all the degrees of freedom are frozen. The fluctuating degrees of freedom outside the frozen region are described by a massless, but not conformal, field theory.

We will see how these conclusions change for the staggered magnetization in Sec. IV C and the domain walls in Sec. V C.

IV. EXAMPLE II: THE STAGGERED TRANSVERSE MAGNETIZATION

Another observable whose ground state fluctuations can be fully characterized within our formalism is the transverse staggered magnetization, defined as

$$\mathfrak{M}_s = \sum_{l \in A} (-1)^{l+1} \sigma_l^z. \tag{38}$$

In this section we present an exact and comprehensive study of its fluctuations for the XY chain. Our results also apply in the limit $\gamma \to 0$, which corresponds to the zero anisotropy case of the XXZ spin chain (Sec. IV C). Partial computations of the staggered magnetization FCS have been done in Ref. [26] for this model in the scaling limit, by relying on field theoretical tools.

A. Full counting statistics

For the staggered magnetization [cf. Eq. (10)], we have $M = 2I_s$, where $I_s = \text{diag}(1, -1, 1, -1, ...)$ and N = 0. The length of the interval A will be taken for convenience 2L. By applying the results in Sec. II, we end up with the following determinant representation for the ground state FCS,

$$\chi_{\mathfrak{M}_{s}}(\lambda) = (-\sinh^{2}\lambda)^{L} \det[G_{s}], \tag{39}$$

where G_s is a block Toeplitz matrix, built from the 2×2 blocks g_{lm} $(l, m = 1 \dots L)$, given by

$$g_{lm} = \begin{bmatrix} \coth(\lambda) + (G_{ba})_{2(l-m)} & (G_{ba})_{2(l-m)-1} \\ (G_{ba})_{2(l-m)+1} & -\coth(\lambda) + (G_{ba})_{2(l-m)} \end{bmatrix}.$$
(40)

Generalizing the discussion of Sec. III A, the symbol of the block Toeplitz matrix G_s is the Fourier transform $\tau(\phi)$ of the 2×2 matrix g_{lm} , that is,

$$\tau(\phi) = \begin{bmatrix} \coth(\lambda) + h_{+}(\phi) & e^{-i\phi/2}h_{-}(\phi) \\ e^{i\phi/2}h_{-}(\phi) & -\coth(\lambda) + h_{+}(\phi) \end{bmatrix}, \quad (41)$$

with $h_{\pm}(\phi) = (e^{i\theta(\phi/2)} \pm e^{i\theta(\phi/2-\pi)})/2$. For $\lambda \in \mathbb{R}$, the matrix elements of τ have a winding number zero and the large-L limit of the FCS can be then computed by recalling a generalization of the Szegő theorem due to Widom [59–61] and a conjecture formulated in Ref. [62] (see again Appendix A).

In particular, for $|h| \neq 1$, the matrix elements of $\tau(\phi)$ do not have zeros or jump discontinuities for $\phi \in [0, 2\pi]$. The Szegő-Widom theorem [59] then applies and one obtains

$$\ln \chi_{\mathfrak{M}_s}(\lambda) = L \left[\ln(-\sinh^2 \lambda) + \int_0^{2\pi} \frac{d\phi}{2\pi} \ln[\det \tau(\phi)] \right] + O(1). \tag{42}$$

The O(1) term in Eq. (42) can be also estimated numerically [see Eq. (A11)].

At the quantum critical point, the matrix elements of the symbol $\tau(\phi)$ have a jump discontinuity at $\phi = 0$. We can then apply a generalization of Fisher-Hartwig theorem nonrigorously derived in Ref. [62] [see Eqs. (A12) and (A13)], and it turns out

$$\ln \chi_{\mathfrak{M}_s}(\lambda) = L \left[\ln(-\sinh^2 \lambda) + \int_0^{2\pi} \frac{d\phi}{2\pi} \ln[\det \tau(\phi)] \right]$$
$$-\beta_s^2(\lambda) \ln(L) + O(1), \tag{43}$$

where $\beta_s(\lambda) = \frac{1}{\pi} \arctan(\tanh^2 \lambda)$.

Universal terms in the critical FCS. In the limit $|\lambda| \to \infty$, the FCS is proportional to the probability of observing an antiferromagnetic domain of length 2L in the ground state. More explicitly, from Eqs. (7) and (38), it turns out that

$$\langle e^{\lambda \mathfrak{M}_S} \rangle \stackrel{\lambda \gg 1}{\to} e^{2\lambda L} \langle P_{\uparrow \downarrow \dots \uparrow \downarrow} \rangle,$$
 (44)

where $P_{\uparrow\downarrow\cdots\uparrow\downarrow}$ is the projector onto an antiferromagnetic configuration of transverse spins of length 2L. The ground state expectation value of such a projector will be denoted by $\mathcal{E}_s(h)$.

Therefore, in the limit $|\lambda| \to \infty$, the prefactor of the logarithmic term in Eq. (43) has a CFT interpretation, since a staggered sequence of spins in the z direction renormalizes to a linear combination of fixed boundary conditions for the longitudinal spins [44]. Consistently one has $\beta_s^2(\pm \infty) = c/8 = 1/16$ as for the transverse magnetization (cf. Sec. III A). At criticality, one expects [32] also subleading $O(L^{-1} \ln L)$ corrections to Eq. (43). By generalizing the method of Ref. [32] [see Appendix A below Eq. (A13)], we are able to determine them for $\gamma > 0$ and it turns out that

$$-\frac{\gamma^2 + 1}{2\pi^3 \nu} \frac{\tanh^2 \lambda}{\tanh^4 \lambda + 1} \arctan^2(\tanh^2 \lambda) L^{-1} \ln L. \tag{45}$$

Details of the derivation of Eq. (45), together with a numerical check, are given in Appendix C. Notice that for $|\lambda| \to \infty$, Eq. (45) agrees with the CFT prediction given in Eq. (22) provided $\xi_{\text{fixed}}(\gamma) = (\gamma^2 + 1)/(8\gamma)$.

B. The probability distribution at criticality

The probability distribution of the staggered magnetization is defined as in Eq. (24). Because all the eigenvalues of \mathfrak{M}_s are even integers, the relation $\chi_{\mathfrak{M}_s}(i\lambda) = \chi_{\mathfrak{M}_s}(i\lambda + \pi)$ still holds and therefore also Eq. (25). We will then be interested in estimating the large-L limit of the Fourier transform,

$$\mathcal{P}_s(M) = \int_0^{\pi} \frac{d\lambda}{2\pi} e^{-iM\lambda} \chi_{\mathfrak{M}_s}(i\lambda). \tag{46}$$

The analytic continuation of the symbol in Eq. (41) to imaginary λ introduces a winding when |h| < 1 for $\lambda \in [\pi/4, 3\pi/4]$. At criticality instead, the Wick rotation $\lambda \to i\lambda$ is allowed and the large-L limit of Eq. (46) can be obtained in complete analogy to what is done in Sec. III B (see also Appendix B). One finds

$$\mathcal{P}_s(M) = \frac{e^{-\frac{M^2}{2\sigma^2 L}}}{\sqrt{2\pi\sigma^2 L}} \left[1 + B\cos\frac{\pi M}{2} L^{-\frac{1}{4}} \right],\tag{47}$$

with

$$\sigma^2 = 2 - \frac{4(\gamma^2 + 1)^2 \arccos[2\gamma/(\gamma^2 + 1)]}{\pi |\gamma^4 - 1|}.$$
 (48)

In this case, $\mu=0$ and $\ln B$ is the O(1) term in the expansion (43) of $\ln \chi_{\mathfrak{M}_s}(i\pi/2)$. Note that $\chi_{\mathfrak{M}_s}(i\pi/2)=\det[G_{ba}]$, and the correlation matrix G_{ba} is Toeplitz. Hence, in this particular case, one can use the Fisher-Hartwig conjecture (A3) instead of (A12), which allows us to determine B. In fact, applying (A3), we obtain $\chi_{\mathfrak{M}_s}(i\pi/2) \sim BL^{-1/4}$, and B is given by Eq. (A4). For $\gamma=1$, its expression is especially compact, $B=2^{-1/6}e^{1/4}\mathfrak{A}^{-3}$.

The Gaussian form of the probability distribution implies that the Shannon entropy of the staggered magnetization also scales as $O(\ln L)$ for large L.

C. The case $\gamma = 0$

The fluctuations of the staggered magnetization at $\gamma = 0$ are also interesting, since they depend on the value of the transverse field. Let us assume, without loss of generality, $0 \le h < 1$ and define, as in Sec. III D, $k_F = \arccos h$; also we will refer to the case h = 0 as half filling.

At $\gamma=0$ and away from half filling, the matrix elements in Eq. (41) are piecewise functions of ϕ with two jump discontinuities at $\phi=\{2k_F,2\pi-2k_F\}$. By applying the conjecture in Eq. (A12) and in particular Eq. (A13), it is possible to calculate the large-L limit for the FCS of the staggered magnetization as follows,

$$\ln \chi_{\mathfrak{M}_s}(\lambda)|_{\gamma=0} = \frac{2k_F L}{\pi} \ln(\cosh 2\lambda) + \frac{1}{2\pi^2} \ln^2(\cosh 2\lambda) \ln L + O(1). \tag{49}$$

For h = 0 instead, the matrix elements of the symbol in Eq. (41) when evaluated at $\gamma = 0$ are piecewise functions of ϕ

but with only one jump discontinuity located at $\phi = 2k_F$. The results in Eqs. (A12) and (A13) are still valid but the large-L asymptotics is now

$$\ln \chi_{\mathfrak{M}_s}^{h=0}(\lambda)|_{\gamma=0} = L \ln(\cosh 2\lambda) - 2\beta^2(\lambda) \ln L + O(1), (50)$$

with $\beta(\lambda)$ defined below Eq. (20).

As we already observed in (44), in the limit $|\lambda| \to \infty$, the FCS is proportional to the probability of finding an antiferromagnetic string in the ground state. There is a qualitative difference between the two limits $|\lambda| \to \infty$ of Eq. (44) at half filling and away from it. In the first case, the large-L limit commutes with the large-L limit and the latter can be calculated directly from Eq. (50) with the result

$$\ln \mathcal{E}_s(h=0) = -L \ln 2 - \frac{1}{8} \ln L + O(1). \tag{51}$$

At h=0, the probability of observing a region with antiferromagnetic order within the ground state of the XX spin chain is exponentially suppressed by its length, i.e., is $O(e^{-L})$. It also contains a logarithmic correction $O(\ln L)$ whose prefactor is compatible with the CFT interpretation recalled at the end of Sec. III A. For $h=\gamma=0$, an antiferromagnetic string of transverse spins renormalizes [63] at large distances to a Dirichlet boundary condition for a compactified boson with a central charge c=1. The prefactor of the subleading logarithmic contribution in Eq. (51) is then -c/8=-1/8. It is natural to expect the same logarithmic correction with a prefactor -1/8 also in the gapless phase [8] of the XXZ spin chain. To the authors' best knowledge, this has yet to be verified.

Away from half filling, the large-L limit and the large- λ limit no longer commute. Mathematically, this is due to the fact that the determinant of the symbol in Eq. (41) in the limit $|\lambda| \to \infty$, and for $\gamma = 0$, h > 0, vanishes along the interval $I \equiv [2k_F, 2\pi - 2k_F]$. Then, Eqs. (A12) and (A13) cannot be used to derive its large-L asymptotics. For scalar symbols which vanish on an interval $I \subset [0, 2\pi]$, the asymptotics of the corresponding Toeplitz determinant was worked out by Widom in Ref. [64] [see Eq. (A10)]. By generalizing such a result [see Eq. (A14)], we conjecture that

$$\ln \mathcal{E}_s(h > 0) = L^2 \ln \sin k_F - L \ln 2 - \frac{1}{4} \ln L + O(1). \quad (52)$$

In Fig. 2, we check numerically the above conjecture. The points are the values for $\ln \mathcal{E}_s(h > 0)$ obtained from the numerical computation of Eq. (39) at $\gamma = 0$ and h > 0 while the curves correspond to the analytical prediction in Eq. (52).

The physical explanation of Eq. (52) mimics the discussion in Sec. III D. For h > 0, the conservation law $[H_{XY}|_{\gamma=0}, \mathfrak{M}_z] = 0$ requires all the eigenstates of the XX Hamiltonian to be eigenstates of $N^{-1}\mathfrak{M}_z$ with an eigenvalue different from zero in the thermodynamic limit $N \to \infty$. Therefore the probability of observing a large region with antiferromagnetic order at zero temperature must fall off more quickly, as $O(e^{-L^2})$, than at h = 0. At half filling, instead, the Néel state $|\uparrow\downarrow\cdots\uparrow\downarrow\rangle$ is not orthogonal to the ground state and its overlap [44] decays exponentially as $O(e^{-N})$, leading to an exponential decay of $\mathcal{E}_s(h=0)$ in Eq. (51).

Finally, we note that at criticality Eqs. (49) and (50) imply that the probability distribution of the staggered magnetization is Gaussian at $\gamma = 0$, with a variance of O(L). Therefore its

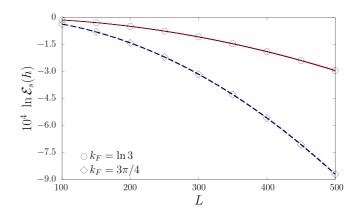


FIG. 2. Numerical check of the expansion conjectured in Eq. (52) for the formation probability of an antiferromagnetic domain in an XX spin chain with Fermi momentum $k_F \neq \pi/2$. The dots have been obtained by calculating numerically the determinant in Eq. (39) in the limit $\lambda \to -\infty$. The curves correspond to the conjectured expansion (52); the O(1) term has been determined from $\ln \mathcal{E}_s(L=500)-500^2 \ln \sin k_F-500 \ln 2-1/4 \ln(500)$, taking as $\mathcal{E}_s(L=500)$ the value obtained numerically for this quantity at L=500 for each Fermi momentum considered.

Shannon entropy is $O(\ln L)$ for large L. There are also subleading power-law corrections of the type $L^{-\alpha}$ as in Eq. (47) but with an exponent $\alpha = 1/2$.

V. EXAMPLE III: THE DOMAIN WALLS

We characterize exactly at large L the fluctuations of the number of domain walls in the XY spin chain, that is,

$$\mathfrak{K} = \sum_{l \in A} \left(1 - \sigma_l^x \sigma_{l+1}^x \right). \tag{53}$$

At $\gamma=1$, this observable can be accessed by a Kramers-Wannier transformation applied to the transverse magnetization [10]. Our analysis will be more general and valid for any values of the anisotropy $\gamma>0$. Eventually, we will also show how our results for the FCS allow determining analytically the EFP of the longitudinal magnetization $\mathfrak{M}_x=\sum_{l\in A}\sigma_l^x$. The latter has been recently discussed in Ref. [27] resorting to certain numerical approximations.

A. Full counting statistics

By applying the Jordan-Wigner transformation in Eq. (13), the operator \Re of Eq. (53) can be put in the form of Eq. (6) with

$$(M)_{lm} = \delta_{|l-m|,1}, \quad (N)_{lm} = \delta_{|l-m|,1} \operatorname{sgn}(m-l), \quad (54)$$

for l, m = 1, ..., L + 1. Even if the matrix N in Eq. (54) is nonzero, it is simple enough to carry over the calculation of the matrix exponential in Eq. (11). One finds (see Appendix C) the following determinant representation for the domain wall FCS,

$$\chi_{\mathfrak{K}}(\lambda) = \det[G_{\mathfrak{K}}]. \tag{55}$$

The $L \times L$ matrix $G_{\mathfrak{K}}$ is of Toeplitz type with a symbol [cf. Eq. (18)],

$$g_{\mathfrak{K}}(\phi) = \frac{e^{2\lambda} + 1}{2} + \frac{e^{2\lambda} - 1}{2} e^{-i\phi} e^{i\theta(\phi)}.$$
 (56)

The analysis of its large-L behavior is then straightforward. Indeed, the same Eqs. (19) and (20) hold for the large-L limit of the domain wall FCS upon the replacement of the symbols: $g_{\mathfrak{M}_{e}}(\phi) \rightarrow g_{\mathfrak{K}}(\phi)$.

EFP of the order parameter. The exact expression derived in Eq. (55) for the domain wall FCS is in accordance with the Kramers-Wannier duality between longitudinal and transverse spin configurations analyzed in Ref. [44] for the Ising spin chain. In particular, by comparing Eq. (56) with Eq. (18) at $\gamma = 1$ and taking for simplicity h > 0, one concludes that

$$\chi_{\mathfrak{K}}(\lambda)|_{h} = e^{\lambda L} \chi_{\mathfrak{M}_{z}}(-\lambda)|_{1/h}, \quad h > 0.$$
 (57)

In the limit $\lambda \to -\infty$, Eq. (57) implies

$$\lim_{\lambda \to -\infty} \chi_{\mathfrak{K}}(\lambda) = \langle P_{\to \dots \to} + P_{\leftarrow \dots \leftarrow} \rangle, \tag{58}$$

where $P_{\rightarrow \dots \rightarrow}$ and $P_{\leftarrow \dots \leftarrow}$ are projectors onto states that contain a ferromagnetic region of length L with spins aligned along the x axis. The Kramers-Wannier duality maps both these configurations to one where all the spins are polarized along the positive z axis [44]. Notice that such a conclusion follows directly from Eq. (57). Analogously, an antiferromagnetic domain of longitudinal spins is the Kramers-Wannier dual of a ferromagnetic domain of negatively polarized transverse spins [44]. This last statement is implied by the limit $\lambda \to \infty$ of Eq. (57).

In the absence of a longitudinal field coupling to σ_l^x , the two projectors in Eq. (58) have the same ground state expectation value. The latter is the EFP, $\mathcal{E}_x(h)$, of the order parameter $\mathfrak{M}_x|_A = \sum_{l \in A} \sigma_l^x$ restricted to the subsystem A. For the Ising spin chain, and positive transverse field, after some contour integral manipulations outlined in Appendix C, we obtain the compact expressions for $\mathcal{E}_x(h)$,

$$\ln \mathcal{E}_{x}(h) = \begin{cases} L\left[\int_{0}^{1/h} \frac{dy}{\pi} K(y^{2}) - \ln 2\right] + O(1), & h > 1, \\ L\left(\frac{2\mathfrak{C}}{\pi} - \ln 2\right) - \frac{1}{16} \ln L + O(1), & h = 1, \\ -L\int_{0}^{h} \frac{dy}{\pi} \frac{1}{y} \left[K(y^{2}) - \frac{\pi}{2}\right] + O(1), & h < 1. \end{cases}$$

The function K(y) is the complete elliptic integral of the first kind, written in MATHEMATICA notations, while $\mathfrak{C} = \frac{1}{2} \int_0^1 dy \, K(y^2)$ is the Catalan constant. The first few terms of the series expansion about h=0 of Eq. (59) reproduce the approximate formula proposed recently in Ref. [27]. Of course the calculation of the EFP for the order parameter could be extended to any $\gamma > 0$, simply by considering the limit $\lambda \to -\infty$ of the symbol in Eq. (56), though the extension of Eq. (59) to $\gamma \neq 1$ does not have a nice compact form.

Universal terms in the critical FCS. As expected from the discussion at the end of Sec. III A, the prefactor of the $O(\ln L)$ term of the critical domain wall FCS in the limit $\lambda \to \pm \infty$ is γ independent and with a value of $-\frac{1}{16}$. By pushing the asymptotics analysis of the Toeplitz determinant in Eq. (55) further, one can single out along the critical lines also an

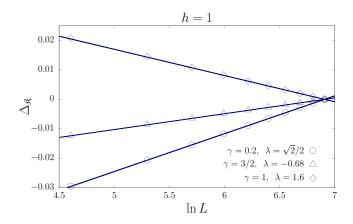


FIG. 3. Numerical check of the $O(L^{-1} \ln L)$ term in the expansion of $\ln \chi_{\mathfrak{K}}(\lambda)$ along the critical line h=1. We plot $\Delta_{\mathfrak{K}}$, defined in Eq. (C7), as a function of $\ln L$ for several fixed values of γ and λ , and choosing $L_0=10^3$. The dots have been obtained by calculating numerically $\chi_{\mathfrak{K}}(\lambda)$ through Eq. (55). The lines represent $d_{\mathfrak{K}} \ln(L/L_0)$, taking for $d_{\mathfrak{K}}$ the coefficient of the $O(L^{-1} \ln L)$ term predicted in Eq. (60).

 $O(\ln L/L)$ term [see Eq. (A6)],

$$-\frac{2\gamma - 1}{2\pi^3 \gamma} \tanh(2\lambda) \arctan^2(\tanh \lambda) L^{-1} \ln L, \qquad (60)$$

whose presence can be checked numerically (see Fig. 3 and Appendix C).

Notice however that the lattice result in Eq. (60) does not have a definite sign as a function of $\gamma > 0$; it vanishes for $\gamma = 1/2$. These considerations suggest that the limit $\lambda \to \pm \infty$ of Eq. (60) does not have an immediate CFT interpretation [32] and deserves futher study.

Painlevé V equation in the scaling limit. An interesting consequence of Eq. (56) is that the same analysis of the scaling limit discussed in Sec. III C for the transverse magnetization also applies to the domain walls. In the limits $|h| \to 1, L \to \infty$ keeping $x = 2L|\ln|h||/\gamma$ finite, the domain wall FCS interpolates from the critical $(x \ll 1)$ asymptotics given in Eq. (A3) to the off-critical asymptotics $(x \gg 1)$ in Eq. (31). The crossover is again analytically captured by Eq. (32) after replacing $g_{\mathfrak{M}_z}(\phi)$ with $g_{\mathfrak{K}}(\phi)$. In particular, since the Fisher-Hartwig exponent $\beta(\lambda)$ in Eq. (32) is the same for the transverse magnetization and the domain walls, the expansion of the Painlevé V τ function in Eq. (34) is also identical. A numerical check of the interpolation formula in Eq. (32) adapted to the domain wall fluctuations is given in Fig. 4.

B. The probability distribution at criticality

The eigenvalues of the operator \mathfrak{K} in Eq. (53) are the even integers $2n_w$ where $n_w=0,\ldots,L$ is the number of domain walls present in the subsystem A. Therefore, the probability distribution $P_{\mathfrak{K}}(W)=\langle \delta(\mathfrak{K}-W) \rangle$ can be recast in the form of Eq. (25) and we will calculate here

$$\mathcal{P}_K(W) = \int_0^\pi \frac{d\lambda}{2\pi} e^{-iW\lambda} \chi_{\mathfrak{K}}(i\lambda), \tag{61}$$

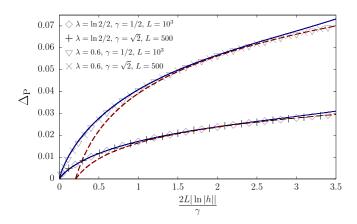


FIG. 4. Numerical analysis of the crossover between the noncritical and the critical behavior of the FCS of the number of domain walls, $\chi_{\mathfrak{K}}(\lambda)$. We study the quantity Δ_{P} , defined in Eq. (C2) but replacing $\chi_{\mathfrak{M}_{z}}$ and $g_{\mathfrak{M}_{z}}$ by $\chi_{\mathfrak{K}}, g_{\mathfrak{K}}$, vs the ratio $x = 2L|\ln|h||/\gamma$; we vary h, keeping γ , λ , and L fixed. The dots correspond to calculate numerically $\chi_{\mathfrak{K}}(\lambda)$ using Eq. (55). As we point out in Appendix C, we expect $\Delta_{P} \sim \ln \tau_{V}(x)$ when L is large enough. The solid curves represent the expansion (34) of the logarithm of the Painlevé V τ function around x = 0 up to order $O(x^4)$. The dashed curves are the asymptotic behavior (35) of this function for $x \to \infty$.

at the quantum critical point |h| = 1. The exponential decay for large L of the domain wall FCS already implies that $\mathcal{P}_K(W)$ is a Gaussian, as pointed out in Sec. III B. More formally, by applying the saddle-point analysis of Appendix B, one finds

$$\mathcal{P}_K(W) = \frac{e^{-\frac{(W-\mu L)^2}{2\sigma^2 L}}}{\sqrt{2\pi\sigma^2 L}} \left[1 + B\cos\frac{\pi W}{2} L^{-\frac{1}{4}} \right], \tag{62}$$

with parameters μ , σ given by

$$\mu = 1 - \frac{2\gamma}{\pi(\gamma + 1)} \left(1 + \frac{\operatorname{arccosh}(\gamma)}{\sqrt{\gamma^2 - 1}} \right), \tag{63}$$

and

$$\sigma^2 = \frac{\gamma^2(\gamma - 1) + 7\gamma + 1}{(\gamma + 1)^3}.$$
 (64)

The coefficient $\ln B$ is the O(1) term in the expansion of $\ln \chi_{\mathfrak{K}}(\lambda)$ at $\lambda = i\pi/2$. Therefore, it can be calculated from Eq. (A4). We omit to write here the explicit form of B since it is a lengthy expression. In Fig. 5, we check numerically the probability distribution in Eq. (62).

At the critical point |h|=1, $\gamma \neq 0$, the Shannon entropy of the domain wall probability distribution scales as $O(\ln L)$ for large L. In fact, the same conclusion also applies to the other critical point of the XY chain: $\gamma=0$ and |h|<1. This will be discussed in detail in the next section.

In the noncritical regions, $|h| \neq 1$, $\gamma > 0$, $\mathcal{P}_K(W)$ is also a Gaussian for large L, but there is no $L^{-1/4}$ subleading correction [see Eqs. (B4) and (B5) of Appendix B]. In that Appendix, we give the technical details to obtain those results.

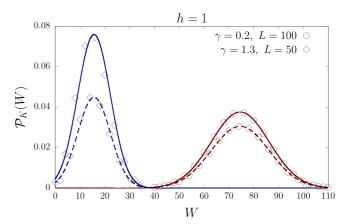


FIG. 5. Probability distribution $\mathcal{P}_K(W)$ of domain walls in an interval of length L along the critical line h=1. The dots correspond to the direct numerical integration of Eq. (61), considering for $\chi_{\mathfrak{K}}(\lambda)$ the asymptotic expansion obtained by applying the Fisher-Hartwig conjecture. The solid and dashed curves represent the analytical approximation found in Eq. (62) for W=4n and W=4n+2, respectively, with $n \in \mathbb{N}$. For the case $\gamma=0.2$ and L=100, B=0.327387, while for $\gamma=1.3$ and L=50, B=0.682844.

C. The case $\gamma = 0$

We investigate the FCS of the domain walls for the XX spin chain [cf. Eq. (36)]. For simplicity, we assume $0 \le h < 1$ and define $k_F = \arccos h$ as in Sec. III D. In the limit $\gamma \to 0$, the symbol in Eq. (56) is a piecewise function of ϕ with two jump discontinuities at $\phi = \{k_F, 2\pi - k_F\}$. We can then apply Eq. (A3) and obtain the following large-L asymptotics of the Toeplitz determinant in Eq. (55),

$$\begin{split} \ln \chi_{\mathfrak{K}}(\lambda)|_{\gamma=0} &= a(\lambda)L \\ &+ \frac{2}{\pi^2} \text{Re}[\operatorname{arctanh}^2(\tanh \lambda e^{-ik_F})] \ln L + O(1). \end{split}$$

Equation (65) shows that the domain wall FCS decays exponentially with the subsystem length L. The coefficient $a(\lambda)$ and the O(1) term in Eq. (65) can be explicitly determined but their expressions are rather lengthy. For |h| < 1, the logarithm of the FCS also contains an $O(\ln L/L)$ subleading contribution that can be calculated from Eq. (A6) with the result

$$\frac{4}{\pi^3} \operatorname{Re} \left[\frac{i e^{ik_F} \tanh \lambda}{e^{2ik_F} - \tanh^2 \lambda} \operatorname{arctanh}^2 \left[e^{-ik_F} \tanh \lambda \right] \right] L^{-1} \ln L. \quad (66)$$

Contrary to the case of the transverse magnetization discussed in Sec. III D, Eqs. (65) and (66) are finite in the limits $\lambda \to \pm \infty$. They can then be used to test the universality and semi-universality of the prefactors of the $O(\ln L)$ and $O(\ln L/L)$ terms.

In particular for $\lambda \to -\infty$, the FCS in Eq. (65) is proportional to the formation probability of a ferromagnetic domain of longitudinal spins. This spin configuration flows toward a Neumann boundary condition for a free boson compactified on a circle [65]. In this case, as also pointed out in Sec. IV C, CFT [32] predicts that the prefactor of the $O(\ln L)$ term is -1/8. It is easy to realize that the exact lattice result in Eq. (65) agrees with the field theory conjecture only at

half filling. A similar discrepancy for $k_F \neq \pi/2$ was also pointed out in other comparisons between CFT expectations and lattice calculations for free fermions (see for instance, Refs. [66,67]). At half filling, the limit $\lambda \to -\infty$ in Eq. (66) is also consistent with Eq. (21) at c=1 if the nonuniversal extrapolation length is $\xi=1$.

In the limit $\lambda \to \infty$, the domain wall FCS is proportional to the formation probability of an antiferromagnetic domain of longitudinal spins. To the authors' best knowledge, it is not clear to which conformal boundary condition of a free bosonic theory this spin configuration should flow. Anyway, the limit $\lambda \to \infty$ of the prefactor in the $O(\ln L)$ in Eq. (65) still admits a c=1 CFT interpretation while Eq. (66) is in agreement with Eq. (22), provided one postulates the presence of a boundary condition changing operator [53] with conformal dimension $h_{\text{bcc}} = 1/8$.

We close this section by highlighting an exact expression for the probability of formation of a ferromagnetic length-L domain of longitudinal spins at half filling and zero temperature. By evaluating the limit $\lambda \to -\infty$ and $k_F \to \pi/2$ in Eqs. (65) and (66), including the O(1) term in Eq. (A4), we obtain

$$\ln \mathcal{E}_{x}(h=0)|_{\gamma=0} = \left(\frac{2\mathfrak{G}}{\pi} - \ln 2\right)L - \frac{1}{8}\ln L$$

$$+ \frac{\mathfrak{G}}{\pi} - \frac{9\ln 2}{8} + 2\ln[G(3/4)G(5/4)]$$

$$- \frac{7\zeta(3)}{8\pi^{2}}$$

$$+ \frac{1}{8\pi}L^{-1}\ln L + O(L^{-1}), \tag{67}$$

where $\zeta(z)$ is the Riemann zeta. We quote the result in Eq. (67) as a mathematical curiosity: The appearance of the Riemann zeta function with an odd argument in the calculations of the formation probabilities in the *XXZ* spin chain is the leitmotif of Ref. [68].

VI. CONCLUSIONS

In this paper, we characterized exactly the quantum fluctuations of the transverse, staggered magnetization, and the domain walls in the ground state of the *XY* spin chain.

We also derived an analytic expression that captures the behavior of the full counting statistics for the transverse magnetization and the domain walls in the scaling limit, close to the quantum phase transition. The interpolation formula is built from the solution of a Painlevé V equation, for which it is possible to write down an explicit power series expansion.

The lattice calculations allow a direct verification of the field theoretical conjectures formulated in Ref. [32] for the $O(\ln L)$ and $O(\ln L/L)$ subleading contributions to the critical formation probabilities. These are extracted as limits for a large value of the coupling λ of the cumulant generating functions. In particular, we showed that the field theory predictions for the semiuniversal $O(\ln L/L)$ term do not have an obvious application to the domain walls when $\gamma < 1/2$. An analogous issue, already observed in Refs. [66,67], is found for their critical fluctuations in the XX spin chain away from half filling.

By determining exactly the domain wall full counting statistics, we have also calculated the probability of observing in the ground state a ferromagnetic and antiferromagnetic domain of transverse and longitudinal spins. Fluctuations of the latter are harder to access since the order parameter is not a quadratic fermionic form.

Our results hinge on the asymptotic expansion of Toeplitz determinants, for which we have also formulated and checked numerically a different conjecture in Appendix A, in particular Eq. (A14). The technique is suitable to detect any pattern of order [69] in the transverse direction, by properly modifying the observable \mathfrak{D} .

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APPENDIX A: ASYMPTOTICS OF DETERMINANTS OF BLOCK TOEPLITZ MATRICES

In this paper we made extensive applications of several results on the determinants of block Toeplitz matrices. We summarize them in this Appendix.

Let \mathcal{G} be an arbitrary matrix valued function of dimension $d \times d$ defined on the unit circle S^1 and with entries in $L^1(S^1)$. The block Toeplitz matrix $T_L[\mathcal{G}]$ with symbol \mathcal{G} is the $L \cdot d$ -dimensional matrix built from the Fourier coefficients of the entries of \mathcal{G} such that

$$(T_L[\mathcal{G}])_{nm} = (\mathcal{G})_{n-m} = \int_0^{2\pi} \frac{d\phi}{2\pi} \mathcal{G}(\phi) e^{i\phi(n-m)}$$

for n, m = 1, ..., L. We shall denote by $D_L[\mathcal{G}]$ the determinant of $T_L[\mathcal{G}]$, i.e., $D_L[\mathcal{G}] = \det(T_L[\mathcal{G}])$.

First, let us consider the case d = 1, in which the symbol g is a scalar function and therefore $T_L[g]$ is a Toeplitz matrix. This is the case of interest in Secs. III and V, where we have expressed the FCS of the magnetization and of domain walls respectively as Toeplitz determinants.

Szegő theorem. If the symbol $g(\phi)$ is a smooth enough, nonvanishing, complex function with zero winding number (i.e., the argument of $g(\phi)$ is continuous and periodic for $\phi \in [0, 2\pi]$), then the (strong) Szegő theorem [51,70] states that

$$\ln D_L[g] = (\ln g)_0 L + \sum_{k=1}^{\infty} k(\ln g)_k (\ln g)_{-k} + o(1).$$
 (A1)

Here, the o(1) terms decay exponentially with L.

Fisher-Hartwig formula. When the symbol $g(\phi)$ presents zeros or jump discontinuities, the Szegő theorem is no longer valid. In this case, the Fisher-Hartwig formula [52,71] gives the asymptotic behavior of the determinant. Suppose that the symbol has R zeros and/or discontinuities at the points

 $0 \leqslant \phi_1, \ldots, \phi_R < 2\pi$, and we can factorize $g(\phi)$ in the form

$$g(\phi) = V(\phi) \prod_{r=1}^{R} [2 - 2\cos(\phi - \phi_r)]^{\alpha_r} e^{i\beta_r [\phi - \phi_r - \pi \, \text{sgn}(\phi - \phi_r)]},$$
(A2)

where $V(\phi)$ is a function satisfying the conditions of the Szegő theorem, and $\operatorname{Re} \alpha_r > -1/2, \beta_r \in \mathbb{C}$ with $\alpha_r \pm \beta_r \neq -1, -2, \ldots$ for all r. Then, according to the Fisher-Hartwig formula,

$$\ln D_L[g] = (\ln V)_0 L + \sum_{r=1}^R (\alpha_r^2 - \beta_r^2) \ln L + E(V, \{\alpha_r\}, \{\beta_r\}, \{\phi_r\}) + o(1), \quad (A3)$$

where

$$E(V, \{\alpha_r\}, \{\beta_r\}, \{\phi_r\})) = \sum_{k=1}^{\infty} k(\ln V)_k (\ln V)_{-k}$$

$$+ \sum_{r=1}^{R} [(-\alpha_r + \beta_r) V_{-}(\phi_r) - (\alpha_r + \beta_r) V_{+}(\phi_r)]$$

$$- \sum_{1 \leq r \neq r' \leq R} (\alpha_r - \beta_r) (\alpha_{r'} + \beta_{r'}) \ln(1 - e^{i(\phi_r - \phi_{r'})})$$

$$+ \sum_{r=1}^{R} \ln \frac{G(1 + \alpha_r + \beta_r) G(1 + \alpha_r - \beta_r)}{G(1 + 2\alpha_r)}, \quad (A4)$$

and

$$V_{\pm}(\phi) = \sum_{k=1}^{\infty} (\ln V)_{\pm k} e^{\mp i\phi k}.$$
 (A5)

If the function $V(\phi)$ is smooth enough, then it is conjectured [72] that the o(1) term in (A3) can be expressed as a power series in L^{-1} . However, here we have numerically found that in some cases the leading o(1) term is of order $O(L^{-1} \ln L)$. Following Ref. [32], we trace back the origin of these terms to the presence of cusps in the function $V(\phi)$ at the Fisher-Hartwig singularities ϕ_r .

Subleading contributions $O(L^{-1} \ln L)$. In order to determine the contribution $L^{-1} \ln L$ to $\ln D_L[g]$, let us take a symbol that can be factorized in the form (A3) such that

$$g(\phi) = V(\phi)e^{i\beta(\phi - \phi_c - \pi \operatorname{sgn}(\phi - \phi_c))}$$

That is, it has a jump discontinuity at $\phi = \phi_c$. Now we further suppose that $V(\phi)$ has a cusp at $\phi = \phi_c$, i.e.,

$$V(\phi) \sim \kappa [1 + \mu^{\pm}(\phi - \phi_c)], \quad \phi \to \phi_c^{\pm},$$

where κ is a constant independent of ϕ and $\mu^+ \neq \mu^-$. Generalizing the analysis performed in Ref. [32] to this case, we factorize $V(\phi)$ in the form

$$V(\phi) = U(\phi)(1+z)^{\nu(z)}(1+1/z)^{\tilde{\nu}(z)}, \quad z \equiv e^{i(\phi-\phi_c-\pi\,\operatorname{sgn}(\phi-\phi_c))},$$

with

$$v(z) = \sum_{p=1}^{\infty} \eta_p(z+1)^p, \quad \tilde{v}(z) = \sum_{p=1}^{\infty} \eta_p(1/z+1)^p.$$

The coefficients η_p must be chosen to smoothen $V(\phi)$ such that $U(\phi)$ be analytic at ϕ_c . Then, in light of Ref. [32], we conjecture that

$$\ln D_L[g] = aL + b \ln L + c - 2\eta_1 \beta^2 L^{-1} \ln L, \tag{A6}$$

where the coefficients a, b, and c can be computed using the Fisher-Hartwig conjecture (A3). The coefficient η_1 can be determined by taking into account that the function $U(\phi)$ is of class C^1 at $\phi = \phi_c$ if and only if

$$\lim_{\phi \to \phi_c^-} U'(\phi) = \lim_{\phi \to \phi_c^+} U'(\phi).$$

From this condition it follows that

$$\eta_1 = \frac{\mu^- - \mu^+}{2\pi}.$$

In some cases, we have to deal with symbols with two jump discontinuities where the function $V(\phi)$ presents cusps. In this case, we perform the above analysis for each cusp separately and, at the end, the coefficient of the $O(L^{-1} \ln L)$ term is the sum of the contribution of the two cusps as we have numerically checked.

Multiple factorizations and nonzero winding. The symbol $g(\phi)$ may admit more than one factorization (A2),

$$g(\phi) = V^{(j)}(\phi) \prod_{r=1}^{R} [2 - 2\cos(\phi - \phi_r)]^{\alpha_r^{(j)}} e^{i\beta_r^{(j)}(\phi - \phi_r - \pi \operatorname{sgn}(\phi - \phi_r))},$$

where j is the label of each factorization. In this case, there is a generalization of the Fisher-Hartwig conjecture, proposed in Ref. [73] and proved in Ref. [74]. It can be stated as follows: For $L \to \infty$,

$$D_{L}[g] \sim \sum_{j \in S} e^{(\ln V^{(j)})_{0}L} L^{\Omega(j)} e^{E(V^{(j)}, \{\alpha_{r}^{(j)}\}, \{\beta_{r}^{(j)}\}, \{\phi_{r}\})}, \quad (A7)$$

where

$$\Omega(j) = \sum_{r=1}^{R} [(\alpha_r^{(j)})^2 - (\beta_r^{(j)})^2],$$

and

$$S = \{j | \operatorname{Re} \Omega(j) = \Omega\}, \quad \text{with} \quad \Omega = \max_{j} \operatorname{Re} \Omega(j).$$

In some situations, the analyzed symbol has a winding number ± 1 , i.e., it can be written as $g(\phi)=e^{\pm i\phi}V(\phi)$ where the function $V(\phi)$ satisfies the hypothesis of the Szegő theorem. This is the case, for instance, of the symbol of the FCS of domain walls $\chi_{\mathfrak{K}}(i\lambda)$, which has a winding number when |h|>1 and $\lambda\in[\pi/4,3\pi/4]$. When this occurs, we must resort to another extension of the Szegő theorem [52,75]. If $g(\phi)$ has a winding number +1, the corresponding determinant behaves for a large dimension as

$$D_L[g] \sim (-1)^L m_L D_{L+1}[V].$$
 (A8)

The asymptotics of the determinant $D_{L+1}[V]$ is given by (A1) and m_L is the L-Fourier coefficient of the function

$$m(\phi) = e^{V_{-}(\phi) - V_{+}(\phi)}$$

with $V_{\pm}(\phi)$ as defined in (A5). Analogously, if $g(\phi)$ has a winding number -1, then we have

$$D_L[g] \sim (-1)^L l_L D_{L+1}[V],$$
 (A9)

where now l_L is the L-Fourier coefficient of

$$l(\phi) = e^{V_{+}(-\phi)-V_{-}(-\phi)}.$$

In order to estimate the leading contribution of l_L and m_L for large L, it is convenient to analytically continue the functions $l(\phi)$ and $m(\phi)$ from the unit circle to the whole Riemann sphere. Let us call $\mathfrak{V}(z)$, $\mathfrak{l}(z)$, and $\mathfrak{m}(z)$ the analytical continuations of $V(\phi)$, $l(\phi)$, and $m(\phi)$, such that $\mathfrak{V}(e^{i\phi}) = V(\phi)$, $\mathfrak{l}(e^{i\phi}) = l(\phi)$, and $\mathfrak{m}(e^{i\phi}) = m(\phi)$. If we now introduce the Wiener-Hopf factorization for $\mathfrak{V}(z)$,

$$\mathfrak{V}(z) = b_{+}(z)e^{(\ln V)_{0}}b_{-}(z), \quad b_{+}(z) = e^{\sum_{k>0}(\ln V)_{\mp k}z^{\pm k}},$$

then

$$l(z) = \frac{b_{-}(1/z)}{b_{+}(1/z)}, \quad \mathfrak{m}(z) = \frac{b_{+}(z)}{b_{-}(z)},$$

and l_L , m_L can be expressed as the contour integrals

$$l_{L} = \oint_{|z|=1} \frac{dz}{2\pi i} \frac{b_{-}(z)}{b_{+}(z)} z^{-(L+1)},$$

$$m_{L} = \oint_{|z|=1} \frac{dz}{2\pi i} \frac{b_{+}(1/z)}{b_{-}(1/z)} z^{-(L+1)}.$$

Note that $b_{+}(z)$ is analytic inside the unit circle while $b_{-}(z)$ is analytic outside it. The idea now is to deform the contour of integration from the unit circle to the point at infinity where the term z^{-L-1} cancels the integrand. In general, the integrand presents singularities such as branch points and/or poles outside the unit circle which must be surrounded by the deformed contour. Therefore, the dominant contribution to l_L and m_L will come from the singularity outside the unit circle closest to it. If this singularity is a pole, we can compute its contribution with the residue theorem. If it is a branch point, we take the branch cuts such that each one connects a branch point outside the unit circle to infinity without intersecting the rest as well as the unit circle. Then, once the contour has been deformed to infinity and runs around the branch cuts, we can apply the Watson lemma for loop integrals (see, e.g., Refs. [76,77]) to obtain the leading contribution.

Widom theorem. Another situation of our interest is when the symbol $g(\phi)$ is periodic and supported on a closed interval $I = [0, \omega] \cup [2\pi - \omega, 2\pi]$ such that, when it is restricted to this arc, $g(\phi)$ is smooth enough and positive. In this case, Widom [64] showed that

$$\ln D_L[g] \sim L^2 \ln \sin \frac{\omega}{2} + L \int_0^{2\pi} \frac{d\phi}{2\pi} \ln g \left[2 \arcsin \left(\sin \frac{\omega}{2} \sin \phi \right) \right] - \frac{1}{4} \ln L.$$
(A10)

Szegő-Widom theorem. We now move on to the case d>1. Genuine block Toeplitz determinants with d=2 appear when we study the FCS of the staggered magnetization in Sec. IV. As we will see, we can formulate analogous results to the Szegő theorem and the Fisher-Harwig conjecture as well as the Widom theorem.

Consider a $d \times d$ symbol \mathcal{G} . If the entries of $\mathcal{G}(\phi)$ are smooth enough, complex functions and $\det \mathcal{G}(\phi) \neq 0$ with zero winding number, then the Szegő-Widom theorem

[59–61] gives the asymptotic behavior of $D_L[\mathcal{G}]$,

$$\ln D_L[\mathcal{G}] = (\ln \det \mathcal{G})_0 L + E[\mathcal{G}] + o(1).$$

The term $E[\mathcal{G}]$ can be written as

$$E[\mathcal{G}] = \ln \det T[\mathcal{G}]T[\mathcal{G}^{-1}], \tag{A11}$$

where $T[\mathcal{G}]$, $T[\mathcal{G}^{-1}]$ are the semi-infinite matrices obtained respectively from $T_L[\mathcal{G}]$ and $T_L[\mathcal{G}^{-1}]$ in the limit $L \to \infty$. The Szegő-Widom theorem reduces to the Szegő theorem for d=1.

Conjecture 1. If the entries of $\mathcal{G}(\phi)$ present jump discontinuities at the points ϕ_1, \dots, ϕ_R , and det $\mathcal{G}(\phi)$ can be factorized in the Fisher-Hartwig form (A2), then $D_L[\mathcal{G}]$ behaves as [62]

$$\ln D_L[\mathcal{G}] = (\ln \det \mathcal{G})_0 L + b \ln L + O(1), \tag{A12}$$

where

$$b = \frac{1}{4\pi^2} \sum_{r=1}^{R} \text{Tr} \left\{ \ln[\mathcal{G}_r^- (\mathcal{G}_r^+)^{-1}] \right\}^2, \tag{A13}$$

with \mathcal{G}_r^{\pm} the lateral limits of $\mathcal{G}(\phi)$ at the point ϕ_r ,

$$\mathcal{G}_r^{\pm} = \lim_{\phi \to \phi_{\pm}^{\pm}} \mathcal{G}(\phi).$$

Note that this result is a generalization for matricial symbols of that in (A3) for nonvanishing, scalar symbols with jump discontinuities.

We have also numerically found that in the expansion of $\ln D_L[\mathcal{G}]$, with jump discontinuities in $\mathcal{G}(\phi)$, may appear terms of order $O(L^{-1} \ln L)$. Inspired by the analysis performed for these corrections in the scalar case, we claim that, when d > 1, they can be related to the presence of cusps in $\det \mathcal{G}(\phi)$ at the discontinuity points ϕ_r . Then, one may repeat the analysis performed for the result conjectured in Eq. (A6), but replacing $V(\phi)$ by $\det \mathcal{G}(\phi)$ and $-\beta^2$ by the coefficient b given in (A13).

Conjecture 2. Finally, we have also studied symbols $\mathcal{G}(\phi)$ for which det $\mathcal{G}(\phi)$ is supported on the arc I, and therefore the previous results cannot be applied. In analogy to the Widom theorem (A10), we conjecture that

$$\ln D_L[\mathcal{G}] \sim L^2 \ln \sin \frac{\omega}{2} + L \int_0^{2\pi} \frac{d\phi}{2\pi} \ln \det \mathcal{G} \left[2 \arcsin \left(\sin \frac{\omega}{2} \sin \phi \right) \right] \frac{1}{4} \ln L,$$
(A14)

if the restriction of $\mathcal{G}(\phi)$ to the interval I satisfies the conditions of the Widom-Szegő theorem.

APPENDIX B: ESTIMATION OF THE CRITICAL PROBABILITY DISTRIBUTIONS

In this Appendix, we describe the way to obtain the behavior for large L of the probabilities $\mathcal{P}_{\alpha}(M)$ along the critical lines $h = \pm 1$, $\gamma > 0$. The discussion is qualitatively similar for the three observables considered in the paper: The transverse magnetization ($\alpha = z$), the staggered transverse magnetization ($\alpha = s$), and the number of domain walls ($\alpha = K$).

In all the cases, $\ln \chi_{\mathfrak{O}}(i\lambda) = Lf_{\mathfrak{O}}(\lambda) + o(L)$ ($\mathfrak{O} = \{\mathfrak{M}_z, \mathfrak{M}_s, \mathfrak{K}\}$). This condition already implies that the

fluctuations around the mean value of the measurements of the observable $\mathfrak O$ are Gaussian in the large-L limit. More explicitly, we assume $M=L\mu+\delta M$, with $\delta M/L\to 0$ for $L\to\infty$. The probability distribution is then the integral

$$\mathcal{P}_{\alpha}(M) = \int_{0}^{\pi} \frac{d\lambda}{2\pi} e^{-i\lambda(L\mu + \delta M) + Lf_{\mathfrak{D}}(\lambda) - \delta_{\mathfrak{D}}(\lambda)\ln L}, \quad (B1)$$

which can be evaluated by the saddle point. The saddle-point equation $f_{\mathfrak{D}}'(\lambda_s) = i\mu$, requires Re $f_{\mathfrak{D}}'(\lambda_s) = 0$, with solutions $\lambda_s = \{0, \pi/2\}$ and Im $f_{\mathfrak{D}}'(\lambda_s) = \mu$. As expected, μ is the mean value $\lim_{L \to \infty} \langle \mathfrak{D} \rangle / L$ and moreover $f_{\mathfrak{D}}''(\lambda_s) = -\sigma^2$ for both $\lambda_s = \{0, \pi/2\}$ with $\sigma^2 = \lim_{L \to \infty} \langle (\mathfrak{D} - \langle \mathfrak{D} \rangle)^2 \rangle / L$, the variance.

Finally one also has the following: $f_{\mathfrak{D}}(0) = 0$ with $\delta_{\mathfrak{D}}(0) = 0$; $f_{\mathfrak{D}}(\pi/2) = iv\pi/2$, with v = 1 for $\mathfrak{D} = \mathfrak{M}_z$ and v = 0 for $\mathfrak{D} = \{\mathfrak{M}_s, \mathfrak{K}\}$ and $\delta_{\mathfrak{D}}(\pi/2) = \frac{1}{4}$.

Inserting the expansions of $f_{\mathfrak{D}}(\lambda)$ up to second order in $\lambda - \lambda_s$ for $\lambda_s = \{0, \pi/2\}$ into Eq. (B1) we can easily derive

$$\mathcal{P}_{\alpha}(M) = \frac{1}{\sqrt{2\pi L\sigma^2}} e^{-\frac{(\delta M)^2}{2\sigma^2 L}} \left(1 + B\cos\frac{\pi (vL - M)}{2} L^{-1/4} \right), \tag{B2}$$

with B = O(1).

Probability distribution outside the critical lines. In the noncritical regions $|h| \neq 1, \gamma > 0$, the probability distribution of the observables studied in the paper can be obtained by applying the saddle-point analysis described before. Therefore, their fluctuations outside the critical regions are also Gaussian in the large-L limit, but there is no a subleading power-law correction $L^{-1/4}$ since $\delta_{\mathfrak{D}}(\lambda) = 0$. Nevertheless, outside the critical lines, we have to be careful when we take the analytic continuation of $\chi_{\mathfrak{D}}(\lambda)$ to imaginary λ (i.e., $\lambda \to i\lambda$) since the corresponding symbol may acquire a winding number. Let us consider, for example, the domain walls. When we replace λ by $i\lambda$ in Eq. (56), the resulting symbol $g_{\mathfrak{K}}(\phi)|_{i\lambda}$ has a winding number -1 if |h| > 1 and $\lambda \in [\pi/4, 3\pi/4]$. For these particular values, the asymptotic behavior predicted for $\chi_{\mathfrak{K}}(i\lambda)$ by using the Szegő theorem is not valid and we must apply the modification of it for symbols with a winding number -1, which is written in Eq. (A9). Following the discussion presented below that equation, we then conclude that

$$\ln \chi_{\mathfrak{K}}(i\lambda)|_{|h|>1} \sim L \left[\int_0^{2\pi} \frac{d\phi}{2\pi} \ln[e^{i\phi}g_{\mathfrak{K}}(\phi)|_{i\lambda}] - \ln(-z_0) \right],$$
(B3)

for $\lambda \in [\pi/4, 3\pi/4]$. If we consider the analytic continuation of $\ln g_{\mathfrak{K}}(\phi)|_{i\lambda}$ from the unit circle to the Riemann sphere, then z_0 is the closest singularity of that function to the unit circle with $|z_0| > 1$.

Taking into account the previous issue in the saddle-point analysis of Eq. (B1), we obtain that, for |h| > 1,

$$\mathcal{P}_K(W) = \frac{e^{-\frac{(W-\mu L)^2}{2\sigma^2 L}}}{\sqrt{2\pi\sigma^2 L}},$$
 (B4)

while, for |h| < 1, there is an oscillatory term,

$$\mathcal{P}_{K}(W) = \frac{e^{-\frac{(W-\mu L)^{2}}{2\sigma^{2}L}}}{\sqrt{2\pi\sigma^{2}L}} \left[1 + B\cos\frac{\pi W}{2} \right],$$
 (B5)

where

$$B = \exp\left(\sum_{k>0} k(\ln g_{\mathfrak{K}})_k (\ln g_{\mathfrak{K}})_{-k}\right)\bigg|_{\lambda = i\pi/2}.$$
 (B6)

In both cases, the mean and the variance can be computed from

$$\mu = \int_0^{2\pi} \frac{d\phi}{2\pi} (e^{i(\theta(\phi) - \phi)} + 1)$$
 (B7)

and

$$\sigma^2 = \int_0^{2\pi} \frac{d\phi}{2\pi} (1 - e^{2i(\theta(\phi) - \phi)}).$$
 (B8)

An analogous result was found in Ref. [10] for the transverse magnetization, with the difference that the oscillatory term of Eq. (B5) appears in the region |h| > 1 instead of |h| < 1.

APPENDIX C: ADDITIONAL TECHNICAL DETAILS

1. The O(1) term in the interpolation formula [Eq. (32)]. The complete interpolation formula in Eq. (32), including the O(1) terms, is

$$\ln \chi_{\mathfrak{M}_z}(\lambda; x) = (\ln g_{\mathfrak{M}_z})_0 L - \beta^2(\lambda) \ln(x) + \ln \tau_V(x)$$

$$+ \sum_{k=1}^{\infty} k (\ln g_{\mathfrak{M}_z})_k (\ln g_{\mathfrak{M}_z})_{-k}$$

$$+ \ln[G(1 + \beta(\lambda))G(1 - \beta(\lambda))] + o(1), (C1)$$

where $(\ln g_{\mathfrak{M}_z})_k$ is the *k*-Fourier mode of $\ln g_{\mathfrak{M}_z}$, and o(1) is uniform for $0 < |\ln |h|| < \varepsilon$ with ε small enough.

In Figs. 1 and 4, we test numerically the validity of this expression by introducing the following quantity,

$$\Delta_{P} = \ln \chi_{\mathfrak{M}_{z}}(\lambda; x) - (\ln g_{\mathfrak{M}_{z}})_{0}L + \beta^{2}(\lambda) \ln(x)$$

$$- \sum_{k=1}^{\infty} k (\ln g_{\mathfrak{M}_{z}})_{k} (\ln g_{\mathfrak{M}_{z}})_{-k}$$

$$- \ln[G(1 + \beta(\lambda))G(1 - \beta(\lambda))]. \tag{C2}$$

Therefore, if Eq. (32) is correct, then Δ_P should behave for large L as

$$\Delta_{\rm P} \sim \ln \tau_V(x),$$
 (C3)

as we check in Figs. 1 and 4.

2. The subleading contribution for the staggered magnetization [Eq. (45)]. If one numerically investigates the subleading terms in the expansion of Eq. (43) for $\ln \chi_{\mathfrak{M}_s}(\lambda)$, the conclusion is that the first o(1) term is of order $L^{-1} \ln L$, as happens in the transverse magnetization and for the number of domain walls. However, here we are dealing with a block Toeplitz matrix and the analysis based on the presence of cusps in the symbol described in Appendix A [see Eq. (A6)] cannot directly be applied now. Nevertheless, we may relate this term to the existence of a cusp in the determinant of the symbol $\tau(\phi)$, given in Eq. (41). In fact, the function $|\det \tau(\phi)|_{h=1}|$ presents a cusp at $\phi=0$, the point where the entries of the symbol $\tau(\phi)|_{h=1}$ are discontinuous. We conjecture that this cusp gives rise to the $O(L^{-1} \ln L)$ term in the expansion of

TABLE I. The columns c_s^{fit} and d_s^{fit} contain the coefficients of the function in Eq. (C6) obtained when we fit it to the numerical values of Δ_s for the γ , λ indicated in the first column, h = 1, and L = 1000, 1100, 1200, ..., 2000 [Δ_s is defined in Eq. (C5), and here we take $L_0 = 2000$]. In the last column, d_s expected from Eq. (45).

	$c_s^{ m fit}$	$d_s^{ m fit}$	d_s
$\lambda = -2.1, \gamma = \sqrt{3}$	0.0458770695997351	-0.0106671484603713	-0.010606911294100373
$\lambda = 1.2, \gamma = 1$	-0.0306456874870144	-0.00559008728446244	-0.005575179303697452
$\lambda = -0.69, \gamma = 1/2$	-0.0136641140511327	-0.0015081064892357	-0.001507352503438705

Eq. (43), and its coefficient can be determined in a similar way as in the scalar case with the conjecture given in Eq. (A6), replacing now the symbol by the determinant of the symbol. For the cusp in $|\det \tau(\phi)|_{h=1}|$, we have that

$$\eta_1 = \frac{\gamma^2 + 1}{4\pi\gamma} \frac{\tanh^2(\lambda)}{\tanh^4(\lambda) + 1}.$$
 (C4)

By analogy with the scalar case, we assume that $-\beta^2$ is now the coefficient of the logarithmic term in the expansion of $\ln \chi_{\mathfrak{M}_s}(\lambda)$, which is produced by the discontinuity of the entries of $\tau(\phi)|_{h=1}$ at the point of the cusp, i.e., $\beta = \arctan[\tanh^2(\lambda)]/\pi$. Therefore, pushing further the conjecture of Eq. (A6), we expect in the expansion of Eq. (43) a $O(L^{-1} \ln L)$ term with coefficient $-2\eta_1\beta^2$, that is, the one written in Eq. (45).

In order to check this claim, we define

$$\Delta_s = L[\ln \chi_{\mathfrak{M}_s}(\lambda) - a_s L - b_s \ln L]$$
$$-L_0[\ln \chi_{\mathfrak{M}_s}(\lambda)|_{L=L_0} - a_s L_0 - b_s \ln L_0], \quad (C5)$$

where $\ln \chi_{\mathfrak{M}_s}(\lambda)|_{L=L_0}$ is the FCS evaluated at a fixed length L_0 and a_s, b_s are the coefficients written in Eq. (43). If our conjecture is correct, then we expect

$$\Delta_s \sim c_s(L - L_0) + d_s \ln(L/L_0) \tag{C6}$$

for large L. The coefficient c_s is the O(1) term in Eq. (43) and d_s should be the predicted coefficient for the $O(L^{-1} \ln L)$ term. Unfortunately, we do not know any method to obtain an analytical expression for c_s . Therefore, we have calculated numerically Δ_s for the intervals $L=1000,\,1100,\,1200,\,\ldots,\,2000$ with $L_0=2000$ and different λ and γ . Then we have fitted the curve $c_s^{\rm fit}(L-L_0)+d_s^{\rm fit}\ln(L/L_0)$ to these points. In Table I, we collect the values for $c_s^{\rm fit}$ obtained in the fits as well as the value for d_s expected in Eq. (45).

In Fig. 6, we plot the numerical values of Δ_s subtracting $c_s^{\rm fit}(L-L_0)$ as a function of $\ln L$. The lines correspond to $d_s \ln(L/L_0)$ with d_s the coefficient of the $O(L^{-1} \ln L)$ term predicted in Eq. (45). Note that the lines overlap the points, and this is especially remarkable if we take into account that the fit for $c_s^{\rm fit}$ and $d_s^{\rm fit}$ has been performed with the points in the range between L=1000 and 2000 and we have extended the plot up to points with L=100.

3. Numerical check of the subleading term in the number of domain walls [Eq. (60) and Fig. 3]. In Fig. 3, we study numerically the presence of the $O(L^{-1} \ln L)$ term (60) in the expansion of $\ln \chi_{\Re}(\lambda)$. For this purpose, we consider the quantity

$$\begin{split} \Delta_{\mathfrak{K}} &= L[\ln \chi_{\mathfrak{K}}(\lambda) - a_{\mathfrak{K}}L - b_{\mathfrak{K}}\ln L - c_{\mathfrak{K}}] \\ &- L_0[\ln \chi_{\mathfrak{K}}(\lambda)|_{L=L_0} - a_{\mathfrak{K}}L_0 - b_{\mathfrak{K}}\ln L_0 - c_{\mathfrak{K}}], \end{split}$$
 (C7)

where $a_{\mathfrak{K}}$, $b_{\mathfrak{K}}$, $c_{\mathfrak{K}}$ are the coefficients of the linear, logarithmic, and O(1) terms in the expansion of $\ln \chi_{\mathfrak{K}}(\lambda)$, which can be determined from Eq. (A3), and $\ln \chi_{\mathfrak{K}}(\lambda)|_{L=L_0}$ is the FCS evaluated at an interval of length L_0 . Therefore, if Eq. (60) is the $O(L^{-1} \ln L)$ term in the expansion of $\ln \chi_{\mathfrak{K}}(\lambda)$, then

$$\Delta_{\mathfrak{K}} \sim d_{\mathfrak{K}} \ln(L/L_0)$$
 (C8)

for large L, with $d_{\mathfrak{K}}$ the coefficient predicted in Eq. (60), as we actually observe in Fig. 3.

4. The derivation of the domain wall symbol [Eq. (56)]. Applying Eq. (10), we obtain, after a little massage,

$$\chi_{\mathfrak{K}}(\lambda) = e^{\lambda L} \sqrt{\det e^{-Y}} \det(P_{+} + G_{ba} P_{-})$$

$$= e^{\lambda L} \sqrt{\det e^{-Y}} \det P_{+} \det(I_{L+1} + G_{ba} P_{-} P_{+}^{-1}), \quad (C9)$$

where $P_{\pm} = \frac{1}{2}(T_{22}^{-1} - X \pm I_{L+1})$ and I_{L+1} is the L+1-dimensional identity matrix. The matrix $e^{-Y} = T_{22}$ is tridiagonal,

$$\begin{bmatrix} \cosh^2(\lambda) & -\frac{\sinh(2\lambda)}{2} & \cdots & 0 & 0 \\ -\frac{\sinh(2\lambda)}{2} & \cosh(2\lambda) & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cosh(2\lambda) & -\frac{\sinh(2\lambda)}{2} \\ 0 & 0 & 0 & -\frac{\sinh(2\lambda)}{2} & \cosh^2(\lambda) \end{bmatrix},$$

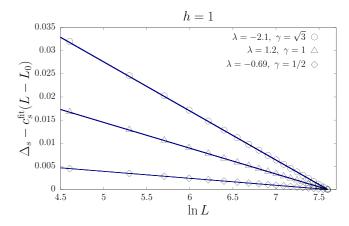


FIG. 6. Numerical check of the term of order $O(L^{-1} \ln L)$ in the expansion of Eq. (43) for the FCS of the staggered magnetization along the critical line h=1. We plot Δ_s [defined in Eq. (C5)] with $L_0=2000$, subtracting $c_s^{\rm fit}(L-L_0)$, and taking for $c_s^{\rm fit}$ the values collected in the corresponding column of Table I. The dots correspond to Δ_s obtained by computing numerically $\chi_{\mathfrak{M}_s}(\lambda)$ from Eq. (39). The lines represent $d_s \ln(L/L_0)$, where d_s is the coefficient of the $O(L^{-1} \ln L)$ term predicted in Eq. (45).

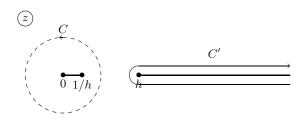


FIG. 7. Contours in the complex z plane discussed in the main text.

while the matrix P_+ is triangular,

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ \tanh(\lambda) & 1 & 0 & \cdots & 0 \\ \tanh^2(\lambda) & \tanh(\lambda) & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \tanh^L(\lambda) & \tanh^{L-1}(\lambda) & \tanh^{L-2}(\lambda) & \cdots & 1 \end{bmatrix},$$

and $P_{-} = P_{+} - I_{L+1}$. Therefore, Eq. (C9) simplifies to

$$\chi_{\mathfrak{K}}(\lambda) = e^{\lambda L} \cosh^{L}(\lambda) \det(I_{L+1} + G_{ba}P_{-}P_{\perp}^{-1}). \tag{C10}$$

Taking now into account that $(P_-P_+^{-1})_{nm} = \delta_{n,m+1} \tanh(\lambda)$, we have that $I_{L+1} + G_{ba}P_-P_+^{-1}$ is the matrix

$$\begin{bmatrix} 1+g_{-1}\tanh(\lambda) & \cdots & g_{-L}\tanh(\lambda) & 0 \\ g_0\tanh(\lambda) & \cdots & g_{-L+1}\tanh(\lambda) & 0 \\ \vdots & \ddots & \vdots & \vdots \\ g_{L-2}\tanh(\lambda) & \cdots & 1+g_{-1}\tanh(\lambda) & 0 \\ \hline g_{L-1}\tanh(\lambda) & \cdots & g_0\tanh(\lambda) & 1 \end{bmatrix}$$

with $g_{n-m} = (G_{ba})_{nm}$. Hence, we can write (C10) as

$$\chi_{\mathfrak{K}}(\lambda) = \det G_{\mathfrak{K}},$$
 (C11)

where $G_{\mathfrak{K}}$ is the $L \times L$ matrix with entries

$$(G_{\mathfrak{K}})_{nm} = \int_0^{2\pi} \frac{d\phi}{2\pi} g_{\mathfrak{K}}(\phi) e^{i\phi(n-m)}, \quad n, m = 1, \dots, L,$$

with $g_{\mathfrak{K}}(\phi)$ as in Eq. (56).

5. The derivation of the EFP in the x direction for the Ising spin chain [Eq. (59)]. At $\gamma = 1$ [see Eq. (56)], the logarithm of the EFP in the x direction is given by

$$\ln \mathcal{E}_x(h) = L[F(h) - \ln 2] + O(1),$$

where F(h) is the integral,

$$F(h) = \int_0^{2\pi} \frac{d\phi}{2\pi} \ln\left(1 - \frac{he^{-i\phi} - 1}{\sqrt{1 + h^2 - 2h\cos\phi}}\right). \quad (C12)$$

We then consider the derivative with respect to h of Eq. (C12) and continue analytically the integrand to the complex plane of $z = e^{i\phi}$. We end up with

$$F'(h) = \frac{1}{2\pi i} \oint_C dz f(z), \tag{C13}$$

where the function f(z) is given by

$$f(z) = \frac{1 - z^2}{2z(hz - 1)\left(z - h + z\sqrt{\frac{(h-z)(hz - 1)}{z}}\right)},$$
 (C14)

and the contour C is a circumference of unit radius encircling the origin anticlockwise (Fig. 7). For h > 1, the domain of analyticity of f is the complex plane with cuts along the segments (0, 1/h) and (h, ∞) . The contour C can be then deformed into C' depicted in Fig. 7 without crossing any singularities. One obtains the integral representation

$$F'(h) = \int_{h}^{\infty} \frac{dx}{\pi} \frac{1}{2h\sqrt{x(x-h)(hx-1)}} = \frac{1}{\pi h^2} K(h^{-2}),$$
(C15)

with K(y) the complete elliptic integral of the first kind, written in MATHEMATICA conventions. By integrating back Eq. (C15) with respect to h and observing that $F(\infty) = 0$ [see Eq. (C12)], the first line of Eq. (59) follows. An analogous calculation can be also performed for h < 1. In this case, however, when deforming the contour, one shall extract the pole contribution at z = 1/h of f(z) in Eq. (C14). Finally, the critical EFP is obtained by taking the $h \to 1$ limit, which is well defined.

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