Determination of the Critical Manifold Tangent Space and Curvature with Monte Carlo Renormalization Group

Yantao Wu and Roberto Car

1 The Department of Physics, Princeton University
2 The Department of Chemistry, Princeton University

(Dated: April 5, 2019)

We show that the critical manifold of a statistical mechanical system around 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 and anisotropic Ising model on a two-dimensional square lattice, and the isotropic Ising model on a cubic lattice to illustrate the method.

I. INTRODUCTION

The critical manifold of a statistical mechanical system is defined as the set of coupling constants from which successive renormalization group (RG) transformations flow into a critical fixed-point. It contains all the coupling constants at which the system becomes scale invariant. It can be defined in any space of coupling constants as

\[ S(T) \]

where

\[ S(T) \]

the critical manifold is not known. With Monte Carlo (MC) simulations, one can determine isolated points on the critical manifold, i.e. the critical couplings of the system, one by one. In this paper, we present a method to determine the critical manifold, i.e. the critical couplings of the system, one by one. In this paper, we present a method to determine the tangent space and curvature of the critical manifold at these isolated points with Variational Monte Carlo Renormalization Group (VMCRG) [5]. The method is based on the assumption that a critical fixed-point Hamiltonian exists under successive coarse-graining transformations of the system at criticality, as required by the general theory of RG [2]. We will show that unlike the computation of the critical exponents in Monte Carlo Renormalization Group [2] or VMCRG, the determination of the critical manifold tangent space (CMTS) and curvature does not suffer truncation error no matter how few the 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.

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 dimension with spins \( \sigma \) and Hamiltonian \( H^{(0)}(\sigma) \),

\[ H^{(0)}(\sigma) = \sum_{\beta} K^{(0)}_{\beta} S_{\beta}(\sigma) \tag{1} \]

where \( S_{\beta}(\sigma) \) are the coupling terms of the system, such as nearest neighbor products, next nearest neighbor products, etc., and \( \{K^{(0)}_{\beta}\} \) 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 defined in the space of \( K^{(0)}_{\beta} \) in reference to a finite set of couplings \( S_{\beta}(\sigma) \) such that \( H^{(0)} \) is critical.

In a real-space RG calculation, one defines the coarse-grained spins \( \sigma’ \) in the renormalized system with a conditional probability \( T(\sigma’|\sigma) \) that effects a scale transformation with scale factor \( b \). \( T(\sigma’|\sigma) \) is the probability of \( \sigma’ \) given spin configuration \( \sigma \) in the original system. The majority rule block spin in the Ising model proposed by Kadanoff [2] is one example of the coarse-grained variables. \( T(\sigma’|\sigma) \) can be iterated \( n \) times to define the \( n \)-th level coarse-graining \( T^{(n)}(\mu|\sigma) \) realizing a scale transformation with scale factor \( b^n \):

\[ T^{(n)}(\mu|\sigma) = \sum_{\sigma^{(n-1)}} \ldots \sum_{\sigma^{(1)}} T(\mu|\sigma^{(n-1)}) \ldots T(\sigma^{(1)}|\sigma) \tag{2} \]

\( T^{(n)} \) defines the \( n \)-th level renormalized Hamiltonian \( H^{(n)}(\mu) \) up to a constant \( g(K) \) independent of \( \mu \):

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

\[ = \sum_{\alpha} K^{(n)}_{\alpha} S_{\alpha}(\mu) + g(K) \tag{3} \]

where \( \{K^{(n)}_{\alpha}\} \) are the \( n \)-th level renormalized coupling constants associated with the coupling terms \( S_{\alpha}(\mu) \) defined for the \( n \)-th level coarse-grained spins. Modulo
the constant coupling term, $T^{(n)}(\mu|\sigma)$ defines $H^{(n)}(\mu)$ 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, $H^{\ast}(\mu)$, as $n$ increases.

To probe $H^{\ast}(\mu)$ in a Monte Carlo (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 finite-size effect becomes negligible with $L$. It is generally impossible to determine all of the coupling constants of $H^{(n)}(\mu)$ because their number increases combinatorially with the lattice size. In practice, one adopts a certain truncation because they are the truncation approximation to two Hamiltonians, $H^{(n)}$ and $H^{(n)} + \delta H^{(n)}$, whose difference is exponentially small in $n$. Because they are the truncation approximation to two Hamiltonians, $H^{(n)}$ and $H^{(n)} + \delta H^{(n)}$, whose difference is exponentially small in $n$. Thus, the spanning set of CMTS, $\{\delta K_{\beta}^{(n)}\}$, satisfies the following equation for sufficiently large $n$,

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

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

$$A^{(n,0)}_{\alpha,\beta} = \frac{\partial K_{\alpha,\text{truncate}}^{(n)}}{\partial K_{\beta}^{(0)}}$$

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

As shown in [1], 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 $V(\mu)$ of the coarse-grained variables, expanded in a finite set of renormalized couplings $S_{\alpha}(\mu)$ with variational parameters $J_{\alpha}$:

$$V_{\beta}(\mu) = \sum_{\alpha} J_{\alpha} S_{\alpha}(\mu),$$

and a variational function in $J = \{J_{\alpha}\}$:

$$\Omega(J) = \ln \sum_{\mu} e^{-(H^{(n)}(\mu)+V_{\beta}(\mu))} + \sum_{\mu} V_{\beta}(\mu)p_{\beta}(\mu)$$

where $p_{\beta}(\mu)$ is a preset target probability distribution, which will be taken as the uniform distribution in the following. As proved in [2], $\Omega$ is convex in each $J_{\beta}$, and if one excludes the constant coupling term, it has a unique minimizer, $J_{\text{min}}$, which satisfies the minimizing condition: for every renormalized coupling $S_{\alpha}(\mu)$,

$$\langle S_{\gamma}(\mu) \rangle_{V_{\text{min}}} = \langle S_{\gamma}(\mu) \rangle_{p_{\gamma}}$$

where $V_{\text{min}} = \sum_{\alpha} J_{\alpha,\text{min}} S_{\alpha}(\mu)$ and $\langle \cdot \rangle_{V_{\text{min}}}$ denotes the ensemble average where $\mu$ distributes according to the biased ensemble:

$$P(\mu) \propto \sum_{\sigma} \exp(-H^{(0)}(\sigma))T^{(n)}(\mu|\sigma)\exp(-V_{\text{min}}(\mu))$$

and $\langle \cdot \rangle_{p_{\gamma}}$ denotes the ensemble average in the target distribution $p_{\beta}(\mu)$. If the set of the coupling terms $S_{\alpha}$ is complete, $V_{\text{min}}(\mu) = \sum_{\alpha} J_{\alpha,\text{min}} S_{\alpha}(\mu) = -H^{(n)}(\mu)$, thus we identify for each $\alpha$,

$$K_{\alpha,\text{truncate}}^{(n)} = -J_{\alpha,\text{min}}$$

Because the set of $S_{\alpha}(\mu)$ is not complete, a truncation error in computing $K_{\alpha,\text{truncate}}^{(n)}$ is incurred. However, because the minimizer of $\Omega$ is unique, the truncation scheme is well-defined. Within VMCRG, $A^{(n,0)}_{\alpha,\beta}$ can be obtained by expanding Eq. [3] to linear order in $\delta K_{\beta}^{(0)}$ and $\delta K_{\alpha}^{(n)}$. The result of the expansion is that [1], for a given $\beta$, one requires for every $S_{\gamma}(\mu)$,

$$\sum_{\alpha} \langle [S_{\gamma}(\mu), S_{\alpha}(\mu)] \rangle_V \delta K_{\alpha}^{(n)} = \langle [S_{\gamma}(\mu), S_{\beta}(\sigma)] \rangle_V$$

for any well-defined truncation scheme with respect to $K_{\beta}^{(0)}$ within the truncation scheme, and thus the CMTS determined as the kernel of the matrix $A^{(n,0)}_{\alpha,\beta} = \frac{\partial K_{\alpha,\text{truncate}}^{(n)}}{\partial K_{\beta}^{(0)}}$, viewed as a column vector indexed by $\alpha$, can be obtained from matrix inversion of Eq. [12].

We stress that Eq. [12] gives the exact derivative of the truncated renormalized constants $K_{\alpha}^{(n)}$ with respect to $K_{\beta}^{(0)}$ within the truncation scheme, and the CMTS determined as the kernel of the matrix $A^{(n,0)}_{\alpha,\beta} = \frac{\partial K_{\alpha,\text{truncate}}^{(n)}}{\partial K_{\beta}^{(0)}}$ is free of truncation error.

We also note that the method described above works for any target distribution $p_{\beta}(\mu)$ in VMCRG. A different
\( p_t(\mu) \) will result in a different bias potential \( V_{\text{min}}(\mu) \) to be used in the sampling of the matrix \( \mathcal{A}^{(n,0)} \). We use the uniform distribution here because then \( V_{\text{min}}(\mu) \) acts to eliminate the long-range correlation in a critical system and the resultant ensemble for the sampling of \( \mathcal{A}^{(n,0)} \) enjoys a much faster MC relaxation \([1]\). However, one can impose any arbitrary bias potential of the coarse-grained variables, \( V(\mu) \), and declare 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 \( V(\mu) \). 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, then \( V_{\text{min}} \) 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 \( K^{(n)}_\alpha \) be equal to \( K^{(n+1)}_\alpha \). Now suppose both \( K^{(0)}_\beta \) and \( K^{(0)}_\beta + \delta K^{(0)}_\beta \) are on the critical manifold, respectively giving rise to the truncated renormalized constants \( K^{(n)}_\alpha \) and \( K^{(n)}_\alpha + \delta K^{(n)}_\alpha \). Then, the spanning set of CMTS, \( \{ \delta K^{(0)}_\beta \} \), instead of satisfying Eq. 5 satisfies the following condition,

\[
K^{(n)}_\alpha + \sum_\beta \frac{\partial K^{(n)}_\alpha}{\partial K^{(0)}_\beta} \delta K^{(0)}_\beta = K^{(n+1)}_\alpha + \sum_\beta \frac{\partial K^{(n+1)}_\alpha}{\partial K^{(0)}_\beta} \delta K^{(0)}_\beta
\]

for every \( \alpha \). But \( K^{(n)}_\alpha \) and \( K^{(n+1)}_\alpha \) 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 will be the kernel of the matrix,

\[
\mathcal{A}^{(n,0)}_{\alpha\beta} - \mathcal{A}^{(n+1,0)}_{\alpha\beta}
\]

D. The Normal Vector 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, and in the even subspace which we will focus on, the co-dimension of the critical manifold is one. 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 all orthogonal to this hyperplane. This means that the row vectors of \( \mathcal{A}^{(n,0)} \) or \( \mathcal{A}^{(n+1,0)} - \mathcal{A}^{(n,0)} \) must all be the normal vector to CMTS and thus be parallel to one another, and that the matrix \( \mathcal{P} \) defined below, which contains the normalized row vectors of \( \mathcal{A}^{(n,0)} \) or \( \mathcal{A}^{(n+1,0)} - \mathcal{A}^{(n,0)} \), should have identical rows:

\[
\mathcal{P}_{\alpha\beta} = \frac{\mathcal{A}^{(n,0)}_{\alpha\beta}}{\mathcal{A}^{(n,0)}_{\alpha1}} \text{ or } \frac{\mathcal{A}^{(n+1,0)}_{\alpha\beta} - \mathcal{A}^{(n,0)}_{\alpha\beta}}{\mathcal{A}^{(n+1,0)}_{\alpha1} - \mathcal{A}^{(n,0)}_{\alpha1}}
\]

If all the rows of \( \mathcal{P} \) are indeed the same, it is a testament of the validity of the RG theory which predicts the existence of a critical fixed-point Hamiltonian and that the co-dimension of the critical manifold is 1 for the models considered in this paper. In general, the CMTS computed from different renormalized couplings will have different statistical uncertainty 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. 2D Isotropic Ising Model

Consider the isotropic Ising model on a 2D square lattice with Hamiltonian \( H(\sigma) \)

\[
H(\sigma) = -K^{(0)}_{nn} \sum_{(i,j)} \sigma_i \sigma_j - K^{(0)}_{nnn} \sum_{[i,j]} \sigma_i \sigma_j
\]

where \( (i,j) \) denotes the nearest neighbor pairs and \( [i,j] \) the next nearest neighbor pairs. \( K^{(0)}_{nn} \) and \( K^{(0)}_{nnn} \) are the corresponding coupling constants. This model is analytically solvable when \( K^{(0)}_{nn} = 0 \) and is critical at the Ousager point with \( K^{(0)}_{nn} = 0.4407... \). Three critical points are first located with VMCRG in the coupling space of \( \{ K^{(0)}_{nn}, K^{(0)}_{nnn} \} \). 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 \( K^{(0)}_{nn} \), the next nearest product \( K^{(0)}_{nnn} \), and the smallest plaquette \( K^{(0)}_{nnnn} \). The model is known to have no marginal operators. The CMTS are determined on these critical points in a four-dimensional coupling space spanned by \( K^{(0)}_{nn}, K^{(0)}_{nnn}, K^{(0)}_{nnnn} \), and the third nearest neighbor products, \( K^{(0)}_{nnnn} \). The \( \mathcal{P}_{\alpha\beta} \) is shown in Table. In addition, the CMTS is analytically solvable at the Ousager point \( \mathcal{S} \), which we also show for comparison.

B. 3D Isotropic Ising Model

Consider now the same model on a 3D square lattice with \( K^{(0)}_{nnn} = 0 \), i.e. the 3D isotropic nearest neighbor
and the 3D anisotropic Ising model. The α index in the table refers to the three renormalized constants: nn, nnn, and n. The fourth row of the table at the Onsager point shows the exact values. β = 2, 3, and 4 respectively indexes the component of the normal vector to CMTS corresponding to coupling terms nn, nnn, and nnn. β = 1 corresponds to the nn coupling term and Pα3 is always 1 by definition. The simulations were performed on 16 cores independently, each of which ran 3 × 10^5 Metropolis MC sweeps. The standard error are cited as the statistical uncertainty.

Ising model. This model does not have an analytical solution, but is known to experience a continuous transition at K_{nn}^{(0)} = 0.22165... [9]. To compute the CMTS at this nearest neighbor critical point, we use n = 3, L = 64, and the b = 2 majority rule with a random pick on tie. The CMTS is computed in an eight-dimensional coupling space \{K^{(0)}\} from the nearest-neighbor and next-nearest-neighbor renormalized coupling constants, K_{nn}^{(n)} and K_{nnn}^{(n)}, shown in Table. III.

| K_{nnn}^{(0)} | P_{α2} | P_{α3} | P_{α4} | P_{α5} | P_{α6} | P_{α7} | P_{α8} |
|---------------|--------|--------|--------|--------|--------|--------|--------|
| 0.4407        | 1.4134 | 0.5135 | 1.794(7)| 1.794(7)| 1.8006 |
| 0.4167        | 0.5134 | 1.799(2)| 1.794(7)|        |
| 0.4133        | 0.5113 | 1.794(7)|        |        |

Exact

0.37
0.0509
0.3717(4)
0.524(3)
1.7664(8)
1.773(2)
1.773(6)

0.228
0.1612
1.252(7)
0.530(3)
1.654(8)
0.657(2)
1.651(1)

TABLE II. P_{αβ} for the 3D isotropic Ising model. α indexes rows corresponding to the two renormalized constants: nn, nnn, and n. The fourth row of the table at the Onsager point shows the exact values. β = 2, 3, and 4 respectively indexes the component of the normal vector to CMTS corresponding to coupling terms nn, nnn, and nnnn. β = 1 corresponds to the nn coupling term and Pα3 is always 1 by definition. The simulations were performed on 16 cores independently, each of which ran 3 × 10^5 Metropolis MC sweeps. The standard error are cited as the statistical uncertainty.

C. 2D Anisotropic Ising Model

Consider then the anisotropic Ising model on a 2D square lattice with Hamiltonian H(σ)

\[ H(σ) = -K_{nn}^{(0)} \sum_{(i,j)_x} σ_i σ_j - K_{nn}^{(0)} \sum_{(i,j)_y} σ_i σ_j \] (17)

where \(⟨i, j⟩_x\) and \(⟨i, j⟩_y\) respectively denote the nearest neighbor pairs along the horizontal and the vertical direction. In the space of \{K_{nn}^{(0)}, K_{nnn}^{(0)}\}, the model is exactly solvable and is critical along the line [10]

\[ \sinh(2K_{nn}^{(0)}) \cdot \sinh(2K_{nn}^{(0)}) = 1 \] (18)

With the 2 × 2 majority rule, the system admits a marginal operator due to anisotropy in the RG transformation [11]. We performed VMCRG calculations on two critical points of the system with \(K_{nn}^{(0)}/K_{nn}^{(0)} = 2\), and 3 with four renormalized couplings: \(K_{nn}^{(n)}, K_{nnn}^{(n)}, K_{nnnn}^{(n)}, K_{nnn}^{(n)}\). The CMTS is computed in the coupling space \(\{K_{nn}^{(n)}, K_{nn}^{(n)}, K_{nnn}^{(n)}, K_{nnn}^{(n)}\}\) by Eq. [14] which is shown as P_{αβ} in Table. III.

| K_{nnn}^{(n)} | P_{α2} | P_{α3} | P_{α4} | P_{α5} | P_{α6} | P_{α7} | P_{α8} |
|---------------|--------|--------|--------|--------|--------|--------|--------|
| 0.304689      | 0.6538 | 2.387(10)| 0.814(8)| 1.749(8)| 1.21(1) |
| 0.646(4)      | 2.381(5)| 0.807(4)| 1.755(4)| 1.20(5) |
| 0.647(4)      | 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) | 2.241(5) | 0.68(1) | 1.736(14) | 0.940(14) |
0.500(16) | 2.23(3) | 0.67(3) | 1.75(4) | 0.94(2) |

TABLE III. P_{αβ} for the 2D anisotropic Ising model. α indexes rows corresponding to the four renormalized constants: nnx, nny, nnn, and n. β = 2 − 6 respectively indexes the component of the normal vector to CMTS corresponding to coupling terms nny, nn, nnnx, and nnnny. β = 1 corresponds to the nn coupling term and P_{α1} is always 1 by definition.

IV. CURVATURE OF THE CRITICAL MANIFOLD

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

\[ δK^{(n)}_{α} = \sum_{β} A_{αβ}^{(n,0)} δK_{β}^{(0)} + \frac{1}{2} \sum_{β, η} B_{αβη}^{(n,0)} δK_{β}^{(0)} δK_{η}^{(0)} \] (19)

where \(A_{αβ}^{(n,0)}\) and \(B_{αβη}^{(n,0)}\) can be determined by substituting Eq. [14] in Eq. [6] and enforcing equality to the second order of \(δK_{β}^{(0)}\). \(A_{αβ}^{(n,0)}\) is already given in Eq. [12]. The result for \(B\) is that for given \(β\) and \(η\), for every γ, one
requires
\[
\sum_{\alpha} \left( \langle S_\gamma(\mu), S_{\alpha}(\mu) \rangle \right)_V B_{\alpha\beta\eta}^{(n,0)} = \left( \langle S_\gamma(\mu), S_{\beta}(\sigma)S_{\eta}(\sigma) \rangle \right)_V
\]
\[
+ \sum_{\alpha\nu} A_{\alpha\beta\nu}\eta\langle S_\gamma(\mu), S_{\alpha}(\mu)S_{\nu}(\mu) \rangle_V
\]
\[
- 2\sum_{\alpha} A_{\alpha\beta}\eta\langle S_\gamma(\mu), S_{\beta}(\sigma)S_{\alpha}(\mu) \rangle_V
\]
(20)

where the connected correlation functions are again sampled in the biased ensemble \( \langle \gamma \rangle_V \). Note that \( B_{\alpha\beta\eta} \) given above is not symmetric in \( \beta \) and \( \eta \). In order for it to be interpreted as a second-order derivative, it needs to be symmetrized:
\[
\frac{\partial^2 K_{\alpha}^{(n)}}{\partial K_{\beta}^{(0)} \partial K_{\eta}^{(0)}} = \frac{1}{2} \left( B_{\alpha\beta\eta}^{(n,0)} + B_{\alpha\eta\beta}^{(n,0)} \right)
\]
(21)

In the coupling space of any pair \( \beta \) and \( \eta \): \{ \( K_{\beta}^{(0)}, K_{\eta}^{(0)} \) \}, 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 by the curvature formula (12) of the implicit curve
\[
K_{\alpha}^{(n)}(K_{\beta}^{(0)}, K_{\eta}^{(0)}) = \text{constant}
\]
(22)

with the second-order derivatives given in Eq. (21). Again, this curvature is determined separately by each renormalized constant \( \alpha \). The result is given Table IV Here we only quote the result calculated from the nearest neighbor renormalized constants \( K_{\alpha}^{(n)} \), \( \alpha = \text{nn} \). The curvature computed from other renormalized constants has statistical uncertainty much larger than the ones in Table IV.

The difficulty in sampling the curvature, or generally any higher-order derivatives, compared to the tangent space, can be seen from Eq. (20). Note that on the left side of Eq. (20) the connected correlation function \( \langle S_\gamma, S_{\alpha} \rangle \) are 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 due to the different terms in Eq. (20) 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 \( S_{\alpha} \) is of order \( N \). (For CMTS, the connected correlation functions of interest are also of the order \( N \), but the statistical uncertainties are those typical for \( O(N^2) \) quantities, as seen in Eq. (14) in general, as an \( n \)-th 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 \( N^{n+1} \), giving an exceedingly large variance. Thus, although in principle arbitrarily high order information about the critical manifold is available by expanding Eq. (9) in practice only low-order knowledge on the critical manifold can be obtained with small statistical uncertainty by a simulation around a single critical point.

V. CONCLUSION

We have described an MC procedure to obtain the geometrical information about the critical manifold that is local around 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 an RG trajectory. Because of such decay, the truncated RG Jacobian matrix, \( A^{(n,0)} \), obtains 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 the one hand, it is immune to the truncation of the renormalized Hamiltonian. On the other hand, it does not depend on what biased potential of the coarse-grained variables is added to the system.

From the perspective of connected correlation functions between the original spin \( \sigma \) and the coarse-grained spin \( \mu \), the aforementioned structure means the following. Given any bias potential \( V(\mu) \) at any critical point, each local observable \( S_{\beta} \) of \( \sigma \) can be viewed as an linear functional \( \langle \cdot, S_{\beta}(\sigma) \rangle \) of the space of local observables of \( \mu \):
\[
\langle \cdot, S_{\beta}(\sigma) \rangle : S_{\gamma}(\mu) \rightarrow \langle S_{\gamma}(\mu), S_{\beta}(\sigma) \rangle_V
\]
(23)

The presence of CMTS implies that many distinct linear functionals are linearly dependent. In fact, by Eq. (12) for any \( \delta K_{\beta}^{(0)} \) in CMTS,
\[
\sum_{\beta} \langle \cdot, S_{\beta}(\sigma) \rangle \delta K_{\beta}^{(0)} = 0
\]
(24)

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

| \( K_{\alpha}^{(0)} \) | \( \beta \) | \( \eta \) | \( \text{nn} \) | \( \text{nnn} \) | \( \Box \) |
|----------------|--------|--------|--------|--------|--------|
| 0.4407 | 0.143(8) | 0.27(2) | 0.21(2) | 0.34(8) | 0.20(2) |
| 0.37 | 0.18(1) | 0.23(1) | 0.30(3) | 0.35(2) | 0.32(2) |
| 0.228 | 0.35(2) | 0.27(3) | 0.49(3) | 0.35(4) | 0.29(2) |
| Exact (nn, nnn) | 0.148 | | | | |

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

\( \Box \)
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 the 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. [24]? In the former case, what are the reasons why all these conditions can be satisfied altogether?

ACKNOWLEDGMENTS

All the codes used in this project were written in C++, and will be available upon request. We acknowledge support from DOE Award [de-sc0017865].

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