

Finite-size scaling at quantum transitions

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We develop the finite-size scaling (FSS) theory at quantum transitions. We consider various boundary conditions, such as open and periodic boundary conditions, and characterize the corrections to the leading FSS behavior. Using renormalization-group (RG) theory, we generalize the classical scaling ansatz to describe FSS in the quantum case, classifying the different sources of scaling corrections. We identify nonanalytic corrections due to irrelevant (bulk and boundary) RG perturbations and analytic contributions due to regular backgrounds and analytic expansions of the nonlinear scaling fields. To check the general predictions, we consider the quantum XY chain in a transverse field. For this model exact or numerically accurate results can be obtained by exploiting its fermionic quadratic representation. We study the FSS of several observables, such as the free energy, the energy differences between low-energy levels, correlation functions of the order parameter, etc., confirming the general predictions in all cases. Moreover, we consider bipartite entanglement entropies, which are characterized by the presence of additional scaling corrections, as predicted by conformal field theory.

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I. INTRODUCTION

Finite-size effects in critical phenomena have been the object of theoretical studies for a long time [1–5]. Finite-size scaling (FSS) describes the critical behavior around a critical point, when the correlation length ξ of the critical modes becomes comparable to the size L of the system. For large sizes, this regime presents universal features, shared by all systems whose transition belongs to the same universality class. Although formulated in the classical framework, FSS also holds at zero-temperature quantum transitions [6], in which the critical behavior is driven by quantum fluctuations.

The FSS approach is one of the most effective techniques for the numerical determination of the critical quantities. While infinite-volume methods require that the condition $\xi \ll L$ is satisfied, FSS applies to the less demanding regime $\xi \sim L$. More precisely, FSS theory provides the asymptotic scaling behavior when both $L, \xi \rightarrow \infty$ keeping their ratio ξ/L fixed. However, knowledge of the asymptotic behavior may not be enough to estimate the critical parameters, because data are generally available for limited ranges of parameter values and system sizes, which are often relatively small. Under these conditions, the asymptotic FSS predictions are affected by sizable scaling corrections. Thus, reliably accurate estimates of the critical parameters need a robust control of the corrections to the asymptotic behavior. This is also important for a conclusive identification of the universality class of the quantum critical behavior when it is *a priori* uncertain.

An understanding of the finite-size effects is also relevant for experiments, when relatively small systems are considered (see, e.g., Ref. [7]), or in particle systems trapped by external (usually harmonic) forces, as in recent cold-atom experiments (see, e.g., Refs. [8–12]).

In this paper we study FSS at quantum transitions [13]. For this purpose, the renormalization-group (RG) approach [3,4,14] to FSS at classical transitions (generally driven by thermal fluctuations) is generalized to quantum transitions driven by quantum fluctuations. This allows us to characterize the corrections to the asymptotic FSS behavior. We predict nonanalytic scaling corrections due to the irrelevant

RG perturbations and analytic contributions which are due to regular backgrounds and to the expansions of the nonlinear scaling fields in terms of the Hamiltonian parameters.

To verify the RG predictions, we consider the quantum XY chain in a transverse field, which represents a standard theoretical laboratory for the understanding of quantum transitions. Its Hamiltonian can be rewritten as a quadratic Hamiltonian of spinless fermions [15,16]. Using this representation, several quantities can be computed either exactly or very precisely by numerical methods. This allows us to check the FSS predictions for the scaling corrections of several observables. We consider the free energy, the energy differences between the lowest-energy levels, and the correlation functions of the order parameter, confirming the RG results in all cases.

Finally, we discuss the FSS behavior of bipartite entanglement entropies in one-dimensional systems with an isolated critical point with $z = 1$. We perform a detailed study in the XY model, verifying the presence of further peculiar corrections related to conical singularities in conformal field theory [17,18], besides those associated with the usual bulk and boundary RG irrelevant perturbations.

The paper is organized as follows. In Sec. II we discuss the general RG approach to the study of FSS at quantum transitions, considering, in particular, the case of isolated quantum critical points between different quantum phases. In Sec. III we present a thorough FSS analysis of the quantum XY chain in a transverse field at the Ising transition, checking the general asymptotic FSS predictions for several physically interesting quantities. Section IV is devoted to a FSS analysis of the bipartite entanglement entropy at the quantum transition of the quantum XY chain, focusing again on the nature of the scaling corrections. Finally, in Sec. V we summarize our main results and draw some conclusions. Two appendices report some formulas which are used in the paper.

II. FINITE-SIZE SCALING AT A QUANTUM TRANSITION

In this section we summarize the main RG ideas behind FSS, providing the framework to analyze critical finite-size

effects in continuous quantum transitions. As their classical counterparts, they are characterized by a diverging length scale ξ and show universal scaling properties, which can be analyzed in the framework of RG theory. Guided by the quantum-to-classical mapping, we generalize Wegner's scaling ansatz [3,4,14,19] to quantum systems, and then use it to predict the type of subleading corrections that are expected in finite systems and/or at finite T , close to a continuous transition. We will consider different types of boundary conditions, focusing mainly on periodic or antiperiodic boundary conditions (PBC and ABC, respectively) and on open boundary conditions (OBC).

We consider the standard case in which the quantum zero-temperature transition of a d -dimensional system is characterized by two relevant parameters μ and h , defined so that they vanish at the critical point. Therefore, the quantum critical point is at

$$T = 0, \quad \mu = 0, \quad h = 0. \quad (1)$$

We assume the presence of a paritylike \mathbb{Z}_2 symmetry, as it occurs, for instance, in Ising or $O(N)$ transitions which separate a paramagnetic phase with $\mu > 0$ from a ferromagnetic phase with $\mu < 0$. The parameter μ is coupled to a RG perturbation that is invariant under the symmetry, while h is associated with the leading odd perturbation, generally related to the order parameter of the transition. As usual, we express the RG dimensions of the perturbations associated with μ and h in terms of the critical exponents ν and η , as [13]

$$y_\mu \equiv \frac{1}{\nu}, \quad y_h \equiv \frac{1}{2}(d + z + 2 - \eta), \quad (2)$$

where z is the dynamic critical exponent associated with time and temperature. At the critical point the low-energy scales vanish: The gap Δ behaves as $\Delta \sim |\mu|^{z\nu}$ at $T = 0$ and $h = 0$. The length scale ξ associated with the critical modes diverges as $\xi \sim |\mu|^{-\nu}$ at $T = 0$ and $h = 0$, and as $\xi \sim T^{-1/z}$ at $\mu = 0$ and $h = 0$.

A. Scaling law of the free energy

Under the quantum-to-classical mapping, the inverse temperature corresponds to the system size in an imaginary time direction. Thus, the temperature scaling at a quantum critical point in d dimensions is analogous to FSS in a corresponding $d + 1$ classical system. If $z = 1$, which holds for transitions described by two-dimensional (2D) conformal field theories (CFTs) [20] and for paramagnetic-ferromagnetic transitions in d -dimensional $O(N)$ symmetric spin systems [21] (Ising systems correspond to $N = 1$), the quantum transition corresponds to a classical $(d + 1)$ -dimensional equilibrium transition, in which $1/T$ plays the role of an additional spatial dimension. There are also interesting cases in which $z \neq 1$. For instance, superfluid-to-vacuum and Mott transitions of lattice particle systems described by the Hubbard and Bose-Hubbard models have $z = 2$ when driven by the chemical potential [13]. In this case, the classical system is strongly anisotropic since $L \rightarrow \lambda L$, $1/T \rightarrow \lambda^z/T$ under a RG rescaling. Also for this class of transitions, which include many dynamic off-equilibrium transitions [22], FSS is quite well established. We can, therefore, extend those results to the quantum case.

According to RG, close to a continuous transition the free energy satisfies a general scaling law. Extending the classical FSS ansatz [3,4,6,14,19,23], we generally write the free-energy density as

$$F(L, T, \mu, h) = F_{\text{reg}}(L, T, \mu, h^2) + F_{\text{sing}}(u_l, u_t, u_\mu, u_h, \{v_i\}, \{\tilde{v}_i\}), \quad (3)$$

where F_{reg} is a nonuniversal function, which is analytic at the critical point (it must also be even with respect to the parameter h related to the odd perturbation), and F_{sing} bears the nonanalyticity of the critical behavior and its universal features. The arguments of F_{sing} are the so-called nonlinear scaling fields [14]. They are analytic nonlinear functions of the model parameters, which are associated with the eigenoperators that diagonalize the RG flow close to the RG fixed point.

1. Nonlinear scaling fields

The scaling fields u_μ and u_h are the relevant scaling fields related to the model parameters μ and h . The scaling fields u_l and u_t are also relevant, with RG dimensions

$$y_l = 1, \quad y_t = z, \quad (4)$$

respectively, and are associated with the finite spatial size L ($u_l \sim 1/L$) and with the temperature ($u_t \sim T$).

Besides the relevant scaling fields, we should also consider an infinite number of irrelevant scaling fields with negative RG dimensions. We distinguish them into two families, the bulk scaling fields $\{v_i\}$ and the surface scaling fields $\{\tilde{v}_i\}$, with RG dimensions y_i and \tilde{y}_i , respectively. The first set is the only one that occurs in the infinite-volume limit and whenever there are no boundaries in the system, for instance, for PBC or ABC. They are responsible for the scaling corrections to the leading critical behavior in the infinite-volume limit. Using standard notation, assuming that they are ordered so that $|y_1| \leq |y_2| \leq \dots$, we set

$$\omega = -y_1. \quad (5)$$

In the presence of a surface, an additional set of boundary RG perturbations should be included. Their RG dimensions depend on the type of boundary conditions and, in particular, on the type of surface critical behavior one is considering. We set

$$\omega_s = -\tilde{y}_1, \quad (6)$$

where \tilde{y}_1 is the dimension of the leading boundary operator.

To go further we must discuss how the nonlinear scaling fields depend on the control parameters μ , h , L , and T . First, it is natural to assume that the bulk scaling fields u_μ , u_h , and v_i do not depend on the temperature and the size of the system, i.e., they do not mix with $1/L$ and T . This hypothesis is quite natural for systems with short-range interactions. Under a RG transformation, the transformed bulk couplings only depend on the local Hamiltonian, hence they are independent of the boundary. Taking into account the assumed \mathbb{Z}_2 symmetry and the even/odd properties of μ/h , close to the critical point the relevant scaling fields u_μ and u_h can be generally

expanded as

$$u_\mu = \mu + b_\mu \mu^2 + O(\mu^3, h^2 \mu), \quad (7)$$

$$u_h = h + b_h \mu h + O(h^3, \mu^2 h), \quad (8)$$

where b_μ and b_h are nonuniversal constants. As for the irrelevant scaling fields, they are usually nonvanishing at the critical point.

The scaling fields u_l and u_t are associated with the size of the $(d+1)$ -dimensional system. For classical systems in a box of size L^d with PBC or ABC and, more generally, for translation-invariant boundary conditions, it is usually assumed that $u_l = 1/L$, exactly. This assumption, which has been verified in many instances—for instance, in the two-dimensional Ising model—and extensively discussed in Ref. [19], can be justified as follows. Consider a lattice system and a decimation transformation which reduces the number of lattice sites by a factor 2^d . In the absence of boundaries and for short-range interactions, the new (translation-invariant) couplings are only functions of the couplings of the original lattice and are independent of L , while $L \rightarrow L/2$. Since the flow of L is independent of the flow of the couplings, we expect

$$u_l = L^{-1} \quad (9)$$

for PBC or ABC. This condition does not generally hold for nontranslation-invariant systems. We thus assume that u_l is an arbitrary function of $1/L$. For $L \rightarrow \infty$ it can be expanded as

$$u_l = L^{-1} + bL^{-2} + \dots \quad (10)$$

Note that, if we define an effective size

$$L_e = L - b, \quad (11)$$

the scaling field becomes

$$u_l = 1/L_e + O(L_e^{-3}). \quad (12)$$

Hence, by using L_e , all subleading corrections due to b/L^2 are eliminated in *any* observable. Of course, this does not imply that $1/L$ corrections are absent in *any* observable, as such type of corrections may have other origins (we will come back to this point in Sec. III F). Such an observable-independent shift is often considered in FSS studies of systems with boundary conditions that differ from the periodic ones (see, e.g., Refs. [24–26]), which also provide some evidence of the presence of L^{-2}, L^{-3} corrections in the scaling field u_l .

Let us now consider the thermal scaling field u_t . To clarify the issue, let us first assume that $z = 1$, so that the quantum system is equivalent to a classical $(d+1)$ -dimensional system. The classical system is, however, weakly anisotropic: Couplings in the thermal direction differ from those in the spatial one. Moreover, the anisotropy depends on the model parameters. In classical weakly anisotropic systems, universality is obtained only after transforming them to an isotropic system by means of a scale transformation (see Refs. [27,28], and references therein). Therefore, we define

$$u_t = \frac{T}{c(\mu, h)} \approx \frac{T}{c_0} [1 + b_t \mu + O(\mu^2, h^2)], \quad (13)$$

where $c(\mu, h)$ is an appropriate nonuniversal function, $c_0 \equiv c(0, 0)$, and b_t is a constant. The function c may be identified

with the speed of sound. More precisely, if $E(\mathbf{k})$ is the dispersion relation of the model, which is assumed to be spatially isotropic, we define $c = |\nabla_{\mathbf{k}} E|_{k_{\min}}$, where k_{\min} is the value of k where the energy has an absolute minimum. Relation (13) is expected to hold also when $z \neq 1$, although in this case the rescaling factor is not related to the sound velocity.

2. Asymptotic expansion of the singular free energy

The singular part of the free energy (3) is expected to satisfy the scaling equation

$$F_{\text{sing}}(u_l, u_t, u_\mu, u_h, \{v_i\}, \{\tilde{v}_i\}) = \lambda^{-(d+z)} F_{\text{sing}}(\lambda u_l, \lambda^z u_t, \lambda^{y_\mu} u_\mu, \lambda^{y_h} u_h, \{\lambda^{y_i} v_i\}, \{\lambda^{\tilde{y}_i} \tilde{v}_i\}), \quad (14)$$

where λ is arbitrary. In the FSS case it is useful to take $\lambda = 1/u_l$, obtaining

$$F_{\text{sing}} = u_l^{d+z} \mathcal{F} \left[\frac{u_t}{u_l^z}, \frac{u_\mu}{u_l^{y_\mu}}, \frac{u_h}{u_l^{y_h}}, \left\{ \frac{v_i}{u_l^{y_i}} \right\}, \left\{ \frac{\tilde{v}_i}{u_l^{\tilde{y}_i}} \right\} \right]. \quad (15)$$

The scaling variables $v_i u_l^{-y_i}$ and $\tilde{v}_i u_l^{-\tilde{y}_i}$, corresponding to the irrelevant scaling fields, vanish for $L \rightarrow \infty$ since y_i and \tilde{y}_i are negative. Thus, provided that F_{sing} is finite and nonvanishing in this limit, we can expand the singular part of the free energy as

$$F_{\text{sing}} \approx u_l^{d+z} \mathcal{F}_0(u_t/u_l^z, u_\mu/u_l^{y_\mu}, u_h/u_l^{y_h}) + v_1 u_l^{d+z+\omega} \mathcal{F}_\omega(u_t/u_l^z, u_\mu/u_l^{y_\mu}, u_h/u_l^{y_h}) + \dots + \tilde{v}_1 u_l^{d+z+\omega_s} \mathcal{F}_s(u_t/u_l^z, u_\mu/u_l^{y_\mu}, u_h/u_l^{y_h}) + \dots, \quad (16)$$

where we retain only the contributions of the dominant (least) irrelevant bulk and surface scaling fields, of RG dimensions $-\omega$ and $-\omega_s$, respectively. Note that expansion (16) is only possible below the upper critical dimension [29]. Above it, F_{sing} is singular and cannot be expanded as in Eq. (16). The breakdown of this expansion causes a breakdown of the hyperscaling relations and allows us to obtain the mean-field exponents.

As usual, we introduce the scaling variables

$$w \equiv \mu L^{1/\nu}, \quad \kappa \equiv h L^{y_h}, \quad \tau \equiv \frac{1}{c_0} T L^z, \quad (17)$$

and

$$w_e \equiv \mu L_e^{1/\nu}, \quad \kappa_e \equiv h L_e^{y_h}, \quad \tau_e \equiv \frac{1}{c_0} T L_e^z, \quad (18)$$

where L_e is defined in Eq. (11). Then, we have

$$\begin{aligned} \frac{u_\mu}{u_l^{y_\mu}} &\approx w \left(1 - \frac{b_1}{\nu} \frac{1}{L} \right) + \frac{b_\mu}{L^{1/\nu}} w^2 \approx w_e + \frac{b_\mu}{L^{1/\nu}} w_e^2, \\ \frac{u_h}{u_l^{y_h}} &\approx \kappa \left(1 - y_h b_1 \frac{1}{L} \right) + \frac{b_h}{L^{1/\nu}} w \kappa \approx \kappa_e + \frac{b_h}{L^{1/\nu}} \kappa_e w_e, \\ \frac{u_t}{u_l^z} &\approx \tau \left(1 - z b_1 \frac{1}{L} \right) + \frac{b_t}{L^{1/\nu}} \tau w \approx \tau_e + \frac{b_t}{L^{1/\nu}} \tau_e w_e, \end{aligned} \quad (19)$$

where we have included the leading scaling correction. If $\nu < 1$ and w , κ , and τ are used as FSS variables, the leading

correction is of order $1/L$. If instead, one uses w_e , κ_e , and τ_e , the leading correction decreases faster, as $L^{-1/\nu}$.

3. The regular part of the free energy

Finally, we should also take into account the regular part F_{reg} of the free energy [see Eq. (3)]. For classical systems, in the absence of boundaries, e.g., for PBC or ABC, F_{reg} is assumed to be independent of L , or, more plausibly, to depend on L only through exponentially small corrections [3,4,19]. We extend this conjecture to the quantum case. Since PBC or ABC are always taken in the thermal direction, it is natural to assume that F_{reg} does not depend on the size $1/T$ of the thermal direction: F_{reg} does not depend on temperature. Instead, we see no reason why F_{reg} should not depend on L for generic spatial boundary conditions. Therefore, we assume a regular expansion in powers of $1/L$ such as

$$F_{\text{reg}}(L, \mu, h^2) = F_{\text{reg},0}(\mu, h^2) + \frac{1}{L} F_{\text{reg},1}(\mu, h^2) + \dots, \quad (20)$$

where $F_{\text{reg},0}(\mu, h^2)$ is the bulk contribution, the only one present when PBC or ABC are considered in the spatial direction.

4. Universality

An important question concerns the universality of the function \mathcal{F} related to the singular part of the free energy [cf. Eq. (15)]. Since scaling fields are arbitrarily normalized, universality holds apart from a normalization of each argument and an overall constant. Therefore, given two different models, if \mathcal{F}_1 and \mathcal{F}_2 are the corresponding scaling functions, we have

$$\mathcal{F}_1(x_1, x_2, x_3, \{y_i\}, \{\tilde{y}_i\}) = A \mathcal{F}_2(c_1 x_1, c_2 x_2, c_3 x_3, \{d_i y_i\}, \{\tilde{d}_i \tilde{y}_i\}), \quad (21)$$

where all constants A , c_i , d_i , and \tilde{d}_i are nonuniversal.

The universality properties of \mathcal{F} imply analogous relations for \mathcal{F}_0 , \mathcal{F}_ω , and \mathcal{F}_s , entering its asymptotic expansion (16), which are expected to be universal, apart from multiplicative normalizations and normalizations of the scaling fields. This implies that, within the given universality class, they are independent of the microscopic features of the model. However, they depend on the nature of the boundary conditions. Note also the presence of the variable u_t/u_t^z , which corresponds to the so-called shape factor in classical transitions: The universal scaling functions depend on the shape of the finite system that is considered.

5. Summary

Expansions (16), (19), and (20) allow us to compute all scaling corrections. Collecting all terms and using L_e as basic length scale, we can write

$$\begin{aligned} F(L, T, \mu, h) = & F_{\text{reg},0}(\mu, h^2) + L_e^{-(d+z)} \mathcal{F}_0(\tau_e, w_e, \kappa_e) \\ & + v_1 L_e^{-(d+z+\omega)} \mathcal{F}_\omega(\tau_e, w_e, \kappa_e) \\ & + \tilde{v}_1 L_e^{-(d+z+\omega_s)} \mathcal{F}_s(\tau_e, w_e, \kappa_e) \\ & + \frac{1}{L} F_{\text{reg},1}(\mu, h^2) + \frac{1}{L^2} F_{\text{reg},2}(\mu, h^2) + \dots, \end{aligned} \quad (22)$$

where v_1 and \tilde{v}_1 are computed at the critical point. The missing corrections are of order (relative to the leading singular term $L_e^{-(d+z)}$) $L_e^{-1/\nu}$, $L_e^{-|y_2|}$, $L_e^{-|\tilde{y}_2|}$ (they are due to the singular part of the free energy), and of order L^{d+z-3} (they are due to the regular part of the free energy). The last three terms appearing in Eq. (22) represent boundary contributions, hence they should not be present for PBC or ABC. Moreover, in this case we also have $L_e = L$. Finally, note that, since the corrections of order $L_e^{-1/\nu}$ are due to the expansion of the scaling fields, they are always proportional to w [see Eq. (19)], thus they vanish for $\mu = 0$.

To summarize, the RG expansion (22) provides information on the corrections to the asymptotic behavior. There are several different sources of scaling corrections:

(i) The irrelevant RG perturbations which generally give rise to $O(L^{-\omega})$ corrections, where ω is a universal exponent associated with the leading irrelevant RG perturbation.

(ii) Corrections arising from the expansion of the scaling fields u_μ , u_h , and u_t in terms of the Hamiltonian parameters. They give rise to corrections of order $L^{-1/\nu}$ and are absent for $\mu = 0$.

(iii) Corrections arising from the analytic background term of the free energy.

(iv) The irrelevant RG perturbations associated with the boundary conditions, which are of order $L^{-\omega_s}$. They are absent in the absence of boundaries, such as PBC or ABC.

(v) The $O(1/L)$ boundary corrections arising from the nontrivial analytic L dependence of the scaling field u_t , Eq. (10). They are absent in the absence of boundaries. The leading correction can be taken into account by simply redefining the length scale L , i.e., by using L_e instead of L [cf. Eq. (11)].

Equations (15) and (16) give the generic scaling form of the free-energy density. However, in certain cases the behavior is more complex due to the appearance of logarithmic terms [14]. They may be due to the presence of marginal RG perturbations, as happens in Berezinskii-Kosterlitz-Thouless transitions in U(1)-symmetric systems [30–33], or to resonances between the RG eigenvalues, as occurs in transitions belonging to the 2D Ising universality class [14,34] or to the three-dimensional $O(N)$ -vector universality class in the large- N limit [26,35]. We should also mention that peculiar FSS behaviors—for instance, a modulation of the leading amplitudes—are observed in quantum particle systems at fixed chemical potential when an infinite number of level crossings occurs as the system size varies, and in the so-called XX chain in a transverse external field [36–38].

Several interesting quantities can be obtained by taking derivatives of the free energy. For example, in particle systems whose relevant parameter μ is a linear function of the chemical potential, the FSS of the particle density is obtained by differentiating Eq. (22) with respect to μ , i.e., $\rho \sim \partial F / \partial \mu$. Therefore, for $h = 0$, we obtain

$$\rho = \rho_{\text{reg}}(\mu) + \frac{1}{L} \rho_{\text{reg},1}(\mu) + \dots + L_e^{-(d+z-y_\mu)} \mathcal{D}(w_e, \tau_e) + \dots \quad (23)$$

We note that the regular term represents the leading term when $d + z - y_\mu > 0$, which is the case for most physically

interesting systems. The compressibility can be obtained by taking an additional derivative with respect to μ .

B. Scaling law in the infinite-volume limit

We can also write down general scaling laws for the quantum critical behavior in the infinite-volume limit. We start again from Eq. (14), setting in this case $u_l = 0$ and $\lambda = u_t^{-1/z}$. The free-energy density scales as

$$F = F_{\text{reg}}(\mu, h^2) + u_t^{d/z+1} \mathcal{F}(u_\mu u_t^{-y_\mu/z}, u_h u_t^{-y_h/z}, \{v_i u_t^{-y_i/z}\}), \quad (24)$$

where, as explained above, we assume that $F_{\text{reg}}(\mu, h^2)$ is T independent. For $h = 0$ and $u_t \rightarrow 0$, we can expand the free energy as

$$F \approx u_t^{d/z+1} \mathcal{A}(u_\mu u_t^{-1/(zv)}) + u_t^{d/z+1+\omega/z} v_1 \mathcal{A}_\omega(u_\mu u_t^{-1/(zv)}) + F_{\text{reg}}(\mu, 0) + \dots \quad (25)$$

The specific heat is obtained by differentiating the previous expression:

$$C_V \equiv T \frac{\partial^2 F}{\partial T^2} = \frac{u_t^{d/z}}{c} [\mathcal{C}(u_\mu u_t^{-1/(zv)}) + u_t^{\omega/z} \mathcal{C}_\omega(u_\mu u_t^{-1/(zv)}) + \dots]. \quad (26)$$

Notice that there are no contributions from the regular part of the free energy. At the critical point $\mu = 0$, Eq. (26) predicts

$$C_V \sim T^{d/z} [1 + O(T^{\omega/z})]. \quad (27)$$

C. FSS of the low-energy scales

The singular part of the free energy is essentially determined by the behavior of the low-energy levels at the quantum transition. Therefore, the low-energy scales, and in particular the energy difference Δ of the lowest-energy levels, should show an analogous asymptotic behavior, besides the leading term [13] $\Delta \sim L^{-z}$. Thus, at $T = 0$ and $h = 0$, they are expected to show the asymptotic FSS behavior

$$c(\mu)\Delta(L, \mu) = L_e^{-z} [\mathcal{D}(w_e) + v_1 L_e^{-\omega} \mathcal{D}_\omega(w_e) + \tilde{v}_1 L_e^{-\omega_s} \mathcal{D}_s(w_e) + \dots], \quad (28)$$

where c is the function providing the relation of u_t with T [cf. Eq. (13)]. Such a factor is needed to take into account that energies are expressed in terms of the temperature T , while the right-hand side contains the spatial dimension L_e . The neglected corrections are of order $L^{-2}, L^{-1/\nu}, L^{-|y_2|}, L^{-|\tilde{y}_2|}$. The scaling functions $\mathcal{D}_\#$ are universal, apart from multiplicative factors and a normalization of their argument. For $w_e \rightarrow \infty$, $\mathcal{D}(w) \sim w^{z\nu}$ to ensure $\Delta \sim \mu^{z\nu}$ for $\mu > 0$ (paramagnetic phase) in the infinite-volume limit.

D. FSS of the two-point correlation function

We now consider the correlation functions of the order-parameter field $\phi(\mathbf{x}, t)$, for example, the equal-time two-point function,

$$G(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}, t) \phi(\mathbf{y}, t) \rangle. \quad (29)$$

For vanishing magnetic field, the leading scaling behavior is given by

$$G(\mathbf{x}, \mathbf{y}; T, \mu, L) \approx u_l^{d+z-2+\eta} \mathcal{G}(u_l \mathbf{x}, u_l \mathbf{y}; u_t/u_l^z, u_\mu/u_l^{y_\mu}). \quad (30)$$

Equation (30) is only valid for $L \rightarrow \infty$, $|\mathbf{x} - \mathbf{y}| \rightarrow \infty$ with $|\mathbf{x} - \mathbf{y}|/L$ fixed. Instead, if one takes the limit at fixed $|\mathbf{x} - \mathbf{y}|$, no singular behavior is observed in the FSS limit. Corrections to Eq. (30) arise from two different sources. First of all, there are the corrections due to the scaling fields with negative RG dimensions. Moreover, there are corrections which we will call *field-mixing* terms. Indeed, the order-parameter field ϕ is in general a linear combination,

$$\phi = \sum_{i=1} a_i \mathcal{O}_{h,i}, \quad (31)$$

of the odd fixed-point operators $\mathcal{O}_{h,i}$, which satisfy

$$\langle \mathcal{O}_{h,i}(\mathbf{r}) \mathcal{O}_{h,j}(\mathbf{s}) \rangle \sim |\mathbf{r} - \mathbf{s}|^{-d_i-d_j} \quad (32)$$

at the critical point, where the associated dimensions d_i (we assume here $d_1 < d_2 < d_3 \dots$) are related to the RG dimensions $y_{h,i}$ of the odd (leading and subleading) RG operators by $d_i = d + z - y_{h,i}$. The leading odd operator $\mathcal{O}_h \equiv \mathcal{O}_{h1}$ is associated with the leading nonlinear scaling field of RG dimension y_h given in Eq. (2). Equation (30) represents the contribution of the leading operator \mathcal{O}_h since

$$d + z - y_h = \frac{1}{2}(d + z - 2 + \eta). \quad (33)$$

Furthermore, we should also consider the contributions of all subleading operators that have the same symmetry properties of the order parameter. Hence, we end up with the expansion

$$G(\mathbf{x}, \mathbf{y}; T, \mu, L) \approx \sum_{jk} u_l^{2(d+z)-y_{hj}-y_{hk}} \mathcal{G}_{jk}(u_l \mathbf{x}, u_l \mathbf{y}; u_t/u_l^z, u_\mu/u_l^{y_\mu}, \{v_i u_l^{-y_i}\}, \{\tilde{v}_i u_l^{-\tilde{y}_i}\}). \quad (34)$$

In the case of OBC, also boundary operators should be considered.

Let us consider the space integral of the correlation function (29), defined as

$$\chi_{\mathbf{y}} \equiv \sum_{\mathbf{x}} G(\mathbf{y}, \mathbf{x}). \quad (35)$$

In the case of PBC or ABC, since translation invariance holds, $\chi_{\mathbf{y}}$ is independent of \mathbf{y} . In the presence of a boundary, this is no longer the case. As long as \mathbf{y} is fixed in the FSS limit, the leading scaling behavior is always the same, while scaling corrections are expected to depend on \mathbf{y} . The asymptotic FSS expansion of $\chi_{\mathbf{y}}$ for $h = 0$ and $T = 0$ is expected to be

$$\chi_{\mathbf{y}}(\mu, L) = L^{2-z-\eta} [\mathcal{X}(w) + L^{-\omega} \mathcal{X}_\omega(w) + L^{-1} \mathcal{X}_{s1}(w) + L^{-\omega_s} \mathcal{X}_{s2}(w) + L^{-1/\nu} \mathcal{X}_\mu(w) + L^{y_{h2}-y_h} \mathcal{X}_h(w) + \dots] + B_\chi(\mu, L), \quad (36)$$

where w is defined in Eq. (17), the scaling functions $\mathcal{X}_\#$ are universal apart from multiplicative factors and a normalization of the argument, and y_{h2} is the RG dimension of the next-to-leading operator which is odd under $h \rightarrow -h$ (this term is due to the field mixing). The corrections of order $L^{-1/\nu}$ arise from the expansion (7) of the scaling field u_μ . Finally, B_χ is an

analytic background term which represents the contribution to the integral of points \mathbf{x} such that $|\mathbf{x} - \mathbf{y}| \ll L$. It is the analog of the analytic part of the free energy [see Eq. (3)]. Therefore, the leading scaling corrections for χ scale as $L^{-\zeta}$ with

$$\zeta = \min[\omega, 1, \omega_s, 1/\nu, 2 - z - \eta, y_h - y_{h2}]. \quad (37)$$

It is important to note that χ_y should not be confused with the magnetic susceptibility, which is a macroscopic quantity obtained by differentiating the free energy with respect to the magnetic field.

One can also consider a correlation length ξ associated with the critical modes. Since ξ has RG dimension 1, in the FSS limit we obtain an expansion analogous to Eq. (36), i.e.,

$$\begin{aligned} \xi(\mu, L) = & L[\mathcal{Y}(w) + L^{-\omega}\mathcal{Y}_\omega(w) + L^{-1}\mathcal{Y}_{s1}(w) \\ & + L^{-\omega_s}\mathcal{Y}_{s2}(w) + L^{-1/\nu}\mathcal{Y}_u(w) \\ & + L^{y_{h2}-y_h}\mathcal{Y}_h(w) + \dots] + B_\xi(\mu, L). \end{aligned} \quad (38)$$

Here $B_\xi(\mu, L)$ is a background term depending on the explicit definition of the correlation length. For example, we may define a second-moment correlation length by using the two-point function (29), as

$$\xi^2 = \frac{1}{2d\chi_0} \sum_{\mathbf{x}} \mathbf{x}^2 G(\mathbf{0}, \mathbf{x}), \quad (39)$$

where the point $\mathbf{y} = 0$ is at the center of the system. In the case of PBC or ABC, one may consider the more convenient definition

$$\xi^2 \equiv \frac{1}{4 \sin^2(p_{\min}/2)} \frac{\tilde{G}(\mathbf{0}) - \tilde{G}(\mathbf{p})}{\tilde{G}(\mathbf{p})}, \quad (40)$$

where $\mathbf{p} = (p_{\min}, 0, \dots)$, $p_{\min} \equiv 2\pi/L$, and $\tilde{G}(\mathbf{p})$ is the Fourier transform of $G(\mathbf{x})$. For these definitions there are two background contributions. One contribution is due to χ_0 and scales as $L^{\eta+z-2}$. A second one is due the sum appearing in the numerator of expression (39) and scales as $L^{\eta+z-4}$. This second contribution is subleading with respect to the first one, hence

$$B_\xi(\mu, L) = L^{\eta+z-1} B_\chi(\mu, L). \quad (41)$$

We thus conclude that scaling corrections are analogous to those for χ , i.e., scale as $L^{-\zeta}$, where ζ is given in Eq. (37).

E. Dimensionless RG invariant quantities

Dimensionless RG invariant quantities are particularly useful to investigate the critical region. Examples of such quantities are the ratio

$$R_\xi \equiv \xi/L, \quad (42)$$

where ξ is any length scale related to the critical modes, for example the one defined in Eq. (39), and ratios of the correlation function G at different distances, e.g.,

$$R_g(\mathbf{X}, \mathbf{Y}) = \ln[G(\mathbf{0}, \mathbf{XL})/G(\mathbf{0}, \mathbf{YL})], \quad (43)$$

where the point $\mathbf{x} = 0$ is at the center of the system. We denote them generically by R .

According to FSS, at $T = 0$ and $h = 0$, they must behave as

$$\begin{aligned} R(\mu, L) = & \mathcal{R}(w) + L^{-1/\nu} \mathcal{R}_u(w) + L^{-\omega} \mathcal{R}_\omega(w) \\ & + L^{-1} \mathcal{R}_{s1}(w) + L^{-2} \mathcal{R}_{s2}(w) + L^{-\omega_s} \mathcal{R}_{\omega_s}(w) \\ & + L^{-(y_h - y_{h2})} \mathcal{R}_h(w) + \dots, \end{aligned} \quad (44)$$

where $w = \mu L^{1/\nu}$. Note the presence of the corrections of order L^{-1} , which are related to the fact that L is used as a normalizing length scale in Eqs. (42) and (43). One could have equally used L_e or u_l^{-1} , obtaining RG invariant quantities that have the same universal scaling behavior, but that differ by corrections of order $1/L$.

The scaling function $\mathcal{R}(w)$ is universal apart from a trivial normalization of the argument. In particular, the limit

$$\lim_{L \rightarrow \infty} R(0, L) = \mathcal{R}(0) \quad (45)$$

is universal within the given universality class, i.e., it is independent of the microscopic details of the model, although it depends on the shape of the finite volume and on the boundary conditions. Since \mathcal{R}_u arises from the next-to-leading $O(\mu^2)$ term of the expansion (7) of the scaling fields, we have $\mathcal{R}_u \sim w^2 \mathcal{R}'(w)$ (with an unknown coefficient because the expansion of the scaling field is usually unknown). Thus, this term does not contribute at $\mu = 0$. Note also that the boundary term is absent for PBC. Moreover, in the case of R_ξ with ξ defined as in Eq. (39), there is also a $L^{-2+z+\eta}$ correction due to the background B_ξ [this term is absent in the case of R_g as defined in Eq. (43)].

A popular method [5,39] to determine the critical point uses the finite-size behavior of R as a function of L and μ . Indeed, if

$$\lim_{\mu \rightarrow 0^-} \lim_{L \rightarrow \infty} R(\mu, L) > \lim_{L \rightarrow \infty} R(0, L) > \lim_{\mu \rightarrow 0^+} \lim_{L \rightarrow \infty} R(\mu, L) \quad (46)$$

or vice versa, one can define μ_{cross} by requiring

$$R(\mu_{\text{cross}}, L) = R(\mu_{\text{cross}}, 2L). \quad (47)$$

The crossing point μ_{cross} converges to $\mu = 0$ with corrections of order $L^{-1/\nu-\zeta}$. Here $\zeta = \min[\omega, 1, \omega_s, (y_h - y_{h2})]$ for generic boundary conditions breaking translation invariance and $\zeta = \min[\omega, (y_h - y_{h2})]$ for PBC. In the presence of backgrounds, we should also include the background corrections. For instance, in the case of R_ξ [cf. Eq. (42)], we have

$$\zeta = \min[\omega, 1, \omega_s, 2 - z - \eta, y_h - y_{h2}]. \quad (48)$$

III. FSS IN THE QUANTUM XY CHAIN

A. The 1D XY model

The quantum XY chain in a transverse field is a standard theoretical laboratory for quantum transitions. In the case of OBC, its Hamiltonian is

$$\begin{aligned} H_{\text{OBC}}(J, g) = & - \sum_{x=-L/2+1}^{L/2-1} \mathcal{H}_{x, x+1} - g \sum_{x=-L/2+1}^{L/2} \sigma_x^{(3)}, \\ \mathcal{H}_{x, x+1} = & \frac{J}{2} [(1 + \gamma) \sigma_x^{(1)} \sigma_{x+1}^{(1)} + (1 - \gamma) \sigma_x^{(2)} \sigma_{x+1}^{(2)}], \end{aligned} \quad (49)$$

where $\sigma^{(i)}$ are the Pauli matrices. In the case of PBC and ABC, respectively, we have

$$H_{\text{PBC/ABC}}(J, g) = H_{\text{OBC}}(J, g) \pm \mathcal{H}_{-L/2+1, L/2}, \quad (50)$$

where the upper sign refers to PBC and the lower one to ABC. It is not restrictive to set $J = 1$. We always take L even, setting the origin at the center of the domain, more precisely at one of the two central sites, so that $-L/2 + 1 \leq x \leq L/2$. For $\gamma = 0$ we recover the so-called XX chain in a transverse external field.

For any $\gamma \neq 0$ the model undergoes a quantum transition at

$$\mu \equiv g - 1 = 0, \quad (51)$$

separating a quantum paramagnetic phase for $\mu > 0$ from a quantum ferromagnetic phase for $\mu < 0$. The transition belongs to the 2D Ising universality class, hence its critical behavior is associated with a 2D CFT with central charge $c = 1/2$. The critical exponents take the values $z = 1$, $\nu = 1$, and $\eta = 1/4$. The structure of the subleading corrections for Ising systems was discussed in Refs. [34,40–42]. In particular, Reinicke [42] analyzed the subleading corrections for the XY chain at the critical point. If the finite system is translation invariant—this is the case of PBC—the most relevant subleading operators have RG dimension -2 . They belong to the identity family and can be expressed by using the Virasoro generators [43,44] as $Q_2^I \bar{Q}_2^I$ and $Q_4^I + \bar{Q}_4^I$, where $Q_2 = L_{-2}|I\rangle$, $Q_4 = (L_{-2} - \frac{3}{5}L_{-4})|I\rangle$. The analysis of Ref. [42] shows that the spin-zero operator $Q_2^I \bar{Q}_2^I$ (which can be related to the energy-momentum tensor) is absent, as also occurs in the classical 2D Ising model [34]. The second (spin-four) operator gives rise instead to scaling corrections that are proportional to $3/4 - \gamma^2$. The primary field associated with the energy family controls the off-critical behavior. The corresponding scaling field is $u_\mu \sim \mu/\gamma$ [41,45].

According to the analysis of Ref. [34], the next subleading operator ($Q_4^\epsilon + \bar{Q}_4^\epsilon$ in their notations) gives correction of order L^{-3} . Such an operator is odd under duality transformations, which also hold for the XY model to some extent, as we discuss below. Hence, we expect it to contribute only at quadratic order (hence it gives corrections of order L^{-6}), as occurs in the 2D Ising model [34]. If this term is absent, the next-to-leading correction is related to the leading spin-six operator in the identity family, which has RG dimension -4 .

The quantum XY Hamiltonian can be mapped onto a quadratic Hamiltonian of spinless fermions by a Jordan-Wigner transformation [15,16], which can be straightforwardly diagonalized. One obtains [16]

$$H = \sum_k E(k) \left(a_k^\dagger a_k - \frac{1}{2} \right), \quad (52)$$

where a_k^\dagger and a_k are fermionic creation-annihilation operators and

$$E(k) = 2[g^2 + \gamma^2 - 2g \cos k + (1 - \gamma^2) \cos^2 k]^{1/2}. \quad (53)$$

The set of values of k which must be summed over and the allowed states depend on the boundary conditions [15,16,46,47].

In the limit $T \rightarrow 0$, the relevant modes are those with the lowest energy, i.e., those with $k \approx 0$. For $k \rightarrow 0$, the energy

$E(k)$ can be expanded as

$$E(k)^2 = c(\mu, \gamma)^2 [u_\mu(\mu, \gamma)^2 + k^2 + v_1(\mu, \gamma)k^4 + O(k^6)], \quad (54)$$

where

$$c(\mu, \gamma) = 2\sqrt{\gamma^2 + \mu}, \quad (55)$$

$$u_\mu(\mu, \gamma) = \frac{\mu}{\sqrt{\gamma^2 + \mu}}, \quad (56)$$

$$v_1(\mu, \gamma) = \frac{3 - 4\gamma^2 - \mu}{12(\gamma^2 + \mu)}. \quad (57)$$

As we shall see, $u_\mu(\mu, \gamma)$ and $v_1(\mu, \gamma)$ play the role of the nonlinear scaling fields associated with μ and with the leading irrelevant operator. Note that

$$v_1(0, \gamma) = 0 \quad \text{for } \gamma = \gamma_i = \sqrt{3}/2. \quad (58)$$

Therefore, provided that $v_1(\mu, \gamma)$ is the correct scaling field, no corrections of order $L^{-\omega} = L^{-2}$ due to the leading bulk irrelevant operator are expected for the particular value $\gamma = \gamma_i$ in any observable (note, however, that corrections of order $L^{-\omega-1}$ do not cancel out). The identification of u_μ and v_1 as scaling fields is in full agreement with the CFT results of Refs. [41,42], but it goes beyond that, since it specifies the expression of the scaling field also away from the critical point, i.e., for $\mu \neq 0$.

B. Duality in the XY model

Duality transformations play an important role in Ising systems, hence it is important to discuss duality in the XY model [48,49]. An exact transformation can be defined for the model with $\gamma = 1$. In this case, one should consider slightly modified Hamiltonians with OBC. One can consider [49]

$$H_{d1}(J, g) = -J \sum_{x=-L/2+1}^{L/2} \sigma_x^{(1)} \sigma_{x+1}^{(1)} - g \sum_{x=-L/2+1}^{L/2-1} \sigma_x^{(3)}, \quad (59)$$

which differs from Hamiltonian (49) because of the absence of the magnetic field on site $L/2$, or

$$H_{d2}(J, g) = -J \sum_{x=-L/2+1}^{L/2} \sigma_x^{(1)} \sigma_{x+1}^{(1)} - g \sum_{x=-L/2+1}^{L/2} \sigma_x^{(3)} - J \sigma_{L/2}^{(1)}, \quad (60)$$

in which there is an additional magnetic field along the x direction at site $x = L/2$. For these Hamiltonians a transformation U exists [49] such that

$$UH(J, g)U^\dagger = H(g, J) = gH(1, J/g). \quad (61)$$

It follows that there exists an exact correspondence between the energy levels for $g > 1$ and those for $g < 1$ (again we set $J = 1$). The presence of a symmetry can be guessed from the expression of $E(k)$ [see Eq. (53)]. Indeed, for $\gamma = 1$ the energy levels satisfy

$$E(k, g) = gE(k, 1/g), \quad (62)$$

where we have written explicitly the g dependence. It is important to note that exact duality holds only for Hamiltonians (59) and (60). For different types of boundary conditions, boundary terms break duality, hence there is no direct correspondence between the states with $g < 1$ and those with $g > 1$.

It is interesting to understand physically why boundary conditions break duality. This is due to the different nature of the ground states for $g > 1$ and $g < 1$. Indeed, if g is large, we expect the XY Hamiltonian to have a nondegenerate ground state with the spins aligned in the z direction. On the other hand, if g is small we expect a doubly degenerate ground state, with the spins aligned either in the x direction or in the $-x$ direction. Since the degeneracy of the ground state is different for $g > 1$ and $g < 1$, there cannot be an exact duality symmetry. In order to have exact duality, one must therefore change the model so that (at least) the degeneracy of the ground state does not depend on g . If we consider Hamiltonian (60), this condition is realized by lifting the degeneracy of the ground state for $g < 1$: The magnetic field along the x direction at site $x = L/2$ makes the ground state nondegenerate, with all spins pointing in the $+x$ direction. If we instead consider Hamiltonian (59), duality is obtained at the price of making the ground state doubly degenerate for any value of g . To show this, note that $[\sigma_{L/2}^{(1)}, H_{d1}] = 0$. Thus, the Hilbert space can be decomposed into two subspaces \mathcal{H}_\pm , such that $\sigma_{L/2}^{(1)}\psi_\pm = \pm\psi_\pm$. If we restrict H_{d1} to \mathcal{H}_+ we obtain Hamiltonian (60) for a chain of length $L - 1$. Hence, the ground state in \mathcal{H}_+ is nondegenerate for all values of g . If we restrict H_{d1} to \mathcal{H}_- we obtain $UH_{d2}U^+$, where $U = \prod_{x=-L/2+1}^{L/2-1} \sigma_x^{(3)}$, hence we obtain the same spectrum as that of H_{d1} restricted to \mathcal{H}_+ . Thus, for Hamiltonian (59) duality is obtained by making each state doubly degenerate.

Finally, let us note that a remnant of duality is also present for $\gamma \neq 1$. This guarantees that the transition always occurs at $g = 1$. Indeed, consider the transformation

$$\mu = -\frac{\mu'}{1 + \mu'/\gamma^2}. \quad (63)$$

Then, we have

$$u_\mu(\mu, \gamma) = -u_\mu(\mu', \gamma), \quad c(\mu) = \frac{4\gamma^2}{c(\mu')}, \quad (64)$$

so that, at points that only differ by the sign of u_μ , the low- k behavior of $E(k)$ is the same, apart from a change of normalization.

C. Free energy

The free energy of the quantum XY model can be directly related to the finite-size free energy of the 2D Ising model. If we consider a strip of width M , the Ising free-energy density is given by (we use K instead of β to avoid confusion with the quantum case and write $F = -Tf_{\text{Is}}$) [50,51]

$$f_{\text{Is}}(K, M) = \frac{1}{2} \ln(2 \sinh 2K) + \frac{1}{2} \int_0^{2\pi} \frac{dk}{2\pi} \epsilon(k) + \frac{1}{M} \int_0^{2\pi} \frac{dk}{2\pi} \ln[1 + e^{-M\epsilon(k)}], \quad (65)$$

where

$$\begin{aligned} \epsilon(k) &= \ln[\zeta(k) + \sqrt{\zeta(k)^2 - 1}], \\ \zeta(k) &= \cosh 2K \coth 2K - \cos k/2. \end{aligned} \quad (66)$$

For large values of M , the leading behavior of the finite-size correction term is obtained by expanding $\epsilon(k)$ for $k \rightarrow 0$, since $\epsilon(k)$ is positive and has an absolute minimum at $k = 0$. Close to the critical point $K_c = (1 + \sqrt{2})/2$, if $\delta = K_c - K > 0$ (paramagnetic phase), we obtain

$$\epsilon(k) = 4(\delta^2 + k^2/64)^{1/2}. \quad (67)$$

This expression allows us to rewrite

$$f_{\text{Is}}(K, M) = F_{\text{reg}}(K) - \frac{2\delta^2}{\pi} \ln \delta^2 + \delta^2 g_{\text{Is}}(\delta M), \quad (68)$$

where

$$\begin{aligned} F_{\text{reg}}(K) &= \frac{2G}{\pi} + \frac{\ln 2}{2} - \delta\sqrt{2} \\ &+ \frac{2}{\pi} \delta^2 (1 + \ln 2 - \pi/2) + O(\delta^2), \\ g_{\text{Is}}(x) &= \frac{4}{\pi x^2} \int_0^\infty dy \ln[1 + \exp[-4(x^2 + y^2)^{1/2}]], \end{aligned} \quad (69)$$

and G is Catalan's constant. For the XY model we obtain a similar result. Defining

$$F_{XY} = -T \ln \text{Tr} e^{-\beta H}, \quad \beta = 1/T, \quad (70)$$

we obtain [16]

$$\begin{aligned} F_{XY}(\mu, T, \gamma) &= -\frac{1}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} E(k) \\ &- \frac{1}{\beta} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \ln[1 + e^{-\beta E(k)}], \end{aligned} \quad (71)$$

where $E(k)$ is given in Eq. (53). Also in this case the large β behavior is obtained by expanding $E(k)$ around $k = 0$, i.e., by using Eq. (54). At leading order, we reobtain Eq. (68) with some different normalization constants:

$$\begin{aligned} F_{XY}(\mu, T, \gamma) &= F_{XY, \text{reg}}(\mu, \gamma) \\ &+ \frac{2a u_\mu^2}{\pi} \ln u_\mu^2 - a u_\mu^2 g_{\text{Is}}(b u_\mu / u_t), \end{aligned} \quad (72)$$

where $u_t = T/c$, c defined in Eq. (55), and

$$a = \frac{c}{16}, \quad b = \frac{1}{4}. \quad (73)$$

Note the presence of the logarithmic term, which is due to a resonance between the identity operator of RG dimension 2 and the thermal operator of RG dimension 1 [14]. In principle, logarithmic terms should appear in all observables and both at leading and at subleading order. However, extensive analyses of the 2D Ising model [19,34,52–59] have identified logarithmic corrections only in a very few cases. Note also that the regular function $F_{XY, \text{reg}}(\mu, \gamma)$ in Eq. (72) does not depend on T as conjectured in Sec. II A 3.

We wish now to compute the corrections to Eq. (72). For this purpose we set $\lambda = u_\mu/u_t$ and consider the expansion of

$$B(x, \lambda, T) = \frac{E(xu_t)}{E_c(xu_t, u_\mu)}, \quad (74)$$

where $E_c(x, u_\mu) = (x^2 + u_\mu^2)^{1/2}$, in powers of u_t , keeping x and λ fixed. We obtain

$$\frac{1}{c} B(x, \lambda, T) = 1 + B_c(x, \lambda, T) = 1 + \sum_{n=2} u_t^n B_{c,n}(x, \lambda). \quad (75)$$

Since $\beta E_c(xu_t, u_\mu) = E_c(x, \lambda)/c$ is independent of u_t and $B_c(x, \lambda, T) \sim u_t^2$, we can write

$$\begin{aligned} & \beta \int_0^\pi dk \ln(1 + e^{-\beta E(k)}) \\ &= \int_0^{\beta\pi} dx \left\{ \ln[1 + e^{-E_c(x, \lambda)}] \right. \\ & \quad \left. + \ln \left[1 - \frac{e^{-E_c(x)} E_c(x, \lambda) B_c(x, \lambda, T)}{1 + e^{-E_c(x, \lambda)}} + \dots \right] \right\}. \quad (76) \end{aligned}$$

Each term $B_{c,n}(x, \lambda)$ of Eq. (75) increases as a power of x for $x \rightarrow \infty$. Therefore, the integrand vanishes exponentially as $x \rightarrow \infty$ order by order, and we can extend the upper limit of integration to $+\infty$, making an exponentially small error. The second term in braces can then be expanded in powers of u_t , proving that the free energy admits an expansion in powers of u_t at λ fixed.

Let us now compute the first correction of order u_t^2 . Proceeding as discussed above, we obtain

$$\begin{aligned} & \beta \int_0^\pi dk \ln[1 + e^{-\beta E(k)}] \\ &= \int_0^\infty dx \ln[1 + e^{-E_c(x, \lambda)}] \\ & \quad - \frac{u_t^2}{2} v_1(\mu, \gamma) \int_0^\infty dx \frac{x^4 (x^2 + \lambda^2)^{-1/2}}{1 + \exp \sqrt{x^2 + \lambda^2}}. \quad (77) \end{aligned}$$

Note that the corrections of order u_t^2 are proportional to $v_1(\mu, \gamma)$. Hence, it is natural to identify this quantity as the scaling field associated with the leading irrelevant operator. We will confirm this conjecture in the next sections.

D. Scaling of the energy gap: Periodic and antiperiodic boundary conditions

We wish now to compute the finite-size behavior of the difference Δ between the energy of the lowest excited states and that of the ground state, extending the results of Ref. [40]. For PBC we shall show that Δ admits an expansion of the form

$$\Delta_P = \frac{c(\mu, \gamma)}{2L} \left[\Delta_{P0}(\tilde{w}) + \frac{v_1(\mu, \gamma)}{L^2} \Delta_{P2}(\tilde{w}) + O(L^{-4}) \right], \quad (78)$$

where

$$\tilde{w} = u_\mu L. \quad (79)$$

An analogous expansion holds also for ABC. Such a result confirms the identification of u_μ and v_1 as nonlinear scaling

fields. Note that, if

$$w \equiv \frac{\mu L}{\gamma} \quad (80)$$

is used as scaling variable and c is replaced by its leading behavior 2γ , then we have

$$\Delta = \frac{\gamma}{L} \left[\Delta_{P0}(w) + \frac{1}{L} \Delta_{P1}(w) + O(L^{-2}) \right]. \quad (81)$$

The corrections of order L^{-1} , which vanish at the critical point $w = 0$, are due to the expansion of the nonlinear scaling field u_μ and of the sound velocity c (in the general case, they would be of order $L^{-1/\nu}$).

To compute the energy levels, we use the results of Katsura [16]. They are obtained by using Eq. (52), with a proper identification of the allowed values of k . The energy levels can be divided in two sectors: the even one in which $k = 2m\pi/L$, $m = 0, \dots, L-1$, and the odd one in which $k = (2m+1)\pi/L$, $m = 0, \dots, L-1$. The corresponding ground-state energies are

$$\begin{aligned} \mathcal{E}_0^{\text{odd}} &= -\frac{1}{2} \sum_{m=0}^{L-1} E \left(\frac{2m+1}{L} \pi \right), \\ \mathcal{E}_0^{\text{even}} &= -\frac{1}{2} \sum_{m=0}^{L-1} E \left(\frac{2m}{L} \pi \right), \end{aligned} \quad (82)$$

where $E(k)$ is given in Eq. (53). Note that, for $\gamma \neq 0$, we have $\mathcal{E}_0^{\text{odd}} < \mathcal{E}_0^{\text{even}}$. Half of the states belong to the odd sector. They can be written as $a_{k_1}^\dagger a_{k_2}^\dagger \dots a_{k_m}^\dagger |\text{odd}\rangle$, where k_1, k_2, \dots, k_m belong to the odd sector, m is even for PBC and odd for ABC. The allowed states in the even sector can also be written as $a_{k_1}^\dagger a_{k_2}^\dagger \dots a_{k_m}^\dagger |\text{even}\rangle$, but now m depends both on the boundary conditions and on the value of g . For $g \geq 1$, m is odd (even) for PBC (ABC). For $g \leq 1$ the opposite condition holds: m is even for PBC, odd for ABC. For $g = 1$ the parity of m can be chosen arbitrarily, obtaining the same spectrum in all cases as a result of the fact that $E(0) = 0$. Therefore, for $g > 1$ and PBC, the lowest energy states are

$$\begin{aligned} E_0^P &= \mathcal{E}_0^{\text{odd}}, \\ E_1^P &= \mathcal{E}_0^{\text{even}} + E(0), \\ E_2^P &= \mathcal{E}_0^{\text{odd}} + E(\pi/L) + E(\pi - \pi/L), \end{aligned} \quad (83)$$

while for $g \leq 1$ we obtain

$$\begin{aligned} E_0^P &= \mathcal{E}_0^{\text{odd}}, \\ E_1^P &= \mathcal{E}_0^{\text{even}}, \\ E_2^P &= \mathcal{E}_0^{\text{odd}} + E(\pi/L) + E(\pi - \pi/L). \end{aligned} \quad (84)$$

For ABC we have for $g \geq 1$

$$\begin{aligned} E_0^A &= \mathcal{E}_0^{\text{even}}, \\ E_1^A &= \mathcal{E}_0^{\text{odd}} + E(\pi/L) = \mathcal{E}_0^{\text{odd}} + E(\pi - \pi/L), \\ E_2^A &= \mathcal{E}_0^{\text{even}} + E(0) + E(2\pi/L) \\ &= \mathcal{E}_0^{\text{even}} + E(0) + E(\pi - 2\pi/L), \end{aligned} \quad (85)$$

while for $g \leq 1$

$$\begin{aligned} E_0^A &= \mathcal{E}_0^{\text{even}} + E(0), \\ E_1^A &= \mathcal{E}_0^{\text{odd}} + E(\pi/L) = \mathcal{E}_0^{\text{odd}} + E(\pi - \pi/L), \\ E_2^A &= \mathcal{E}_0^{\text{even}} + E(2\pi/L) = \mathcal{E}_0^{\text{even}} + E(\pi - 2\pi/L). \end{aligned} \quad (86)$$

Note that the first two excited states are doubly degenerate. Then, Δ and $\Delta^{(2)}$, the energy gaps for the first and second excited state, respectively, are given by

$$\begin{aligned} \Delta_P &= \mathcal{E}_0^{\text{even}} - \mathcal{E}_0^{\text{odd}} + \theta(g-1)E(0), \\ \Delta_A &= \mathcal{E}_0^{\text{odd}} - \mathcal{E}_0^{\text{even}} + E(\pi/L) - \theta(1-g)E(0) \\ &= -\Delta_P + E(\pi/L) + 2(g-1), \\ \Delta_P^{(2)} &= 2E(\pi/L), \\ \Delta_A^{(2)} &= E(2\pi/L) + \theta(g-1)E(0), \end{aligned} \quad (87)$$

with $\theta(x) = 1$ for $x \geq 0$, $\theta(x) = 0$ for $x < 0$. The behavior of these quantities in the FSS limit, in which $\mu = g-1 \rightarrow 0$, $L \rightarrow \infty$ at μL fixed, was considered in Ref. [40]. We have performed the calculation again, using the general method discussed in Appendix B of Ref. [60]. We obtain

$$\begin{aligned} \frac{1}{\gamma} \mathcal{E}_0^{\text{odd}} &\approx -\frac{L}{\gamma} J + \frac{1}{L} \left[\frac{\pi}{3} - w - 4\pi G_1(w/2\pi) \right] \\ &\quad - \frac{w^2}{4\pi L} \left(\ln \frac{w^2}{16\pi^2} + 2\gamma_E - 1 \right), \end{aligned} \quad (88)$$

$$\begin{aligned} \frac{1}{\gamma} \mathcal{E}_0^{\text{even}} &\approx -\frac{L}{\gamma} J + \frac{1}{L} \left[-\frac{\pi}{6} + 4\pi G_1(w/2\pi) - 2\pi G_1(w/\pi) \right] \\ &\quad - \frac{w^2}{4\pi L} \left(\ln \frac{w^2}{\pi^2} + 2\gamma_E - 1 \right), \end{aligned} \quad (89)$$

where $w = \mu L/\gamma$, $\gamma_E \approx 0.5772157$ is Euler's constant,

$$J = \int_0^\pi \frac{dk}{2\pi} E(k), \quad (90)$$

and $G_1(x)$ is a remnant function [61]:

$$G_1(x) = \sum_{n=1}^{\infty} \left(\sqrt{n^2 + x^2} - n - \frac{x^2}{2n} \right). \quad (91)$$

For $x \rightarrow 0$, $G_1(x) \approx -x^4 \zeta(3)/8$, while for $|x| \rightarrow \infty$ we have [60]

$$\begin{aligned} G_1(x) &= \frac{1}{12} + \frac{x^2}{4} \left(-\ln \frac{x^2}{4} + 1 - 2\gamma_E \right) - \frac{|x|}{2} \\ &\quad - \frac{|x|}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} K_1(2\pi n|x|), \end{aligned} \quad (92)$$

where K_1 is a modified Bessel function. Using these results we obtain [62]

$$\begin{aligned} L\Delta_P/\gamma &\approx \Delta_{P0} \\ &= \frac{\pi}{2} + w + \frac{w^2}{\pi} \ln 2 \\ &\quad + 2\pi G_1(w/\pi) - 8\pi G_1(w/2\pi), \end{aligned} \quad (93)$$

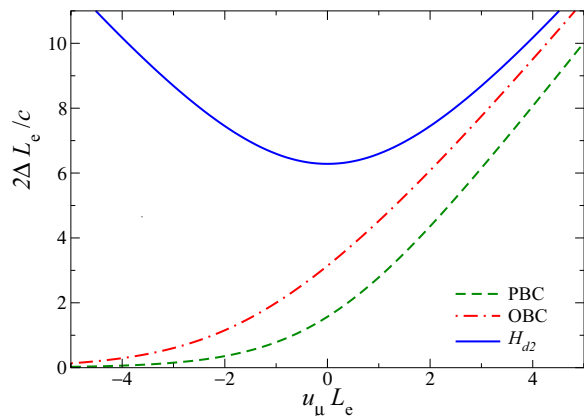


FIG. 1. (Color online) We report the energy difference Δ between the lowest energy levels. We plot $2\Delta L_e/c$ versus $\tilde{w}_e = u_\mu L_e$ in the scaling limit for PBC ($L_e = L$ for PBC), OBC, and for the self-dual Hamiltonian (60).

$$L\Delta_A/\gamma \approx \Delta_{A0} = -\Delta_{P0} + 2w + 2\sqrt{\pi^2 + w^2}. \quad (94)$$

These results are consistent with Eq. (78) since $\tilde{w} \approx w$ and $c \approx 2\gamma$ for $\mu \rightarrow 0$. The PBC curve is shown in Fig. 1. For $w \rightarrow 0$, Eqs. (93) and (94) give $\Delta_{P0}(w) = \pi/2$ and $\Delta_{A0}(w) = 3\pi/2$, in agreement with Ref. [47]. For $|w| \rightarrow \infty$, using Eq. (92) we obtain

$$\Delta_{P0} = w + |w| - 2\frac{|w|}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} [K_1(2n|w|) - 2K_1(n|w|)], \quad (95)$$

which shows that $L\Delta_P \approx 2\mu L$ for $w \rightarrow +\infty$ and $L\Delta_P \approx 0$ for $w \rightarrow -\infty$, with exponentially small corrections. In the same limit, $L\Delta_A$ behaves as $L\Delta_P$, but corrections are now of order w^{-2} .

Let us now focus on the corrections. For this purpose, in the PBC case we consider the combination

$$\widehat{\Delta}_{P2}(\tilde{w}, L, \gamma) = \frac{L^2}{v_1(0, \gamma)} \left[\frac{2L\Delta_P}{c} - \Delta_{P0}(\tilde{w}) \right]. \quad (96)$$

If Eq. (78) is correct, such a combination should converge to $\Delta_{P2}(\tilde{w})$ as $L \rightarrow \infty$ at fixed \tilde{w} . Moreover, the limiting curve should be independent of γ . The results for $\gamma = 0.4$ and 0.8 shown in Fig. 2 are in full agreement, confirming Eq. (78) at order L^{-3} . These curves are obtained by computing Δ using high-precision arithmetic for values of L in the range $10^3 \lesssim L \lesssim 10^5$ at fixed \tilde{w} . On the scale of the figures the results fall on top of each other, providing the limiting scaling curve.

To verify that the neglected corrections in Eq. (78) decay as L^{-4} , we consider the case $\gamma = \gamma_i = \sqrt{3}/2$, for which $v_1(\mu, \gamma_i) \approx -\mu/(12\gamma_i^2)$, and compute

$$\widehat{\Delta}_{P4}(\tilde{w}) = L^4 \left[\frac{2L\Delta_P}{c} - \Delta_{P0}(\tilde{w}) - \frac{\tilde{w}}{12\gamma_i L^3} \Delta_{P2}(\tilde{w}) \right]. \quad (97)$$

If corrections are of order L^{-4} , this quantity should have a finite limit as $L \rightarrow \infty$ at fixed \tilde{w} . If corrections are instead of order L^{-3} , this quantity should diverge linearly in L as $L \rightarrow \infty$. The results shown in Fig. 3 are consistent with a finite limit, and hence confirm that corrections decay as L^{-4} .

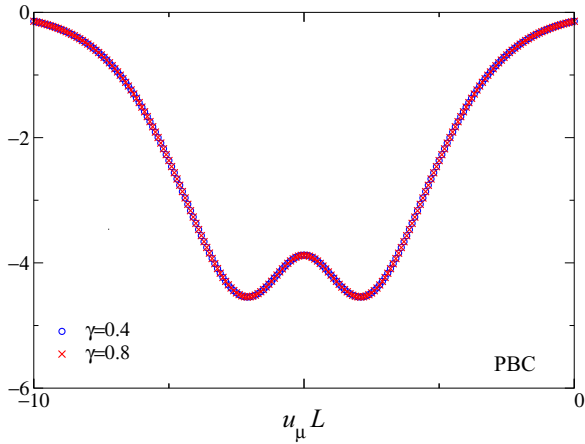


FIG. 2. (Color online) Plot of the correction $\widehat{\Delta}_{P2}$ to the lowest-energy spectral gap, as defined in Eq. (96), versus $\tilde{w} = u_\mu L$ for $\gamma = 0.4$ and 0.8 . The two sets of data appear to follow a unique curve.

E. Scaling of the energy gap: Open boundary conditions

Let us now consider the OBC case. This case is more complex than the PBC one, since we must take into account boundary irrelevant corrections and the fact that u_l is a nontrivial function of L . The latter type of corrections can be taken into account by using an effective size L_e . Boundary irrelevant operators give rise to corrections of order L^{-2} , hence $\omega_s = 2$. The latter corrections are generally expected in systems belonging to the 2D Ising universality class [63,64]. In practice, we will show that

$$\Delta = \frac{c(\mu, \gamma)}{2L_e} \left[\Delta_0(\tilde{w}_e) + \frac{1}{L^2} \Delta_2(\tilde{w}_e, \gamma) + O(L^{-3}) \right], \quad (98)$$

where

$$\tilde{w}_e = u_\mu L_e. \quad (99)$$

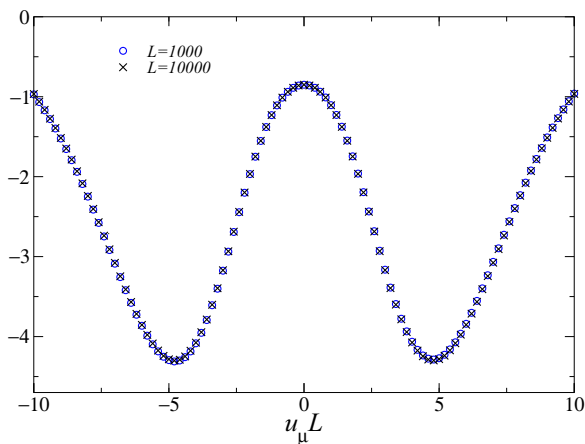


FIG. 3. (Color online) To confirm the absence of terms of order L^{-3} in the expansion (78), the combination $\widehat{\Delta}_{P4}$ defined in Eq. (97) is plotted versus \tilde{w} for two values of L , $L = 10^3$ and $L = 10^4$. The two sets of data are hardly distinguishable, showing that $\widehat{\Delta}_{P4}$ has a nontrivial finite large- L limit.

The function $\Delta_2(\tilde{w}_e, \gamma)$ is not proportional to $v_1(0, \gamma)$ (for instance, it does not vanish for $\gamma = \gamma_t = \sqrt{3}/2$), indicating the presence of boundary contributions with $\omega_s = 2$. For $\gamma = 1$ the effective length L_e is equal to $L + 1/2$. From the analysis of the numerical data, we will conjecture a general expression for L_e , valid for all values of γ (see below).

We first consider the case $\gamma = 1$, for which we can use the analytic expressions reported in Ref. [46]. The gap Δ is given by $E(k_0)$, where k_0 is the smallest (in absolute value) k that satisfies the secular equation [46]

$$\frac{\sin(L+1)k}{\sin Lk} = \frac{1}{g}. \quad (100)$$

In the scaling limit at fixed $w = \mu L/\gamma$, the solution of the secular equation depends on w . For $w > -1$, we have

$$k_0 = \frac{\delta_1}{L} + \frac{\delta_2}{L^2} + O(L^{-3}), \quad (101)$$

where δ_1 is the solution in $]0, \pi[$ of the equation

$$\delta_1 = -w \tan \delta_1, \quad (102)$$

and δ_2 is given by

$$\delta_2 = -\frac{\delta_1(\delta_1^2 + 2w^2)}{2(\delta_1^2 + w + w^2)}. \quad (103)$$

For $w < -1$, we have instead

$$k_0 = \frac{i\delta_1}{L} + \frac{i\delta_2}{L^2} + O(L^{-3}), \quad (104)$$

where δ_1 is the solution in $]0, +\infty[$ of the equation

$$\delta_1 = -w \tanh \delta_1, \quad (105)$$

and

$$\delta_2 = -\frac{\delta_1(\delta_1^2 - 2w^2)}{2(\delta_1^2 - w - w^2)}. \quad (106)$$

For $w \rightarrow +\infty$, we have $\delta_1 \approx \pi - \pi/w$ and $\delta_2 \approx -\pi + 2\pi/w$; for $w \rightarrow 0$, we have $\delta_1 \rightarrow \pi/2$ and $\delta_2 \rightarrow -\pi/4$; for $w \rightarrow -1$, δ_1 and δ_2 both vanish, while for $w \rightarrow -\infty$ we obtain $\delta_1 \approx -w[1 + O(e^{-2|w|})]$ and $\delta_2 \approx w/4$.

Using the expansion of k_0 and Eq. (54) we obtain in the limit $L \rightarrow \infty$ at w fixed

$$\frac{L^2 \Delta^2}{c^2} = \pm \delta_1^2 + w^2 \pm 2\delta_1 \delta_2 \frac{1}{L}, \quad (107)$$

where the upper signs should be used for $w > -1$ and the lower signs for $w < -1$. As in the PBC case, the gap δ_1 vanishes as $w \rightarrow -\infty$, while for $w \rightarrow +\infty$ we have $L\Delta/c \approx w$. The resulting curve is reported in Fig. 1.

To get rid of the analytic corrections, we express $L^2 \Delta^2/c^2$ as a function of \tilde{w} . Since $w = \tilde{w} + \tilde{w}^2/(2L)$, we obtain

$$\frac{L^2 \Delta^2}{c^2} = \pm \delta_1^2 + \tilde{w}^2 \mp \left(\frac{\delta_1^2(\delta_1^2 + \tilde{w})}{\delta_1^2 \pm \tilde{w}(1 + \tilde{w})} \right) \frac{1}{L}, \quad (108)$$

where δ_1 is now a function of \tilde{w} and we used

$$\frac{d\delta_1}{dw} = \frac{\delta_1}{w + w^2 \pm \delta_1^2}. \quad (109)$$

The $1/L$ correction can be eliminated by rescaling the size L . Indeed, if we define

$$L_e = L + \frac{1}{2}, \quad (110)$$

we obtain

$$\frac{L_e^2 \Delta^2}{c^2} = \pm \delta_1^2 + \tilde{w}_e^2 + O(L^{-2}), \quad (111)$$

where δ_1 is now a function of $\tilde{w}_e = u_\mu L_e$. Actually, the same rescaling (110) eliminates the $1/L$ corrections for any energy level. This result can be derived immediately if we rewrite the secular equation in terms of u_μ and L_e :

$$\frac{\tilde{w}_e}{L_e} = \frac{2 \cot(L_e k) \sin k/2}{[1 - (\sin^2 k/2)(\sin L_e k)^{-2}]^{1/2}}. \quad (112)$$

This equation is symmetric under $L_e \rightarrow -L_e$ and $k \rightarrow -k$, implying the k has an expansion in odd powers of $1/L_e$. No even powers appear, confirming the absence of corrections of order L_e^{-1} in the expansion of the gap.

The previous analysis was restricted to the first correction. It is important to stress that it is not possible to eliminate the corrections of order L^{-3} in the expansion of k_0 by redefining $L_e = L + 1/2 + a/L$, with a suitable a . Indeed, at the critical point the secular equation gives $k_0 = 2\pi/(L + 1/2)$ exactly. Therefore, for $\tilde{w} = 0$, there are no L_e^{-3} corrections only if $a = 0$. But, if we take $a = 0$, corrections are present for $\tilde{w} \neq 0$.

Let us now consider the energy gap for $\gamma \neq 1$. In the absence of analytic results, we compute the difference Δ of the two lowest energy levels numerically for $L \leq 4096$ and for $\gamma = \sqrt{3}/2, 0.8$, and 0.4 . Also for these values of γ we find that the leading scaling correction can be eliminated by using an appropriate γ -dependent L_e . An accurate numerical guess for L_e is

$$L_e = L + \frac{1}{2} + \frac{(\gamma + 2)(\gamma - 1)}{2\gamma}. \quad (113)$$

With this choice Δ has an expansion of the form

$$\frac{2L_e \Delta(\mu, L, \gamma)}{c} = \Delta_0(\tilde{w}_e) + O(L^{-2}). \quad (114)$$

We can estimate the correction term by considering

$$\hat{\Delta}_2 = \frac{4}{3} \left[\frac{2L_{e1} \Delta(\mu_1, L, \gamma)}{c(\mu_1)} - \frac{2L_{e2} \Delta(\mu_2, 2L, \gamma)}{c(\mu_2)} \right], \quad (115)$$

where L_{e1} and L_{e2} correspond to L and $2L$, respectively, and μ_1 and μ_2 are obtained by solving $u_\mu(\mu_1, \gamma)L_{e1} = \tilde{w}_e$ and $u_\mu(\mu_2, \gamma)L_{e2} = \tilde{w}_e$. The resulting quantity has a finite limit for $L \rightarrow \infty$ at fixed \tilde{w}_e , reported in Fig. 4. Note that corrections do not vanish for $\gamma_i = \sqrt{3}/2$, where $v_1(0, \gamma_i) = 0$, hence they cannot be only due to the bulk subleading operator with $\omega = 2$. Moreover, there is no rescaling that allows us to obtain a collapse of all data onto a single curve. Therefore the data show the presence of corrections due to a boundary subleading operator with exponent $\omega_s = 2$, in agreement with the RG analyses of Refs. [63,64].

Finally, it is interesting to consider the self-dual Hamiltonian (60). The secular equation turns out to be particularly simple. The allowed values of k are simply $k = \pi n/(L + 1)$, $n = 1, \dots, L$ for all values of g . Therefore, if we define

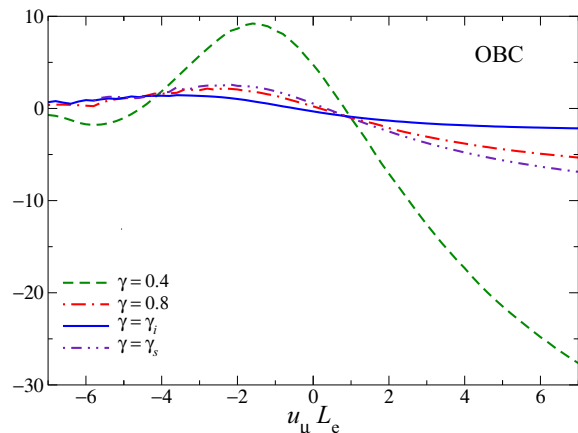


FIG. 4. (Color online) Leading correction $\hat{\Delta}_2$ defined in Eq. (115) versus $\tilde{w}_e = u_\mu L_e$ for OBC. Results for $\gamma = \gamma_i = \sqrt{3}/2$, $\gamma = 0.8, 0.4$, and $\gamma = \gamma_s = \sqrt{3} - 1$ (for $\gamma = \gamma_s$ we have $L_e = L$).

$L_e = L + 1$, we have

$$\frac{L_e^2 \Delta^2}{c^2} = \pi^2 + \tilde{w}_e^2 + \frac{\pi^4 v_1(\mu, \gamma)}{L_e^2} + O(L^{-4}). \quad (116)$$

The scaling function for $L \rightarrow \infty$ is reported in Fig. 1. Note that Δ_1 does not vanish for $\tilde{w}_e \rightarrow -\infty$, a consequence of the fact that the degeneracy for $g < 1$ is lifted by the added magnetic field. A second peculiarity of the result is the absence of boundary corrections, once length scales are expressed in terms of L_e .

F. RG invariant ratios

In Secs. III C–III E we have shown that the data for the free energy and energy gap are consistent with the assumption that u_μ and v_1 are nonlinear scaling fields. Moreover, in the case of OBC the leading boundary correction can be eliminated by redefining $L \rightarrow L_e$.

We wish now to verify these conjectures by studying different observables related to the correlation function of the order parameter $\sigma_x^{(1)}$. We consider the equal-time correlation function

$$G(x, y) = \langle \sigma_x^{(1)} \sigma_y^{(1)} \rangle, \quad (117)$$

then we define

$$\chi \equiv \sum_x G(0, x), \quad (118)$$

$$\xi^2 \equiv \frac{1}{2\chi} \sum_x x^2 G(0, x), \quad (119)$$

and the RG invariant quantities

$$R_\xi \equiv \xi/L, \quad R_g \equiv \ln[G(0, L/8)/G(0, L/4)]. \quad (120)$$

We compute R_g for PBC and OBC, for several values of L and \tilde{w} (L_e and \tilde{w}_e in the OBC case) and extrapolate the results to $L \rightarrow \infty$. The results are reported in Fig. 5. Note that in the scaling limit, all scaling variables are equivalent, i.e., $w \approx \tilde{w} \approx \tilde{w}_e$, but this is not true when considering the scaling corrections. The value of R_g at the critical point for $L \rightarrow \infty$ can be computed by using the exact expression of the two-point

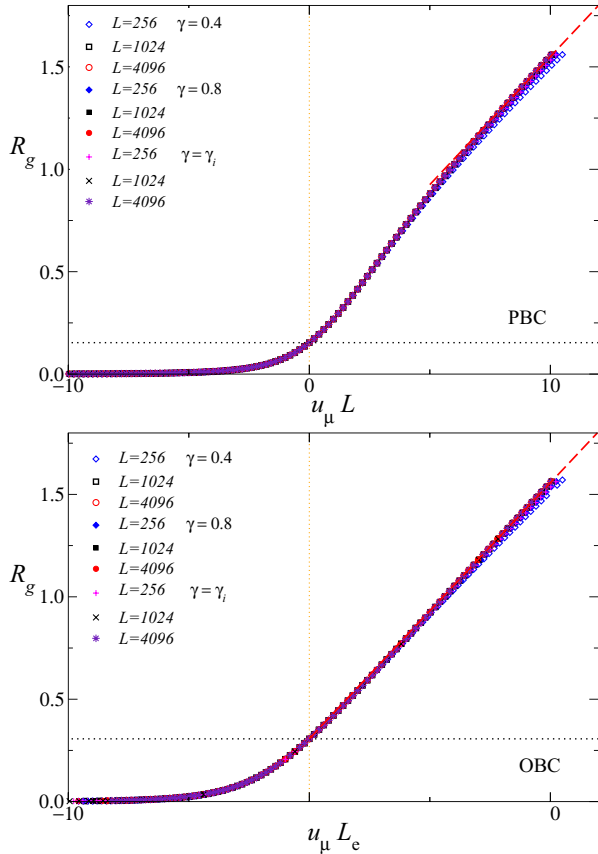


FIG. 5. (Color online) Plots of the RG invariant quantity R_g , defined in Eq. (120), versus $\tilde{w} = u_\mu L$ for PBC (top) and versus $\tilde{w}_e = u_\mu L_e$ for OBC (bottom). We report data for $\gamma = 0.4, 0.8$, and $\gamma_i = \sqrt{3}/2$. They approach a universal curve with increasing L . The horizontal dotted lines correspond to the exact value at $\mu = 0$. The dashed lines show the asymptotic behavior $R_g \approx w/8$ for $w \rightarrow \infty$.

function at the critical point in the scaling limit. The numerical values are reported in Appendix A. We can also predict the large- w behavior by using the known expression of $G(x)$ in the infinite-volume limit for $\mu > 0$. Since $G(x) \sim K_0(x\mu)$ for $\gamma = 1$ [13], where $K_0(x)$ is a modified Bessel function, we obtain $R_g \approx w/8$ for $w \rightarrow \infty$.

Let us now discuss the leading corrections in the PBC case. According to the general analysis, in the limit $L \rightarrow \infty$, $\mu \rightarrow 0$ at fixed \tilde{w} , we expect corrections of order $L^{-\omega} = L^{-2}$ due to the leading irrelevant operator and corrections due to field mixings. We will show that the latter also scale as L^{-2} , obtaining an expansion of the form

$$R_g(\mu, L, \gamma) = R_{g0}(\tilde{w}) + \frac{1}{L^2} R_{g2}(\tilde{w}, \gamma) + O(L^{-3}), \quad (121)$$

with

$$R_{g2}(\tilde{w}, \gamma) = v_1(\mu, \gamma) R_{g21}(\tilde{w}) + v_2(\mu, \gamma) R_{g22}(\tilde{w}), \quad (122)$$

where $v_1(\mu, \gamma)$ is the nonlinear scaling field reported in Eq. (57). To verify this expansion, we consider the combination

$$\begin{aligned} \widehat{R}_{g2}(\tilde{w}, L, \gamma) &= \frac{4L^2}{3} [-R_g(\tilde{w}, L) + 9R_g(\tilde{w}, 2L) \\ &\quad - 8R_g(\tilde{w}, 4L)]. \end{aligned} \quad (123)$$

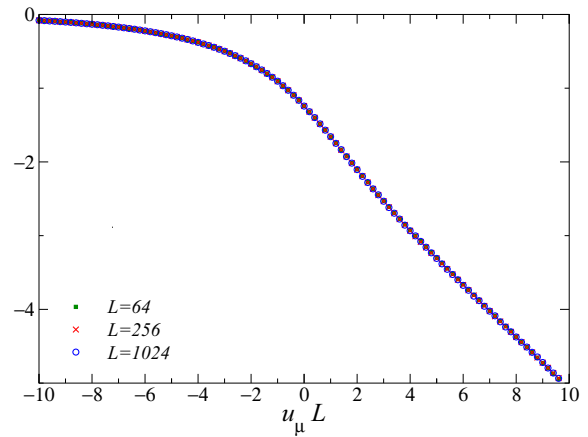


FIG. 6. (Color online) Plot of the leading correction \widehat{R}_{g2} , defined in Eq. (123), to the RG invariant quantity R_g versus $\tilde{w} = u_\mu L$ for PBC. We report data for $\gamma_i = \sqrt{3}/2$, and some values of L . Data clearly converge toward an asymptotic large- L curve.

If Eq. (121) holds, $\widehat{R}_{g2}(\tilde{w}, L, \gamma)$ converges to $R_{g2}(\tilde{w}, \gamma)$ with corrections of order L^{-2} . If instead Eq. (121) does not hold and corrections to the leading scaling behavior are of order $1/L$, $\widehat{R}_{g2}(\tilde{w}, L, \gamma)$ diverges as $L \rightarrow \infty$. In Fig. 6 we show the results for $\gamma_i = \sqrt{3}/2$ for which $v_1(0, \gamma_i) = 0$. The combination $\widehat{R}_{g2}(\tilde{w}, L, \gamma)$ has a finite limit for $L \rightarrow \infty$, confirming that the leading scaling corrections decay as $1/L^2$.

Since $v_1(0, \gamma_i) = 0$, the corrections we observe cannot be due to the operator $\mathcal{Q}_2^2 + \bar{\mathcal{Q}}_2^2$ which controls the leading scaling correction for the free energy and the spectrum. Corrections are instead a field-mixing effect. The lattice operator is a combination of conformal fields:

$$\sigma_{\text{LAT}}^{(1)} = \mathcal{O}_\sigma + \sum_{i=1} \mathcal{O}_{\sigma,i}, \quad (124)$$

where \mathcal{O}_σ is the primary CFT field and $\mathcal{O}_{\sigma,i}$ are the secondary fields that belong to the σ family, the leading one being $\mathcal{O}_{\sigma_1} = L_{-1}|\sigma\rangle$ and $y_\sigma - y_{\sigma_1} = 1$. To provide additional evidence for the validity of Eq. (121), we consider

$$\begin{aligned} \widehat{R}_{g21} &= \frac{4L^2}{3} [R_g(\mu, L, \gamma) - R_g(\mu, 2L, \gamma)] \\ &\quad - \frac{4L^2}{3} \frac{v_2(0, \gamma)}{v_2(0, \gamma_i)} [R_g(\mu, L, \gamma_i) - R_g(\mu, 2L, \gamma_i)]. \end{aligned} \quad (125)$$

If Eq. (121) holds, then

$$\widehat{R}_{g21}(\mu, L, \gamma) \approx v_1(0, \gamma) R_{g21}(\tilde{w}). \quad (126)$$

Since $v_1(\mu, \gamma)$ is known, this relation gives us a recipe to identify $v_2(0, \gamma)$. We determine $v_2(0, \gamma)$ by requiring $\widehat{R}_{g21}(\mu, L, \gamma)/v_1(0, \gamma)$ to be independent of γ . By using numerical results for $\gamma = 0.4$ and $\gamma = 0.8$, we find that this condition is satisfied by simply taking

$$v_2(0, \gamma)/v_2(0, \gamma_i) = 1. \quad (127)$$

This is shown by the data in Fig. 7. The scaling field $v_2(\mu, \gamma)$ is independent of γ for $\mu \rightarrow 0$.

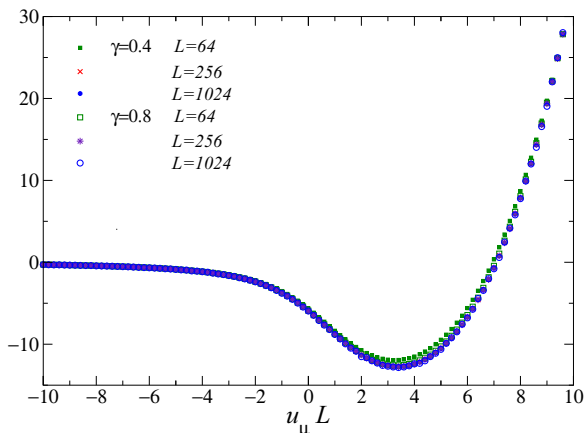


FIG. 7. (Color online) Test of Eq. (121) for PBC. The ratio $\widehat{R}_{g21}(\mu, L, \gamma)/v_1(0, \gamma)$ —the combination $\widehat{R}_{g21}(\mu, L, \gamma)$ is defined in Eq. (125)—is plotted versus $\tilde{w} = u_\mu L$. We use Eq. (127). The data for different values of γ appear to approach the same curve with increasing L .

Let us now consider the scaling corrections in the OBC case. In this case we find that scaling corrections of order $1/L$ are present even if the limit $L \rightarrow \infty$ is taken at fixed \tilde{w}_e . Indeed, the numerical data are consistent with

$$R_g(\mu, L, \gamma) = R_{g0}(\tilde{w}_e) + \frac{1}{L} R_{g1}(\tilde{w}_e, \gamma). \quad (128)$$

To estimate the $1/L$ correction, we consider

$$\widehat{R}_{g1}(L, \tilde{w}_e, \gamma) = \frac{2L}{3} [R_g(L, \tilde{w}_e) - 13R_g(2L, \tilde{w}_e) + 44R_g(4L, \tilde{w}_e) - 32R_g(8L, \tilde{w}_e)]. \quad (129)$$

For $L \rightarrow \infty$, we have

$$\widehat{R}_{g1}(L, \tilde{w}_e, \gamma) \rightarrow R_{g1}(\tilde{w}_e, \gamma) \quad (130)$$

with corrections of order L^{-3} [65]. We have computed $\widehat{R}_{g1}(L, \tilde{w}_e, \gamma)$ for $64 \leq L \leq 512$, obtaining, for all values of γ , a nonzero result. The function $\widehat{R}_{g1}(L, \tilde{w}_e, \gamma)$ for $L = 512$ (it is essentially asymptotic) is reported in Fig. 8. Note that it has

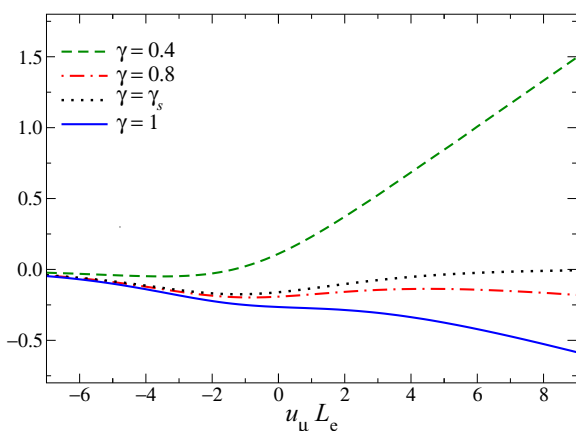


FIG. 8. (Color online) Plot of the $1/L$ correction $\widehat{R}_{g1}(L, \tilde{w}_e, \gamma)$, defined in Eq. (129), versus $\tilde{w}_e = u_\mu L_e$. OBC results for $L = 512$ and several values of γ ($\gamma_s = \sqrt{3} - 1$).

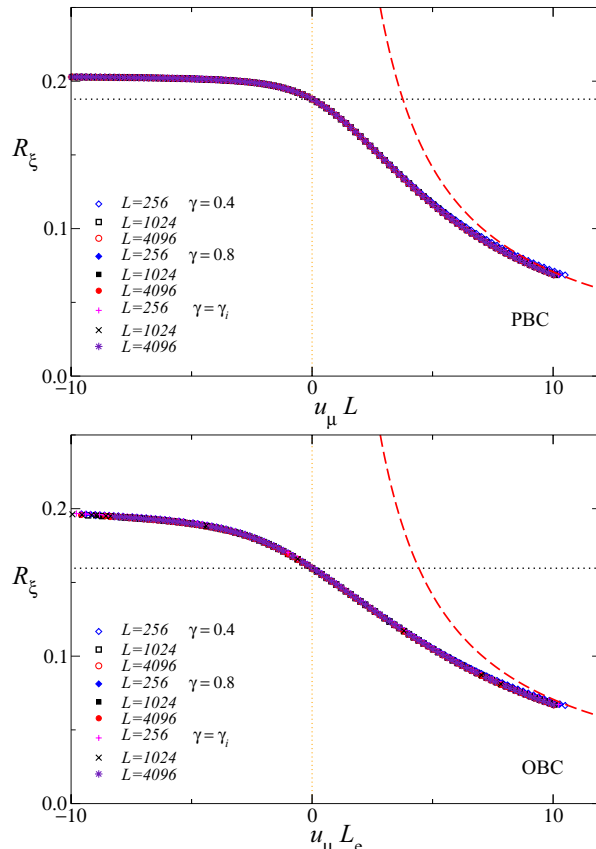


FIG. 9. (Color online) Plot of $R_\xi \equiv \xi/L$ [ξ is defined in Eq. (120)] versus $\tilde{w} = u_\mu L$ for PBC (top) and versus $\tilde{w}_e = u_\mu L_e$ for OBC (bottom). We report data for $\gamma = 0.4, 0.8$, and $\gamma_s = \sqrt{3}/2$. For both OBC and PBC the data for different values of γ approach a universal curve with increasing L . The horizontal dotted lines correspond to the exact value at $\mu = 0$. The dashed lines show the asymptotic behavior $R_\xi \approx 1/(\sqrt{2}\tilde{w})$ for $\tilde{w} \rightarrow \infty$ (for OBC we should replace \tilde{w} with \tilde{w}_e).

a nontrivial dependence on γ : No rescaling exists that makes the curves corresponding to different values of γ fall one on top of the other. This implies that such correction cannot be ascribed to a single subleading operator. We can also exclude that the $1/L$ correction can be eliminated by using L_e in the definition of R_g , i.e., by defining

$$R'_g \equiv \ln[G(0, L_e/8)/G(0, L_e/4)]. \quad (131)$$

Indeed, for $\gamma = \gamma_s = \sqrt{3} - 1$, we have $L_e = L$, hence $R_g = R'_g$. But also in this case $1/L$ corrections are present. They may be explained by the presence of field mixings with the boundary operators.

Let us finally consider R_ξ . Its behavior in the scaling limit is shown in Fig. 9. The finite-size behavior of R_ξ is more complex, since one must also take into account the background term which gives corrections of order $L^{-2+z+\eta} = L^{-3/4}$, independent of the type of boundary conditions. For OBC next-to-leading corrections are of order L^{-1} , while for PBC, if the scaling limit is taken at fixed \tilde{w} , they are of order $L^{-7/4}$ and

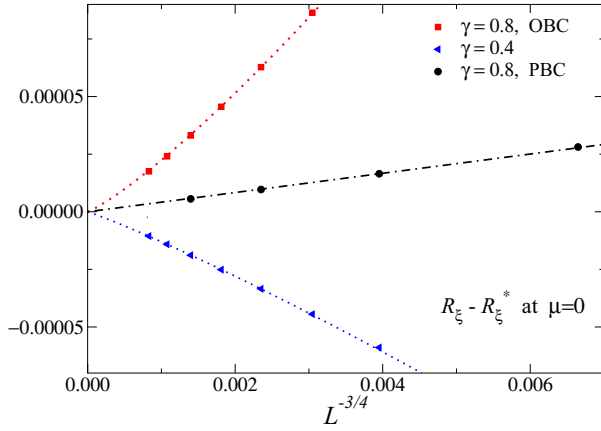


FIG. 10. (Color online) Plot of $R_\xi - R_\xi^*$ at $\mu = 0$ vs $L^{-3/4}$. The dotted lines are fits to $aL^{-3/4} + bL^{-1}$, while the dot-dashed one is a fit to $aL^{-3/4}$ only. Results for OBC and PBC and for $\gamma = 0.4$ and 0.8 . $R_\xi^* = 0.159622\dots$ and $R_\xi^* = 0.187790\dots$ in the OBC and PBC case, respectively (see Appendix A).

are due to the L dependence of the background term. These predictions are well confirmed by the data shown in Fig. 10.

IV. FINITE-SIZE SCALING OF BIPARTITE ENTANGLEMENT ENTROPIES

In a quantum system the reduced density matrices of subsystems and, in particular, the corresponding entanglement entropies and spectra, provide effective probes of the nature of the quantum critical behavior (see, e.g., Refs. [66–70]). Their dependence on the finite size of the system may be exploited to determine the critical parameters of a quantum transition [71–76].

The spatial entanglement of systems near their quantum critical point can be quantified by computing von Neumann or Rényi entanglement entropies of the reduced density matrix of a subsystem. They generally satisfy the area law, with some notable exceptions presenting logarithmic corrections, such as free Fermi gases in arbitrary dimensions [68]. Moreover, in a homogeneous one-dimensional (1D) system of length L whose quantum critical behavior is described by a 2D CFT, the bipartite entanglement entropy $S(I_A, L)$ increases logarithmically [77–80] with increasing the size I_A of the subsystem at the critical point, i.e., $S \sim \ln I_A$, or with increasing the spatial length scale ξ when approaching the critical point, i.e., $S \sim \ln \xi$ (if $1 \ll \xi \ll I_A$). In both cases the coefficients of the logarithms are related to the central charge of the corresponding CFT.

In this section we discuss the finite-size behavior of the entanglement entropy of spatial bipartitions of the system. We restrict the discussion to zero temperature and to one-dimensional systems with an isolated quantum critical point with $z = 1$ and central charge c . The general FSS behavior is then compared with exact and numerical results for the XY chain.

A. FSS in 1D systems at a quantum critical point

We consider a 1D lattice system, and divide it into two connected parts A and B of length ℓ_A and $\ell_B = L - \ell_A$, and

consider the Rényi entropy

$$S_\alpha(\ell_A, L) = S_\alpha(L - \ell_A, L) = \frac{1}{1 - \alpha} \ln \text{Tr} \rho_A^\alpha, \quad (132)$$

where α is a positive constant, ρ_A is the reduced density matrix of the subsystem A , i.e.,

$$\rho_A = \text{Tr}_B \rho, \quad (133)$$

and ρ is the density matrix of the ground state. For $\alpha \rightarrow 1$, the Rényi entropy coincides with the von Neumann (vN) entropy

$$S_1(\ell_A, L) = S_1(L - \ell_A, L) = -\text{Tr} \rho_A \ln \rho_A. \quad (134)$$

The asymptotic behavior of bipartite entanglement entropies is known at the critical point $\mu = 0$ [77–80]. We have

$$S_\alpha(\ell_A, L) \approx cq \frac{1 + \alpha^{-1}}{12} [\ln L + \ln \sin(\pi \ell_A / L) + e_\alpha], \quad (135)$$

where c is the central charge, q counts the number of boundaries between the two parts of the system, thus, $q = 2$ and $q = 1$ in the PBC and OBC case, respectively. The constant e_α is nonuniversal and depends on the boundary conditions [79–81].

The corrections to Eq. (135) may have various origins. Beside the corrections discussed in Sec. II, there are additional corrections. They are related to the operators associated with the conical singularities at the boundaries between the two parts, which appear in the α -sheeted Riemann surface introduced to compute $\text{Tr} \rho_A^\alpha$ [17,18]. In the limit $L, \ell_A \rightarrow \infty$ at fixed ℓ_A / L , these new operators give rise to terms of order $L^{-\varepsilon/\alpha}$ in the case of OBC [17,18] and of order $L^{-2\varepsilon/\alpha}$ in the case of PBC [82,83]. Here $\varepsilon > 0$ is the RG dimension [17,18] of the leading conical operator. The results for a number of 1D models suggest that the energy operator plays a major role in this respect [74,82–84], hence

$$\varepsilon = 1/\nu. \quad (136)$$

Moreover, the analysis of exactly solvable models shows the presence of other corrections suppressed by integer powers of L [82]. The general predictions are confirmed by the exact results for the XY chain at the critical point, for both OBC and PBC. They are summarized in Appendix B.

The asymptotic behavior of the bipartite entanglement entropies is also known in the thermodynamic limit close to the transition point [18,79], i.e., for $L, \ell_A \ll \xi$, where ξ is the length scale of the critical modes, such as that defined in Eq. (39). One obtains [18,79,85]

$$S_\alpha(\ell_A, L; \mu) \approx cq \frac{1 + \alpha^{-1}}{12} \ln \xi + a_\alpha, \quad \xi \ll \ell_A, L, \quad (137)$$

where again $q = 2$ in the case of PBC and $q = 1$ in the case of OBC, and a_α is a nonuniversal constant. The corrections to the asymptotic behavior (137) are expected to be [18] of order $\xi^{-\varepsilon/\alpha}$, where ε is the same exponent controlling the finite-size corrections at the critical point. Additional corrections of order ξ^{-2} should also be present [86].

In the general FSS regime, the bipartite entanglement entropy has been conjectured to satisfy the asymptotic scaling equation [79]

$$S_\alpha(\ell_A, L; \mu) - S_\alpha(\ell_A, L; 0) \approx \Sigma_\alpha(\ell_A / L, \mu L^{1/\nu}). \quad (138)$$

Consistency with Eqs. (135) and (137) implies

$$\Sigma_\alpha(\ell_A/L, w) \approx -\nu c q \frac{1 + \alpha^{-1}}{12} \ln w \quad (139)$$

for $w \rightarrow \infty$. If we include the scaling corrections, we expect

$$\begin{aligned} S_\alpha(\ell_A, L; \mu) - S_\alpha(\ell_A, L; 0) \\ \approx \Sigma_\alpha(\ell_A/L, u_\mu/u_l^{1/\nu}) \\ + b_\alpha u_l^{\varepsilon/\alpha} \Sigma_{\alpha,c}(\ell_A/L, u_\mu/u_l^{1/\nu}) + \dots, \end{aligned} \quad (140)$$

where the ellipsis corresponds to other corrections of order $u_l^{\omega_s}$, $u_l^{\omega_s}$, \dots , which may be more relevant than the conical ones in some cases.

Starting from the entanglement entropies, one can define RG invariant quantities, which can be used to determine the critical behavior in a finite volume. For this purpose, we consider

$$Q_\alpha(X, Y) = \frac{12}{q(1 + \alpha^{-1})} \left[\frac{S_\alpha(XL, L, \mu) - S_\alpha(YL, L, \mu)}{\ln \sin(\pi X) - \ln \sin(\pi Y)} \right] \quad (141)$$

with $0 < Y < X < 1$. According to Eq. (135), at the critical point $\mu = 0$

$$\lim_{L \rightarrow \infty} Q_\alpha(X, Y) = c. \quad (142)$$

On the other hand, for $\mu \neq 0$ and $\xi \ll L$, since $S_\alpha(\ell_A, L, \mu)$ is independent of ℓ_A in this limit, we have $Q_\alpha(X, Y) = 0$.

The quantity Q_α may be used to determine the transition point and critical exponents, as the RG invariant quantities R considered in Sec. II E. For any boundary condition, Eq. (140) implies

$$Q_\alpha(\mu, L) = Q_\alpha(u_\mu u_l^{-1/\nu}) + b_\alpha u_l^{\varepsilon/\alpha} Q_{\alpha,c}(u_\mu u_l^{-1/\nu}) + \dots \quad (143)$$

with $Q_\alpha(0) = c$, where the dependence on the interval coordinates X, Y is understood. The scaling functions Q_α and $Q_{\alpha,c}$ depend only on X, Y , and the boundary conditions, apart from a trivial normalization of their argument, while b_α is a nonuniversal constant. In the PBC case, we have

$$Q_{\alpha,c}(0) = 0, \quad (144)$$

since corrections decay as $L^{-2\varepsilon/\alpha}$ at the critical point. Besides the corrections of order $L^{-\varepsilon/\alpha}$, one should also consider the standard corrections related to the usual bulk and boundary irrelevant operators, and analytic corrections.

B. FSS in the XY chain

To verify the general FSS behaviors presented in Sec. IV A, we consider again the XY chain. In this case $\nu = 1$, so that $\varepsilon = 1$. Therefore, for $\alpha > 1$ the corrections associated with the Rényi entanglement entropies of order $L^{-1/\alpha}$ are stronger than the standard ones discussed in the previous sections, which scale as $1/L$ at least. We consider the quantity

$$Q_\alpha \equiv Q_\alpha(X = 1/2, Y = 1/4), \quad (145)$$

i.e., we take $X = 1/2$ and $Y = 1/4$ in Eq. (141). In the following we present results for the Rényi and vN entanglement entropies, for several values of γ , OBC, and PBC, and lattice sizes up to $L = O(10^4)$.

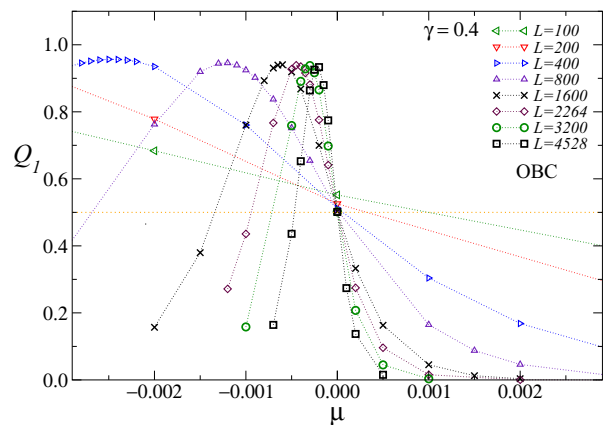


FIG. 11. (Color online) The RG invariant quantity Q_1 , derived from the vN entanglement entropy using Eqs. (141) and (145), for $\gamma = 0.4$. We consider OBC and several values of L . The dotted lines connecting the data corresponding to the same value of L are only meant to guide the eye.

Figure 11 shows Q_1 for $\gamma = 0.4$ and several values of L for OBC. The curves show a maximum for $\mu < 0$ and cross each other approximately at $\mu = 0$. Using Eq. (143), one can easily establish that the crossing point $\mu_{\text{cross}}(L)$, defined by

$$Q_\alpha[\mu_{\text{cross}}(L), L] = Q_\alpha[\mu_{\text{cross}}(L), 2L], \quad (146)$$

approaches the critical point as

$$\mu_{\text{cross}} = O(L^{-1/\nu-1/\alpha}). \quad (147)$$

This is confirmed by the results for Q_α (see, e.g., Fig. 11).

Figures 12 and 13 show plots of Q_1 and Q_2 , for OBC and PBC, respectively, versus the scaling variable $w = \mu L/\gamma$ for $\gamma = 0.4$ and $\gamma = 0.8$. The data appear to approach universal curves with increasing L , clearly supporting the universality of the asymptotic function $Q_\alpha(w)$ [cf. Eq. (143)], for both OBC and PBC. Note that the maximum of the PBC scaling curve is at $w \equiv \mu L/\gamma = 0$ and equals $c = 1/2$, while the OBC maximum is larger than $c = 1/2$ —we obtain $Q_{1,\text{max}} \approx 0.9358$ and $Q_{2,\text{max}} \approx 1.248$ —and it is located in the region $w < 0$. The scaling curves vanish exponentially for $|w| \rightarrow \infty$. As expected, scaling corrections appear larger for Q_2 than Q_1 .

Let us now investigate the corrections to the leading term. To begin with, we consider the Rényi entanglement entropies for $\alpha > 1$, whose leading corrections are expected to be due to the conical singularities, i.e., the $O(L^{-1/\alpha})$ term explicitly reported in Eq. (143). We use the asymptotic formulas reported in Appendix B to derive the finite-size behavior of Q_α at $\mu = 0$. We obtain

$$Q_\alpha = 1/2 + b_\alpha L^{-1/\alpha} + O(L^{-2/\alpha}) + O(L^{-1}), \quad (148)$$

where

$$\begin{aligned} b_\alpha &= \bar{b}_\alpha \gamma^{-1/\alpha}, \\ \bar{b}_\alpha &= \frac{12(\pi/8)^{1/\alpha} \Gamma[1/2 + 1/(2\alpha)](2^{1/(2\alpha)} - 1)}{(1 + \alpha)\Gamma[3/2 - 1/(2\alpha)] \ln 2}. \end{aligned} \quad (149)$$

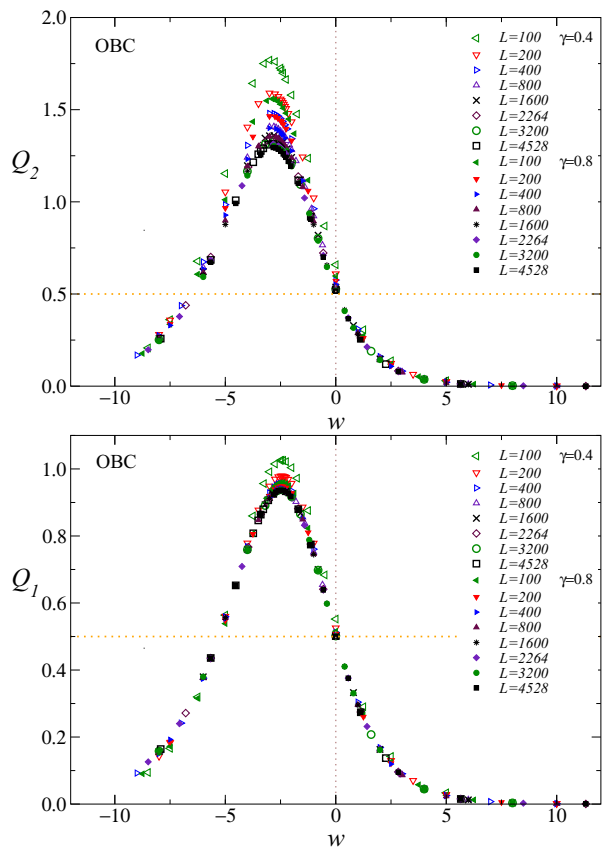


FIG. 12. (Color online) Scaling behavior of Q_1 (bottom) and Q_2 (top) for OBC vs $w \equiv \mu L/\gamma$, for $\gamma = 0.4$ and $\gamma = 0.8$. In both cases the data for different values of γ approach a universal large- L curve.

In particular $\bar{b}_2 = 0.925\,049\dots$ for $\alpha = 2$. Instead, for PBC with $\mu = 0$, we find

$$Q_\alpha = 1/2 + p_\alpha L^{-2/\alpha} + O(L^{-4/\alpha}) + O(L^{-2}), \quad (150)$$

$$p_\alpha = \frac{3(\alpha - 1)(\pi/4)^{2/\alpha}(2^{1/\alpha} - 1)\Gamma[1/2 + 1/(2\alpha)]^2}{\alpha(\alpha + 1)\Gamma[3/2 - 1/(2\alpha)]^2 \ln 2}$$

for $\gamma = 1$. In particular $p_2(\gamma = 1) = 0.428\,928\dots$

The FSS limit is taken at fixed $\tilde{w}_e = u_\mu L_e$ for OBC and $\tilde{w} = u_\mu L$ for PBC [see Eqs. (56) and (113) for the definitions of u_μ and L_e], to avoid analytic corrections due to the expansion of the scaling fields. The numerical data of the $\alpha = 2$ Rényi entropy are in full agreement with Eq. (143): for both PBC and OBC scaling corrections decay as $L^{-1/2}$. Moreover, for both OBC and PBC, the corrections are proportional to $\gamma^{-1/2}$ as found at the critical point [cf. Eq. (149)]. This is clearly demonstrated by the analysis of the large- L behavior of the quantity

$$\widehat{Q}_{2,c} \equiv 2(\gamma L)^{1/2} [Q_2(\tilde{w}, L, \gamma) - Q_2(\tilde{w}, 4L, \gamma)]. \quad (151)$$

If corrections are of order $(\gamma L)^{-1/2}$, in the limit $L \rightarrow \infty$ at fixed \tilde{w} or \tilde{w}_e , $\widehat{Q}_{2,c}$ converges to a nontrivial γ -independent scaling function, i.e., to the function $\widehat{Q}_{2,c}(\tilde{w})$ appearing in Eq. (143). Figures 14 and 15 show the extrapolation of $\widehat{Q}_{2,c}$ for OBC and PBC, respectively. They are obtained by using results for chains of length $L \leq 4096$. The resulting tiny differences that are hardly visible in Figs. 14 and 15 are plausibly due

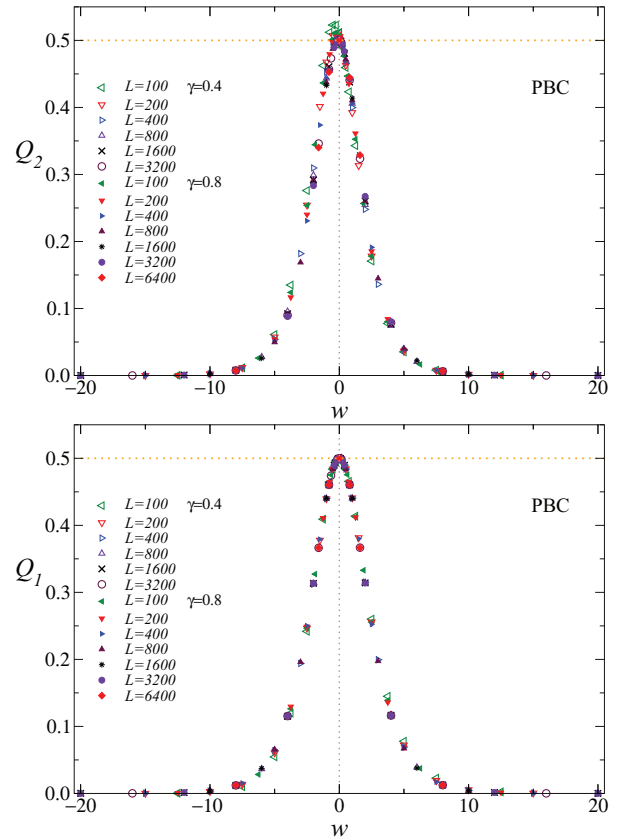


FIG. 13. (Color online) Scaling behavior of Q_1 (bottom) and Q_2 (top) for PBC vs $w = \mu L/\gamma$, for $\gamma = 0.4$ and $\gamma = 0.8$. In both cases the data clearly converge toward an asymptotic large- L curve which is independent of γ .

to tiny numerical errors affecting the raw data and to the extrapolation uncertainty. The curves for different values of γ appear to approach a unique curve, thus supporting our general scenario. Analogous results are expected for any $\alpha > 1$.

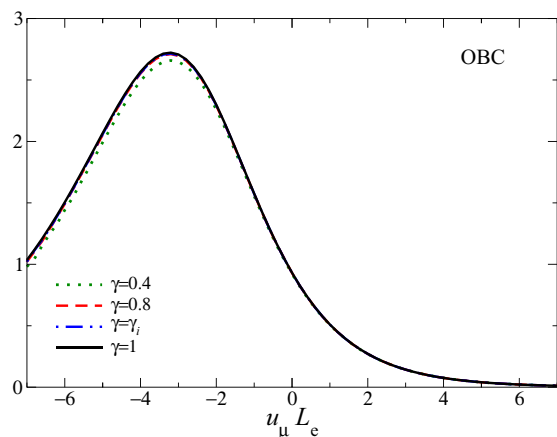


FIG. 14. (Color online) Check of the scaling of the corrections to the asymptotic behavior of Q_2 for OBC: Plot of the large- L limit of $\widehat{Q}_{2,c}$, defined in Eq. (151), versus $\tilde{w}_e = u_\mu L_e$, for several values of γ ($\gamma_i = \sqrt{3}/2$). The different curves are hardly distinguishable: The small differences are within the accuracy of the large- L extrapolation of the data up to $L = 1024$.

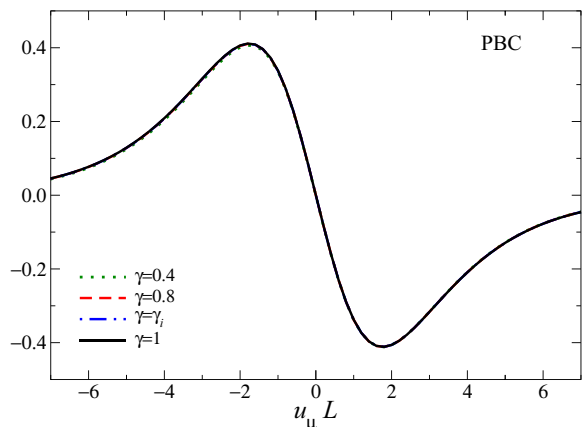


FIG. 15. (Color online) The large- L limit of $\widehat{Q}_{2,c}$ for PBC, defined in Eq. (151), versus $\tilde{w} = u_\mu L$, for several values of γ . Here $\gamma_i = \sqrt{3}/2$. On the scale of the figure, the different curves are hardly distinguishable. The small differences are within the extrapolation errors. For $w = 0$ the numerical data are consistent with zero, i.e., with the absence of $L^{-1/2}$ corrections, in agreement with the exact results at the critical point.

The analysis of the leading corrections for the vN entanglement entropy is more complicated, essentially because, in the limit $\alpha \rightarrow 1$, the leading corrections may have different origins. This is already shown by the results at the critical point. The asymptotic expansion of the vN entanglement entropy at the critical point for OBC and $\gamma = 1$ is reported in Appendix B. This allows us to derive

$$Q_1(0, L) = 1/2 + b_{\text{vN}} L^{-1} + O(L^{-2}), \quad (152)$$

$$b_{\text{vN}} = \frac{\pi(6\sqrt{2} - 7)}{8 \ln 2} \quad \text{for } \gamma = 1.$$

Note that b_{vN} does not coincide with the $\alpha \rightarrow 1$ limit of the coefficient b_α appearing in Eq. (149). Thus, other corrections contribute at order $1/L$. To understand better the subleading FSS behavior, we computed the corrections of order L^{-1} at fixed $\tilde{w}_e = u_\mu L_e$. They can be estimated by considering

$$\widehat{Q}_{1,c} = 2L[Q_1(\tilde{w}_e, L, \gamma) - Q_1(\tilde{w}_e, 2L, \gamma)]. \quad (153)$$

This quantity is constructed so that it approaches a nontrivial function if the leading corrections are of order L^{-1} . Figure 16 shows the large- L extrapolations [87] of \widehat{Q}_1 for several values of γ . We verify that the γ dependence cannot be eliminated by rescaling $\widehat{Q}_{1,c}(\tilde{w}_e, L, \gamma)$ by a function of γ . Hence, besides the conical contribution, there must be other corrections due to the boundaries. They may be interpreted as analytic corrections related to the length ℓ of the domain. Analogously to the nonlinear scaling field u_l associated with $1/L$ which has an expansion in powers of $1/L$ [cf. Eq. (10)], it is natural to introduce a scaling field u_ℓ associated with ℓ , with $u_\ell \approx 1/\ell + a/\ell^2$. The expansion of u_ℓ would contribute additional boundary corrections of order $1/L$, when the limit is taken at fixed ℓ/L . This is confirmed by the asymptotic behavior of the vN entanglement entropy at the critical point

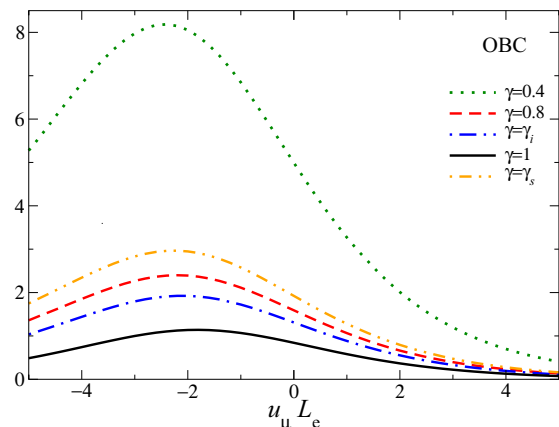


FIG. 16. (Color online) Scaling corrections for the vN entanglement quantity Q_1 for OBC: The large- L limit of $\widehat{Q}_{1,c}$ defined in Eq. (153) is plotted versus $\tilde{w}_e = u_\mu L_e$, for several values of γ . Here $\gamma_i = \sqrt{3}/2$ and $\gamma_s = \sqrt{3} - 1$.

(see Appendix B). Indeed, for $\gamma = 1$ it can be written as

$$S_1(\ell, L) = \frac{1}{12} \left[\ln L_e + \ln \sin \frac{\pi \ell_e}{L_e} + e_1 \right] - \frac{\pi}{16 \sin(\pi \ell_e / L_e)} \frac{1}{L_e} + O(L_e^{-2}), \quad (154)$$

where $L_e = L + 1/2$ and $\ell_e = \ell + 1/4$, e_1 is a constant, and the term of order L^{-1} is the $\alpha \rightarrow 1$ limit of the corrections of order $L^{-1/\alpha}$ occurring for generic $\alpha > 1$. Equation (154) allows us to identify the origin of the correction terms: There are conical corrections that give rise to the L_e^{-1} term appearing in Eq. (154), and boundary terms that can be eliminated by introducing L_e and ℓ_e .

In the case of PBC, the results of Appendix B at the critical point lead to

$$Q_1(0, L, \gamma) = 1/2 + p_{\text{vN}} L^{-2} + O(L^{-4}), \quad (155)$$

$$p_{\text{vN}} = \frac{\pi^2}{80 \ln 2} \quad \text{for } \gamma = 1.$$

The constant p_{vN} is unrelated to the constant p_α defined in Eq. (150). Indeed, p_α vanishes for $\alpha = 1$. These results apparently indicate that conical singularities are not related to the L^{-2} corrections at the critical point. Let us now extend the analysis away from the critical point, computing Q_1 in the FSS limit at fixed \tilde{w} . A detailed numerical analysis shows that there are no scaling corrections of order $1/L$. The function $Q_{1,c}$ appearing in Eq. (143) vanishes identically: Corrections for $\tilde{w} \neq 0$ decay as L^{-2} as occurs at the critical point. A detailed analysis of the numerical data for several values of γ shows that we can write

$$Q_1(\mu, L, \gamma) = Q_1(\tilde{w}) + L^{-2}[Q_{1,c1}(\tilde{w}) + v_1(0, \gamma)Q_{1,c2}(\tilde{w})] + O(L^{-3}), \quad (156)$$

where $v_1(\mu, \gamma)$, defined in Eq. (57), is the scaling field associated with the leading bulk subleading corrections. Notice that if we replace $\tilde{w} \equiv u_\mu L$ with its linear approximation $w \equiv \mu L / \gamma$ in Eq. (156), the leading term does not change but now the corrections are of order L^{-1} . They are due to

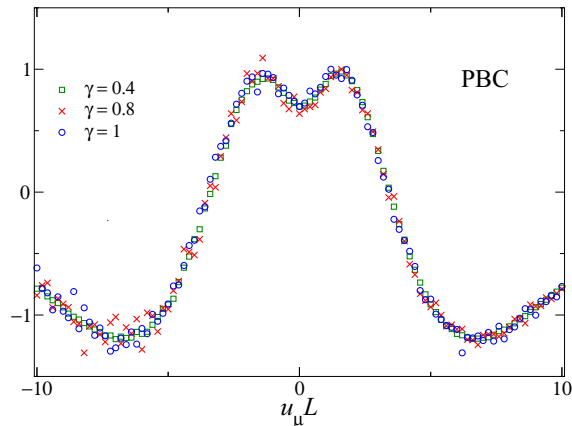


FIG. 17. (Color online) Scaling corrections for the vN entanglement quantity Q_1 for PBC: The large- L limit of $\widehat{Q}_{1,c2}$ defined in Eq. (157) is plotted versus $\tilde{w} = u_\mu L$ for several values of γ . The data collapse onto a single curve; the apparent oscillations, which are particularly visible for $\tilde{w} < 0$ and $\gamma = 0.8$, are essentially due to numerical errors in the computation of the raw data for $L \leq 512$.

the next-to-leading term appearing in the expansion of \tilde{w} in powers of w . To verify Eq. (156), we consider

$$\widehat{Q}_{1,c2}(\tilde{w}, L, \gamma) = \frac{L^2}{v_1(0, \gamma)} [Q_1(\tilde{w}, L, \gamma) - Q_1(\tilde{w}, L, \gamma_i)], \quad (157)$$

where $\gamma_i = \sqrt{3}/2$ [we remind the reader that $v_1(0, \gamma_i) = 0$]. If Eq. (156) holds, $\widehat{Q}_{1,c2}(\tilde{w}, L, \gamma)$ should converge to $Q_{1,c2}(\tilde{w})$, hence it should be independent of γ for large values of L . As shown in Fig. 17, a straightforward extrapolation [87] of data up to $L = 4096$ supports it. The second correction term in Eq. (156) is associated with the bulk irrelevant operator. The origin of the first term, which is independent of γ , is instead less clear. As we have already discussed, at the critical point the conical corrections of order $L^{-2/\alpha} = L^{-2}$ vanish, hence $Q_{1,c1}(0)$ can only be an analytic correction. It is natural to conjecture that the same is true away from the critical point. Indeed, if conical and analytic corrections were both present, one would expect them to have different γ dependencies. Hence, one would expect two different scaling functions with different γ -dependent coefficients.

V. SUMMARY AND CONCLUSIONS

We study FSS at quantum zero-temperature transitions, focusing on the corrections to the leading asymptotic behavior. This issue is relevant for numerical and experimental studies of quantum transitions, where the data are generally available for a limited range of system sizes, which are often relatively small. In these cases, the finite-size results show sizable corrections with respect to the leading FSS asymptotic behavior. Such corrections must be taken into account to obtain reliably accurate estimates of the critical parameters and, if needed, to identify the universality class of the transition.

We present a RG analysis of FSS at quantum zero-temperature transitions of d -dimensional systems characterized by two relevant parameters μ and h , which are, respectively, even and odd with respect to an assumed paritylike

symmetry. Well-known examples of such quantum transitions are those occurring in quantum XY (Ising) systems and general $O(N)$ -symmetric spin models, superfluid or metallic transitions in particle systems, etc. (see, e.g., Ref. [13]).

To characterize the scaling corrections, we generalize the classical scaling ansatz [3,4,14] to quantum transitions. This allows us to predict the type of subleading corrections that are expected in finite systems and/or at finite temperature. First, there are corrections associated with the bulk and boundary irrelevant RG perturbations, that decay as $L^{-\kappa}$, where κ is generally a noninteger exponent. For example, in the case of the quantum transitions of two-dimensional quantum Ising and Heisenberg models, the leading bulk $O(L^{-\omega})$ corrections have $\omega \approx 0.8$ (see, e.g., Ref. [5]). Then, one should consider analytic corrections due to the regular backgrounds. Finally, since the RG predictions are expressed in terms of the nonlinear scaling fields, one should also consider the correction terms arising from their expansion in powers of the Hamiltonian parameters, the spatial size L , and the temperature T . We also name these terms analytic corrections, since they arise from the analytic dependence of the nonlinear scaling fields on the system parameters, though, in general, they decay as $L^{-\rho}$ with noninteger ρ .

To check the general predictions, we consider the quantum XY chain in a transverse field, which is a standard theoretical laboratory to understand issues concerning quantum transitions. In particular, it is an ideal testing ground, since its Hamiltonian can be exactly diagonalized [16], allowing us to compute several interesting quantities either exactly or very accurately by using numerical methods.

The analytic computation of the finite-size behavior of the energy spectrum and of the free energy allows us to infer the exact form of the nonlinear scaling fields associated with the relevant Hamiltonian parameter $\mu \equiv g - 1$ and with the leading irrelevant operator with RG dimension -2 . Moreover, we can also determine the *speed of sound* c , which enters the relation between the temperature T and the corresponding scaling field. We provide a complete analysis of the asymptotic FSS behavior of the energy gap Δ (i.e., the difference between the energies of the two lowest levels) up to $O(L^{-4})$ for PBC and to $O(L^{-2})$ for OBC [cf. Eqs. (78) and (98), respectively]. In the PBC case, we show that all terms up to L^{-4} are due to the expansion of the nonlinear scaling field u_μ associated with μ and to the leading irrelevant RG perturbation. In the OBC case the corrections of order L^{-1} in the expansion of Δ are due to the L dependence of the nonlinear scaling field u_l associated with the spatial size L ; they can be eliminated by introducing an effective spatial size $L_e = L + l(\gamma)$ [cf. Eq. (113)]. Instead, the corrections of order L^{-2} show contributions associated with boundary irrelevant RG perturbations of RG dimension $\tilde{\gamma}_1 = -2$. Then, we perform an analogous analysis for some RG invariant quantities derived from the two-point function of the order parameter, i.e., $G(x, y) = \langle \sigma_x^{(1)} \sigma_y^{(1)} \rangle$, pointing out the presence of further corrections, arising from mixings of the operator $\sigma_x^{(1)}$ with other odd subleading operators. These results for the XY chains are in full agreement with the general RG framework put forward in Sec. II, which generalizes Wegner's scaling theory to quantum transitions.

Finally, we discuss the FSS behavior of bipartite entanglement Rényi and vN entropies in one-dimensional systems

with an isolated quantum critical point with $z = 1$ and central charge c . They present further peculiar corrections to the asymptotic FSS behavior predicted by conformal field theory, arising from operators associated with conical singularities in the corresponding conformal mapping [17]. The FSS predictions are compared with results for the XY chain. We show that the leading FSS corrections for the Rényi entropies with $\alpha > 1$ [cf. Eq. (132)] are always of order $L^{-1/\alpha}$, for any boundary conditions [see Eq. (140)]. In particular, in the PBC case corrections are of order $L^{-2/\alpha}$ only at the critical point $\mu = 0$. The behavior of the vN entanglement entropy is more complex. In the OBC case, the leading correction of order L^{-1} is the sum of terms of different origin: we find contributions from the conical operators and boundary corrections as well. In the PBC case, the leading FSS corrections are of order L^{-2} when the asymptotic scaling behavior is expressed in terms of nonlinear scaling fields [cf. Eq. (156)]; otherwise, for $\mu \neq 0$, corrections of order $L^{-1/\nu}$ arise from the expansion of the nonlinear scaling field \tilde{w} in powers of the relevant model parameters. Apparently, the $O(L^{-2})$ corrections in Eq. (156) are the sum of an analytic contribution and of a term due to the bulk irrelevant RG operator.

In our FSS study of the entanglement properties we introduce the RG invariant quantity Q_α . It is defined in terms of the Rényi entanglement entropy S_α [see Eq. (141)] in such a way as to have a universal FSS behavior (in particular, it approaches the central charge c at the critical point). The quantity Q_α may be useful to investigate 1D quantum transitions exploiting entanglement properties.

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APPENDIX A: USEFUL CFT FORMULAS

The 2D Ising universality class is associated with a CFT with central charge $c = 1/2$. CFT provides the asymptotic FSS behavior of the two-point function at the critical point [43]. We report some useful CFT formulas for the critical two-point function which are used in the paper. In the CFT (classical) framework we consider strips $L \times \infty$ with PBC and OBC, i.e., with coordinates $-L/2 \leq x \leq L/2$ and $y \in \mathbb{R}$.

1. Open boundary conditions

Setting $z_i \equiv x_i + L/2$, and

$$Z_\pm \equiv (z_2 \pm z_1)/L, \quad Y \equiv (y_2 - y_1)/L, \quad (\text{A1})$$

the critical two-point function on a strip for a classical system with OBC in one direction reads [43,44]

$$G_{\text{CFT}}(\vec{r}_1, \vec{r}_2) = \frac{(\pi/L)^{1/4}}{[\sin(\pi z_2/L) \sin(\pi z_1/L)]^{1/8}} \times \left[\frac{|\sin \pi(Z_+ + iY)/2|^{1/2}}{|\sin \pi(Z_- + iY)/2|^{1/2}} - \frac{|\sin \pi(Z_- + iY)/2|^{1/2}}{|\sin \pi(Z_+ + iY)/2|^{1/2}} \right]^{1/2}. \quad (\text{A2})$$

The two-point function $G(x_1, x_2)$ of the quantum system at the critical point is obtained by setting $Y = 0$. This result allows us to exactly compute the universal large- L limit of the RG invariant quantities $R_\xi \equiv \xi/L$ and R_g , defined in Eqs. (119) and (120), respectively, at the critical point. We obtain the critical values

$$R_g^* = 0.306\,462\dots, \quad R_\xi^* = 0.159\,622\dots \quad (\text{A3})$$

For the XY chain we may also consider the connected equal-time two-point function of the operator $\sigma_x^{(3)}$, i.e.,

$$G_n(x, y) = \langle \sigma_x^{(3)} \sigma_y^{(3)} \rangle - \langle \sigma_x^{(3)} \rangle \langle \sigma_y^{(3)} \rangle. \quad (\text{A4})$$

For $T = h = 0$, we obtain

$$G_n(0, x) \sim \frac{\cos(\pi x/L)}{L^2 \sin^2(\pi x/L)}. \quad (\text{A5})$$

Note that $G_n(0, x) \sim x^{-2}$ for $|x| \ll L$.

2. Periodic boundary conditions

In the case of PBC we have

$$G_{\text{CFT}}(\vec{r}_1, \vec{r}_2) = \frac{(\pi/L)^{1/4}}{|\sin \pi(Z_- + iY)|^{1/4}}. \quad (\text{A6})$$

Again, setting $Y = 0$, we obtain the two-point function $G(x_1, x_2)$ at the critical point, from which we can compute

$$R_g^* = 0.153\,493\dots, \quad R_\xi^* = 0.187\,790\dots \quad (\text{A7})$$

if ξ is defined as in Eq. (119). If instead the correlation length is defined as

$$\xi^2 \equiv \frac{\tilde{G}(0) - \tilde{G}(k_{\min})}{k_{\min}^2 \tilde{G}(k)}, \quad (\text{A8})$$

where \tilde{G} is the Fourier transform of G , and $k_{\min} = 2\pi/L$, we obtain $R_\xi^* = 0.389\,848\dots$

APPENDIX B: SOME EXACT RESULTS FOR THE ENTANGLEMENT ENTROPIES

In this Appendix we report some exact results for the entanglement entropies of the XY chain at the critical point. For this purpose, we also exploit known results for the XX model,

$$H_{XX} = -\frac{1}{2} \sum_{i=1}^L [\sigma_i^{(1)} \sigma_{i+1}^{(1)} + \sigma_i^{(2)} \sigma_{i+1}^{(2)}], \quad (\text{B1})$$

and the exact relation [81]

$$S_\alpha^{\text{XY}}(\ell, L) = \frac{1}{2} S_\alpha^{\text{XX}}(2\ell, 2L) \quad (\text{B2})$$

between the entanglement entropies of the XY model (49) with $g = 1$ and $\gamma = 1$, and those of the XX model (B1).

Some results for the corrections to the leading behavior for OBC were already reported in Ref. [88]. Using also the results

of Ref. [83] for the XX model, we can write the large- L behavior of the Rényi entropy with $\alpha > 1$ at fixed ℓ/L as

$$S_\alpha(\ell, L) = C_\alpha [\ln L + \ln \sin(\pi X) + e_\alpha(\gamma)] - \frac{\Gamma[1/2 + 1/(2\alpha)]}{2\alpha\Gamma[3/2 - 1/(2\alpha)]} \left[\frac{\pi}{8\gamma L \sin(\pi X)} \right]^{1/\alpha} + O(L^{-2/\alpha}) + O(L^{-1}), \quad (\text{B3})$$

where

$$C_\alpha \equiv c \frac{1 + \alpha^{-1}}{12}, \quad c = 1/2, \quad X \equiv \ell/L, \quad (\text{B4})$$

$$e_\alpha(\gamma) = \ln \gamma + \ln(8/\pi) + \int_0^\infty \frac{dt}{t} \left[\frac{6}{1 - \alpha^{-2}} \times \left(\frac{1}{\alpha \sinh t/\alpha} - \frac{1}{\sinh t} \right) \frac{1}{\sinh t} - e^{-2t} \right]. \quad (\text{B5})$$

Note that scaling corrections are proportional to $\gamma^{-1/\alpha}$, a property which also holds away from the critical point (see Sec. IV B). Equation (B3) does not allow us to compute the corrections for the vN entropy. Indeed, for $\alpha = 1$, there are two sources of L^{-1} terms: the conical corrections and the analytic boundary corrections. For $\gamma = 1$ we have [88]

$$S_1(\ell, L) = \frac{1}{12} [\ln L_e + \ln \sin \pi X_e + e_1(1)] - \frac{\pi}{16L \sin(\pi X)} + O(L^{-2}), \quad (\text{B6})$$

where $L_e = L + 1/2$, and $X_e \equiv \ell_e/L_e$ with $\ell_e = \ell + 1/4$. Thus, after appropriately shifting ℓ and L to ℓ_e and L_e ,

respectively, the remaining L^{-1} correction term turns out to be equal to the limit $\alpha \rightarrow 1$ of the correction of order $L^{-1/\alpha}$ appearing in Eq. (B3). Therefore, at the critical point the leading $O(L^{-1})$ correction in the vN entropy shows both conical and boundary contributions. However, the latter can be reabsorbed by redefining both length scales L and ℓ . Actually, for $\gamma = 1$, replacing $L \rightarrow L_e = L + 1/2$ and $\ell \rightarrow \ell_e = \ell + 1/4$ in Eq. (B3), we also obtain the $O(L^{-1})$ corrections for general S_α .

In the case of PBC, using the results for the XX model reported in Refs. [37,82], we obtain for $\alpha > 1$ and $\gamma = 1$,

$$S_\alpha(\ell, L)|_{\gamma=1} = 2C_\alpha [\ln L + \ln \sin(\pi X) + \tilde{e}_\alpha(1)] - (\alpha - 1) \frac{\Gamma[1/2 + 1/(2\alpha)]^2}{4\alpha^2\Gamma[3/2 - 1/(2\alpha)]^2} \left[\frac{\pi}{4L \sin(\pi X)} \right]^{2/\alpha} + O(L^{-4/\alpha}) + O(L^{-2}), \quad (\text{B7})$$

where $\tilde{e}_\alpha(\gamma) = e_\alpha(\gamma) - \ln 2$. For the vN entropy we instead obtain

$$S_1(\ell, L)|_{\gamma=1} = \frac{1}{6} [\ln L + \ln \sin(\pi X) + \tilde{e}_1(1)] - \frac{\pi^2}{480L^2 \sin^2(\pi X)} + \frac{\pi^2}{144L^2} + O(L^{-4}). \quad (\text{B8})$$

Note that the limit $\alpha \rightarrow 1$ of the corrections of order $L^{-2/\alpha}$ in Eq. (B7) vanishes, hence in the PBC case the leading conical singularities do not contribute at the critical point.

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