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Finite-size scaling of the Shannon-Rényi entropy in two-dimensional systems with spontaneously broken continuous symmetry

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We study the scaling of the (basis-dependent) Shannon entropy for two-dimensional quantum antiferromagnets with Néel long-range order. We use a massless free-field description of the gapless spin wave modes and phase space arguments to treat the fact that the finite-size ground state is rotationally symmetric, while there are degenerate physical ground states which break the symmetry. Our results show that the Shannon entropy (and its Rényi generalizations) possesses some universal logarithmic term proportional to the number N_{NG} of Nambu-Goldstone modes. In the case of a torus, we show that $S_{n>1} \simeq \text{const.} \times N + \frac{N_{\text{NG}}}{4} \frac{n}{n-1} \ln N$ and $S_1 \simeq \text{const.} \times N - \frac{N_{\text{NG}}}{4} \ln N$, where N is the total number of sites and n the Rényi index. The result for $n > 1$ is in reasonable agreement with the quantum Monte Carlo results of Luitz *et al.* [*Phys. Rev. Lett.* **112**, 057203 (2014)], and qualitatively similar to those obtained previously for the *entanglement* entropy. The Shannon entropy of a line subsystem (embedded in the two-dimensional system) is also considered. Finally, we present some density-matrix renormalization group (DMRG) calculations for a spin- $\frac{1}{2}$ XY model on the square lattice in a cylinder geometry. These numerical data confirm our findings for logarithmic terms in the $n = \infty$ Rényi entropy (also called $-\ln p_{\text{max}}$). They also reveal some universal dependence on the cylinder aspect ratio, in good agreement with the fact that, in that case, p_{max} is related to a noncompact free-boson partition function in dimension $1+1$.

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I. INTRODUCTION

Recently, there is a growing interest in utilizing information-theoretic quantities to characterize phases, to go beyond the traditional characterizations based on order parameters and correlation functions. The most popular among them is entanglement entropy. In fact, many low-energy and long-distance properties of quantum many-body systems can be extracted from the scaling of the entanglement entropy of some large subsystem. Two prototypical examples are critical spin chains, where the central charge can be read off from the scaling of the entanglement of a segment [1–3], and that of gapped topologically ordered states in dimension two, which have some universal subleading contributions related to the nature of the fractionalized excitations (quantum dimensions) of the phase [4,5].

It was also realized that a somewhat simpler entropy, the (basis-dependent) Shannon entropy, share some similar properties (see Ref. [6] for a review). It is defined as follows. When expanded in some discrete basis $\{|i\rangle\}$, a quantum state $|\psi\rangle$ defines a set of probabilities

$$p_i = |\langle\psi|i\rangle|^2 \quad (1)$$

that can, in turn, be used to define a Shannon entropy:

$$S_1 = - \sum_i p_i \ln p_i. \quad (2)$$

In the following, it will also be useful to consider a generalization of this entropy, the Shannon-Rényi entropy (SRE):

$$S_n = \frac{1}{1-n} \ln \left(\sum_i p_i^n \right), \quad (3)$$

with Eq. (1). For one-particle problems described by a wave function $\psi(r)$ in real space, the entropies are simply related by $S_n = \frac{1}{1-n} \ln P_n$ to the so-called inverse participation ratios: $P_n = \int d^D \mathbf{r} |\psi(r)|^{2n}$. The latter measure how spatially localized is the particle. In the presence of disorder it can be used to detect Anderson metal-insulator transitions [7], as follows: in the delocalized phase one has $P_n \simeq L^{-D(n-1)}$, where D is the spatial dimension, and L the linear system size (thus L^D is the Hilbert space dimension). In contrast, one has instead $P_n \simeq L^0$ in the localized phase. At the transition point it scales like $P_n \simeq L^{-\alpha_n(n-1)}$ where α_n defines a continuous family of critical exponents (multifractality). In the notation of Eq. (3), it means $S_n \simeq \alpha_n \ln L$.

The situation is quite different for many-body systems, which have exponentially many [$\propto \exp(\text{const.} \times L^D)$] basis states. A generic many-body wave function has some nonzero weights on a finite fraction of these basis states. As a consequence, the leading behavior of the SRE [Eq. (3)] is generically a *volume law*, which means $S_n \simeq \alpha_n L^D$. This may also be interpreted as “multifractality” [8] with interesting features at phase transitions [9]. However, it should be noted that, contrary to that in one-body wave functions, the “multifractality” is generic for wave functions living in a many-body Hilbert space, even for featureless product states. Consider for instance N independent spin- $\frac{1}{2}$ in the same state $\cos(\theta)|\uparrow\rangle + \sin(\theta)|\downarrow\rangle$. The SRE of that tensor product state is $S_n = \frac{N}{1-n} \ln(\cos^{2n} \theta + \sin^{2n} \theta)$, which is a nonlinear function of n . Here, the number of spins N corresponds to the volume L^D of the system. In fact, the coefficient of the leading volume-law term in the SRE is generally nonuniversal and depends on microscopic details, as it is evident in the above simple example. Thus it is not an interesting quantity from the viewpoint of elucidation of universal behavior in a quantum phase. Nevertheless, subleading terms can contain

universal information which are determined by the long-distance properties of the system. This has been studied in quantum spin chains in particular, and these corrections are typically $\mathcal{O}(1)$ for periodic chains [10–12] and $\mathcal{O}(\ln L)$ for open chains [13,14].

In this paper, we are interested in two-dimensional (2D) quantum antiferromagnets, where the spin rotation symmetry— $U(1)$ or $SU(2)$ —is spontaneously broken at zero temperature in the thermodynamic limit. In such systems with magnetic long-range order and gapless Nambu–Goldstone modes, it was observed, using (modified) spin-wave calculations [15] and quantum Monte Carlo (QMC) on Heisenberg models [16] that the *entanglement* entropy possesses some additive $\ln L$ corrections to the boundary law. Soon after, these results were explained by some analytical calculations (quantum rotor model and a nonlinear sigma model) [17], leading to the prediction that, in two dimensions, the coefficient of $\ln L$ is $N_{\text{NG}}/2$, where N_{NG} is the number of Nambu–Goldstone modes. We note that a related discussion was also made for Heisenberg ferromagnets in Refs. [18–20]. The situation is however quite different from antiferromagnets of our interest, which have linearly dispersing Nambu–Goldstone modes and a unique ground state in a generic finite-size system.

Recently, the SRE of several 2D magnets were computed using QMC [6,21,22]. By simulating spin- $\frac{1}{2}$ XXZ and Heisenberg models, $U(1)$ and $SU(2)$ broken symmetries were investigated. The SRE for the complete system (torus), as well as the entropy of a line subsystem were measured. In these studies, the basis states $|i\rangle$ chosen to define the probabilities p_i (and the SRE) are eigenstates of the local magnetization $S^x(r)$. This basis choice requires to select a particular spin direction in the xy (easy) plane of the system, and such a choice therefore explicitly breaks the spin rotation symmetry about the z axis. In the present work, we will also focus on such a situation, where the quantization axis used to define the local basis is not invariant under the rotation symmetry of the Hamiltonian, but corresponds to a possible ordering direction for the order parameter (i.e., the sublattice magnetization).

In all the cases studied in Refs. [6,21,22], some additive $\ln L$ corrections were observed in the SRE in presence of magnetic long-range order. Some of these results are summarized in Table I. Motivated by these numerical results, we study in this paper the SRE of these systems by using an effective relativistic (free boson) field theory of the Nambu–Goldstone modes. While we are primarily interested in the cases with a spontaneously broken $U(1)$ or $SU(2)$ symmetry, our analysis can be applied to the cases with a more general spontaneously broken continuous symmetry.

It should be noted that, Nambu–Goldstone modes, which accompany a spontaneous breaking of a continuous symmetry, are classified into two categories: type I and type II [23] or type A and type B [24]. In this paper, we focus on the cases only with the type-I (type-A with a linear dispersion) Nambu–Goldstone modes, which can be described by the relativistic free boson field theory. In such cases, we can identify the number of the Nambu–Goldstone modes N_{NG} with the number of broken symmetry generators. We leave the analysis of the cases with type-II or type-B modes to the future, although some part of our discussion could be applied to these cases as well.

TABLE I. Subleading logarithmic terms in the SRE of the 2D Heisenberg and XY models, possibly with ferromagnetic second neighbor interaction J_2 (which strengthens the magnetic order). n is the Rényi (noted q in Ref. [21]). The numerical values obtained by Toulouse’s group (Supplemental Material of Ref. [21]) are given in the third column. We selected the best fit only for simplicity—which does not do justice to their extensive and detailed data analysis. The last column is the present theoretical prediction [Eq. (48)], which combines the oscillators [Eq. (15)] and TOS (degeneracy factor) contributions [Eq. (47)]. The number N_{NG} of Nambu–Goldstone modes is 2 for Heisenberg and 1 for XY.

Model	n	$\ln(N)$ coef. Ref. [21]	$\frac{N_{\text{NG}}}{4} \frac{n}{n-1}$
Heisenberg			
$J_2 = 0$	∞	0.460(5)	0.5
$J_2 = -5$	∞	0.58(2)	0.5
$J_2 = 0$	2	1.0(2)	1
$J_2 = -5$	2	1.25(4)	1
$J_2 = -5$	3	1.06(3)	0.75
$J_2 = -5$	4	1.0(1)	0.666
XY			
$J_2 = 0$	∞	0.281(8)	0.25
$J_2 = -1$	∞	0.282(3)	0.25
$J_2 = 0$	2	0.585(6)	0.5
$J_2 = -1$	2	0.598(4)	0.5
$J_2 = 0$	3	0.44(2)	0.375
$J_2 = -1$	3	0.432(7)	0.375
$J_2 = 0$	4	0.35(8)	0.333
$J_2 = -1$	4	0.38(2)	0.333

We find a universal logarithmic term in the SRE with respect to the system size, governed by the number of modes N_{NG} . Our theory is consistent with the numerical results obtained by the Toulouse group, even though the quantitative agreement is not perfect. We will also provide new numerical results for the SRE on cylinders, to be compared with the theory. We believe that our approach is on the right track and could be extended for further quantitative improvements.

The paper is organized as follows. In Sec. II, we analyze the contribution to the SRE of the fluctuations due to Nambu–Goldstone modes. We first focus on the $n = \infty$ limit of the SRE, $S_\infty \sim -\ln p_{\text{max}}$, where p_{max} is the largest among the probabilities of finding a particular basis configuration upon the corresponding projective measurement of the ground state. As far as the universal terms are concerned, we show that this problem is closely related to the determinant of the Laplacian in 2D (Sec. II C). While we find a universal logarithmic term, its coefficient has the opposite sign to that obtained with QMC. The discrepancy is attributed to the degeneracy of the ground states in the presence of spontaneous breaking of a continuous symmetry, as discussed in Sec. III. In Sec. IV, we combine the results from earlier sections to derive the universal logarithmic term in SRE for $n > 1$ and $n = 1$. In Sec. V, we also discuss the logarithmic terms in the SRE of a subsystem which has the geometry of a straight line embedded in a 2D system, for which Luitz *et al.* [22,25] have some QMC data indicating clearly the presence of universal log

terms. Section VI presents some 2D DMRG calculations of the ground state of the spin- $\frac{1}{2}$ XX model on cylinders, from which we extract $-\ln(p_{\max})$, the associated $\ln L$ term, as well as an universal aspect-ratio-dependent contribution of order $\mathcal{O}(1)$ that we compare to an analytical free-field calculation. Section VII is devoted to conclusions and discussion.

II. OSCILLATOR/SPIN-WAVE CONTRIBUTIONS

A. Massless free scalar field

We first assume that the system is in a broken symmetry state, with a well-defined direction of the order parameter (say x). At low energy the interactions between spin-waves are irrelevant and each mode can be described by a free gapless scalar boson with a linear dispersion relation. As a consequence we can consider the case of a single mode [i.e., broken $U(1)$] and the final result for the SRE will simply have to be multiplied by the number of Nambu-Goldstone modes.

At each point \mathbf{r} in space an angle $\phi_{\mathbf{r}}$ describes the local orientation of the order parameter with respect to its average direction. At low energies and when coarse grained over sufficiently long distances, these deviations are small and one can treat them as real numbers (instead of angles in $]-\pi, \pi[$), therefore neglecting the compactness of $\phi_{\mathbf{r}}$. This leads to the Hamiltonian of a massless free scalar field:

$$H = \frac{1}{2} \int d^2\mathbf{r} [\chi_{\perp} \Pi_{\mathbf{r}}^2 + \rho_s (\nabla \phi_{\mathbf{r}})^2], \quad (4)$$

where ρ_s is the stiffness, $\chi_{\perp} = \frac{c^2}{\rho_s}$ is the transverse susceptibility, c the spin-wave velocity, and $\Pi_{\mathbf{r}} = \frac{\rho_s}{c} \dot{\phi}_{\mathbf{r}}$ is canonically conjugate to $\phi_{\mathbf{r}}$. This is a collection of harmonic oscillators, one for each momentum \mathbf{k} :

$$H = \frac{1}{2} \sum_{\mathbf{k}} \left(\frac{c^2}{\rho_s} \Pi_{\mathbf{k}}^2 + \rho_s \mathbf{k}^2 |\phi_{\mathbf{k}}|^2 \right). \quad (5)$$

B. Configuration with the highest probability

We start by considering the $n = \infty$ SRE, which amounts to evaluate the probability of the “most likely” configuration. As a warm up let us first recall that the (normalized) ground-state wave function ψ of an harmonic oscillator with the Hamiltonian $H = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 x^2$ is

$$\psi(x) = \left(\frac{m\omega}{\pi} \right)^{1/4} \exp\left(-\frac{m\omega}{2} x^2\right). \quad (6)$$

The probability density p_{\max} to find the particle at its “most likely” location, which is the square of the wave function at $x = 0$, is the square of the normalization factor:

$$p_{\max} = |\psi(0)|^2 = \left(\frac{m\omega}{\pi} \right)^{1/2}. \quad (7)$$

Comparing this to Eq. (5), the mode \mathbf{k} of the free field has a mass $m_{\mathbf{k}} = \frac{\rho_s}{c^2}$ and frequency $\omega_{\mathbf{k}} = c|\mathbf{k}|$. So, the probability $p_{\max}(\mathbf{k})$ for the mode \mathbf{k} to be “at the origin” is

$$p_{\max}(\mathbf{k}) = \left(\frac{m_{\mathbf{k}} \omega_{\mathbf{k}}}{\pi} \right)^{1/2} = \left(\frac{\rho_s |\mathbf{k}|}{\pi c} \right)^{1/2}. \quad (8)$$

We are interested in the probability density to observe $\phi_{\mathbf{r}} = 0$ everywhere in space, so we impose $\phi_{\mathbf{k}} = 0$ for all \mathbf{k} and get

$$p_{\max}^{\text{osc}} = \prod_{\mathbf{k} \neq 0} p_{\max}(\mathbf{k}) = \prod_{\mathbf{k} \neq 0} \left(\frac{\rho_s |\mathbf{k}|}{\pi c} \right)^{1/2}. \quad (9)$$

Taking the logarithm, we obtain

$$-\ln(p_{\max}^{\text{osc}}) = -\frac{1}{2} \sum_{\mathbf{k} \neq 0} \ln\left(\frac{\rho_s}{\pi c}\right) - \frac{1}{4} \sum_{\mathbf{k} \neq 0} \ln \mathbf{k}^2. \quad (10)$$

The zero mode $\mathbf{k} = 0$ is omitted since we assume that the system is in a broken-symmetry state. Including the zero mode would, in a finite volume, “delocalize” the order parameter and restore the rotation symmetry. We will take later into account the rotational symmetry of the finite-size ground state by a correcting factor associated with the “degeneracy” of the Anderson tower of states (TOS), see Sec. III. The first sum in Eq. (10) is simply a volume term ($\sim L^2$) but the universal contribution comes from the second sum, which we analyze now.

C. Determinant of Laplacian

Since the $-\mathbf{k}^2$ are the eigenvalues of the Laplacian Δ , the Eq. (10) is a lattice regularization of $\ln \det' \Delta$, where \det' means that the zero eigenvalue is removed from the calculation of the determinant.

One can regularize the sum by using a periodic $L \times L$ lattice (torus), in which case the universal terms in the $L \rightarrow \infty$ asymptotics can be extracted by means of an Euler-Maclaurin expansion. A possible way to regularize $\ln \det' \Delta$ is indeed to use the Brillouin zone of an $L \times L$ square lattice:

$$\Sigma(L) = \sum_{\mathbf{k} \neq 0} \ln(\mathbf{k}^2) = \sum_{n,m=-\frac{L}{2} \dots \frac{L}{2}-1} \ln(k_n^2 + k_m^2), \quad (11)$$

where the discrete momenta are given by $k_n = \frac{2\pi n}{L}$ and the zero-mode ($n = m = 0$) is omitted. Using twice the Euler-Maclaurin expansion at the trapezoid order gives

$$\Sigma(L) = \left(\frac{1}{2} \pi - 3 - \ln(2) + 2 \ln(2\pi) \right) L^2 + \ln(L^2) + \mathcal{O}(1). \quad (12)$$

While the term proportional to L^2 can be shown to depend on the regularization scheme, the $\ln(L^2)$ is universal.

In fact, $\det' \Delta$ is a quantity which has been studied extensively in the literature (see for instance Refs. [26,27]). In particular, on a compact surface without boundary and with Euler characteristics χ , one has

$$\ln \det' \Delta \simeq \text{const.} \times L^2 + \left(1 - \frac{\chi}{6} \right) \ln(L^2). \quad (13)$$

This result is remarkable since the coefficient of the $\ln(L^2)$ term is purely topological. It can be derived using the heat-kernel method and zeta regularization for instance [28]. An explicit calculation, in cylinder geometry, is presented in Appendix A. We also note that on a cylinder or on a torus, the quantity $\ln \det' \Delta$ will also contain some finite aspect-ratio dependent term, directly related to the one appearing in free boson partition functions which are well studied in the context conformal

field theory [29]. The aspect-ratio-dependent correction turns out to be very important in the analysis of the numerical data presented in Sec. VI.

We therefore have

$$-\ln(p_{\max}^{\text{osc}}) = \text{const.} \times L^2 + \frac{1}{4} \left(\frac{\chi}{6} - 1 \right) \ln(L^2) + \mathcal{O}(1) \quad (14)$$

and, specializing to the torus ($\chi = 0$),

$$-\ln(p_{\max}^{\text{osc}}) = \text{const.} \times L^2 - \frac{1}{4} \ln(L^2) + \mathcal{O}(1). \quad (15)$$

In the following, we are often interested only in the universal logarithmic contribution and express, for example, Eq. (15) as

$$-\ln(p_{\max}^{\text{osc}}) \sim -\frac{1}{4} \ln(L^2). \quad (16)$$

If compared directly with the numerical QMC results for the $n = \infty$ SRE (Table I), the log coefficient $-\frac{N_{\text{NG}}}{4}$ obtained above is clearly off, with a wrong sign in particular. As we argue later, this is due to the fact that the oscillator contribution provides only one part of the logarithmic terms. The other part, discussed in Sec. III, is due to the fact that the ground state of a system of finite volume (as is the case in the simulations) is rotationally invariant, contrary to the initial assumption of a broken-symmetry state. We note that this rotational symmetry of finite systems also plays an important role concerning logarithmic terms in the entanglement entropy [17,30]. Before dealing with this important point (in the context of SRE), we discuss the n dependence of the oscillator contribution to the SRE.

D. Finite Rényi index

So far we only considered one probability, p_{\max} , of observing the configuration with $\phi_r = 0$. We will now discuss the $\ln(L)$ contribution to the finite- n SRE.

Each probability p_i [Eq. (1)] can be obtained in a path integral formalism, by imposing the state $|i\rangle$ at $\tau = 0$, the plane corresponding to the imaginary time origin. As already discussed in the context of spin chains [14,31], the quantity

$$Z_n = \sum_i p_i^n \quad (17)$$

can be represented as an imaginary time path integral for the field theory with n replica fields $\phi^{(1)}, \phi^{(2)}, \dots, \phi^{(n)}$. Except at $\tau = 0$, replica fields are decoupled, and each of them is described by the same free boson field Lagrangian. At $\tau = 0$, we impose the “gluing condition”

$$\phi^{(1)} = \phi^{(2)} = \dots = \phi^{(n)}. \quad (18)$$

This condition can be solved exactly, in a similar manner to the analysis in 1 spatial dimension. In fact, in general, we need to include possible boundary perturbations, which turn out to be very important as we will discuss below.

1. Without boundary perturbations

Keeping the caveat in mind, first let us discuss what would be the SRE in the absence of boundary perturbations. In terms of the field theory, we can simply introduce the new basis of

the replica fields:

$$\Phi^{(0)} = \frac{1}{\sqrt{n}} \sum_j \phi^{(j)}, \quad (19)$$

$$\Phi^{(1)} = \frac{1}{\sqrt{2}} (\phi^{(1)} - \phi^{(2)}), \quad (20)$$

$$\vdots \quad (21)$$

That is, $\Phi^{(0)}$ the “center of mass” field, and the remaining $n - 1$ fields $\Phi^{(1)}, \dots, \Phi^{(n-1)}$ are difference fields. The gluing condition (18) amounts to imposing the Dirichlet boundary condition $\Phi^{(j)} = 0$ for the difference fields but leave the center-of-mass field $\Phi^{(0)}$ free [32,33]. It then follows that

$$Z_n^{\text{osc}} = \left(\frac{z_D}{z_0} \right)^{n-1}, \quad (22)$$

where z_D is the partition function for the single free boson field with the Dirichlet boundary condition imposed at $\tau = 0$, and z_0 is the partition function of the single free boson without imposing any boundary condition at $\tau = 0$. Precisely speaking, the “boundary” $\tau = 0$ is in the middle of the entire system defined for $-\infty < \tau < \infty$ we consider. Nevertheless, it can still be regarded as a boundary of $2n$ -component boson field after a folding procedure [31]. Since imposing the Dirichlet boundary condition is equivalent to freezing the fluctuation of the order parameter,

$$p_{\max}^{\text{osc}} = \frac{z_D}{z_0}. \quad (23)$$

Thus we find

$$Z_n^{\text{osc}} \sim (p_{\max}^{\text{osc}})^{n-1}, \quad (24)$$

concerning the universal subleading contribution to S_n . This would give

$$S_n^{\text{osc}} = \frac{1}{1-n} \ln Z_n^{\text{osc}} \sim -\ln p_{\max}^{\text{osc}} \sim -\frac{N_{\text{NG}}}{4} \ln N. \quad (25)$$

which is actually the same as S_{∞} . For the free boson field theory in 1+1 dimensions, the resolution of the gluing condition is in fact tricky because of the subtlety in the compactification of the boson field [31], leading to a correction to the result as derived by the above argument. However, in two spatial dimensions, the boson field can be regarded as noncompact and the simple derivation as given above stands correct.

The same result can be also derived without using replica trick, following the analysis in 1 spatial dimension given in Ref. [10]. Ignoring the possible boundary perturbations is equivalent to consider the purely Gaussian wave function:

$$\psi(\{\phi_{\mathbf{k}}\}) = \prod_{\mathbf{k} \neq \mathbf{0}} \left(\frac{\rho_s |\mathbf{k}|}{\pi c} \right)^{1/4} \exp \left(-\frac{\rho_s |\mathbf{k}|}{2c} |\phi_{\mathbf{k}}|^2 \right). \quad (26)$$

For such a state, the calculation of Z_n is just a Gaussian integration, and it can therefore be performed explicitly. The result has a simple expression in terms of p_{\max}^{osc} Eq. (15):

$$Z_n^{\text{Gauss}} = \frac{(p_{\max, \rho_s}^{\text{osc}})^n}{P_{\max, n \rho_s}^{\text{osc}}}, \quad (27)$$

where we have explicitly kept the dependence on the stiffness, and where the denominator is evaluated at a modified value of the stiffness $\tilde{\rho}_s = n\rho_s$. For the massless oscillators discussed previously, the universal logarithm in $\ln p_{\max, \rho_s}^{\text{osc}}$ is actually independent of ρ_s [see Eq. (15)]. Thus we find the same result as Eqs. (24) and (25). This derivation has an advantage that it is exact for an arbitrary real n and does not rely on the analytic continuation in n which is usually required in a replica trick. However, it should be still noted that it does rely on the assumption of purely Gaussian wave function. Even though such a Gaussian form correctly captures the long-wavelength fluctuations of the order parameter, it does not describe exactly the short-distance degrees of freedom on the lattice. Neglecting the non-Gaussian terms in the wave function corresponds to ignoring the effects of possible boundary perturbations in the replica formulation.

2. With the relevant boundary perturbation

In the preceding analysis, we ignored the possible boundary perturbations, which can be important. In the replica field formulation, the replica fields are decoupled in the bulk and each replica is described by the same Lagrangian density. For the bulk, we already know the asymptotically exact low-energy effective theory, which corresponds to the infrared fixed point of the renormalization group. However, at the “boundary” ($\tau = 0$), which is introduced by taking the inner product with the basis states, the replica fields are coupled and other boundary perturbations can arise. In the presence of a relevant boundary perturbation, the boundary condition is renormalized into a different one, leading to a different SRE. The general principle is that all the boundary perturbations which are allowed by symmetries would arise, unless they are eliminated by fine-tuning. In SRE, because of the choice of the basis, the $U(1)$ symmetry is generally broken explicitly.

In fact, the change of boundary condition induced by the boundary perturbation and the resulting “phase transition” in SRE were studied in 1 spatial dimension [14]. There, the leading boundary perturbation which is allowed by the breaking of the $U(1)$ symmetry and is consistent with the compactification of the boson field is $\cos \frac{\phi}{R}$, where R is the compactification radius. This implies, for the center-of-mass field, the boundary perturbation $\cos \frac{\Phi^{(0)}}{\sqrt{n}R}$. This is relevant for $n > n_c$. Once relevant, it locks the center-of-mass field at the boundary, giving rise to the Dirichlet boundary condition.

In contrast, in the 2D case discussed here, the boson field describes a small fluctuation on the broken symmetry states, and thus it can be regarded as noncompact. Therefore we expect the boundary mass term $\sim \phi^2$ to appear, once the $U(1)$ symmetry is broken. The important difference from 1 dimension is that, the boundary mass term is always relevant (but see Sec. IV). Its effect is still similar to one-dimensional case, locking the center-of-mass field at the boundary. This results in the Dirichlet boundary condition on *all* the n replica fields. Thus the partition function reads

$$Z_n^{\text{osc}} = \left(\frac{z_D}{z_0} \right)^n \quad (28)$$

[compare with Eq. (22) in the absence of the boundary perturbation]. This leads to the universal logarithmic

correction as

$$S_n^{\text{osc}} \sim -\frac{n}{n-1} \ln p_{\max}^{\text{osc}} \sim -\frac{N_{\text{NG}}}{4} \frac{n}{n-1} \ln(N). \quad (29)$$

III. DEGENERACY FACTOR

We have derived the universal oscillator contribution to SRE in the previous section. The final result for SRE, however, also requires a consideration of the ground-state degeneracy due to the spontaneous symmetry breaking.

Let us briefly review the standard concept of tower of states (TOS) [34–37], which reconciles the fact that the finite-size (antiferromagnetic) eigenstates are rotationally invariant while, in $D \geq 2$, the system can break the rotational symmetry in the infinite volume limit at $T = 0$.

If a spin Hamiltonian \mathcal{H} has a continuous rotation symmetry, say $U(1)$ for simplicity, the total angular momentum $S_{\text{tot}}^z = \sum_{\mathbf{r}} S_{\mathbf{r}}^z$ (generator of the rotations) is a conserved quantity, and one can choose the eigenstates of \mathcal{H} such that they are also eigenstates of S_{tot}^z . For an antiferromagnetic system, the finite-size ground state has $S_{\text{tot}}^z = 0$ and is thus rotationally invariant.¹

This may seem in contradiction with the possible spontaneous symmetry breaking. However, the symmetry of the finite-size ground state of course does not rule out the possibility of the spontaneous symmetry breaking. Indeed, the spontaneous symmetry breaking is, rigorously speaking, a concept which applies to the thermodynamic limit, where ground states that break the symmetry must be degenerate.

In order to realize some spontaneous symmetry breaking in the thermodynamic limit, the finite-size spectrum must contain low-energy eigenstates above the symmetric ground state. Generic finite-size eigenstates of the Hamiltonian are also eigenstates of S_{tot}^z , and thus each of them does not break the symmetry. The “physical” ground states in the thermodynamic limit, which do break the symmetry, correspond to superpositions of the finite-size low-energy eigenstates. In the case of the spontaneous breaking of a continuous symmetry, which is the focus of the present paper, there must be an infinite number of such symmetry-breaking physical ground states in the thermodynamic limit. In order to produce these symmetry-breaking physical ground states as superpositions, the number of the low-energy eigenstates in the finite-size spectrum must grow as the system size is increased. The set of these low-energy states (including the ground state) which reflect the spontaneous breaking is commonly called Anderson TOS.

As discussed above, the finite-size counterpart of the symmetry-breaking ground states (hereafter finite-size symmetry-breaking states for brevity) are given by appropriate superpositions of the finite-size eigenstates belonging to the Anderson TOS. This also implies that the symmetric finite-size ground state is given by a superposition of the symmetry-breaking states.

¹This was shown rigorously for an Heisenberg-like (or XXZ) model on a bipartite lattice (with the same number of sites on both sublattices): the Lieb-Mattis theorem [44].

It is helpful for understanding to map the spin system with S_{tot}^z conservation to an interacting many-boson problem, by identifying $S_{\mathbf{r}}^+$ with the creation operator $\psi^\dagger(\mathbf{r})$ and $S_{\mathbf{r}}^-$ with the annihilation operator $\psi(\mathbf{r})$. Then S_{tot}^z corresponds to the total number of particles, with a constant offset per site. In a symmetry-breaking ground state in the thermodynamic limit $|\phi\rangle$, $\psi(\mathbf{r})$ is thought to have a nonvanishing expectation value, which can be regarded as an order parameter. Specifically,

$$\langle\phi|\psi(\mathbf{r})|\phi\rangle = \sqrt{\rho_s}e^{i\phi}, \quad (30)$$

where $\rho_s > 0$ represents the superfluid density and ϕ represents the phase of the condensate. The symmetry-breaking ground state $|\phi\rangle$ is labeled by the phase ϕ , a continuous parameter, and thus is infinitely degenerate.

Now let us consider a finite-size system. A finite-size symmetry-breaking state would also satisfy Eq. (30). Such a state may be given as a coherent state satisfying

$$\psi(\mathbf{r})|\phi\rangle \sim \sqrt{\rho_s}e^{i\phi}|\phi\rangle. \quad (31)$$

The expectation of the total number of particles N_{tot}^p in such a state is

$$\langle N_{\text{tot}}^p \rangle = \sum_{\mathbf{r}} \langle\phi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\phi\rangle = N\rho_s. \quad (32)$$

Likewise, we can also evaluate

$$\begin{aligned} \langle (N_{\text{tot}}^p)^2 \rangle &= \sum_{\mathbf{r}, \mathbf{r}'} \langle\phi|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')|\phi\rangle \\ &= (N\rho_s)^2 + N\rho_s. \end{aligned} \quad (33)$$

This implies a nonvanishing fluctuation

$$\langle (\Delta N_{\text{tot}}^p)^2 \rangle = N\rho_s. \quad (34)$$

The fluctuation of N_{tot}^p (fluctuation of S_{tot}^z in the spin-system context) is actually required by the uncertainty relation

$$\Delta N_{\text{tot}}^p \Delta\phi \gtrsim \frac{1}{2}, \quad (35)$$

which is a consequence of the noncommutativity

$$[N_{\text{tot}}^p, \phi] \sim i. \quad (36)$$

Equations (34) and (35) implies that the finite-size symmetry-breaking state also has an uncertainty in its phase:

$$\Delta\phi = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right). \quad (37)$$

In other words, a symmetry-breaking state ‘‘occupies’’ a finite patch on the circle representing all the possible order parameter directions, as illustrated in Fig. 1.² This implies that two finite-size symmetry-breaking states are distinguishable only if their phases differ by more than $\Delta\phi = \mathcal{O}(\frac{1}{\sqrt{N}})$.

This can be also confirmed with the explicit construction of the coherent state

$$|\phi\rangle = e^{-\frac{\rho_s}{2}} \exp\left[\frac{\sqrt{\rho_s}e^{i\phi}}{\sqrt{N}} \sum_{\mathbf{r}} \psi^\dagger(\mathbf{r})\right] |\text{vac}\rangle, \quad (38)$$

²Note that this scaling for the transverse fluctuations can also be obtained using a linear spin-wave calculation.

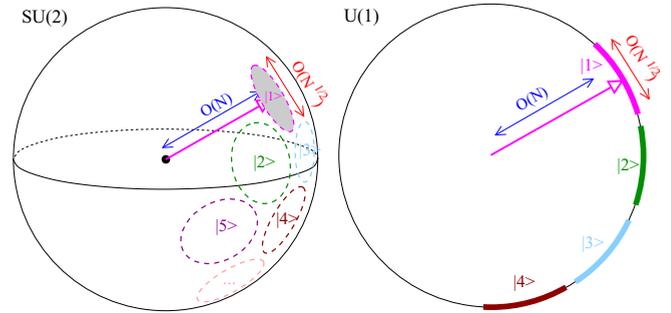


FIG. 1. (Left) The order parameter fluctuations in the broken symmetry states $|i\rangle$ of a collinear SU(2) antiferromagnet are schematically represented as patches on a sphere (the order parameter manifold). Since the typical transverse fluctuations of the order parameter (sublattice magnetization) are $\sim N\Delta\phi = \mathcal{O}(N^{\frac{1}{2}})$ [Eq. (37)], each patch occupies an area $\sim \mathcal{O}(N)$. From the fact that the area of the sphere is $\sim N^2$, we get that the number Q of nonoverlapping patches scales as $\mathcal{O}(N)$. (Right) Case of a U(1) order parameter, where each broken symmetry state $|i\rangle$ is represented by a (colored) arc on the circle. Knowing that the transverse fluctuations are also $\sim N^{\frac{1}{2}}$, the phase space argument leads to $Q \sim N^{\frac{1}{2}}$ independent states.

where $|\text{vac}\rangle$ is the vacuum with no boson present. Using this expression, we find

$$\begin{aligned} |\langle\phi|\phi'\rangle| &= \exp[-\rho_s N(1 - \cos|\phi - \phi'|)] \\ &\sim \exp\left[-\frac{1}{2}\rho_s N(\phi - \phi')^2\right], \end{aligned} \quad (39)$$

which is small when $|\phi - \phi'| \gtrsim \mathcal{O}(\frac{1}{\sqrt{N}})$. Therefore, in a finite-size system of N sites, there are $\mathcal{O}(\sqrt{N})$ linearly-independent symmetry-breaking states in the case of the spontaneous breaking of a U(1) symmetry.³ It should be noted that the oscillator modes discussed in Sec. II are not included in the above construction of the coherent states, which are only used for counting the number of (almost) independent symmetry-breaking ground states. The final result on the SRE is obtained by combining the counting of the symmetry-breaking ground states and the contribution from the oscillator modes, as it will done later in this paper. We also note that, the simple coherent states discussed above do not precisely represent physical symmetry-breaking ground states in the presence of interactions (which is always the case for quantum antiferromagnets) [38]. Here those simple coherent states are used for simplicity, as they should lead to the same number of independent symmetry-breaking ground states. The same

³From Eq. (34), we see that the states in the TOS have a typical spin $S_{\text{tot}}^z \sim \sqrt{N}$. Since the energies of the eigenstates in the TOS scale as $E \simeq (S_{\text{tot}}^z)^2/N$ [37] (the kinetic energy of a quantum rotor with angular momentum S_{tot}^z and a moment of ‘‘inertia’’ proportional to the total number of spins), these states have a typical energy $E \sim \mathcal{O}(1)$ relative to the finite-size symmetric ground state. This corresponds to a vanishing energy density in thermodynamic limit, as it should. Finally, in the broken U(1) case, the TOS is known to contain one eigenstate per value of S_{tot}^z [37]. The fact that the typical value of S_{tot}^z scales as \sqrt{N} then implies a total number of state is also $\mathcal{O}(\sqrt{N})$. This is consistent with what we found using the coherent state ansatz.

argument, when applied to an SU(2) symmetry broken down to U(1) (collinear antiferromagnet) leads to the conclusion that a low-energy symmetry-breaking state occupies a solid angle $\delta\Omega \sim 4\pi N^{-1}$ on the Bloch sphere representing the order parameter manifold (see Fig. 1).

In a more general situation, we expect (phase space volume argument) the TOS dimension Q to scale as $\sim N^\alpha$, with an exponent α which only depends on the number of Nambu-Goldstone modes:

$$\alpha = N_{\text{NG}}/2. \quad (40)$$

As discussed in Introduction, throughout this paper we consider systems with only type-I (type-A with linear dispersion) Nambu-Goldstone modes, where the number of Goldstone modes is equal to the number of broken symmetry generators.

IV. RÉNYI PARAMETER (n) DEPENDENCE OF THE SRE

Now that we have all the necessary ingredients, we shall give the final results on the universal log correction to the SRE. As we will discuss below, the results depends on the Rényi parameter n .

A. $n > 1$

The choice of the x basis explicitly breaks the U(1) symmetry of the XXZ model (or SU(2) symmetry of the Heisenberg model). This symmetry breaking appears in the fact that, upon re-weighting the basis configurations according to $p_i \rightarrow p_i^n$, the order parameter will preferentially be aligned with the x direction. This is obvious in the limit $n \rightarrow \infty$, where the only configuration left is the one with the largest probability p_{max} and corresponds to a perfectly ordered state with order parameter pointing in the x direction. While such a preferential direction is nontrivial for a finite n , we expect it to hold for $n > 1$ since, as we will discuss later, the exact rotational symmetry is restored at $n = 1$ only. In terms of the field theory, such a preference is represented by a boundary mass term. Since such a mass term is always a relevant perturbation, we expect Eq. (29) to hold for general $n > 1$. However, as we have mentioned earlier, Eq. (29) contains only the oscillator contributions.

What enters in the SRE is the probability p_{max} , and, for the x -basis measurement of the antiferromagnetic XXZ model we consider in this paper, we note $|+\rangle$ the associated spin configuration. That is,

$$p_{\text{max}} = |\langle \Psi | + \rangle|^2. \quad (41)$$

As we have discussed in Sec. III, the symmetric finite-size ground state $|\Psi\rangle$, with $S_{\text{tot}}^z = 0$, is built as a linear superposition of $Q \sim N^\alpha$ symmetry-breaking states noted $\{|1\rangle, |2\rangle, \dots, |Q\rangle\}$. The U(1) case would correspond to $\alpha = \frac{1}{2}$ and SU(2) \rightarrow U(1) would be $\alpha = 1$ (see Fig. 1). We thus write

$$|\Psi\rangle = \frac{1}{\sqrt{Q}}(|1\rangle + |2\rangle + \dots + |Q\rangle). \quad (42)$$

As a consequence,

$$p_{\text{max}} = |\langle \Psi | + \rangle|^2 = \frac{1}{Q} \left| \sum_{i=1}^Q \langle i | + \rangle \right|^2. \quad (43)$$

We can choose the states appearing in Eq. (42) so that only one, say $|1\rangle$, has an order parameter direction which matches that of the classical configuration $|+\rangle$. We argue that $\sum_{i=1}^Q \langle i | + \rangle$ is dominated by the $i = 1$ term, and that the others may be ignored in the limit $N \rightarrow \infty$, as they are exponentially suppressed as a function of the system size N relative to the dominant $i = 1$ term.

On the other hand, since the state $|1\rangle$ is “aligned” with the classical state $|+\rangle$, $\langle 1 | + \rangle$ will precisely have the oscillator contribution as in Eq. (15). So, as far as the universal part is concerned, we may thus write

$$p_{\text{max}} \simeq \frac{1}{Q} |\langle 1 | + \rangle|^2 = \frac{1}{Q} p_{\text{max}}^{\text{osc}} \quad (44)$$

with $Q \sim N^{N_{\text{NG}}/2}$. We finally get

$$\begin{aligned} -\ln(p_{\text{max}}) &\sim -\ln(p_{\text{max}}^{\text{osc}}) + \frac{1}{2} N_{\text{NG}} \ln(N) \\ &\sim +\frac{1}{4} N_{\text{NG}} \ln(N). \end{aligned} \quad (45)$$

As already discussed in Sec. IID, we argue that, for $n > 1$ where the boundary mass is relevant, the universal contribution to the SRE is dominated by that of p_{max} so that $S_n \sim \frac{n}{1-n} \ln(p_{\text{max}})$. Now p_{max} receives $\ln N$ contributions from the gapless oscillator modes, as well as from the degeneracy factor Q discussed above. We may thus write

$$S_{n>1} \sim \frac{n}{n-1} (\ln(Q) - \ln(p_{\text{max}}^{\text{osc}})). \quad (46)$$

Replacing Q by $N^{N_{\text{NG}}/2}$ and $-\ln(p_{\text{max}}^{\text{osc}})$ by Eq. (15), we finally obtain

$$S_{n>1} \sim \frac{N_{\text{NG}}}{4} \frac{n}{n-1} \ln(N). \quad (47)$$

In Table I, the result above is compared to the QMC results obtained by Luitz *et al.* (Toulouse group) [21] at $n = 2, 3, 4$, and ∞ . The agreement is reasonable, and especially good for $n = \infty$, although not perfect. We also note that their results for models *without* continuous symmetry breaking (gapped phase of the XXZ model) indicate the absence of $\ln N$ correction, which is of course consistent with the present analysis. We stress that the error bars given in Table I do not include the (significant) variations when larger system sizes are included. For this reason, we believe that the numerical data are consistent with our predictions. The apparently larger discrepancy between the theoretical prediction and the numerical estimate is partly attributed to the smallness of the boundary mass perturbation for smaller Rényi parameter n . In fact, as we will discuss in Sec. VB, the boundary mass perturbation should vanish at $n = 1$. Thus the crossover to the asymptotic behavior predicted theoretically for $n > 1$ would occur at larger lengthscale when n is decreased towards 1. We hope that further progress in numerical methods and theoretical understanding of finite-size effects will improve the agreement.

An important support to the above reasoning is provided by the exact result for the SRE of the Lieb-Mattis model [21]. The latter has an SU(2) \rightarrow U(1) TOS (hence $\alpha = 1$ and $Q \sim N$) but no gapless spin-waves (hence no oscillator contribution to the entropy). The ground state of this model was shown to have

$S_{n>1} = \frac{n}{n-1} \ln N + \mathcal{O}(1)$ [21], which is in agreement with the first term (TOS contribution) in the right-hand side (r.h.s.) of Eq. (47).

B. $n = 1$

The case $n = 1$ requires a special consideration. When $n = 1$, the boundary still retains the exact symmetry of the Hamiltonian. This can be seen because

$$Z_1 = \sum_i p_i = \sum_i \langle \Psi | i \rangle \langle i | \Psi \rangle = \langle \Psi | \Psi \rangle = 1. \quad (49)$$

Namely, there is no particular boundary condition imposed at $\tau = 0$; it is rather a fictitious cut of the Euclidean space-time.

Even for $n = 1$, the boundary mass could be added as a perturbation. However, the exact symmetry discussed above implies that the boundary mass perturbation is absent in the present problem for $n = 1$. The absence of boundary mass corresponds to the quadratic action and thus to the Gaussian wave function, Eq. (26). The Shannon entropy is then calculated using the Gaussian wave function trick as the $n \rightarrow 1$ limit of Eq. (25).

The exact symmetry means that there is no preference given to the direction of the order parameter. Thus, all the Q symmetry-breaking ground states contained in the finite-size ground state [as in Eq. (42)] contribute to the universal part of p_{\max} . Therefore, unlike in the case of $n > 1$, the $1/Q$ factor is missing, and the final result is given by

$$S_1 \sim -\ln p_{\max}^{\text{osc}} \sim -\frac{N_{\text{NG}}}{4} \ln N, \quad (50)$$

where the universal logarithmic correction entirely comes from the oscillator contribution. The lack of the degeneracy factor can be indeed confirmed with the exact result

$$S_1 \sim 0 \quad (51)$$

for the Lieb-Mattis model [21], in which there is no oscillator contribution. The logarithmic correction in the Lieb-Mattis model comes only from the degeneracy factor; the fact that the $\ln N$ term precisely vanishes at $n = 1$ implies that the degeneracy factor is also absent there, reflecting the exact symmetry as discussed above.

C. $n < 1$

The SRE is still well-defined for $n < 1$. In fact, it has been studied numerically for 1 spatial dimension, using exact numerical diagonalization [14]. On the other hand, estimate of the SRE using Quantum Monte Carlo simulation is more difficult for smaller n , as contributions of smaller probabilities p_i are more pronounced. It is also difficult to perform simulations when n is not an integer greater than one, since this prevents the use of replica-based algorithms. In fact, to our knowledge, no numerical data for the SRE at $n < 1$ is yet available in 2D. Since analytical prediction of the SRE is also subtle for $n < 1$, in this paper, we refrain from making a prediction in this regime and leave this question for future studies.

V. LINE SUBSYSTEM

So far we considered the configurations of the whole system, but it is also possible to consider the probabilities (and associated entropies) of the configurations of a *subsystem*, noted Ω . For instance, the SRE of a segment in a critical spin chain was found to have some striking similarities with the entanglement entropy of that segment [39,40]. In this section, we will specialize to the case where Ω is a line embedded in a 2D system. In that case, using QMC and spin-wave calculations [41], the *entanglement* entropy was recently shown to have some logarithmic correction. We show here that the SRE possesses some very similar universal subleading term.

A. Oscillators

We first study the oscillator contribution to p_{\max}^{Ω} , the probability of the most likely configuration of the region Ω (in the chosen basis). For this, we consider the reduced density matrix of a subsystem in the framework of Eq. (4). Since the Hamiltonian is Gaussian for the variables ϕ_r , the reduced density matrix ρ_{Ω} is also Gaussian. But to get the SRE entropies, and p_{\max}^{Ω} in particular, we do not need the full reduced density matrix but only its diagonal elements. The latter, being again Gaussian, must have the following form:

$$\langle \phi | \rho_{\Omega} | \phi \rangle = \frac{1}{Z_{\Omega}} \exp \left\{ -\frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}' \in \Omega} \phi_{\mathbf{r}} [(G_{|\Omega})^{-1}]_{\mathbf{r}-\mathbf{r}'} \phi_{\mathbf{r}'} \right\}, \quad (52)$$

where the state $|\phi\rangle$ has a fixed ‘‘angle’’ $\phi_{\mathbf{r}}$ at each site and $(G_{|\Omega})_{\mathbf{r}, \mathbf{r}'}$ is the correlation function for two sites inside the region Ω . Using $\text{Tr} \rho_{\Omega} = 1$ and Gaussian integration, the normalization factor can be expressed using the determinant of the correlation matrix $G_{|\Omega}$:

$$Z_{\Omega} = \sqrt{\det(2\pi G_{|\Omega})}. \quad (53)$$

So, we already see that the probability $p_{\max}^{\Omega, \text{osc}}$ to observe $\phi_{\mathbf{r}} = 0$ everywhere in Ω is given by

$$p_{\max}^{\Omega, \text{osc}} = 1/Z_{\Omega} = [\det(2\pi G_{|\Omega})]^{-1/2}, \quad (54)$$

or, in terms of the eigenvalues $g_{\mathbf{k}}$ of $G_{|\Omega}$,

$$-\ln(p_{\max}^{\Omega, \text{osc}}) = \frac{1}{2} \sum_{\mathbf{k}} \ln(2\pi g(\mathbf{k})). \quad (55)$$

Now we specialize the above calculation to the case where Ω is a line. Due to the linear dispersion relation of the Goldstone mode, the long-distance behavior of the (transverse) correlation $G_{|\Omega}(r)$ is related to the (two-dimensional) Fourier transform of $1/k$, that is,

$$G_{|\Omega}(r \rightarrow \infty) = G(r \rightarrow \infty) \sim 1/r. \quad (56)$$

Now we transform this correlation back to real space, but restricting to the one-dimensional momentum \mathbf{k} along the line. We get

$$g(\mathbf{k} \rightarrow 0) \sim -\ln(|\mathbf{k}|). \quad (57)$$

If we replace $g(\mathbf{k})$ by $\sim -a \ln(|\mathbf{k}|)$ in Eq. (55) ($a > 0$ is some nonuniversal factor) and if we regularize the sum by taking a

finite line with L sites, we obtain

$$-\ln(p_{\max}^{\text{line,osc}}) = \frac{1}{2} \sum_{\substack{n=-L/2 \\ n \neq 0}}^{L/2-1} \ln \left[-2\pi a \ln \left(\frac{2\pi n}{L} \right) \right], \quad (58)$$

This sum can be analyzed using an Euler-Maclaurin expansion. The dominant part turns out to be proportional to L , and the first subleading correction turns out to be very slowly diverging:

$$-\ln(p_{\max}^{\text{line,osc}}) = \text{const.} \times L - \ln(\ln(L)) + \mathcal{O}(1). \quad (59)$$

In other words, there is *no* $\ln(L)$ term, contrary to the largest probability for the full system [compare with Eq. (15)].

B. Degeneracy factor

The phase space argument of Sec. III to treat the TOS contribution needs to be adapted for the probability p_{\max}^{line} to observe an ordered configuration along a line. Indeed, if we specify an ordered configuration $|\text{ord}\rangle$ only on a line, it involves L sites only and the order parameter direction is fixed with a lower “precision”. Consequently, we expect that *several* broken symmetry states $|i\rangle$ (of the whole system) could have some significant “overlap” with $|\text{ord}\rangle$.

Let us examine the case of the U(1) symmetry breaking. The symmetry-breaking ground state may be represented by a coherent state. The explicit expression (38) can be also written as

$$|\phi\rangle = e^{-\frac{\phi_s}{2}} \prod_{\mathbf{r}} \left[\exp \left(\frac{\sqrt{\rho_s} e^{i\phi}}{\sqrt{N}} \psi^\dagger(\mathbf{r}) \right) |\text{vac}\rangle_{\mathbf{r}} \right]. \quad (60)$$

This shows that the coherent state is a product state.

Fixing the spin configurations on the line amounts to taking the partial trace of the ground-state density matrix $|\Psi\rangle\langle\Psi|$ over the spin variables *outside* the line, and then projecting on the fixed spin configuration on the line. As we argued earlier, the finite-size symmetric ground state $|\Psi\rangle$ may be written as a superposition of almost independent symmetry-breaking (coherent) states as in Eq. (42). We thus first write the reduced density matrix of the line:

$$\rho_{\text{line}} = \frac{1}{Q} \sum_{i,j=1}^Q \text{Tr}_{\text{line}}(|i\rangle\langle j|), \quad (61)$$

where the trace is performed over the degrees of freedom lying outside the line. Because the exterior of the line is a large subsystem ($\sim N$ sites) it seems clear that no state $|e\rangle$ outside the line can achieve a significant overlap simultaneously with $|i\rangle$ and $|j\rangle$ if $i \neq j$. Furthermore, since the coherent state is a product state, the partial trace can be carried out to obtain

$$\rho_{\text{line}} \sim \frac{1}{Q} \sum_{j=1}^Q \left| \phi = \frac{2\pi j}{Q} \right\rangle_{\text{line}} \rho_{\text{line}} \left\langle \phi = \frac{2\pi j}{Q} \right|, \quad (62)$$

where $|\phi\rangle_{\text{line}}$ is a coherent state defined on the line. However, an evaluation of the overlap between the coherent states on the line similar to Eq. (39) reveals that they are independent only if the angle parameters differ by $O(1/\sqrt{L})$ or more. Thus, in

terms of the (almost) independent coherent states on the line,

$$\rho_{\text{line}} \sim \frac{1}{\tilde{Q}} \sum_{j=1}^{\tilde{Q}} \left| \phi = \frac{2\pi j}{\tilde{Q}} \right\rangle_{\text{line}} \rho_{\text{line}} \left\langle \phi = \frac{2\pi j}{\tilde{Q}} \right|, \quad (63)$$

where $\tilde{Q} = \mathcal{O}(\sqrt{L})$ and the overall factor is determined by the condition $\text{Tr}_{\text{line}} \rho_{\text{line}} = 1$.

Thus we find

$$p_{\max}^{\text{line}} \simeq \frac{1}{\tilde{Q}} p_{\max}^{\text{line,osc}} \quad (64)$$

or, equivalently,

$$-\ln(p_{\max}^{\text{line}}) \simeq -\ln(p_{\max}^{\text{line,osc}}) + \frac{1}{2} \ln(L). \quad (65)$$

Similar arguments can be constructed for the SU(2) case, leading to a $\ln(L)$ term. More generally, we may conjecture that the result only depends on the number of Goldstone modes:

$$-\ln(p_{\max}^{\text{line}}) \simeq -\ln(p_{\max}^{\text{line,osc}}) + \frac{N_{\text{NG}}}{2} \ln(L). \quad (66)$$

C. Final result and comparison with the numerics

As just done for the whole system, we can combine the oscillator contribution [i.e., no $\ln L$ term, see Eq. (59)], the TOS contribution [Eq. (66)] and the argument of Sec. IV to get the n dependence. The final result for the SRE is

$$S_{n>1}^{\text{line}} \sim \frac{N_{\text{NG}}}{2} \frac{n}{n-1} \ln(L). \quad (67)$$

For $n = \infty$, Luitz *et al.* [22] found the coefficient of $\ln(L)$ to be $\gtrsim 0.7$ for a system with $N_{\text{NG}} = 2$ (to be compared to 1 from the formula above). In a more recent work [25], the QMC calculations were pushed up to $L = 40$ for $n = 2, 3, 4$, up to $L = 128$ for $n = \infty$ and up to $L = 30$ for noninteger values n . In all cases, the QMC results are in good agreement with Eq. (67).

VI. p_{\max} FOR THE 2D SPIN- $\frac{1}{2}$ XY MODEL ON THE SQUARE LATTICE

In order to provide some additional check for our predictions concerning p_{\max} , we consider the ferromagnetic XY model on the square lattice:

$$H = - \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y), \quad (68)$$

which spontaneously breaks the U(1) symmetry in the thermodynamic limit ($N_{\text{NG}} = 1$). The ground state $|\psi\rangle$ in the $S_{\text{tot}}^z = 0$ sector was obtained numerically using 2D DMRG [42] (using the C++ ITENSOR library [43]) on cylinders of length L_x and circumference L_y , up to $L_y = 12$. The probability p_{\max} is defined by projection onto the state where all spins point in the (say) x direction:

$$p_{\max} = |\langle |\psi\rangle \rightarrow \cdots \rightarrow \rangle|^2. \quad (69)$$

Once $|\psi\rangle$ is in a matrix-product form (as produced by the DMRG algorithm), p_{\max} is easily obtained by computing the scalar product with the ferromagnetic configuration above (a product state). The numerical results are given in Table II

TABLE II. DMRG results for p_{\max} in the 2D XY ferromagnet. L_x is the length of the cylinder, and L_y is the perimeter. E is the ground-state energy. Due to the area-law scaling of the entanglement entropy, χ should grow exponentially with L_y to ensure an accurate description of the wave function. The last column provides the largest truncation error measured during the last DMRG sweep.

L_x	L_y	E	$-\ln(p_{\max})$	χ	sweeps	error
4	4	-8.0167741	1.864172	256	17	0
6	4	-12.4272461	2.285488	800	15	5.96×10^{-14}
8	4	-16.8429370	2.675768	800	16	2.44×10^{-13}
10	4	-21.2608268	3.049265	800	16	7.944×10^{-13}
12	4	-25.6798523	3.412229	100	20	3.753×10^{-13}
6	6	-18.4620013	2.701232	1000	33	1.17×10^{-9}
8	6	-25.0549930	3.155927	1000	29	1.83×10^{-9}
10	6	-31.6501154	3.594168	1000	26	2.85×10^{-9}
12	6	-38.2463365	4.021994	2000	41	1.65×10^{-10}
14	6	-44.8431957	4.442731	2600	30	6.43×10^{-11}
16	6	-51.4404602	4.858276	2600	36	9.10×10^{-11}
24	6	-77.8315765	6.488096	2600	31	2.32×10^{-10}
4	8	-15.7729479	2.570953	3000	22	5.33×10^{-9}
8	8	-33.3327539	3.674920	3000	50	4.47×10^{-9}
9	8	-37.7249437	3.936932	3000	41	5.07×10^{-9}
10	8	-42.1174937	4.195792	3000	33	5.91×10^{-9}
11	8	-46.5103127	4.452070	4000	50	2.04×10^{-9}
12	8	-50.9033297	4.706283	4000	50	2.36×10^{-9}
13	8	-55.2965038	4.958716	4500	40	1.73×10^{-9}
14	8	-59.6898005	5.209670	4500	50	1.98×10^{-9}
15	8	-64.0831974	5.459323	4800	50	1.73×10^{-9}
16	8	-68.4766749	5.707869	4800	50	1.93×10^{-9}
20	8	-86.0511590	6.693276	4800	50	3.00×10^{-9}
24	8	-103.626222	7.668465	4800	50	3.92×10^{-9}
4	10	-19.6833386	2.921201	4000	38	9.21×10^{-8}
5	10	-25.1667352	3.252921	4000	46	6.61×10^{-8}
7	10	-36.1399647	3.891643	4000	50	6.70×10^{-8}
8	10	-41.6279980	4.202464	4000	49	6.83×10^{-8}
9	10	-47.1165448	4.509336	4000	50	7.40×10^{-8}
10	10	-52.60545201	4.813080	4000	50	8.13×10^{-8}
11	10	-58.0946827	5.114146	5000	45	4.60×10^{-8}
12	10	-63.5840956	5.413127	6000	40	2.90×10^{-8}
13	10	-69.0736369	5.710448	6000	45	3.12×10^{-8}
14	10	-74.5633010	6.006292	6000	46	3.40×10^{-8}
4	12	-23.5988117	3.268168	6000	45	3.64×10^{-7}
5	12	-30.1784875	3.644283	6000	50	2.88×10^{-7}
6	12	-36.7611498	4.012780	6000	50	2.81×10^{-7}
7	12	-43.3450519	4.374877	5000	50	4.34×10^{-7}
8	12	-49.9299175	4.732248	5000	42	4.36×10^{-7}
9	12	-56.5153082	5.085815	5000	50	4.56×10^{-7}
10	12	-63.1010587	5.436351	5000	50	4.85×10^{-7}
11	12	-69.6874332	5.784312	6000	37	3.28×10^{-7}
12	12	-76.2736890	6.130302	6000	34	3.47×10^{-7}

and plotted in Fig. 2. The matrix dimensions (up to $\chi = 6000$) were chosen to ensure that the maximum truncation error stays below 10^{-7} for $L_y < 12$ and below 5×10^{-7} for $L_y = 12$. This insures a precision of at least four digits on p_{\max} for the largest systems.

We now discuss the theoretical prediction for p_{\max} in the cylinder geometry. First, the TOS contribution is expected to be independent of the geometry and should therefore be [single

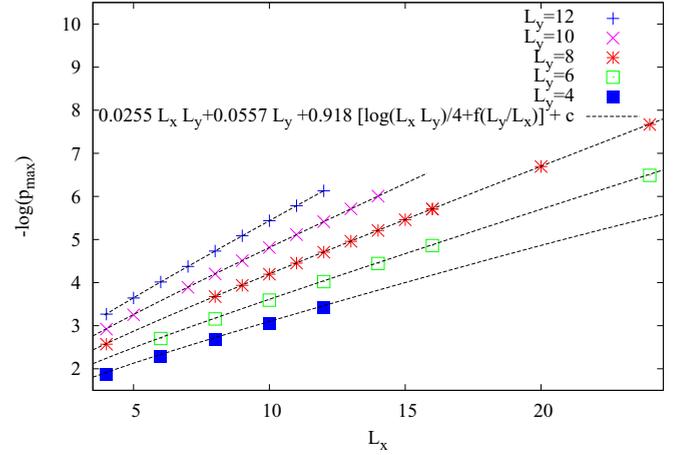


FIG. 2. DMRG results for p_{\max} in the 2D XY ferromagnet (data given in Table II). The fitting function (fit restricted to the data points with $L_{x,y} \geq 10$, see text) is shown with dashed lines. The prefactor of the logarithm term, here 0.918/4 is in good agreement with the theoretical prediction for a single Nambu-Goldstone mode (1/4). The aspect ratio-dependent term $f_N(L_y/L_x)$, defined in Eq. (78), contains no free parameter.

Nambu-Goldstone mode, see Eq. (45)]:

$$-\ln(p_{\max}^{\text{TOS}}) = \frac{1}{2} \ln N, \quad (70)$$

where $N = L_x L_y$. As for the torus, the oscillator contribution to $-\ln(p_{\max})$ has a nonuniversal const. $\times N$ term, and some universal part related to the determinant of the Laplacian:

$$-\ln(p_{\max}^{\text{osc}}) \sim -\frac{1}{4} \ln \det' \Delta. \quad (71)$$

The leading universal part is a $\ln(N)$ term related to the Euler characteristics χ [see Eq. (13)]. From the fact that $\chi = 0$ on cylinder, we have $\ln \det' \Delta \sim \ln(N)$. Adding the TOS contribution, one gets

$$-\ln(p_{\max}^{\text{osc+TOS,cyl.}}) \sim \frac{1}{4} \ln(N). \quad (72)$$

In practice, the accessible system sizes are not large enough to extract from $-\ln(p_{\max})$ the coefficient of the $\ln(N)$ directly and reliably. To analyze the finite-size data of Table II, it is therefore interesting and useful to look also for the next subleading term in $\ln \det' \Delta$. The latter is finite in the thermodynamic limit, and it depends in some universal manner on the aspect ratio $r = L_y/L_x$ of the cylinder. Such terms are well known in the context of partition functions in 2D conformal field theory, since the determinant of the Laplacian is related to the (noncompact) free-boson partition function (see Eq. (10.16) in Ref. [29]):

$$Z_{\text{free boson}} = \sqrt{\frac{A}{\det' \Delta}}, \quad (73)$$

where A is the area (here $A = N = L_x L_y$).

In our case, we have a cylinder with free spins at the boundaries. This translates to some free boundary conditions (BC) for the oscillators, and such conditions are expected to flow (in the renormalization group sense) to some Neumann BC for the free field. So, we need to compute the determinant of the Laplacian on a cylinder with Neumann BC. This quantity can be computed using zeta-regularization [28], as detailed in

Appendix A. The result is

$$\det' \Delta = Ar \left| \eta \left(\frac{ir}{2} \right) \right|^2, \quad (74)$$

where η is the Dedekind η -function. Plugging this result in Eq. (71) gives

$$-\ln(p_{\max}^{\text{osc.cyl.}}) \sim -\frac{1}{4} \ln(N) - \frac{1}{2} \ln \left[\sqrt{r} \eta \left(\frac{ir}{2} \right) \right]. \quad (75)$$

We finally add the TOS contribution to get

$$-\ln(p_{\max}^{\text{osc+TOS.cyl.}}) \sim \frac{1}{4} \ln(N) - \frac{1}{2} \ln \left[\sqrt{\frac{L_y}{L_x}} \eta \left(\frac{iL_y}{2L_x} \right) \right]. \quad (76)$$

So, we analyzed the data with the following fitting function:

$$-\ln(p_{\max}) \simeq aL_x L_y + bL_y + c + d \left[\ln(L_x L_y)/4 + f_N \left(\frac{L_y}{L_x} \right) \right] \quad (77)$$

$$\text{with } f_N(r) = -\frac{1}{2} \ln \left[\sqrt{r} \eta \left(\frac{ir}{2} \right) \right], \quad (78)$$

and a , b , c , and d are four free parameters. From our theoretical analysis [Eq. (76)], d corresponds to the number of Nambu-Goldstone mode(s) and should be close to 1. The result of the fits is shown in Fig. 2. The dashed lines represent a fit to the data points with $L_{x,y} \geq 10$, and gives $d = 0.918$. We note that, although only the largest system sizes were used in the fit, the function defined in Eq. (77) goes through all the data points with a relatively good accuracy, including the small systems. We also mention that the parameter d we have obtained is relatively stable: we find $d \simeq 0.906$ if we restrict the fit to the cylinders with $L_{x,y} \geq 8$, $d \simeq 0.899$ if we restrict to $L_{x,y} \geq 6$, and $d \simeq 0.915$ if we used all the data (including $L_{x,y}$ as small as 4). Although we have not performed a precise analysis of the error bar, our experience with varying the number of data points included in the fit indicates that the data we described well by $N_{\text{GN}} \simeq d = 0.9(1)$.

To check further the validity of this analysis, we have fitted the data by the function above, but imposing $d = 1$. This leaves three free parameters: the area coefficient a , the linear coefficient b , and a constant c . We have plotted in Fig. 3 the difference between the numerical data and $aL_x L_y + bL_y + \ln(L_x L_y)/4 + c$. These variations, plotted as a function of the aspect ratio $r = L_y/L_x$, appear to be very well described by $f_N(r)$, as expected if there is an underlying free boson system with Neumann boundary conditions. The agreement between the data and f_N is quite good, given the fact the plot contains only three adjustable parameters.

VII. CONCLUSION

We have shown theoretically that a spontaneously broken continuous symmetry leads to some universal logarithmic contribution to the Shannon-Rényi entropies. By connecting the Shannon-Rényi entropy due to Nambu-Goldstone mode

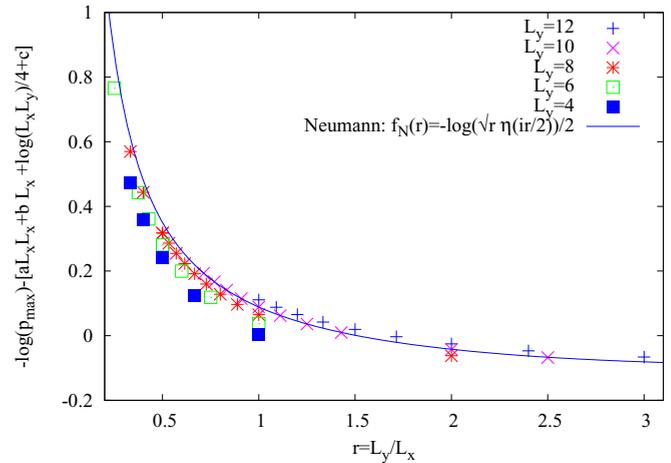


FIG. 3. The DMRG results (Table II and Fig. 2) are fitted to $g(L_x, L_y) = aL_x L_y + bL_y + c + \ln(L_x L_y)/4 + f_N(L_y/L_x)$ (three adjustable parameters: a , b , and c). As for Fig. 2, the fit was restricted to the data points with $L_{x,y} \geq 10$. The plot represents the difference between the data and $aL_x L_y + bL_y + c + \ln(L_x L_y)/4$, as a function of the cylinder aspect-ratio $r = L_y/L_x$. This difference is well described by the aspect-ratio-dependent term $f_N(L_y/L_x)$ [Eq. (78)] that is predicted for Neumann boundary conditions at the edges of the cylinder.

fluctuations with the determinant of the Laplacian, we also showed that the logarithmic contribution to the Shannon-Rényi entropy is topological and depends on the Euler-Poincaré characteristics of the two-dimensional system. As the ground state of a finite-size system is symmetric while the choice of the basis selects a particular symmetry-broken state, there is an additional logarithmic contribution to the Shannon-Rényi entropy corresponding to the ground-state degeneracy. Combining the two contributions together, the universal logarithmic term in the Shannon-Rényi entropy we find is in a good agreement with the numerical result obtained by the Toulouse group. We have also extended our analysis to the Shannon-Rényi entropy defined with respect to a line subsystem.

The situation turns out to be remarkably similar to the logarithms found in the entanglement entropy of a subsystem, where, also, the zero-point motion of the oscillator modes and the rotational symmetry of the finite-size ground state had to be included [17]. This suggests that there is a deep connection between the entanglement and Shannon-Rényi entropies, despite the obvious differences such as partition dependence of the former and the basis dependence of the latter. In fact, the Shannon-Rényi entropy has been also discussed in the context of the entanglement entropy in systems at conformal critical points. There, the entanglement entropy in a certain class of wave functions in $D + 1$ spatial dimensions is mapped to the Shannon-Rényi entropy in a D -dimensional system [10]. On the other hand, given the similarity of the present analysis to that in Ref. [17], there might be a direct connection between the two different entropies in the same D -dimensional system. Elucidation of such a connection would be useful to advance further our understanding on both entropies.

As in the case of the entanglement entropy, our hope is that the Shannon-Rényi entropy will be useful as a diagnostic tool to characterize and classify quantum phases, in particular

those beyond the traditional classification scheme. Our efforts in the present paper is limited to the conventional phases with a spontaneous broken continuous symmetry, which are already understood very well. Nevertheless, the fact that we can extract the number of the Nambu-Goldstone modes from the scaling of the Shannon-Rényi entropy suggests that this could be a novel tool as useful as the entanglement entropy. In order to extend the application of the Shannon-Rényi entropy to less conventional phases, it would be important to develop a new numerical scheme as well as analytical methods, since many of interesting phases arise in the presence of frustration which often makes quantum Monte Carlo simulations difficult.

A relatively straightforward extension of the present work would be to study the effects of sharp corners in the system geometry, which would also contribute to the logarithmic divergence of the Shannon-Rényi entropy. Checking these property numerically would provide valuable tests for the arguments presented here.

The symmetry argument presented in Sec. IV suggests that the value $n = 1$ of the Rényi index corresponds to a phase transition point, with a quite different predicted behavior of the SRE [Eq. (50)]. Numerical verification of our prediction would be an interesting problem. Further elucidation of this phase transition, and exploration into the $n < 1$ phase also seems an interesting direction of research, both from the analytical and numerical point of views.

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APPENDIX A: LAPLACIAN DETERMINANT ON CYLINDER WITH NEUMANN B.C.

We consider a cylinder of length L_x and circumference L_y . In presence of Neumann B.C. at both ends, the eigenmodes and eigenvalues of the Laplacian are

$$\phi_{n,m}(x,y) = \exp\left(2i\pi m \frac{y}{L_y}\right) \cos\left(\pi n \frac{x}{L_x}\right), \quad (A1)$$

$$\begin{aligned} \lambda_{n,m} &= -\left(\frac{2\pi m}{L_y}\right)^2 + \left(\frac{\pi n}{L_x}\right)^2 \\ &= -\left(\frac{2\pi}{L_y}\right)^2 |m + \tau n|^2, \quad \tau = \frac{iL_y}{2L_x}, \end{aligned} \quad (A2)$$

where $n = 0, 1, \dots, \infty$ and $m \in \mathbb{Z}$. This spectrum, with the zero mode omitted, is used to define a generalized zeta function:

$$Z(s) = \sum_{\substack{n \geq 0, m \in \mathbb{Z}, \\ (n,m) \neq (0,0)}} \frac{1}{|\lambda_{n,m}|^s}, \quad (A3)$$

The sum is convergent for $\text{Re}(s) > 1$ and its analytical continuation to $s = 0$ provides a (zeta) regularization for the logarithm of the determinant:

$$Z'(0) = - \sum_{\substack{n \geq 0, m \in \mathbb{Z}, \\ (n,m) \neq (0,0)}} \ln |\lambda_{n,m}| = - \ln \det' \Delta, \quad (A4)$$

To compute $Z(s)$, we introduce another function

$$G(s) = \sum_{\substack{n, m \in \mathbb{Z}, \\ (n,m) \neq (0,0)}} \frac{1}{|n + \tau m|^{2s}}, \quad (A5)$$

such that

$$Z(s) = \frac{1}{2} \left(\frac{L_y}{2\pi}\right)^{2s} (G(s) + 2\zeta(2s)) \quad (A6)$$

and

$$Z'(0) = \ln\left(\frac{L_y}{2\pi}\right) (G(0) + 2\zeta(0)) + \frac{1}{2} (G'(0) + 4\zeta'(0)) \quad (A7)$$

($\zeta(s) = \sum_{n>0} n^{-s}$ is the Riemann zeta function). The analytic continuation of $G(s)$ to $s = 0$ is a standard result (see, for instance, Eq. (4.4) of Ref. [28]):

$$G(0) = -1, \quad (A8)$$

$$G'(0) = - \ln((2\pi)^2 |\eta(\tau)|^4). \quad (A9)$$

As for ζ , we have $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\frac{1}{2} \ln(2\pi)$. Plugging these results into Eq. (A7), we get

$$\begin{aligned} Z'(0) &= -2 \ln\left(\frac{L_y}{2\pi}\right) - \frac{1}{2} (\ln((2\pi)^2 |\eta(\tau)|^4) + 2 \ln(2\pi)) \\ &= - \ln(L_y^2 |\eta(\tau)|^2). \end{aligned} \quad (A10)$$

$$\quad (A11)$$

We finally obtain

$$\ln \det' \Delta_{\text{cyl.}} = \ln(L_y^2 |\eta(\tau)|^2) \quad (A12)$$

$$= \ln(L_x L_y) + \ln\left(\frac{L_y}{L_x} \left| \eta\left(\frac{iL_y}{2L_x}\right) \right|^2\right), \quad (A13)$$

as announced in Eq. (74). Note that the $\ln(L_x L_y)$ term in the equation above corresponds to that of Eq. (13) (with $\chi = 0$).

APPENDIX B: TORUS CASE

For completeness, we also mention that the method above applies directly to the case of the torus. In that case, the result reads [28]

$$\ln \det' \Delta_{\text{torus}} = \ln(L_x L_y) + \ln\left(\frac{L_y}{L_x} \left| \eta\left(\frac{iL_y}{2L_x}\right) \right|^4\right).$$

In terms of p_{\max} , it gives (per Nambu-Goldstone mode)

$$-\ln(p_{\max}^{\text{osc,torus}}) = \text{const.} \times N - \frac{1}{4} \ln(N) - \frac{1}{2} \ln \left[\sqrt{\frac{L_y}{L_x}} \left| \eta \left(\frac{iL_y}{2L_x} \right) \right|^2 \right].$$

We finally add the TOS contribution to get

$$-\ln(p_{\max}^{\text{osc+TOS,torus}}) = \text{const.} \times N + \frac{1}{4} \ln(N) - \frac{1}{2} \ln \left[\sqrt{\frac{L_y}{L_x}} \left| \eta \left(\frac{iL_y}{2L_x} \right) \right|^2 \right].$$

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