Determination of the critical manifold tangent space and curvature with Monte Carlo renormalization group

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We show that the critical manifold of a statistical mechanical system in the vicinity of a critical point is locally accessible through correlation functions at that point. A practical numerical method is presented to determine the tangent space and the curvature to the critical manifold with variational Monte Carlo renormalization group. Because of the use of a variational bias potential of the coarse-grained variables, critical slowing down is greatly alleviated in the Monte Carlo simulation. In addition, this method is free of truncation error. We study the isotropic Ising model on square and cubic lattices, the anisotropic Ising model, and the tricritical Ising model on square lattices to illustrate the method.

I. INTRODUCTION

The introduction of renormalization group (RG) theory in statistical physics [1] has greatly deepened our understanding of phase transitions. Our understanding of RG, however, is far from complete. The actual implementation of the RG procedure remains a highly nontrivial task. The critical manifold of a lattice model is defined as the set of coupling constants for which the long range physics of the system is described by a unique underlying scale-invariant field theory. However, the same lattice model may admit different critical behaviors described by different field theories upon changing the coupling constants. This is the case, for instance, in the tricritical Ising model to be discussed later. Thus, the critical manifold is always defined with respect to the field theory underlying the lattice model. It could be defined in any space of coupling constants associated with a finite number of coupling terms with co-dimension in that space equal to the number of relevant operators of the system. General RG theory requires that the RG flow should go into a unique fixed-point Hamiltonian if the starting point of the flow is on the critical manifold. There are various "natural" RG procedures where different points on a critical manifold do not go to the same critical fixed point, the most well-known example being the decimation rule in dimensions higher than one [2]. By contrast, when an RG procedure satisfies this requirement, the attractive basin of the critical fixed point is the entire critical manifold, and a computational scheme should exist, at least, in principle, to identify the critical manifold. Whether or not this approach can be successfully pursued were a stringent test of the RG procedure under consideration. Conversely, the knowledge of the critical manifold provides a straightforward way to check the validity of any RG procedure: One could simply simulate the RG flow starting from two different points in the critical manifold and verify that they eventually land on the same fixed point. This consideration alone should be enough motivation for developing a method to compute the critical manifold.

Another issue for which the knowledge of the critical manifold would be of interest is the study of the geometry of the coupling constant space, i.e., the parameter manifold of a classical or quantum many-body system. How to define a Riemannian metric in the parameter manifold has been proposed for a long time for both classical [3] and quantum systems [4]. Recently, there have been developments in understanding the significance of the geometry of the parameter manifold for both classical and quantum systems [5–9]. One would expect knowledge of the critical manifold would fit naturally into such developments. We do not pursue further this issue here, but we leave it to future research.

In this paper, we present a method to determine the tangent space and curvature of the critical manifold at the critical points of a system with variational Monte Carlo (MC) renormalization group (VMCRG) [10]. We will show that, unlike the computation of the critical exponents with Monte Carlo renormalization group [11] or VMCRG, the determination of the critical manifold tangent space (CMTS) and curvature does not suffer truncation error no matter how few renormalized coupling terms are used. We discuss first the case where there are no marginal operators along the RG flow and then the case where there are. The examples that we consider in this paper are all classical, but the method can be extended to quantum systems if a sign-free path-integral representation of the quantum system would be available.

II. MONTE CARLO RENORMALIZATION GROUP AND THE CRITICAL MANIFOLD

A. Coarse-graining and renormalized coupling constants

For notational simplicity, we use the terminology for classical magnetic spins on a lattice in the following discussion, although the formalism applies in general. Consider a statistical mechanical system in d-spatial dimensions with spins σ

and Hamiltonian $H^{(0)}(\boldsymbol{\sigma})$,

$$H^{(0)}(\boldsymbol{\sigma}) = \sum_{\beta} K_{\beta}^{(0)} S_{\beta}(\boldsymbol{\sigma}), \tag{1}$$

where $S_{\beta}(\boldsymbol{\sigma})$'s are the coupling terms of the system, such as nearest-neighbor spin products, next-nearest-neighbor spin products, etc., and $\mathbf{K}^{(0)} = \{K_{\beta}^{(0)}\}$ are the corresponding coupling constants. Here, we call the original Hamiltonian before any RG transformation the zeroth level renormalized Hamiltonian, hence, the notation (0) in the superscript. The critical manifold is, then, defined in the space of $K_{\beta}^{(0)}$ corresponding to a finite set of couplings $S_{\beta}(\boldsymbol{\sigma})$.

In a real-space RG calculation, one defines coarse-grained spins $\boldsymbol{\sigma}'$ in the renormalized system with a conditional probability $T(\boldsymbol{\sigma}'|\boldsymbol{\sigma})$ that effects a scale transformation with scale factor b. $T(\boldsymbol{\sigma}'|\boldsymbol{\sigma})$ is the probability of $\boldsymbol{\sigma}'$ given spin configuration $\boldsymbol{\sigma}$ in the original system. The majority rule block spin in the Ising model proposed by Kadanoff *et al.* [12] is one example of the coarse-grained variables. $T(\boldsymbol{\sigma}'|\boldsymbol{\sigma})$ can be iterated n times to define the nth level coarse-graining $T^{(n)}(\boldsymbol{\mu}|\boldsymbol{\sigma})$ realizing a scale transformation with scale factor b^n,

$$T^{(n)}(\boldsymbol{\mu}|\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}^{(n-1)}} \cdots \sum_{\boldsymbol{\sigma}^{(1)}} T(\boldsymbol{\mu}|\boldsymbol{\sigma}^{(n-1)}) \cdots T(\boldsymbol{\sigma}^{(1)}|\boldsymbol{\sigma}). \tag{2}$$

$T^{(n)}$ defines the nth level renormalized Hamiltonian $H^{(n)}(\boldsymbol{\mu})$ up to a constant $g(\mathbf{K}^{(0)})$ independent of $\boldsymbol{\mu}$ [13],

$$H^{(n)}(\boldsymbol{\mu}) \equiv -\ln \sum_{\boldsymbol{\sigma}} T^{(n)}(\boldsymbol{\mu}|\boldsymbol{\sigma}) e^{-H^{(0)}(\boldsymbol{\sigma})} + g(\mathbf{K}^{(0)})$$

$$= \sum_{\alpha} K_{\alpha}^{(n)} S_{\alpha}(\boldsymbol{\mu}) + g(\mathbf{K}^{(0)}), \tag{3}$$

where $\{K_{\alpha}^{(n)}\}$'s are the nth level renormalized coupling constants associated with the coupling terms $S_{\alpha}(\boldsymbol{\mu})$ defined for the nth level coarse-grained spins. Modulo the constant coupling term, $T^{(n)}(\boldsymbol{\mu}|\boldsymbol{\sigma})$ defines $H^{(n)}(\boldsymbol{\mu})$ uniquely. $H^{(n)}$ renormalized from different starting Hamiltonians $H^{(0)}$ will generally be different. However, if no marginal operators appear in the RG transformation, the renormalized Hamiltonians from different initial points on the critical manifold will converge to the same critical fixed-Hamiltonian $H^*(\boldsymbol{\mu})$ as n goes to infinity.

To probe $H^*(\boldsymbol{\mu})$ in a MC simulation, one increases the iteration level n and the system size L until the renormalized Hamiltonian $H^{(n)}$ becomes invariant with n to the desired accuracy and the L dependence becomes negligible. It is generally impossible to determine all of the coupling constants of $H^{(n)}(\boldsymbol{\mu})$ because their number increases combinatorially with the lattice size. In practice, one adopts some truncation scheme and approximates $H^{(n)}$ with a finite number of coupling terms $\{S_{\alpha}(\boldsymbol{\mu})\}$ with coupling constants $K_{\alpha}^{(n)}$,

$$H^{(n)}(\boldsymbol{\mu}) \approx \sum_{\alpha} K_{\alpha}^{(n)} S_{\alpha}(\boldsymbol{\mu}). \tag{4}$$

B. Critical manifold tangent space in the absence of marginal operators

To compute the CMTS, let us suppose that $K_{\beta}^{(0)}$ and $K_{\beta}^{(0)} + \delta K_{\beta}^{(0)}$ belong to the critical manifold and apply the RG proce-

dure starting from these two points. As the difference in the irrelevant directions becomes exponentially suppressed with progressively large n, the corresponding two renormalized Hamiltonians will tend to the same Hamiltonian $H^{(n)}$ in the absence of RG marginal operators. In particular, the truncated coupling constants $K_{\alpha,\text{truncate}}^{(n)}$ and $K_{\alpha,\text{truncate}}^{(n)} + \delta K_{\alpha,\text{truncate}}^{(n)}$, renormalized from $K_{\beta}^{(0)}$ and $K_{\beta}^{(0)} + \delta K_{\beta}^{(0)}$, respectively, will be equal within deviations exponentially small with n because they are the truncation approximation for two Hamiltonians $H^{(n)}$ and $H^{(n)} + \delta H^{(n)}$, whose difference is exponentially small in n. Thus, the spanning set of the CMTS $\{\delta K_{\beta}^{(0)}\}$ satisfies the following equation for sufficiently large n:

$$K_{\alpha,\text{truncate}}^{(n)} + \sum_{\beta} \frac{\partial K_{\alpha,\text{truncate}}^{(n)}}{\partial K_{\beta}^{(0)}} \delta K_{\beta}^{(0)} = K_{\alpha,\text{truncate}}^{(n)} \tag{5}$$

for every α. That is, the CMTS $\{\delta K_{\beta}^{(0)}\}$ is the kernel of the nth level RG Jacobian,

$$\mathcal{A}_{\alpha\beta}^{(n,0)} \equiv \frac{\partial K_{\alpha,\text{truncate}}^{(n)}}{\partial K_{\beta}^{(0)}} \tag{6}$$

for any well-defined truncation scheme. In the following, we will use $K_{\alpha}^{(n)}$ to denote the truncated coupling constants.

As shown in Ref. [10], VMCRG provides an efficient way to compute the renormalized constants and the RG Jacobian matrix with MC under a given truncation scheme. It introduces a bias potential $V(\boldsymbol{\mu})$ of the coarse-grained variables, expanded in a finite set of renormalized couplings $S_{\alpha}(\boldsymbol{\mu})$ with variational parameters J_{α},

$$V_{\mathbf{J}}(\boldsymbol{\mu}) = \sum_{\alpha} J_{\alpha} S_{\alpha}(\boldsymbol{\mu}), \tag{7}$$

and a variational function of $\mathbf{J} = \{J_{\alpha}\}$,

$$\Omega(\mathbf{J}) = \ln \sum_{\boldsymbol{\mu}} e^{-[H^{(n)}(\boldsymbol{\mu}) + V_{\mathbf{J}}(\boldsymbol{\mu})]} + \sum_{\boldsymbol{\mu}} V_{\mathbf{J}}(\boldsymbol{\mu}) p_t(\boldsymbol{\mu}), \tag{8}$$

where $p_t(\boldsymbol{\mu})$ is a preset target probability distribution, which will be taken as the uniform distribution in the following. As proved in Ref. [14], Ω is convex in each J_{β}, and, if one excludes the constant coupling term, has a unique minimizer $\mathbf{J}_{\min}$, which can be found with a stochastic gradient descent algorithm using the Jacobian and the Hessian of $\Omega(\mathbf{J})$ [10],

$$\frac{\partial \Omega(\mathbf{J})}{\partial J_{\alpha}} = -\langle S_{\alpha}(\boldsymbol{\mu}) \rangle_{V_{\mathbf{J}}} + \langle S_{\alpha}(\boldsymbol{\mu}) \rangle_{p_t}, \tag{9}$$

$$\frac{\partial^2 \Omega(\mathbf{J})}{\partial J_{\alpha} \partial J_{\beta}} = \langle S_{\alpha}(\boldsymbol{\mu}) S_{\beta}(\boldsymbol{\mu}) \rangle_{V_{\mathbf{J}}} - \langle S_{\alpha}(\boldsymbol{\mu}) \rangle_{V_{\mathbf{J}}} \langle S_{\beta}(\boldsymbol{\mu}) \rangle_{V_{\mathbf{J}}}. \tag{10}$$

Here $\langle \cdot \rangle_{V_{\mathbf{J}}}$ is the biased ensemble average under $V_{\mathbf{J}}$, and $\langle \cdot \rangle_{p_t}$ is the ensemble average under the target probability distribution p_t. The minimizer $\mathbf{J}_{\min}$ then satisfies the minimizing condition: For every renormalized coupling $S_{\gamma}(\boldsymbol{\mu})$,

$$\langle S_{\gamma}(\boldsymbol{\mu}) \rangle_{V_{\min}} = \langle S_{\gamma}(\boldsymbol{\mu}) \rangle_{p_t}. \tag{11}$$

If the set of the coupling terms S_{α} is complete, $V_{\min}(\boldsymbol{\mu}) = \sum_{\alpha} J_{\alpha,\min} S_{\alpha}(\boldsymbol{\mu}) = -H^{(n)}(\boldsymbol{\mu})$, and we identify for each α,

$$K_{\alpha}^{(n)} = -J_{\alpha,\min}. \tag{12}$$

Because the set of $S_{\alpha}(\boldsymbol{\mu})$ is not complete, a truncation error in computing $K_{\alpha}^{(n)}$ is incurred. However, because the minimizer

of Ω is unique, the truncation scheme is well defined. Within VMCRG, $\mathcal{A}_{\alpha\beta}^{(n,0)}$ can be obtained by expanding Eq. (11) to linear order in $\delta K_\beta^{(0)}$ and $\delta K_\alpha^{(n)}$. The result [10] is that, for a given β, every $S_\gamma(\boldsymbol{\mu})$ must satisfy

$$\sum_\alpha \langle\langle S_\gamma(\boldsymbol{\mu}), S_\alpha(\boldsymbol{\mu})\rangle\rangle_V \frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(0)}} = \langle\langle S_\gamma(\boldsymbol{\mu}), S_\beta(\boldsymbol{\sigma})\rangle\rangle_V, \quad (13)$$

where $\langle\langle X, Y\rangle\rangle_V \equiv \langle XY\rangle_V - \langle X\rangle_V\langle Y\rangle_V$ is the connected correlation function of the observables X and Y in the biased ensemble with the potential $V_{\min}(\boldsymbol{\mu})$. Thus, for any β, the Jacobian matrix element $\mathcal{A}_{\alpha\beta}^{(n,0)} = \frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(0)}}$, viewed as a column vector indexed by α, can be obtained from Eq. (13) by matrix inversion.

We also note that the method described above works for any target distribution $p_t(\boldsymbol{\mu})$ in VMCRG. A different $p_t(\boldsymbol{\mu})$ will result in a different bias potential $V_{\min}(\boldsymbol{\mu})$ to be used in the sampling of the matrix $\mathcal{A}^{(n,0)}$. We use the uniform distribution here because, then, $V_{\min}(\boldsymbol{\mu})$ acts to eliminate the long-range correlation in a critical system, and the resultant ensemble for the sampling of $\mathcal{A}^{(n,0)}$ benefits from a much faster MC relaxation [10]. However, one can impose any arbitrary bias potential of the coarse-grained variables $V(\boldsymbol{\mu})$ and adopt the corresponding biased distribution as the target distribution. All the steps in the above derivation follow, and the CMTS can then be computed in the biased ensemble with the arbitrary $V(\boldsymbol{\mu})$. In particular, if one insists on using the original ensemble with no bias potential, one only needs to set the target distribution to be the original unbiased distribution in which case $V_{\min}$ necessarily vanishes and $\mathcal{A}^{(n,0)}$ is sampled in the unbiased ensemble.

C. Critical manifold tangent space in the presence of marginal operators

When there are marginal operators in the RG transformation, two different points on the critical manifold will converge to different fixed-point Hamiltonians. However, starting from any point on the critical manifold, at sufficiently large n, $H^{(n)}$ will be equal to $H^{(n+1)}$, and so will the truncated renormalized constants $K_\alpha^{(n)}$ be equal to $K_\alpha^{(n+1)}$. Now, suppose that both $K_\beta^{(0)}$ and $K_\beta^{(0)} + \delta K_\beta^{(0)}$ are on the critical manifold giving rise to the truncated renormalized constants $K_\alpha^{(n)}$ and $K_\alpha^{(n)} + \delta K_\alpha^{(n)}$, respectively. Then, the spanning set of CMTS $\{\delta K_\beta^{(0)}\}$, instead of Eq. (5), satisfies the following condition:

$$K_\alpha^{(n)} + \sum_\beta \frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(0)}}\delta K_\beta^{(0)} = K_\alpha^{(n+1)} + \sum_\beta \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(0)}}\delta K_\beta^{(0)} \quad (14)$$

for every α. But $K_\alpha^{(n)}$ and $K_\alpha^{(n+1)}$ are already equal up to an exponentially small difference because they are renormalized from the same point on the critical manifold. Thus, when marginal operators appear in the RG transformation, the CMTS is the kernel of the matrix,

$$\mathcal{A}_{\alpha\beta}^{(n+1,0)} - \mathcal{A}_{\alpha\beta}^{(n,0)}. \quad (15)$$

D. The normal vectors to critical manifold tangent space

Because of the spin-flip symmetry, the renormalization of the even operators and of the odd operators are decoupled in the examples we consider here, so they can be considered separately. In the Ising models that we discuss later, the co-dimension of the critical manifold is one, and the tangent space is, thus, a hyperplane and the row vectors of $\mathcal{A}^{(n,0)}$ or $\mathcal{A}^{(n+1,0)} - \mathcal{A}^{(n,0)}$ for systems with or without marginal operators are orthogonal to this hyperplane. This means that the row vectors of $\mathcal{A}^{(n,0)}$ or $\mathcal{A}^{(n+1,0)} - \mathcal{A}^{(n,0)}$ are all normal vectors to the CMTS and are parallel to one another. Thus, the $\mathcal{P}$ matrix defined as

$$\mathcal{P}_{\alpha\beta} = \frac{\mathcal{A}_{\alpha\beta}^{(n,0)}}{\mathcal{A}_{\alpha 1}^{(n,0)}} \quad \text{or} \quad \frac{\mathcal{A}_{\alpha\beta}^{(n+1,0)} - \mathcal{A}_{\alpha\beta}^{(n,0)}}{\mathcal{A}_{\alpha 1}^{(n+1,0)} - \mathcal{A}_{\alpha 1}^{(n,0)}}, \quad (16)$$

that contains the normalized row vectors of $\mathcal{A}^{(n,0)}$ or $\mathcal{A}^{(n+1,0)} - \mathcal{A}^{(n,0)}$ should have identical rows.

In the tricritical Ising model that we also discuss, the critical manifold in the even subspace has co-dimension two [15]. In this case, we cannot expect all the rows of $\mathcal{P}_{\alpha\beta}$ to be equal. Instead, the rows should form a two-dimensional (2D) vector space to which the CMTS is orthogonal. This outcome can be checked, for example, by verifying that all the row vectors of $\mathcal{P}_{\alpha\beta}$ lie in the vector space spanned by its first two rows. If such consistency checks can be satisfied, it is a testament of the validity of RG theory, which predicts that a critical fixed-point Hamiltonian exists and that the co-dimension of the critical manifold has precisely the assumed value for the models considered in this paper.

In general, the CMTS computed from different renormalized couplings will have different statistical uncertainties because the sampling noise differs for different correlation functions in an MC simulation. One should, thus, trust the result with the least uncertainty and use the values computed from other renormalized constants as a consistency check.

III. NUMERICAL RESULTS FOR CMTS

A. Two-dimensional isotropic Ising model

Consider the isotropic Ising model on a 2D square lattice with Hamiltonian $H(\boldsymbol{\sigma})$,

$$H(\boldsymbol{\sigma}) = -K_{\mathrm{nn}}^{(0)} \sum_{\langle i,j\rangle} \sigma_i\sigma_j - K_{\mathrm{nnn}}^{(0)} \sum_{[i,j]} \sigma_i\sigma_j, \quad (17)$$

where $\langle i, j\rangle$ denotes the nearest-neighbor pairs and $[i, j]$ denotes the next-nearest-neighbor pairs. $K_{\mathrm{nn}}^{(0)}$ and $K_{\mathrm{nnn}}^{(0)}$ are the corresponding coupling constants. This model is analytically solvable when $K_{\mathrm{nnn}}^{(0)} = 0$ and is critical at the Onsager point with $K_{\mathrm{nn}}^{(0)} = 0.4407\cdots$ [16]. Four critical points are first located with VMCRG in the coupling space of $\{K_{\mathrm{nn}}^{(0)}, K_{\mathrm{nnn}}^{(0)}\}$. This task can be achieved by fixing $K_{\mathrm{nnn}}^{(0)}$ and varying $K_{\mathrm{nn}}^{(0)}$ whereas monitoring how the corresponding renormalized coupling constant $K_{\mathrm{nn}}^{(n)}$ varies with n, the RG iteration index. The largest value of the original coupling constant $K_{\mathrm{nn},1}^{(0)}$ for which $K_{\mathrm{nn}}^{(n)}$ decreases with n and the smallest value $K_{\mathrm{nn},2}^{(0)}$ for which $K_{\mathrm{nn}}^{(n)}$ increases with n define the best estimate within statistical errors of the interval $[K_{\mathrm{nn},1}^{(0)}, K_{\mathrm{nn},2}^{(0)}]$ of the location of the critical coupling $K_{\mathrm{nn},c}^{(0)}$. We note that the calculated

TABLE I. $\mathcal{P}_{\alpha\beta}$ for the isotropic Ising model. α indexes rows corresponding to the three renormalized constants: nn, nnn, and $\square$. The fourth row of the table at the Onsager point shows the exact values. $\beta = 2$–4, respectively, indexes the component of the normal vector to the CMTS corresponding to coupling terms nnn, $\square$, and nnnn. $\beta = 1$ corresponds to the nn coupling term, and $\mathcal{P}_{\alpha 1}$ is always 1 by definition. The simulations were performed on 16 cores independently, each of which ran 3×10^6 Metropolis MC sweeps. The standard errors are cited as the statistical uncertainty.

$K_{nn}^{(0)}$	$K_{nnn}^{(0)}$	$\mathcal{P}_{\alpha 2}$	$\mathcal{P}_{\alpha 3}$	$\mathcal{P}_{\alpha 4}$
0.4407	0	1.4134(3)	0.5135(3)	1.7963(5)
		1.4146(7)	0.5134(7)	1.799(2)
		1.413(3)	0.511(3)	1.794(7)
Exact		1.4142	0.5139	1.8006
0.37	0.0509	1.3717(4)	0.5242(3)	1.7664(8)
		1.375(1)	0.5243(7)	1.773(2)
		1.372(4)	0.527(3)	1.773(6)
0.228	0.1612	1.2529(7)	0.5303(4)	1.6545(8)
		1.254(1)	0.5318(8)	1.659(2)
		1.252(5)	0.535(3)	1.65(1)
0.5	−0.0416	1.4441(4)	0.5019(5)	1.816(1)
		1.444(2)	0.503(2)	1.818(4)
		1.441(7)	0.499(6)	1.80(1)

renormalized constants are truncated and we assume here that the truncated $K_{nn}^{(n)}$ increases or decreases monotonically with the exact $K_{nn}^{(n)}$. This assumption is very natural and does not seem to be violated in the present paper. Alternatively, the same procedure can be performed by fixing K_{nn} and varying K_{nnn}. In the following VMCRG calculations, we use $n = 4$, $L = 256$, and the $b = 2$ majority rule with a random pick on tie. We use three renormalized couplings: the nearest-neighbor product $K_{nn}^{(n)}$, the next-nearest product $K_{nnn}^{(n)}$, and the smallest plaquette $K_{\square}^{(n)}$. The model is known to have no marginal operators. The four critical points shown in Table I all belong to the same critical phase as they all flow into the same truncated fixed-point renormalized Hamiltonian. The CMTSs are determined at these critical points in a four-dimensional coupling space spanned by $K_{nn}^{(0)}$, $K_{nnn}^{(0)}$, $K_{\square}^{(0)}$, and the third-nearest-neighbor products $K_{nnnn}^{(0)}$. The $\mathcal{P}_{\alpha\beta}$ is shown in Table I. In addition, we also show the CMTS at the Onsager point, which is analytically solvable [17].

The CMTS can also be computed in the odd coupling subspace as we show here for the Onsager point. In this calculation, we take $n = 5$, $L = 256$, and again the $b = 2$ majority rule for coarse graining. The CMTS in a space of four odd couplings, listed in the legend of Table II, is calculated from the same four renormalized couplings. The result is shown in Table II.

B. Three-dimensional istropic Ising model

Consider now the same model on a three-dimensional (3D) square lattice with $K_{nnn}^{(0)} = 0$, i.e., the 3D isotropic nearest-neighbor Ising model. This model does not have an analytical solution but is known to experience a continuous transition at $K_{nn}^{(0)} = 0.221\,65\cdots$ [18]. To compute the CMTS at this nearest-neighbor critical point, we use $n = 3$, $L = 64$, and

TABLE II. $\mathcal{P}_{\alpha\beta}$ for the odd coupling space of the isotropic Ising model. α indexes rows corresponding to the four renormalized odd spin products: $(0, 0)$, $(0, 0)$-$(0, 1)$-$(1, 0)$, $(0, 0)$-$(1, 0)$-$(-1, 0)$ and $(0, 0)$-$(1, 1)$-$(-1, -1)$ where the pair (i, j) is the coordinate of an Ising spin. The simulations were performed on 16 cores independently, each of which ran 3×10^6 Metropolis MC sweeps. The standard errors are cited as the statistical uncertainty.

$K_{nn}^{(0)}$	$K_{nnn}^{(0)}$	$\mathcal{P}_{\alpha 2}$	$\mathcal{P}_{\alpha 3}$	$\mathcal{P}_{\alpha 4}$
0.4407	0	3.31248(8)	1.65629(4)	1.49852(6)
		3.296(2)	1.649(4)	1.479(2)
		3.315(3)	1.658(2)	1.503(2)
		3.32(5)	1.68(4)	1.51(3)

the $b = 2$ majority rule with a random pick on tie. The CMTS is computed in an eight-dimensional coupling space $\{K^{(0)}\}$ spanned by the nearest-neighbor and the next-nearest-neighbor renormalized coupling constants $K_{nn}^{(n)}$ and $K_{nnn}^{(n)}$ as shown in Table III.

C. Two-dimensional anistropic Ising model

Consider then the anisotropic Ising model on a 2D square lattice with Hamiltonian $H(\boldsymbol{\sigma})$,

$$H(\boldsymbol{\sigma}) = -K_{nn_x}^{(0)} \sum_{\langle i, j \rangle_x} \sigma_i \sigma_j - K_{nn_y}^{(0)} \sum_{\langle i, j \rangle_y} \sigma_i \sigma_j, \qquad (18)$$

where $\langle i, j \rangle_x$ and $\langle i, j \rangle_y$, respectively, denote the nearest-neighbor pairs along the horizontal and the vertical directions. In the space of $\{K_{nn_x}^{(0)}, K_{nn_y}^{(0)}\}$, the model is exactly solvable and is critical along the line [19],

$$\sinh\left(2K_{nn_x}^{(0)}\right) \sinh\left(2K_{nn_y}^{(0)}\right) = 1. \qquad (19)$$

With the 2×2 majority rule, the system admits a marginal operator due to anisotropy in the RG transformation [20]. We performed VMCRG calculations on two critical points of the system with $K_{nn_y}^{(0)}/K_{nn_x}^{(0)} = 2$ and 3 with four renormalized couplings $K_{nn_x}^{(n)}$, $K_{nn_y}^{(n)}$, $K_{nnn}^{(n)}$, and $K_{\square}^{(n)}$. The CMTS is computed in the coupling space $\{K_{nn_x}^{(0)}, K_{nn_y}^{(0)}, K_{nnn}^{(0)}, K_{\square}^{(0)}, K_{nnnn_x}^{(0)}, K_{nnnn_y}^{(0)}\}$ using Eq. (15) as shown by $\mathcal{P}_{\alpha\beta}$ in Table IV.

TABLE III. $\mathcal{P}_{\alpha\beta}$ for the 3D isotropic Ising model. The two rows in the table correspond to the two different α's which index the nn and the nnn renormalized constants, respectively. β runs from 1 to 8, corresponding to the following spin products: $S_\beta^{(0)}(\boldsymbol{\sigma})$: $(0, 0, 0)$-$(1, 0, 0)$, $(0, 0, 0)$-$(1, 1, 0)$, $(0, 0, 0)$-$(2, 0, 0)$, $(0, 0, 0)$-$(2, 1, 0)$, $(0, 0, 0)$-$(1, 0, 0)$-$(0, 1, 0)$-$(0, 0, 1)$, $(0, 0, 0)$-$(1, 0, 0)$-$(0, 1, 0)$-$(1, 1, 0)$, $(0, 0, 0)$-$(2, 1, 1)$, and $(0, 0, 0)$-$(1, 1, 1)$ where the triplet (i, j, k) is the coordinate of an Ising spin. Sixteen independent simulations were run, each of which took 3×10^5 Metropolis MC sweeps. The simulations were performed at the nearest-neighbor critical point with $K_{nn} = 0.221\,65$.

$\mathcal{P}_{\alpha 2}$	$\mathcal{P}_{\alpha 3}$	$\mathcal{P}_{\alpha 4}$	$\mathcal{P}_{\alpha 5}$	$\mathcal{P}_{\alpha 6}$	$\mathcal{P}_{\alpha 7}$	$\mathcal{P}_{\alpha 8}$
2.642(8)	1.540(8)	6.61(3)	2.46(1)	0.788(3)	6.92(4)	1.99(1)
2.64(2)	1.55(2)	6.7(1)	2.50(2)	0.795(3)	7.0(1)	1.99(2)

TABLE IV. $\mathcal{P}_{\alpha\beta}$ for the 2D anisotropic Ising model. α indexes rows corresponding to the four renormalized constants: nn_x, nn_y, nnn, and $\Box$. $\beta = 2$–6, respectively, indexes the component of the normal vector to CMTS corresponding to coupling terms nn_y, nnn, $\Box$, $nnnn_x$, and $nnnn_y$. $\beta = 1$ corresponds to the nn_x coupling term, and $\mathcal{P}_{\alpha 1}$ is always 1 by definition.

$K_{nn_x}^{(0)}$	$\mathcal{P}_{\alpha 2}$	$\mathcal{P}_{\alpha 3}$	$\mathcal{P}_{\alpha 4}$	$\mathcal{P}_{\alpha 5}$	$\mathcal{P}_{\alpha 6}$
0.304689	0.653(8)	2.387(10)	0.814(8)	1.749(8)	1.21(1)
	0.646(4)	2.381(5)	0.807(4)	1.755(4)	1.200(5)
	0.647(8)	2.38(1)	0.808(12)	1.747(14)	1.20(1)
	0.63(2)	2.37(3)	0.78(3)	1.76(4)	1.22(3)
Exact	0.6478				
0.240606	0.507(4)	2.241(5)	0.692(7)	1.74(1)	0.957(7)
	0.498(2)	2.236(3)	0.681(3)	1.739(3)	0.946(4)
	0.499(8)	2.24(1)	0.68(1)	1.736(14)	0.940(14)
	0.500(16)	2.23(3)	0.67(3)	1.75(4)	0.94(2)
Exact	0.5				

D. Two-dimensional tricritical Ising model

Finally, let us consider the 2D tricritical Ising model with the Hamiltonian,

$$H(\boldsymbol{\sigma}) = -K_{nn}^{(0)} \sum_{\langle i,j \rangle} \sigma_i \sigma_j - K_{\triangle}^{(0)} \sum_i \sigma_i^2, \qquad (20)$$

where $\sigma = \pm 1, 0$ and $\langle i, j \rangle$ denotes the nearest-neighbor pairs. In the coupling space of $K_{nn}^{(0)}$ and $K_{\triangle}^{(0)}$, the model admits a line of Ising-like continuous phase transitions, which terminates at a tricritical point. At the tricritical point, the underlying conformal field theory (CFT) changes from the Ising CFT with a central charge of $\frac{1}{2}$ to one with a central charge of $\frac{7}{10}$ [21]. Accompanying this phase transition is a change in the co-dimension of the even critical manifold from 1 of the Ising case to 2 of the tricritical case [15]. We compute the CMTS at the tricritical point, which has been determined to occur at $K_{nn}^{(0)} = 1.642(8)$ and $K_{\triangle}^{(0)} = -3.227(1)$ both by MCRG [15] and finite size scaling [22].

The coupling space we consider has six couplings, listed in Table V. We use $n = 5$, $L = 256$, and the $b = 2$ majority rule. The normal vectors to the CMTS are computed using the first five renormalized couplings as the statistical uncertainty of the sixth renormalized coupling is too large. The result is again represented by $\mathcal{P}_{\alpha\beta}$ and shown in Table VI. As can be seen, the rows of $\mathcal{P}$ are not equal within statistical uncertainty, indicating that the co-dimension is higher than one. To verify that the co-dimension is two, one can check whether the row

TABLE V. The couplings used in the computation of CMTS for the 2D tricritical Ising model.

	Coupling
1	σ_i^2
2	$\sigma_i \sigma_j$, i and j nearest neighbors
3	$\sigma_i \sigma_j$, i and j next-nearest neighbors
4	$\sigma_i \sigma_j \sigma_k \sigma_l$, i, j, k, and l in the smallest plaquette
5	$(\sigma_i \sigma_j)^2$, i and j nearest neighbors
6	$(\sigma_i \sigma_j)^2$, i and j next-nearest neighbors

TABLE VI. $\mathcal{P}_{\alpha\beta}$ for the 2D tricritical Ising model. α indexes rows corresponding to the first five renormalized couplings listed in Table V, which also gives the couplings for $\beta = 2$–6.

α	$\mathcal{P}_{\alpha 2}$	$\mathcal{P}_{\alpha 3}$	$\mathcal{P}_{\alpha 4}$	$\mathcal{P}_{\alpha 5}$	$\mathcal{P}_{\alpha 6}$
1	2.085(2)	2.100(5)	0.928(1)	2.079(1)	2.073(2)
2	2.200(2)	2.271(3)	1.046(2)	2.190(2)	2.232(2)
3	2.171(1)	2.2285(2)	1.0160(5)	2.163(1)	2.193(1)
4	2.214(1)	2.283(1)	1.04(1)	2.20(1)	2.24(1)
5	2.038(4)	2.03(1)	0.873(2)	2.03(1)	2.00(1)

vectors for $\alpha = 3$–5 are in the vector space spanned by the first two row vectors. Let $\mathbf{u}_n$ be the nth row vector of $\mathcal{P}$. If the hypothesis of co-dimension two were correct, one could write

$$\mathbf{u}_3 = a\mathbf{u}_1 + b\mathbf{u}_2, \qquad (21)$$

and find a and b from the first two components of the vectors $\mathbf{u}_1$, $\mathbf{u}_2$, and $\mathbf{u}_3$. We could then check that the remaining components of $\mathbf{u}_3$ satisfy the linear relation in Eq. (21) with the so found a and b. A similar check can be carried out for the vectors $\mathbf{u}_4$ and $\mathbf{u}_5$. The vectors $\mathbf{u}_3$, $\mathbf{u}_4$, and $\mathbf{u}_5$ calculated in this way are reported in Table VII. As we can see, the $\mathcal{P}_{\alpha\beta}$ for $\alpha = 3$–5 and $\beta = 2$–6 in Table VII are equal within statistical uncertainty to the corresponding elements in Table VI, consistent with a co-dimension equal to two at the tricritical point.

IV. CURVATURE OF THE CRITICAL MANIFOLD

Next, we compute the curvature of the critical manifold using the isotropic Ising model as an example. For a change $\{\delta K_\beta^{(0)}\}$ in the original coupling constants, we expand the corresponding change in the renormalized constants to quadratic order,

$$\delta K_\alpha^{(n)} = \sum_\beta \mathcal{A}_{\alpha\beta}^{(n,0)} \delta K_\beta^{(0)} + \frac{1}{2} \sum_{\beta\eta} \mathcal{B}_{\alpha\beta\eta}^{(n,0)} \delta K_\beta^{(0)} \delta K_\eta^{(0)}, \qquad (22)$$

where $\mathcal{A}_{\alpha\beta}^{(n,0)}$ and $\mathcal{B}_{\alpha\beta\eta}^{(n,0)}$ can be determined by substituting Eq. (22) in Eq. (11) and enforcing equality to second order in $\delta K_\alpha^{(0)}$. $\mathcal{A}_{\alpha\beta}^{(n,0)}$ is already given in Eq. (13). The result for $\mathcal{B}$ is that for given β and η for every γ, one requires

$$\sum_\alpha \langle\langle S_\gamma(\boldsymbol{\mu}), S_\alpha(\boldsymbol{\mu}) \rangle\rangle_V \mathcal{B}_{\alpha\beta\eta}^{(n,0)}$$
$$= \langle\langle S_\gamma(\boldsymbol{\mu}), S_\beta(\boldsymbol{\sigma}) S_\eta(\boldsymbol{\sigma}) \rangle\rangle_V$$
$$+ \sum_{\alpha\nu} \mathcal{A}_{\alpha\beta} \mathcal{A}_{\nu\eta} \langle\langle S_\gamma(\boldsymbol{\mu}), S_\alpha(\boldsymbol{\mu}) S_\nu(\boldsymbol{\mu}) \rangle\rangle_V$$
$$- 2 \sum_\alpha \mathcal{A}_{\alpha\eta} \langle\langle S_\gamma(\boldsymbol{\mu}), S_\beta(\boldsymbol{\sigma}) S_\alpha(\boldsymbol{\mu}) \rangle\rangle_V, \qquad (23)$$

TABLE VII. $a\mathbf{u}_1 + b\mathbf{u}_2$ computed from Table VI for $\alpha = 3$–5 and $\beta = 2$–6.

α	$\mathcal{P}_{\alpha 2}$	$\mathcal{P}_{\alpha 3}$	$\mathcal{P}_{\alpha 4}$	$\mathcal{P}_{\alpha 5}$	$\mathcal{P}_{\alpha 6}$
3	2.171	2.230	1.019	2.163	2.194
4	2.214	2.284	1.047	2.204	2.245
5	2.038	2.026	0.872	2.033	2.004

TABLE VIII. $\kappa_{\beta\eta}$ at the same three critical points as in Table I, calculated from $\partial^2 K_{nn}^{(n)}/\partial K_\beta^{(0)}\partial K_\eta^{(0)}$. The exact curvature for $\beta = $ nn and $\eta = $ nnn at the Onsager point is also shown [17].

$K_{nn}^{(0)}$	η $\diagdown$ β	nnn	$\square$	nnnn
0.4407	nn	0.143(8)	0.27(2)	0.21(2)
	nnn		0.38(2)	0.341(8)
	$\square$			0.20(2)
Exact (nn, nnn)		0.148		
0.37	nn	0.18(1)	0.23(1)	0.30(3)
	nnn		0.35(2)	0.32(2)
	$\square$			0.18(3)
0.228	nn	0.35(2)	0.27(3)	0.49(3)
	nnn		0.35(4)	0.29(2)
	$\square$			0.20(4)

where the connected correlation functions are again sampled in the biased ensemble $\langle\cdot\rangle_V$. Note that $\mathcal{B}_{\alpha\beta\eta}$ given above is not symmetric in β and η. In order for it to be interpreted as a second-order derivative, it needs to be symmetrized

$$\frac{\partial^2 K_\alpha^{(n)}}{\partial K_\beta^{(0)}\partial K_\eta^{(0)}} = \frac{1}{2}\left(\mathcal{B}_{\alpha\beta\eta}^{(n,0)} + \mathcal{B}_{\alpha\eta\beta}^{(n,0)}\right). \tag{24}$$

In the coupling space of any pair β and η:$\{K_\beta^{(0)}, K_\eta^{(0)}\}$, the critical manifold of the 2D isotropic Ising model is a curve, and the curvature $\kappa_{\beta\eta}$ of the critical curve can be computed from the curvature formula [23] of the implicit curve,

$$K_\alpha^{(n)}\left(K_\beta^{(0)}, K_\eta^{(0)}\right) = \text{constant}, \tag{25}$$

with the second-order derivatives given in Eq. (24). Again, this curvature is determined separately by each renormalized constant α. The result is given Table VIII. Here, we only quote the result calculated from the nearest-neighbor renormalized constants $K_\alpha^{(n)}$, $\alpha = $ nn. The curvature computed from other renormalized constants has statistical uncertainty much larger than the ones in Table VIII.

The difficulty in sampling the curvature, or generally, any higher-order derivatives, compared to the tangent space, can be seen from Eq. (23). Note that, on the left side of Eq. (23), the connected correlation function $\langle\langle S_\gamma, S_\alpha\rangle\rangle$ is of order N, where N is the system size, but each of the terms on the right side is of order N^2. Thus, a delicate and exact cancellation of terms of order N^2 must happen between the terms on the right hand side of Eq. (23) to give a final result only of order N. The variance due to the terms on the right hand side, however, will accumulate and give an uncertainty typical for $O(N^3)$ quantities as each S_α is of order N. [For the CMTS, the connected correlation functions of interest are also of order N, but the statistical uncertainties are those typical of $O(N^2)$ quantities as seen in Eq. (13).] In general, as an mth order derivative of the critical manifold is computed, the connected correlation functions of interest will always be of order N, but the correlation functions that need to sampled will be of order

N^{m+1}, giving an exceedingly large variance. Thus, although, in principle, arbitrarily high-order information about the critical manifold is available by expanding Eq. (11), in practice only low-order knowledge on the critical manifold can be obtained with small statistical uncertainty from a simulation near a single critical point.

V. CONCLUSION

We have presented a MC procedure to obtain the local geometrical information on the critical manifold in the vicinity of a given critical point. The procedure is, in essence, a projector Monte Carlo method that is based on the fact that the irrelevant operators in a system decay exponentially fast along a RG trajectory. Because of such decay, the truncated RG Jacobian matrix $\mathcal{A}^{(n,0)}$ acquires a structure that is asymptotically clearer and clearer as n increases, i.e., its kernel emerges with codimension equal to the number of relevant operators of the system. This structure is quite robust. On one hand, it is immune from the truncation of the renormalized Hamiltonian. On the other hand, it does not depend on what biased potential of the coarse-grained variables is applied to the system.

From the perspective of connected correlation functions between the original spins $\boldsymbol{\sigma}$ and the coarse-grained spins $\boldsymbol{\mu}$, the aforementioned structure means the following. Given any bias potential $V(\boldsymbol{\mu})$ at any critical point, each local observable S_β of $\boldsymbol{\sigma}$ can be viewed as a linear functional $\langle\langle\cdot, S_\beta(\boldsymbol{\sigma})\rangle\rangle$ on the space of the local observables of $\boldsymbol{\mu}$,

$$\langle\langle\cdot, S_\beta(\boldsymbol{\sigma})\rangle\rangle: S_\gamma(\boldsymbol{\mu}) \mapsto \langle\langle S_\gamma(\boldsymbol{\mu}), S_\beta(\boldsymbol{\sigma})\rangle_V. \tag{26}$$

The presence of the CMTS implies that many distinct linear functionals are linearly dependent. In fact, by Eq. (13) for any $\{\delta K_\beta^{(0)}\}$ in the CMTS,

$$\sum_\beta \langle\langle\cdot, S_\beta(\boldsymbol{\sigma})\rangle\rangle\delta K_\beta^{(0)} = 0. \tag{27}$$

This poses an infinite number of conditions which the coarse-graining procedure has to satisfy to generate a proper RG structure. The majority-rule coarse-graining considered in our examples seems to do very well in satisfying these conditions. But a question still remains. Are the conditions satisfied exactly or just approximately but so closely that any violation is overshadowed by the statistical uncertainty? In the latter case, which coarse-graining procedure, preferably with a finite number of parameters, can satisfy all the conditions in Eq. (27)? In the former case, what is the profound reason why all these conditions can be satisfied simultaneously?

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