Rapidly-converging methods for the location of quantum critical points from finite-size data

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We analyze in detail, beyond the usual scaling hypothesis, the finite-size convergence of static quantities toward the thermodynamic limit. In this way we are able to obtain sequences of pseudo-critical points which display a faster convergence rate as compared to currently used methods. The approaches are valid in any spatial dimension and for any value of the dynamic exponent. We demonstrate the effectiveness of our methods both analytically on the basis of the one dimensional XY model, and numerically considering $c = 1$ transitions occurring in non integrable spin models. In particular, we show that these general methods are able to locate precisely the onset of the Berezinskii-Kosterlitz-Thouless transition making only use of ground-state properties on relatively small systems.

PACS numbers: 05.70.Fh, 64.60.an, 75.40.Mg

I. INTRODUCTION

In the study of physical properties of phase transitions a basic prerequisite is a reliable method to locate the critical point, whenever the latter is not known a priori from symmetry or duality arguments. Typically, in numerical or even experimental studies on finite samples one obtains a sequence of pseudocritical points (in the sense specified below) to be extrapolated to the true critical point in the thermodynamic limit (TL). The extrapolation may be done with some polynomial fit in the inverse size of the system or, better, exploiting some fitting function derived on the basis of a scaling ansatz or through the renormalization group (RG). The point is especially relevant in the context of quantum phase transitions (QPT) in lattice systems where the exponential growth of the dimension of the Hilbert space with the number of sites is a strong limitation on the accessible sizes with the current computational power and algorithms. One of the most used algorithms is still the Lanczos method for the virtually exact extraction of the low-lying energy levels; in the most favorable case of spin-1/2 models one cannot go beyond some tens of sites. This limit can be moved to maybe a few thousands of sites using the so-called density matrix renormalization group (DMRG) that has become the method of choice for 1D problems due to its high level of accuracy. Nonetheless, if one considers two or even three dimensional systems the situation is much worse: with the Lanczos algorithm the largest lattices have only a few sites of linear extension and the DMRG is not particularly efficient. At present, the only other choice is Quantum Monte Carlo (QMC) (see, for instance, [3]) that, however, suffers from a sign problem in the case of fermionic or frustrated systems and does not reach the level of accuracy of the DMRG. Very recently there have been attempts to exploit both DMRG-like features and the QMC sampling tricks, to design hybrid methods [4,5] that are however still under verification.

It is generally believed that a sequence of pseudocritical points, for example the loci of maxima of finite-size susceptibilities, converges to the critical point as a power law $L^{-\lambda}$, with a so-called shift exponent $\lambda$ given by the inverse of the correlation length exponent $\nu$. Hence, generally speaking, the larger is $\nu$ the slower is the convergence. This difficulty reaches its maximum for Berezinskii-Kosterlitz-Thouless (BKT) transitions, in which the correlation length diverges with an essential singularity or, loosely speaking, “$\nu = \infty$”. However, already in the seminal paper by Fisher and Barber [6], it was pointed out that the relation $\lambda = 1/\nu$ is not always valid and $\lambda$ depends, among other factors, on the boundary conditions.

The most used method to locate quantum critical points in $d = 1$ by means of finite-size data is the so-called Phenomenological Renormalization Group (PRG), reviewed for instance in [7]. Another convenient approach, the Finite-size Crossing Method (FSCM), was recently proposed in [8]. The aim of this paper is to improve both of them by means of criteria that produce sequences of pseudocritical points that converge more rapidly. We will show that in our sequences the shift exponent will have the form $\lambda = \lambda_0 + \lambda_1/\nu$, where $\lambda_0$ and/or $\lambda_1$ are larger than the corresponding values in the usual methods and therefore allow for a better convergence.

The paper is organized as follows. In Section III we illustrate the general arguments leading to the enhanced sequences, both in the framework of the FSCM and of the PRG (Subsec. III D). Special cases as the BKT transition (Subsec. III C) and that of logarithmic divergences (Subsec. III B) are discussed separately. In Section III we illustrate the usefulness of the methods on the hand of analytic and numerical tests. In Subsec. III A we treat the XY spin-1/2 chain, using a series of exact calculations reported in the Appendix. Then we move to two cases of spin chains for which no exact solution is available: in Subsec. III B we consider a spin-1 model with anisotropies in a parameter range that gives rise to a large value of $\nu$ and in Subsec. III C we study the spin-1/2 model with next to nearest neighbor interactions that is known to undergo a BKT transition. In this case we find a value for the critical coupling in agreement with the accepted ones, which was found using a model-specific investigation of the excited states [9]. Section IV is devoted to conclusions.
II. DERIVATION OF RAPIDLY-CONVERGING SEQUENCES

We consider systems in \( d \) spatial dimensions of linear size \( L \) and periodic boundary conditions (PBC). Let the transition be driven by a linear parameter \( g \) such that the Hamiltonian is

\[
\mathcal{H}(g) = \mathcal{H}_0 + g \mathcal{V}.
\]

Dealing with QPT we consider the case of strictly zero temperature, \( T = 0 \), even if the arguments presented below can be simply extended to the finite-temperature case, replacing the parameter \( g \) with \( T \) (and without using the \textit{dimensional crossover rule} used below). The free energy density reduces to the ground-state (GS) energy density which, close to the critical point \( g_c \), shows a singularity in the second (or higher) derivatives with respect to \( g \):

\[
\frac{1}{L^d} \langle \mathcal{H}(g) \rangle = e(g) = e_{\text{reg}}(g) + e_{\text{sing}}(g),
\]

where \( \xi \approx |g - g_c|^{-\nu} \equiv t^{-\nu} \) is the correlation length. Note that, as a consequence of the scaling hypothesis, the singular part of the energy \( e_{\text{sing}} \) is a universal quantity that depends only on \( \xi \), the relevant length scale close to the critical point. Hence, \( e_{\text{sing}} \) may be considered quite in general an even function of \( (g - g_c) \) that vanishes at the critical point.

On the other hand, the bulk energy density at the critical point behaves as (Primmer-Fisher hypothesis)

\[
e(g_c, L) = e_\infty(g_c) - L^{-(d+\zeta)} F(g_c),
\]

where \( F(g) \) is a sort of Casimir-like term that may depend on the actual geometry of the lattice. Note that this hypothesis has to be changed properly if one or more of the spatial dimensions are of infinite extent. Moreover, Eq. (11.29) of ref. [10] using the dimensional crossover rule according to which the partition function and the thermodynamic (static) properties of a \( d \)-dimensional quantum system are equivalent to those of a \( (d + \zeta) \)-dimensional classical counterpart [11, 10], where \( \zeta \) is the dynamic exponent [1]. Then, for the implementation of our methods we need to know by some other means the value of \( \zeta \) relating the energy gap \( \Delta \) and the correlation length \( \xi \): \( \Delta \propto \xi^{-\zeta} \). Typically, but not always, energy and momentum in the continuum limit at the critical point satisfy a \textit{linear} dispersion relation, \( E = \nu k \), for small \( k \) so that \( \zeta = 1 \) and a relativistic effective field theory can be used to describe the universal features of the transition. In \( d = 1 \) the scale invariance at the critical point is often sufficient to imply also conformal invariance (see Ch. 2 of [11]), thanks to which several exact results can be obtained using the powerful predictions of conformal field theories (CFT). For example, by mapping the space-time complex plane onto a cylinder whose circumference represents the finite chain of length \( L \) we can identify \( F(g_c) = \pi c v_0 /6 \) in Eq. (1) where \( c \) is the central charge of the theory. In the RG sense, moving away from criticality corresponds to perturbing the CFT with a relevant operator that destroys conformal invariance. However, this is not the only effect of varying the microscopic parameter \( g \) out of \( g_c \), in general also the speed of elementary excitations gets renormalized in the unperturbed CFT part. For this reason we say that \( v \) (henceforth \( F \)) depends on \( g \) in the vicinity of \( g_c \).

Scaling and dimensional arguments imply that, in the thermodynamic, off-critical regime \( L \gg \xi \), the singular part of the energy behaves as

\[
e_{\text{sing}} \approx t^{2-\alpha}
\]

with \( \alpha = 2 - (d + \zeta) \nu \). For a second order phase transition \( \alpha < 1 \).

After introducing the scaling variable \( z = (L/\xi)^{1/\nu} = tL^{1/\nu} \), the finite-size scaling (FSS) theory asserts [2] that in a system of length \( L \),

\[
e_{\text{sing}} = C_0 L^{-(d+\zeta)} \Phi_c(z) + \cdots ,
\]

where \( \Phi_c(z) \) is a universal function that, in the off-critical regime \( z \gg 1 \), must behave as \( \Phi_c(z) \approx z^{\nu} \) in order to recover Eq. (2). Instead, for \( L \ll \xi \) we are in the critical regime and \( \Phi_c(z) \) behaves as an analytic function that vanishes for \( z \to 0 \). Here we assume that the leading term in \( \Phi_c(z) \) is quadratic in \( z \) (see below why it cannot be linear), but the following arguments are easily generalizable to higher integer powers. The constant term \( C_0 \Phi_c(0) / L^{d+\zeta} \) is already absorbed in the nonuniversal part of the energy density at \( g_c \) as shown in Eq. (1).

Differentiating \( e(g) \) with respect to \( g \), gives the mean value \( b = \langle \mathcal{V} \rangle / L^d \), whose singular part \( b_{\text{sing}} \) behaves as

\[
b_{\text{sing}} \approx \text{sgn}(g - g_c) t^{1-\alpha} = \text{sgn}(g - g_c) t^{(d + \zeta) \nu - 1}.
\]

Considering FSS for the combination of Eqs. (1) and (3) and then differentiating we find

\[
b(g, L) = b_{\infty, \text{reg}}(g) + \text{sgn}(g - g_c) C_0 L^{1/\nu - (d + \zeta)} \Phi_c'(z) - L^{-(d+\zeta)} [F'(g_c) + F''(g_c) (g - g_c) + \cdots] + O\left(L^{-(d+\zeta+\epsilon)}\right)
\]

where the subscript “\( \infty \), reg” hereafter means regular in the TL. In order to write down the expression above we used \( \partial_g = L^{1/\nu} \partial_z \) and assumed that the powers neglected in the last term are just larger than \( (d + \zeta) \). To illustrate this point we could consider the irrelevant operator with the smallest scaling dimension \( d_{irr} \). At first order in perturbation theory with the renormalized coupling \( g_{irr}(L) = g_{irr}(0)L^{d+\zeta-d_{irr}} \) the corrections to the GS energy density are of the form \( C_{irr} g_{irr}(0) L^{-d_{irr}} \) so that \( \epsilon = d_{irr} - d - \zeta > 0 \). Note also that the amplitude \( C_{irr} \) can vanish and \( O(g_{irr}^2) \) terms have to be included. For these and more details we leave the reader to Ref. [12]. Generically we admit corrections with \( \epsilon \geq 0 \) that may come either from irrelevant operator in the continuum theory or from lattice effects. The case \( \epsilon = 0 \) corresponds to marginal perturbations and typically leads to logarithmic corrections. Notice that now the leading term of \( \Phi_c'(z) \) is linear
in \( z \) in the critical region. If we would have admitted a linear term in \( \Phi_e(z) \) then \( \Phi'_e(0) \neq 0 \) and a finite jump discontinuity at finite \( L \), would be present in \( b(g, L) \).

We can also calculate \( a = \left( \frac{V_0}{\Gamma} \right) = e(g) - g|\partial e(g)/\partial g| \), yielding to a singular part that is similar to Eq. (3) but with a changed sign. In fact, for \( g_c \neq 0 \) the leading singular parts of \( a \) and \( b \) must cancel in the sum that gives back the energy \( e(g) = a(g) + gb(g) \), which does not contain that singularity. In particular, the scaling is

\[
a(g, L) = a_{\infty, \text{reg}}(g) - g\sigma(g - g_c)gC_0L^{\nu -(d + \zeta)\Phi_e(z)} + C_0L^{-(d + \zeta)\Phi_e(z)} - L^{-(d + \zeta)} [F(g) - gF'(g_c) + O(g - g_c)] + \ldots
\]

The FSCM \(^8\) identifies the critical point with the limit of the sequence \( g_L^* \) of single crossing points

\[
b(g_L^*, L) = b(g_L^*, L')
\]

with \( L' = L + \delta L \). Applying this criterion to Eq. (5), we obtain (for \( \delta L \ll L \))

\[
g_L^* - g_c = -\frac{(d + \zeta)F'(g_c)}{2C_0\left[\frac{d}{\nu} - (d + \zeta)\right]} L^{-2/\nu}. \quad \nu \neq \frac{2}{d + \zeta}
\]

This equation defines the shift exponent \( \lambda_{\text{FSCM}} = 2/\nu \) and may converge very slowly when \( \nu \gg 1 \). The extremely difficult case is the BKT transition where formally \( \nu = \infty \), but this latter situation must be treated in a different way (see Subsec. II C).

Now, consider the quantity \( \Gamma(g, L, \gamma) = \gamma e(g, L) - b(g, L) \) and suppose to be able to tune \( \gamma \) exactly at

\[
\gamma^* = \frac{F'(g_c)}{F(g_c)}
\]

It easily seen that \( \Gamma(g_c, L, \gamma^*) \) does not contain the Casimir-like term responsible for the critical point shift. In fact, the scaling of \( \Gamma \) is

\[
\Gamma(g, L, \gamma) = \Gamma_{\infty, \text{reg}}(g, \gamma) - g\sigma(g - g_c)gC_0L^{\nu -(d + \zeta)\Phi_e(z)} - L^{-(d + \zeta)} [F(g) - F'(g) + O(g - g_c)] + O(L^{-(d + \zeta + \epsilon)}).
\]

When \( \gamma \) is equal to \( \gamma^* \) given in Eq. (6), the critical point found by this crossing method is approached as \( g_L^* - g_c \approx L^{-\lambda_{\text{FSCM}}} \), with a shift exponent \( \lambda_{\text{FSCM}} = 2/\nu + \epsilon = \lambda_{\text{FSCM}} + \epsilon \) (again this holds true provided that \( \nu \neq 2/(d + \zeta) \)). The additional term \( \epsilon \) allows, in general, for a better convergence of the sequence \( g_L^* \).

A possible algorithm for finding numerically the critical point in such a way is the following. If \( g_L^* \) is at a crossing point, of \( \Gamma(g, L, \gamma) \), then we have

\[
\gamma(g_L^*, L) = \frac{b(g_L^*, L + \delta L) - b(g_L^*, L)}{e(g_L^*, L + \delta L) - e(g_L^*, L)}.
\]

Notice that putting \( \gamma = 0 \) is equivalent to the FSCM applied to \( b(g, L) \) and the denominator has definite sign about the critical point. Now we find \( g_L^* \) requiring that \( \gamma(g_L^*, L - \delta L) = \gamma(g_L^*, L) \), i.e.

\[
\frac{b(g_L^*, L) - b(g_L^*, L - \delta L)}{e(g_L^*, L) - e(g_L^*, L - \delta L)} = \frac{b(g_L^*, L + \delta L) - b(g_L^*, L)}{e(g_L^*, L + \delta L) - e(g_L^*, L)}
\]

or in the continuum version

\[
\frac{\partial L_b(g, L)}{\partial e(g, L)} = \frac{\partial^2 L_b(g, L)}{\partial^2 e(g, L)}
\]

Calling \( \tau = (g - g_c) = \nu \sigma(g - g_c) \) and rewriting only the essential terms in the scaling ansätze we have the simplified forms

\[
e(g, L) = c_{\infty, \text{reg}}(g) - L^{-(d + \zeta)} F(g) + D_1L^{-(d + \zeta + \epsilon)} + \ldots
\]

\[
b(g, L) = b_{\infty, \text{reg}}(g) + L^{-(d + \zeta)} \left[ 2C_0L^{2/\nu - \tau} - F'(g) \right] + D_2L^{-(d + \zeta + \epsilon)}.
\]

Now, putting these two relations in \(^8\) we obtain

\[
g_L^* - g_c = \frac{D_2F(g_c) - D_1F'(g_c) + \nu(d + \zeta + \epsilon)}{4C_0F(g_c)} L^{-\lambda_{\text{FSCM}}}
\]

that gives a shift exponent \( \lambda_{\text{FSCM}} \) as anticipated.

The main result of this section is the crossing criterion \(^7\) that identifies the rapidly converging sequence \(^9\) to the critical value.

### A. Homogeneity condition

In the previous section we have shown how to obtain a sequence of pseudocritical points with an improved shift exponent \( \lambda_{\text{FSCM}} \). Here we provide another, yet simpler equation for the determination of the critical point. The resulting pseudocritical sequence is characterized by the same shift exponent \( \lambda_{\text{FSCM}} \). However in this case we are able to prove convergence toward the critical point even in the extreme case of a BKT transition (see Subsec. II C).

The idea is to require that at the critical point the \( L \)-dependent part of \( b \) is dominated by the Casimir-like term with power \( (d + \zeta) \) (see Eq. \((5)\)). This condition is translated into the requirement that the \( L \)-derivative of \( b \) is a homogeneous function of degree \( (d + \zeta + 1) \), i.e.

\[
(d + \zeta + 1)\partial_L b(g_L^*, L) + L\partial_L^2 b(g_L^*, L) = 0.
\]

Consequently, the corresponding sequence of pseudocritical points \( g_L^* \) scales as

\[
g_L^* - g_c = \frac{\nu D_2(d + \zeta + \epsilon)}{2C_0\left( d + \zeta + \frac{\epsilon}{\nu} \right)} L^{-\lambda_{\text{FSCM}}}.
\]

The equation \((10)\) represents the homogeneity condition method (HCM) that we are proposing for the efficient location of critical points. We stress here that, being \( b(g, L) \) a GS property, this criterion does not require knowledge of excited states as in the case of the PRG method. This is a point in favor to the HCM since excited states are typically assessed with less numerical accuracy. In addition, the HCM is superior to the PRG in that it produces a faster converging sequence (see Subsec. II D).
B. Case $\nu = 2/(d + \zeta)$ with logarithmic divergences

For completeness we consider the case $\nu = \frac{2}{d + \zeta}$ that was excluded in the previous treatment. In this situation, the ansatz requires the inclusion of logarithmic corrections

$$b(g, L) = b_{\infty,\text{reg}}(g) + C_1 \ln L \tau - L^{-(d+\zeta)} F'(g) + D_2 L^{-(d+\zeta+c)}.$$ 

The calculation of the critical point with the FSCM gives in this case

$$g^*_L - g_c = -\frac{(d + \zeta) F'(g_c)}{C_1} L^{-(d+\zeta)}$$

whereas the HCM Eq. (10) yields

$$g^*_L - g_c = -\frac{\epsilon D_2 (d + \zeta + \epsilon)}{C_1 (d + \zeta)} L^{-(d+\zeta+c)}$$

These results are compatible with the exact calculations of the XY model (see Subsec III A). Note that in general, we should to perform a similar calculation for

$$\nu = \frac{p}{d + \zeta}, \quad p \in \mathbb{N} + 1,$$

namely when the $p$-th derivative of the free energy diverges logarithmically.

C. A scaling ansatz for the BKT case

For $d = 1$ at the BKT the correlation function in the TL behaves like $\xi \approx \exp(at^{-\sigma})$. In the typical example of the classical two dimensional XY model it is known that $\sigma = 1/2$. Instead, for the quantum Heisenberg model with frustration (which we will consider in Subsec III C) Haldane suggested $\sigma = 1/4$ [3]. We also set $\zeta = 1$ because the (effective) dimensionality in the BKT scenario is two. The singular part of the finite-size energy density now is conveniently expressed in terms of $y \equiv L/\xi$ so that

$$e(g, L) = e_{\infty,\text{reg}}(g) + L^{-2} [C_0 \Phi_+(y) - F(g)] + O \left( L^{-(2+\epsilon)} \right)$$

where $\Phi_+(y)$ is a universal function that, in the off-critical regime $y \gg 1$, must behave as $\Phi_+(y) \approx y^2$. Again, in the quasicritical regime $y \ll 1$ at any finite $L$ the energy density and its derivatives must be analytic in $(g - g_c)$. The value $\Phi_+(0)$ can be absorbed in $F(g)$ and it can be checked directly that the first contribution has to be at least quadratic in $t = |g - g_c|$ because otherwise a finite-size discontinuity in $b(g, L)$ would be generated. For $y \ll 1$ we adopt the following ansatz (justified from perturbed conformal field theory [12]):

$$e(g, L) = e_{\infty,\text{reg}}(g) + L^{-2} \left[ K (at^{-\sigma} - \ln L)^{-n/\sigma} - F(g) \right] + \ldots$$

with $K$ a constant and $n$ an integer larger than 1 ($n = 3$ from Eq (22) in [12]). Hence

$$b(g, L) = b_{\infty,\text{reg}}(g) + L^{-2} \left[ n K a^{-n/\sigma} t^{n-1} \frac{\text{sgn}(g - g_c)}{t^{n-1}} \right]$$

$$\left( 1 - \frac{\ln L}{a} t^\epsilon \right)^{-\frac{n}{\sigma} - 1} - F'(g) \right] + O \left( L^{-(2+\epsilon)} \right)$$

Now we want to get rid of all the $O(L^{-2})$ contributions that “hinder” the location of finite-size pseudocritical points. Hence we first differentiate with respect to $L$ to eliminate $b_{\infty,\text{reg}}(g)$, then multiply by $L^3$ to isolate the term in square brackets in Eq (12) and finally set to zero a further difference in $L$ in order to drop $F'(g)$. Formally, in the region $L/\xi \ll 1$, we can write down the condition

$$\partial_L \left( L^3 \partial_L b(g^*_L, L) \right) = 0.$$ \hspace{1cm} (13)

It is worth noticing that the latter condition is equal to the HCM Eq. (10) when $d = \zeta = 1$. Treating $L$ as a continuous variable one can read off the shift exponent for the sequence $g^*_L$ that turns out to be $\Delta (\text{BKT}) = \epsilon/(n - 1 + \sigma)$; if $\epsilon = 0$ then the corrections to scaling are also governed by (another) marginal operator and we expect $g^*_L - g_c \sim (\ln L)^{-(m+1)/(n-1+\sigma)}$ with $m$ a positive integer ($m = 4$ from Eq. (22) in [12]).

Dealing with numerical simulations it is very important to specify how one implements the finite-size differences in $L$. In fact, there are several finite-difference expressions used in the literature to express the derivatives and here the requirement is that they all reproduce Eq. (13) in the limit $L \to \infty$. For example, if one takes a uniform step $\delta L$ then the following symmetric expression can be built

$$b'(g, L) = \frac{b(g, L + \delta L) - b(g, L - \delta L)}{2\delta L},$$

$$b''(g, L) = \frac{b(g, L + \delta L) - 2b(g, L) + b(g, L - \delta L)}{(\delta L)^2},$$

and then the precise condition to cancel the term $O(L^{-2})$ becomes

$$L^3 b''(g^*_L, L) + \left[ 3L^2 - (\delta L)^2 \right] b'(g^*_L, L) = 0.$$ \hspace{1cm} (14)

In the limit of large $L$ we recover (13) as required. Clearly, the correct discretization prescription must be identified not only for the BKT; when $d$ and/or $\zeta$ are not one, the suitable variant of (13) for finite $L$ has to be adopted, with $b''$ weighted by $L^{(d+\zeta+1)b}$ and $b'$ weighted by a polynomial in $L$ of degree $(d+\zeta)$ whose coefficients depend on $(\delta L)$.

D. PRG revisited

The PRG method identifies the critical point with the limit of the sequence $g^*_L$ of crossing points satisfying

$$L^\zeta \Delta (g^*_L, L) - (L + \delta L)^\zeta \Delta (g^*_L, L + \delta L) = 0.$$ \hspace{1cm} (15)
Here $\Delta(g, L)$ is the finite-size energy gap of the spectrum for which we may adopt the following form

$$\Delta(g, L) = L^d [e_1(g, L) - e(g, L)] = L^{-\zeta} \Phi(z) + L^{-(\zeta + \epsilon)} C_{\chi},$$

with $\Phi(z) \approx \Phi_0 + z \Phi_1 + z^2 \Phi_2 + \ldots$ and $C_{\chi}$ a prefactor depending on the excited state $|\chi\rangle$ we are considering. The standard PRG approach in $d = 1$ relies upon Eq. (15) with $\zeta = 1$. More generally, a first test to identify $\zeta$ is done by plotting the usual scaled gaps $L \Delta$ and see if at the critical point they settle to a constant or not. If they do not, one is led to search for a better value of $\zeta \neq 1$ and solve (15) with the correct value of the dynamic exponent. Note that the corrections come from the irrelevant/lattice contributions and the Casimir-like term for the gap is actually the constant term in $\Phi(z)$. For quantum systems in $d = 1$, CFT ($\zeta = 1$) predicts $\Phi_0 = 2 \pi d_\chi v(g)$, where $d_\chi$ is the scaling dimension of the operator $\chi$ that generates the excited state $|\chi\rangle$. In addition $\Phi_1, \Phi_2, \ldots$ can be computed in the framework of perturbed CFT, in the regime $z \ll 1$ when a relevant operator $(g - g_c) R$ with scaling dimension $z = 2 - 1/\nu$ is added to the critical field theory. For instance, from Eqs. (7) and (10) of Ref. [12] we have $\Phi_1 = b_\chi/((2\pi)^2$ where $b_\chi$ is the structure constant that appears as prefactor of the three points correlation function $\langle R(\vec{r}_1) \chi(\vec{r}_2) \chi(\vec{r}_3) \rangle$. 

Now, in general the PRG method gives $|g - g_c| \approx L^{-\lambda_{PRG}}$ with $\lambda_{PRG} = 1/\nu + \epsilon$ [11]. However, it may happen that $\Phi_1 = 0$ in the scaling function (examples are discussed in Subsec. III B and at the end of Subsec. III A for a specific excited state of the XY model). The shift exponent in such a case decreases to $\lambda_{PRG} = 1/\nu + \epsilon/2$. Nonetheless there is a way to improve this behavior. In fact, the “extremum” (instead of the zeroes) of the quantity in left side of Eq. (15) with the ansatz [16] is located exactly at the critical point $z = 0$. In order to appreciate a shift from criticality we have to include higher orders of $\tau = (g - g_c)$ in the irrelevant non-scaling term, i.e.

$$L^\tau \Delta(g, L) = \Phi_0 + L^{2/\nu} \tau^2 \Phi_2 + (C_{\chi}(0) + C_{\chi}'(0) \tau) L^{-\epsilon}.$$

In this case, the convergence is $|g - g_c| \approx L^{-\lambda_{extr}}$ with $\lambda_{extr} = 2/\nu + \epsilon$, which is better than usual PRG not only because of the double exponent but also thanks to the coefficient in front: it is proportional to $C_{\chi}(0)$ which is usually a small quantity. It is also worth noticing that in this case $\lambda_{extr} = \lambda_{\text{fast}}$.

III. TESTING THE METHODS

A. XY model in transverse field

To check our methods analytically, we consider the 1D spin-1/2 XY model given by

$$H = -\sum_{j=1}^{L} \left[ \frac{(1 + \eta)}{2} \sigma_j^x \sigma_{j+1}^x + \frac{(1 - \eta)}{2} \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right].$$

(17)

Throughout the paper we will consider $L$ even and PBC. This model can be solved exactly [11] [13] by means of a Jordan-Wigner transformation from spins to spinless fermions followed by a Bogoliubov transformation to arrive at a Hamiltonian of free quasiparticles. The number of original fermions $N' = \sum_i c_i^\dagger c_i$ is not a conserved quantity, but its parity $P = \exp(i \pi N')$ corresponds to a $\pi$-rotation around the $z$-axis, and therefore is conserved. One should beware of a delicate issue concerning boundary conditions. Starting with PBC in Eq. (17), the fermionic Hamiltonian turns to have PBC in the sector of odd parity $P = -1$. Instead in the even parity sector $P = 1$ which comprises the ground state – antiperiodic boundary conditions must be used. In this sector the model becomes

$$H = \sum_k \Lambda(k) \left( \beta_k^x \beta_k - \frac{1}{2} \right),$$

(18)

where $\beta_k$ are Bogoliubov quasiparticles, $k$ ranges in the first Brillouin zone and the dispersion relation is

$$\Lambda(k) = 2 \sqrt{\eta^2 + h^2 + (1 - \eta^2) \cos^2 k + 2h \cos k}.$$

(19)

For $\eta \neq 0$ this model displays an Ising transition at $h = 1$ with exponents $\nu = \zeta = 1$, which means that the scaling variable is $z = L(h - 1)$. To test our ideas we need to calculate, for finite $L$, the GS energy $e_L(h, \eta)$ and the average potential $b_L(h, \eta) = -\langle \sigma_j^z \rangle = \partial e_L/\partial h$, in the quasi-critical region given by $z \ll 1$. According to Eq. (18) the GS is given by $e_L(h, \eta) = -1/2L \sum_k \Lambda(h_k)$ with $k_n = (2n + 1)\pi/L$, $q = 0, \ldots, L - 1$. We then expand the argument of the sum up to the desired order in $z$. For our purposes we need $e_L(h, \eta)$ up to $O(z^2)$ and $b_L(h, \eta)$ up to $O(z)$. The resulting sums are then evaluated with the aid of Euler-Maclaurin formula [14]. The results and the details are given in the Appendix A. From Eqs. (A2) and (A3), one sees explicitly that terms of order $L^{-3}$ are absent both from $e_L$ and $b_L$ so that according to our definition Eq. (5) we find $\epsilon = 2$. In passing we notice that, from Eq. (A2), the Casimir-like term is $-L^{-2} \pi n |\eta| / 6\nu$ consistent with the CFT formula $-L^{-2} \pi c_2 v^2 / 6$. In fact the central charge is $c = 1/2$ and, from the dispersion relation (19) the spin velocity turns out to be $v = 2|\eta|$. Now, using Eqs. (A2) and (A3), we have all the elements to derive the sequences of pseudocritical points analytically. As far as the FSCM is concerned, the pseudo critical points are obtained imposing $b_L(h_n^\ast) = b_{L+2}(h_n^\ast)$, or formally $\partial_L b_L(h_n^\ast) = 0$. Up to leading order in $L$ the solution is

$$h_n^\ast = 1 + \frac{\pi^2}{6L^2},$$

as already obtained in Ref. [8] for the Ising model ($|\eta| = 1$). This shows explicitly that $\lambda_{\text{FSCM}} = 2$ consistent with our prediction $\lambda_{\text{FSCM}} = 2/\nu$ (remind that $\nu = 1$).

For what concerns the “balancing trick” discussed in Sec. II we can show that the solution of Eq. (6), is given by $\gamma^\ast = -1/2\nu^2$. The pseudocritical points are then given imposing $\partial_L \Gamma(h_n^\ast, L, \gamma^\ast) = 0$. In this case, at leading order, the solution is

$$h_n^\ast = 1 - \frac{7\pi^4 (2\eta^4 + \eta^2 - 3)}{720\eta^2} L^{-4},$$

(20)

as obtained in Ref. [8].
which means $\lambda_{\text{fast}} = 4$ once again consistent with our prediction $\lambda_{\text{fast}} = 2/\nu + \epsilon$ (remind that $\epsilon = 2$). From a numerical point of view it is more profitable to use the HCM. From $3\partial_L b + L b_L^2 b = 0$ we obtain

$$h_L^* = 1 + \frac{7\pi^4 (2\eta^2 - 3)}{20\eta^2} L^{-4}$$

with the same exponent $\lambda_{\text{fast}} = 4$.

Now we proceed to discuss the PRG method for which knowledge of the lowest gap is required. The first excited state belongs to the sector with odd parity. Correspondingly, the finite size gap is given, besides a constant term, by the difference between two Riemann sums where the sampling is taken over odd and even (in units of $\pi/L$) wavenumbers respectively. In analogy with Ref. [15] the lowest gap can be eventually written as $\Delta_L = 2(h - 1) + [T(L) - 2T(L/2)]$, where $T(L) = (1/2) \sum_{j=0}^{L-1} \Lambda(j\pi/L)$. Again we refer to the Appendix for the details. Using the form of the gap Eq. (A4) we can evaluate the various terms of the scaling function in Eq. (16)

$$\Phi(z) = \frac{\pi|\eta|}{2} + \frac{\pi^3}{192|\eta|^3} \left[3(1 - h) - 2(2 + h) \eta^2 + 8\eta^4\right] L^{-2} + \ldots$$

Hence $\Phi_0 = \pi|\eta|/2 = 2\pi v_d \chi$, consistently with Ref. [20] for $|\eta| = 1$ and with the known result $d_\chi = 1/8$ for the first excited state of the $c = 1/2$ minimal model [11]. Moreover, since $\Phi_1 \neq 0$, according to the general analysis in Subsec. II D there is no advantage in searching the minima or maxima in $\tau$ of the left hand side of Eq. (15). Looking for the zeros by imposing the PRG equation $\partial_L (L \Delta_L (h_L^*)) = 0$, yields

$$h_L^* = 1 + \frac{\pi^3 (4\eta^2 - 3)}{48 |\eta|} L^{-3} + O(L^{-5})$$

This result for generic $\eta \neq 0$, shows explicitly that the PRG shift exponent is $\lambda_{\text{PRG}} = 3$ and a conjecture put forward by Hamer and Barber in Ref. [15] for the Ising model. From Eq. (20) together with Eq. (16) we read $\epsilon = 2$ as previously, so that the calculated exponent is consistent with the prediction $\lambda_{\text{PRG}} = 1/\nu + \epsilon$.

The explicit calculation of the various shift exponents, confirms that the HCM given by Eq. (10) is superior to the standard PRG method. However, the things are different if we considered the excitation obtained creating a well-defined quasiparticle with the smallest momentum $k = 2\pi/L$, instead of the very first excitation gap. In that case, the energy gap is given by Eq. (19). Using the method of the extrema of the PRG quantity in the left hand side of Eq. (15), we would have obtained a convergence to the critical point as $L^{-4}$, while with the standard PRG only as $L^{-2}$.

### B. $c = 1$ transition (non BKT)

We choose the spin-1 $J_z - D$ model on a chain ($d = 1$) with PBC

$$H = J \sum_{j=1}^L \vec{S}_j \cdot \vec{S}_{j+1} + (J_z - J) S_j^z S_{j+1}^z + D(S_j^z)^2$$

because the transition from the Haldane phase to the phase at large $D$ is described by a $c = 1$ CFT ($\zeta = 1$) with continuously varying exponents. The Hamiltonian [21] has been used to describe the magnetic properties of different quasi 1D compounds (see [16] for a brief account). Here, by fixing $J = 1$ and $J_z = 0.5$, for which it has been already estimated $\nu = 2.38$ [17], we wish to test the methods described above in a severe case in which a $1/\nu$ scaling would give sub-linear convergence in $L$. Indeed for the FSCM we expect $\lambda_{\text{FSCM}} = 0.84$. The previous estimate using the log-log plots of the finite-size gaps was $D_c = 0.65$ [17], while in Ref. [18] it is found $D_c = 0.635$ using the method of level crossing with antiperiodic boundary conditions, which is however specific to this transition. The first irrelevant operator allowed by the lattice symmetries has scaling dimension $K + 2$ where $K = 2 - \frac{2}{\nu}$ so that $\epsilon = \min(K, \epsilon_{\text{lattice}})$ where with $\epsilon_{\text{lattice}}$ we denote the smallest exponent of corrections arising from lattice contributions at finite $L$ that are not captured in the framework of the (relativistic) continuum theory.

As discussed in Refs. [16, 19] this is a case in which the linear term $\Phi_1$ in the scaling function of the PRG vanishes because $b_\chi = 0$ for the sine-Gordon model, the effective field theory that describe the surroundings of the $c = 1$ line. So it is convenient to use also our improved version of the PRG as discussed in Subsec. II D. The expected shift exponent is $\lambda_{\text{extr}} = 2/\nu + \epsilon$.

In order to have an idea of the range of values of $L$ to be used let us imagine that $\epsilon = K$ so that $\lambda_{\text{fast}} = \lambda_{\text{extr}} = 2 + 1/\nu = 2.42$. With $L > 10$ this exponent leads to variations in the pseudocritical points $D_c$ smaller than $O(10^{-3})$. Hence we prefer to illustrate the method with virtually exact numerical data obtained with the Lanczos algorithm using $L = 8, 10, 12, 14, 16$. The reason is that the DMRG would give rather accurate values for the energies but the estimates for $b = \langle h^2 \rangle$ could not be sufficiently precise to appreciate the variations in $D_c$ obtained from the crossings. So we use the DMRG only to extend the data to $L = 18, 20$ with $3^7$ optimized states. In any case the GS belongs to the $S^z_{\text{tot}} = 0$ sector.

The FSCM with $b = \langle h^2 \rangle$ yields $D_{\text{FSCM}} = 0.647$ with $\lambda_{\text{FSCM}} = 0.79$ in reasonable agreement with the CFT expectations. The high-precision procedure based on Eq. (7) yields $D^\text{fast} = 0.633$ with $\lambda_{\text{fast}} = 7.6$. The value of the shift exponent is definitely larger than what expected, which could be due to the vanishing of the coefficient of the first irrelevant contribution with scaling dimensions $K + 2 < \epsilon_{\text{lattice}}$. In any case, from Fig. 1 we can clearly appreciate that the sequence $D_{\text{FSCM}}^c$ converges more slowly than $D_{\text{fast}}^c$. As far as the PRG is concerned, with the standard procedure of finding the zeroes of Eq. (15), we get $D_{\text{PRG}}^c = 0.640$ with $\lambda_{\text{PRG}} = 1.50$. 


with quantities that inherit a residual (possibly oscillating) in the fourth decimal place about (14). As expected the latter sequence converges in a fashion the extremal value of the quantity on the left side of (15) we instead, using the improved method estimation by looking for the HCM described by Eq. (14). Moreover the sequences have been calculated with PRG methods, both standard and in our improved version. Continuous lines are algebraic best-fits to the data.

Instead, using the improved method estimation by looking for the extremal value of the quantity on the left side of (15) we find a rapidly converging sequence that however also oscillates between 0.636 and 0.635. Finally, a small oscillation in the fourth decimal place about 0.6305 is seen also in the sequence $D_L^{\text{hom}}$ obtained through the homogeneity criterion (14). As expected the latter sequence converges in a fashion similar to $D_L^{\text{fast}}$. All these results are summarized in Fig. 1.

The data show that subtracting out the terms that induce a slow convergence of the pseudocritical points, one remains with quantities that inherit a residual (possibly oscillating) $L$-dependence from the specific lattice model and that could be very difficult to account for. Other factors that affect the extrapolation of the critical points at this level of accuracy are the sampling $\delta D$ and the trade-off between computational accuracy and the maximum available size.

To summarize we observe that our improved methods yield very fast convergence to the critical point that we estimate to be $D_c = 0.633 \pm 0.02$, consistently with Ref. [18].

C. $c = 1$ BKT transition

We consider now the spin-1/2 Heisenberg model with frustration due to next-to-nearest neighbors interaction

$$H = \sum_{j=1}^{L} J_1 \vec{S}_j \cdot \vec{S}_{j+1} + J_2 \vec{S}_j \cdot \vec{S}_{j+2}.$$ 

The model is equivalent to a 2-legs zigzag ladder with $L/2$ rungs. The best estimate of the critical point was made by Okamoto and Nomura using a model-specific crossing method [9]; with exact diagonalizations up to $L = 24$ they determined $J_{2c}/J_1 = 0.2411 \pm 0.0001$. The model is gapless for $J_2 < J_{2c}$ and has a doubly degenerate GS in the TL for $J_2 > J_{2c}$. Again the GS has $S^z_{\text{tot}} = 0$. Without exploiting a priori information about the BKT character of transition (if not the value of the dynamic exponent $\zeta = 1$), we tested the homogeneity criterion (14) using $\delta L = 4$ and 1024 DMRG states that ensure an accuracy of $O(10^{-7})$ on the values of $b = (\vec{S}_j \cdot \vec{S}_{j+2})$. The results reported in Fig. 2 are encouraging: while with the FSCM we would get no crossings at all, the zeroes of Eq. (14) yield a sequence of points converging to $J_2 \sim 0.25$. The main problem comes from the left side of the transition where the truncation DMRG error for $L = 28$ and 32 induces some oscillations on the plotted quantity. We content ourselves with linear fits in $1/L$. If we exclude the point with $L = 12$ the fit is better even if we find $J_{2c}/J_1 = 0.2553 \pm 0.0008$; by selecting all the available points, instead, the fit is visibly worse but the extrapolated value is $J_{2c}/J_1 = 0.242 \pm 0.006$, in agreement with Ref. [9]. As above, apart from the details of the extrapolation procedure, we see that the homogeneity criterion provides a viable procedure to locate the critical point in a BKT transition, where almost all existing generic methods fail. We remark that this analysis is based solely on $b(g, L)$, namely an observable evaluated on the GS, without invoking further assumptions on the nature of the excitations.

IV. CONCLUSIONS

Making only use of finite-size quantities related to the ground state, we show how to generate sequences of pseudocritical points that converge very fast to the infinite-size critical point. The convergence is of the form $L^{-\lambda}$ with a shift exponent $\lambda$. In this article we propose a homogeneity condition method (HCM) which is faster than the standard phenomenological renormalization group (PRG) in locating the critical points. Moreover its validity is more general as it can be applied without modification to the difficult case of a Berezinskii-Kosterlitz-Thouless transition. The homogeneity method requires only the knowledge of $b(g, L) = \langle V \rangle / L^d$, that is, the expectation value of the term that drives the transition.

We also presented an improvement to the PRG method, which allows, under certain conditions, to obtain pseudocritical sequences characterized by the same shift exponent as for the HCM. However, this modification, relying on a particular form of the gap scaling function, is not valid in general. It holds true, for instance for the sine-Gordon model that underlies a variety of transitions in $(1 + 1)$ dimension.

The formulations of the approaches are sufficiently general to be applied in any spatial dimensionality. Even if we are primarily interested in quantum phase transitions ideally at zero temperature, in principle the methods can be extended to problems of finite-temperature statistical mechanics. At variance with other accelerating methods found in the literature, e.g. the van den Broeck-Schwartz or the Bulirsch-Stoer ones (reviewed in Ch. 9 of [11]), the procedures presented here rely on the scaling behavior of thermodynamical quantities expected from physical and renormalization arguments.
Appendix A:

Here we indicate how to compute the mean energy per site $e_L$ and the average potential $b_L$, as require id in Subsec. III A.

Consider for example the energy sum

$$e_L(h, \eta) = -\frac{1}{2L} \sum_{n=0}^{L-1} \Lambda(k_n), \quad k_n = \frac{2n+1}{L} \pi,$$

where $\Lambda(k)$ is given by Eq. (19). We need to investigate the above sum in the quasi-critical region $z = L/\xi \ll 1$ so it is sufficient to expand $e_L(h, \eta)$ in powers of $(h-1) = z/L$.

$$e_L(h, \eta) = -\frac{1}{2L} \sum_{n=0}^{L-1} \left[ \Lambda_{h=1}(k_n) + \frac{z}{L} \partial_h \Lambda|_{h=1}(k_n) \right. \\
+ \left. \left( \frac{z}{L} \right)^2 \frac{1}{2} \partial^2_h \Lambda|_{h=1}(k_n) + O(z^3) \right].$$

The resulting sums can be computed using the Euler-Maclaurin formula (see e.g. [14])

$$\delta \sum_{j=0}^N f(a+j\delta) = \int_a^b f(x)dx + \frac{\delta}{2} [f(a) + f(b)] + \\
\sum_{r=0}^{m} \frac{\delta^{2r}}{(2r)!} B_{2r} \left[ f^{(2r-1)}(b) - f^{(2r-1)}(a) \right] + R_m \quad (A1)$$

valid for a function $f$ with at least $2m$ continuous derivatives in $(a, b)$. Here $B_n$ are the Bernoulli numbers and the remainder $R_m$ depends on $f^{(2m)}$ on $(a, b)$. Some care must be taken when the function $f$ diverges at the border of the Brillouin zone, in this case one must keep $a$ and $b$ away from the borders. Moreover, sending $m$ to infinity in Eq. (A1), some sums must be regularized using a Borel summation technique. The final result for the ground state energy is

$$e_L(h, \eta) = e_\infty(1, \eta) - \frac{\pi |\eta|}{6} L^{-2} - \frac{7\pi^3}{360} \frac{(4\eta^2 - 3)}{|\eta|} L^{-4}$$

$$+ (h - 1) \left[ b_\infty(1, \eta) - \frac{\pi}{12 |\eta|} L^{-2} \right]$$

$$- \frac{(h - 1)^2}{2} \ln(L) + \gamma_C + \ln \left( \frac{8 |\eta|/\pi - 1}{\pi |\eta|} \right) - O(z^3) \quad (A2)$$

where $\gamma_C = 0.577216...$ is the Euler-Mascheroni constant and the thermodynamic values are given by

$$e_\infty(1, \eta) = -\left[ \frac{2|\eta|}{\pi} + \frac{2\arctan(\sqrt{1-\eta^2}/|\eta|)}{\pi\sqrt{1-\eta^2}} \right]$$

$$b_\infty(1, \eta) = -\frac{2\arctan(\sqrt{1-\eta^2}/|\eta|)}{\pi\sqrt{1-\eta^2}}.$$

The validity of the methods has been tested with analytical calculations on the one dimensional XY model in transverse field and numerically on a nontrivial spin-1 chain with anisotropy. As extreme case, we have shown that the homogeneity condition method provides a satisfactory location of the critical point also in the case of Berezinskii-Kosterlitz-Thouless transitions. These confirmations motivate us to consider systems in higher spatial dimensionality. In these cases the numerical data are restricted to smaller system-size and the need for fast-converging pseudo-critical sequences is a prerequisite for the precise location of the critical points.

Acknowledgments

This work was partially supported by the Italian MiUR through the PRIN grant n. 2005021773. M.R. acknowledges support from the EU (SCALA). Numerical calculations were performed on a cluster of machines made available by the Theoretical Group of the Bologna Section of the INFN.
Using similar procedures we obtain the following expression for average potential \( b_L (h, \eta) \):

\[
b_L (h, \eta) = b_\infty (1, \eta) - \frac{\pi}{12 |\eta|} L^{-2} - \frac{7\pi^3 (3 - 2\gamma^2)}{2880 |\eta|^3} L^{-4} \\
- (h - 1) \frac{\ln (L) + \gamma_C + \ln (8|\eta| / \pi) - 1}{\pi |\eta|} + O \left( z^2 \right).
\]

(A3)

Finally, the sum

\[
T(L) = \frac{1}{L} \sum_{j=0}^{L-1} \Lambda \left( \frac{2\pi j}{L} \right)
\]

for the evaluation of the finite-size gap in the PRG method, can be treated along similar lines. The final result for the gap is

\[
\Delta_L = (h - 1) + \frac{\pi (2\eta^2 + h - 1)}{4 |\eta|} L^{-1} \\
+ \frac{\pi^3 \left[ 3(h - 1) - 2(2 + h) \eta^2 + 8\eta^4 \right]}{192 |\eta|^3} L^{-3} + O \left( L^{-5} \right).
\]

(A4)

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