

Real-space renormalization in statistical mechanics

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This review compares the conceptualization and practice of early real-space renormalization group methods with the conceptualization of more recent real-space transformations based on tensor networks. For specificity, it focuses upon two basic methods: the “potential-moving” approach most used in the period 1975–1980 and the “rewiring method” as it has been developed in the last five years. The newer method, part of a development called the *tensor renormalization group*, was originally based on principles of quantum entanglement. It is specialized for computing approximations for tensor products constituting, for example, the free energy or the ground state energy of a large system. It can attack a wide variety of problems, including quantum problems, which would otherwise be intractable. The older method is formulated in terms of spin variables and permits a straightforward construction and analysis of fixed points in rather transparent terms. However, in the form described here it is unsystematic, offers no path for improvement, and of unknown reliability. The new method is formulated in terms of index variables which may be considered as linear combinations of the statistical variables. Free energies emerge naturally, but fixed points are more subtle. Further, physical interpretations of the index variables are often elusive due to a gauge symmetry which allows only selected combinations of tensor entries to have physical significance. In applications, both methods employ analyses with varying degrees of complexity. The complexity is parametrized by an integer called χ (or D in the recent literature). Both methods are examined in action by using them to compute fixed points related to Ising models for small values of the complexity parameter. They behave quite differently. The old method gives a reasonably good picture of the fixed point, as measured, for example, by the accuracy of the measured critical indices. This happens at low values of χ , but there is no known systematic way of getting more accurate results within the old method. In contrast, the rewiring method seems to work poorly in fixed point calculations at low χ . This stands in contrast to the known excellent performance of these newer methods in calculations of free energy, but not fixed points, at large values of χ . Speculations are offered with a particular eye to seeing the reasons why the results of these two approaches are so different.

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CONTENTS

I. Introduction	648	H. Comparisons	651
A. History: The conceptual foundations	648	1. Stochastic variables	651
B. Statistical variables	648	2. Geometric structure	651
C. Renormalization	649	3. Computational strategy	652
D. Fixed point	649	I. Plan of review	652
E. Response analysis and critical indices	649	II. The Renormalization Process	652
F. Requirements on approximations	650	A. Overview	652
G. History of real-space methods	650	1. Introducing new statistical variables	652
		2. Tracing out the original statistical variable	653
		3. Obtaining a recursion relation	653
		B. Basic statistical description	654
		C. Tensor-SVD renormalization	655
		1. Singular value decomposition	655
		2. SVD as an approximation method	655

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3. Gauge invariance and interpretation of fixed-point tensor components	656
D. Zeros in the response matrix	656
1. Errors	656
E. Lower-bound variational renormalization	657
1. Decoration	657
2. Potential-moving theorem	658
3. Using potential moving	658
4. Spatial vectors and tensors	659
III. Results	659
A. Results from block spin calculations	659
1. Block spin renormalization of Ising models	660
2. Block spin renormalization for other models	661
B. SVD results	661
1. Generation of SVD fixed point	661
C. Summary of SVD numerical results	663
1. Square $\chi = 2$	663
2. Hexagonal $\chi = 2$	663
3. Hexagonal $\chi = 3$	664
4. Additional fixed point (hexagonal $\chi = 3$)	664
5. And one more (hexagonal $\chi = 3$)	665
6. Square $\chi = 3$	665
7. Square $\chi = 4$	665
8. Four-state Potts model	665
IV. Discussion	665
A. Error estimates	665
B. Work to be done	667
C. Where do we stand?	667
Acknowledgments	667
Appendix: Gauge freedom and invariance of the recursion step in isotropic TRG	667
Proof	667
References	668

I. INTRODUCTION

A. History: The conceptual foundations

The renormalization group (Nelson, 1977; Maris and Kadanoff, 1978; Cardy, 1996; Kadanoff, 2000) provides a theoretical understanding of singular problems in statistical mechanics (Domb, 1996), particularly ones involving phase transitions. There are two main branches of analysis based upon this method, one involving work in momentum or wave vector space (Wilson and Kogut, 1974), the other involving so-called “real-space” methods. In this review, we follow the latter approach.

Both approaches make extensive use of the following conceptual ideas:

- Scale invariance: Singularities in statistical mechanics tend to be connected with behaviors that are the same at different length scales. Critical points of phase transitions have correlations at all length scales.
- Scale covariance: Near the phase transition, many physical quantities vary as powers of characteristic lengths that describe the system, or of lengths describing the quantities themselves, or as powers of “fields” that measure the deviation of thermodynamic quantities from criticality. These powers characterize the phase transition. They are called *critical indices*.
- Fixed point: The scale invariance is described by a Hamiltonian or free-energy function that has elements

that are independent of length scale. As a result, one might expect that, for example, the Hamiltonian or the free-energy function that describes the system will not change when the length scale changes. This unchanging behavior is described as “being at a fixed point.”

- Renormalization: A transformation that describes the results of changes in the length scale. Usually this transformation will not change the Hamiltonian or free energy describing the fixed point. That is the reason for the name *fixed point*.
- Universality: Near the phase transition, many different physical systems show identical behavior of the quantities that describe critical behavior. Since these quantities are descriptive of scale-invariant behavior, these descriptive quantities can all be seen at large length scales.
- Universality classes: There are many critical points with a wide variety of different origins. Nonetheless these fall into relatively few *universality classes*, each class being fully descriptive of all the details of a given critical behavior.

The behaviors of different critical systems can be, in large measure, classified by describing the dimension and other topological features of the system, and then describing some underlying symmetry that plays a major role at the critical point. For example, the model that Lars Onsager solved, the Ising model (Ising, 1925; Onsager, 1944; Brush, Stephen, 1967), is mostly described by saying it is a two-dimensional system with a spin at each point. The spin can point in one of two directions. The model has a symmetry under flipping the sign of all spins, so that it can describe a magnetic phase transition. It is equally well descriptive of a two-dimensional liquid in which the basic symmetry is in the interchange of high density regions with low density ones, so that it describes a liquid-gas phase transition. Any model with the appropriate symmetry and dimensionality and the right range of interaction strengths is likely to describe both situations, and many others. The Ising model constitutes the simplest model of this kind.

B. Statistical variables

There are many models and real systems that exhibit critical behavior (Green and Sengers, 1966; Kadanoff *et al.*, 1967; Stanley, 1971; Ma, 2000). All of those with short-range interactions and spatial homogeneity have the same kind of characteristic behavior. One starts from a statistical ensemble, that is a very large system of stochastic variables, called $\{\sigma_{\mathbf{r}}\}$, where \mathbf{r} defines a position in space. The statistical calculation is defined by probability distribution, given as an expression of the form $\exp(-\beta\mathbf{H}\{\sigma_{\mathbf{r}}\})$, where β is the inverse temperature and \mathbf{H} is the Hamiltonian for the statistical system. One then uses a sum over all the stochastic variables, defined by the linear operation denoted as a trace, to define a thermodynamic quantity the free energy F as

$$e^{-\beta F} = \text{Tr}_{\{\sigma_{\mathbf{r}}\}}(e^{-\beta\mathbf{H}\{\sigma_{\mathbf{r}}\}}). \quad (1a)$$

Equation (1a) gives the problem formulation for statistical physics introduced by Boltzmann and Gibbs and directly used

for renormalization calculations through the 1980s. Since the Hamiltonian is most often a sum of terms, each containing a few spatially neighboring σ_r values, one can write the free energy as a sum of products of blocks:

$$e^{-\beta F} = \text{Tr}_{\{\sigma_r\}} \prod_{\mathbf{R}} \text{BLOCK}_{\mathbf{R}}, \quad (1b)$$

each block depending on a few statistical variables. This formulation applies equally well to the older and the new formulations of the statistical mechanics. Lately, statistical scientists have realized the advantage of a particular special form of writing the product of blocks, called the *tensor network representation*. In this representation, as well as in vertex models, the statistical Boltzmann weights are associated with vertices (rather than bonds) (Baxter, 2007).

The tensor network representation describes the connectivity and interdependence of blocks and statistical variables. Because of locality the numerical value each block attains depends on a small number of statistical variables. Every statistical variable in turn affects the numerical values in a small number of different blocks. This allows the identification of a statistical variable assuming χ different values with an index assuming the values $\{1, 2, \dots, \chi\}$. The blocks are linked because each index appears in precisely two blocks. The blocks then reduce to tensors whose rank is determined by how many different indices determine the values assumed by a given block. Every configuration corresponds to a specific choice of indices. It is believed, but not proven, that this kind of representation forms a link to the fundamental description of the statistical problem (Vidal, 2003). The free-energy calculation which follows by summation over all possible configurations of the statistical variables reduces to a tensor product tracing out all the mutual index values,

$$e^{-\beta F} = \sum_{i,j,k,\dots} \prod T_{ijkl}. \quad (1c)$$

The tensor indices i, j, k, \dots are indirect representations of the original statistical variables. Each value of a given index may represent a sum, with coefficients that can be positive or negative, of the weights of statistical configurations in the system. Moreover, this representation permits a kind of gauge invariance for each index at each point in space, in which all rotations of any tensor index are a symmetry of the system. Specifically, given that the index i appears in two tensors T_{ijkl}^1 and T_{ipqr}^2 , then the index transformation

$$T_{ijkl}^1 \rightarrow \sum_m O_{i,m} T_{mjkl}^1, \quad T_{ipqr}^2 \rightarrow \sum_m O_{i,m} T_{mpqr}^2, \quad (2)$$

for $\sum_m O_{i,m} O_{j,m} = \delta_{i,j}$, will leave the partition function unchanged. This important formal property underpins the newer statistical calculations.

C. Renormalization

The basic theory describing this kind of behavior was derived by Wilson (1971), based in part upon ideas derived earlier (Gellmann and Low, 1954; Patashinskii and

Pokrovskii, 1964, 1979; Widom, 1964, 1965; Kadanoff, 1966, 2009, 2010, 2013). The first element of the theory is the concept of a *renormalization transformation*. This is a change in the description of an ensemble of statistical systems, obtained by changing the length scale upon which the system is described. Such a transformation can be applied to any statistical system, including ones which are or are not at a critical point. There is a whole collection of methods for constructing such renormalization transformations and describing their properties. This review is concerned with describing one class of such transformations, the real-space transformations. These are ones that employ the description of the ensemble in ordinary space (or sometimes space-time) to construct a description of the renormalization process.

The ensemble is parametrized by a set of coupling constants $\mathbf{K} = \{K_j\}$. These couplings describe the spin interactions of the early renormalization schemes, with the subscripts denoting couplings to different combinations of spin operators s_j via

$$\mathbf{H} = \sum_{\mathbf{r}} \sum_j K_j s_j(\mathbf{r}).$$

Alternatively the K 's may be parameters that determine the tensors. The renormalization transformation increases some characteristic distance describing the system, usually the distance between neighboring lattice points on a lattice defining the spatial structure, so that this distance changes according to $a' = \delta L a$. Correspondingly, the renormalization transformation changes the coupling parameters to new values which we denote by \mathbf{K}' . These new couplings depend upon the values of the old ones, so that

$$\mathbf{K}' = \mathcal{R}(\mathbf{K}). \quad (3)$$

Here the function \mathcal{R} represents the effect of the renormalization transformation.

D. Fixed point

The renormalization theory is particularly powerful at the critical point. This application of the theory is based upon the concept of a fixed point, an ensemble of statistical systems that describes the behavior of all individual statistical systems within a particular universality class. Since the critical point is itself invariant under scaling transformations, the ensemble in question is invariant under a renormalization transformation. It is said to be at a fixed point. The fixed point is represented by a special set of couplings \mathbf{K}^* that obey

$$\mathbf{K}^* = \mathcal{R}(\mathbf{K}^*). \quad (4)$$

E. Response analysis and critical indices

The most important physical effects are obtained by studying the behavior of the renormalization transformation in the vicinity of the critical points. This behavior is quantified by the response matrix relating small changes in the couplings K_j with the small changes they induce in the renormalized couplings K_j' ,

$$B_{ij} = \left. \frac{dK'_i}{dK_j} \right|_{K=K^*}. \quad (5)$$

This matrix has right and left eigenfunctions defined as

$$\sum_j B_{ij} \psi_{j\alpha} = E_\alpha \psi_{i\alpha} \quad \text{and} \quad \sum_i \phi_{\alpha i} B_{ij} = E_\alpha \phi_{\alpha j}. \quad (6)$$

The eigenvalues above directly determine the scaling properties of the exact solution through

$$E_\alpha = (\delta L)^{y_\alpha} = (\delta L)^{d-x_\alpha} \quad (7)$$

with δL being the length rescaling factor produced by the renormalization, d is the dimensionality of the system, and x_α are called the critical exponents.¹ Different authors describe their results in terms of E_α or y_α , or x_α . In this review, we use the last descriptor.

The eigenfunctions ϕ and ψ can be used to construct a linear combination of the coupling constants, namely, $h_\alpha = \phi_{\alpha i} \delta K_i$, which obey the simple scaling transformation rule

$$h'_\alpha = E_\alpha h_\alpha = (\delta L)^{d-x_\alpha} h_\alpha.$$

These eigenfunctions can also be used to construct a set of densities $o_\alpha(\mathbf{r})$ of operators called scaling operators since they have simple properties under scale transformations. The combinations

$$\sum_j s_j(\mathbf{r}) \psi_{j\alpha} = o_\alpha(\mathbf{r}) \quad (8a)$$

define $o_\alpha(\mathbf{r})$ as the densities for the scaling operator. The operators o_α and their extensive counterparts $O_\alpha = \sum_{\mathbf{r}} o_\alpha(\mathbf{r})$, respectively, scale like distances to the power $-x_\alpha$ and y_α , respectively. The other coefficient in the eigenvalue analysis $\phi_{\alpha i}$ can be interpreted by saying that s_i generates a combination of fundamental operators according to

$$s_i(\mathbf{r}) = \sum_\alpha \phi_{\alpha i} o_\alpha(\mathbf{r}). \quad (8b)$$

To make Eqs. (8a) and (8b) work together, we must define the eigenvectors so that they are normalized and complete

$$\sum_i \phi_{\alpha i} \psi_{i\beta} = \delta_{\alpha\beta} \quad \text{and} \quad \sum_\alpha \phi_{\alpha j} \psi_{i\alpha} = \delta_{ij}. \quad (9)$$

The crucial quantity in this analysis is the critical index x_α defining the scaling properties of the scaling operator. For the usual always-finite scaling operators the exponents x_α are positive. Operators for which the corresponding critical

exponents lie between zero and the dimension of the system d are called *relevant operators*. These play a major role in the thermodynamics. Operators for which the corresponding critical exponents are greater than d are called *irrelevant operators* and do not contribute to the singular behavior of the thermodynamic functions (Kadanoff and Wegner, 1971; Wegner, 1976). Below we compare the values of the critical indices x_α as they emerge from the approximate numerical renormalization theory with the exact values that are often known from exact theories as described by Belavin, Polyakov, and Zamolodchikov (1984) and Di Francesco, Mathieu, and Senechal (1997).

F. Requirements on approximations

The concepts of renormalization and scale invariance lead naturally to the identification of scaling and universality and have contributed to the fundamental understanding of critical phenomena. There is also a more practical aspect of the renormalization concepts that allows one to predict the location of phase transitions of specific systems and describe their nature in terms of the critical exponents. However, for most systems, carrying out the actual renormalization cannot be done exactly. Instead, some approximation method must be used to find an approximate renormalization transformation. We hope that the approximation method will give an informative picture of the physical system, that it is numerically accurate, and that it is improvable so that more work can lead to better results.

G. History of real-space methods

The first heuristic definition of a real-space renormalization was given by Kadanoff (1966). Later the viability of the renormalization approach was demonstrated by inventing the ϵ expansion (Wilson and Fisher, 1972; Wilson and Kogut, 1974). This approach was adapted for a numerical calculation of the renormalization function R in terms of a small number of different couplings (Niemeijer and van Leeuwen, 1973; Niemeyer and Van Leeuwen, 1974). These methods were described in one dimension (Nelson and Fisher, 1975; Maris and Kadanoff, 1978) and applied (Kadanoff and Houghton, 1975).

From the point of view of this review, an important advance occurred when a variational method was invented (Kadanoff, 1975) and extensively employed (Kadanoff and Houghton, 1975; Burkhardt, Knops, and den Nijs, 1976; Burkhardt, 1976b; Burkhardt and Knops, 1977; Knops, 1977; den Nijs and Knops, 1978). This method was described as a *lower-bound calculation* since it permitted calculations that gave a lower bound on possible values of the free energy. This approach permitted reasonably accurate and extensive calculations of critical properties in two and higher dimensions.

However, as the 1970s came to an end, the lower-bound method fell into disuse. This turning away was in part because higher accuracy could be obtained by commingling the ideas from real-space renormalization with Monte Carlo simulations (Ma, 1976; Swendsen, 1979; Blote *et al.*, 1996), thereby obtaining excellent representations of fixed points and scalings. Gradually, however, interest turned away from statistical problems and toward problems involving quantum mechanics

¹Scaling indices x_α and y_α are used to represent the natural group properties of scaling operations. If δL_1 and δL_2 are two rescaling factors, then the forms of the eigenvectors as a function of these rescaling factors satisfy $E(\delta L_1 \cdot \delta L_2) = E(\delta L_1)E(\delta L_2)$. It follows that $E(1) = 1$ and $E'(\delta L_1)/E(\delta L_1) = C/\delta L_1$ for some constant C , leading to $E(\delta L) \propto \delta L^y$ (Goldenfeld, 1992).

and zero temperature phase transitions. Although path-integral methods permit one to convert a quantum problem into one in classical statistical mechanics, the statistical methods seemed to work best when the problem had the full rotational symmetry of its lattice and hence did not apply to many quantum problems.

White (1993) invented a quantum mechanical real-space renormalization scheme that worked well for finding the properties of one-dimensional quantum systems via numerical analysis. The success of the density matrix renormalization group started a large school of work aimed at these problems and analogous problems in higher dimensions (Evenbly and Vidal, 2009a; Vidal, 2010; Zhao *et al.*, 2010; Schollwock, 2011).

White's method looked very different from the real-space work of the 1970s. It did, however, have an important provenance in the numerical solution of the Kondo problem (Wilson, 1975). White studied the approximate eigenstates involving long chains of correlated spins and how those long chains interacted with small blocks of spins.

The correlations within wave functions were produced by summing products of correlations on small blocks, producing situations described as “tensor product states” (Cirac and Verstraete, 2009). These tensor product representations facilitated accurate analysis based on the correlations among statistical variables located at a very small number of nearby lattice sites. For example, Vidal (2010) studied a one-dimensional lattice where two or three neighboring lattice sites are used as the basis of the correlations, whereas Levin and Nave (2007) examined higher dimensional systems and used a hexagonal construction in which correlations were constructed from examining the interactions between two neighboring lattice sites and their interactions with their nearest neighbors. Last, in the analysis presented by Gu and Wen (2009), which is closest in structure to the one we carry here and use to compare to the lower-bound calculation, they use a four-index tensor describing the intersections in a square lattice and generate correlations from examining the interaction of a lattice site with all four nearest neighbors. Over the course of time, connections among the different approaches began to be appreciated.

H. Comparisons

Here we focus on differences between the work of the 1970s and that of the last two decades.

1. Stochastic variables

We have already mentioned that the 1975 scheme uses spins while the recent scheme employs much more complex spatial structures labeled by tensor indices. Both approaches need to reflect the underlying symmetry of the problem at hand, for example, the spin flip symmetry of an Ising model. The early work used spin variables that directly reflected the symmetry.²

²However, there were occasional uses of more complex variables. For example, in the Ising model calculation by Burkhardt (1976a), the “spin” variable could take on three values: ± 1 and zero. The last value reflects a hole unoccupied by a magnetic spin.

In contrast, the more recent work has replaced summation over spin variables by sums over tensor indices. The basic symmetries are hidden in the structure of these tensors. In using this tensor representation, recent workers have used universality to say that they can use any problem definition that reflects a desired symmetry. They then also argue that the proper meaning of the tensor indices will give them direct access to the deep structure of the statistical mechanics problem (Swingle and Wen, 2010).

Each tensor index can take on χ possible values, representing the number of different configurations of the system. Recent workers believe, but have not proven, that working with a constant χ [thereby omitting $\chi^2 - \chi$ terms from the singular value decomposition (SVD)] results in an error which tends to zero as $\chi \rightarrow \infty$. Consequently, they reach for approximation methods that permit them to increase χ until it reaches quite large values, and perform the approximation with a high χ value. (Note that these indices with their large number of possible values can simultaneously approximately represent many kinds of different variables: many-component vectors, Ising spins, or continuous variables.) In contrast the earlier workers felt that arbitrary accuracy would not be available to them. The best that was expected was a qualitatively accurate description of the problem.

We use the term *summation variables* to describe both the spins of the earlier work and the stochastic variables linked to the tensor indices more recently used.

2. Geometric structure

Another difference can be seen in the geometric structures used to describe the interactions among the summation variables. In the tensor network formulation the summation variables are associated with bonds and their interactions are associated with vertices, as was done in vertex models; see, for example, Baxter (2007). Each summation variable appears in exactly two tensors, thereby connecting two vertices. The vertices, however, are less constrained and typically group together several indices, thereby forming a rank m vertex.

In the earlier renormalization work, in contrast, the summation variables are associated with vertices and thus may participate in more than two interactions. The interactions are associated with blocks of summation variables allowing each summation variable to participate in more than two interactions.

This difference not only manifests itself in the formulation of the partition function of each of the representations but more importantly restricts the placement of the rescaled summation variables and their interactions. In the earlier work new summation variables could be placed arbitrarily provided the interactions they participate in can be formulated in terms of the old interaction blocks. In the tensor representation the binary interaction structure must be preserved when introducing new summation variables. Thus every introduction of a new summation variable is necessarily associated with changing the interaction connectivity of the old variables, a process called *rewiring*.

3. Computational strategy

The earlier work found the properties of critical points via a method based upon the analysis of fixed points. First the critical system was brought to a fixed point. Critical indices were then calculated by looking at the growth or decay under renormalization of small perturbations about the fixed point, using a method based upon eigenvalues (see Sec. I.E). The main output of the calculation was a set of critical indices which could be compared among calculations and with theoretical results.

In contrast, tensor analysts seldom calculate fixed points.³ Instead they calculate free energies and other thermodynamic quantities by going through a large number of renormalizations, usually increasing the value of χ as they go. (As we shall see, it is natural to square the value of χ in each tensor renormalization.) When they reach a maximum convenient value of χ they employ approximations that enable them to continue to renormalize with fixed χ . These calculations then show the thermodynamic behavior near criticality.

The nonappearance of fixed points in many of the tensor calculations provides an important stylistic contrast between that work and the studies of the 1975 era. The calculation of fixed points for the critical phenomena problems permits the direct calculation of critical indices and thus offers many insights into the physics of the problem. The insights are obtained by keeping track of and understanding every coupling constant used in the analysis. This is easy when there are, as in [Kadanoff \(1975\)](#), sixteen couplings. However, the more recent tensor-style work often employs indices which are summed over hundreds of values, each representing a sum of configurations of multiple spinlike variables. All these indices are generated and picked by the computer. The analyst does not and cannot keep track of the meaning of all these variables. Therefore, even if a fixed point were generated, it would not be very meaningful to the analyst. In fact, the literature does not seem to contain much information about the values and consequences of fixed points for the new style of renormalization.

The fixed-point method seems more fundamental and preferable, but offers major challenges when the value of χ is large.

I. Plan of review

The next section describes the block spin and the rewiring methods employing SVD used for renormalization by [Levin and Nave \(2007\)](#) and [Gu and Wen \(2009\)](#). Section III outlines the results from these calculations, including some new results for both the 1975 method and also the rewiring calculations. The final section suggests further work.

³Notable exceptions include the Hamiltonian work of Vidal and co-workers ([Evenbly and Vidal, 2009a](#); [Vidal, 2010](#)), in which a fixed-point Hamiltonian is indeed calculated. For statistical rather than quantum problems, fixed-point studies were done by [Hinczewski and Nihat Berker \(2008\)](#) and [Aoki, Kobayashi, and Tomita \(2011\)](#). These fixed-point analyses, however, were carried out only for small values of χ .

II. THE RENORMALIZATION PROCESS

A. Overview

We now compare different approximate real-space renormalization schemes. The starting point for the considered methods is a system described by the statistical variables $\{\sigma\}$ and a Hamiltonian $\mathcal{H}\{\sigma\}$. In the 1975 scheme this Hamiltonian is directly used to define the partition function

$$Z = \text{Tr}_{\{\sigma\}} e^{-\beta\mathcal{H}}. \quad (10a)$$

In the newer scheme, the Hamiltonian is used to define a two-, three-, or four-index tensor along the lines described in Sec. II.B. The partition function is then defined as a statistical sum in the form of a sum over indices of a product of such tensors, in the form

$$\text{two index : } Z = \sum_{i,j,k,\dots,n} T_{ij} T_{jk} \cdots T_{ni} \quad (10b)$$

or

$$\text{four index : } Z = \sum_{i,j,k,\dots} \prod T_{ijkl}. \quad (10c)$$

In both cases, the setup of the tensor product is such that each index appears exactly twice. In this way, the system can maintain its gauge invariance. We can then imagine that these partition functions may equally well be described in terms of the values of coupling constants \mathbf{K} or of the value of tensors T .

Working from this starting point, the renormalization scheme is implemented through three steps as follows.

1. Introducing new statistical variables

In the 1975-style scheme, the new variables are defined to be exactly similar to the old variables $\{\sigma\}$, except that the new variables are spaced over larger distances than the old ones (see Fig. 1).⁴ A new Hamiltonian, depending on both old and new variables, is defined by adding to the old Hamiltonian an interaction term⁵ $\tilde{V}(\{\mu\}, \{\sigma\})$. This term is defined so that the partition function remains unchanged by the inclusion of the μ 's. This invariance is enforced by the condition

$$\text{Tr}_{\{\mu\}} e^{-\beta\tilde{V}(\{\mu\}, \{\sigma\})} = 1, \quad \forall \sigma \quad (11a)$$

so that the partition function can be written as

$$Z = \text{Tr}_{\{\sigma\}} e^{-\beta\mathcal{H}(\{\sigma\})} = \text{Tr}_{\{\sigma\}} \text{Tr}_{\{\mu\}} e^{-\beta\mathcal{H}(\{\sigma\}) - \beta\tilde{V}(\{\mu\}, \{\sigma\})}. \quad (11b)$$

A roughly similar analysis can be used in the tensor network scheme. Starting from the definition of the partition function as

⁴In fact, this structural identity of the old and new variable sets is one of the major limitations of the older scheme. The quality of the entire renormalization scheme is determined by the choice of a set of initial variables.

⁵The \sim appears on this V to distinguish it from another use of the symbol V , that is the V that conventionally appears in singular value decomposition analysis.

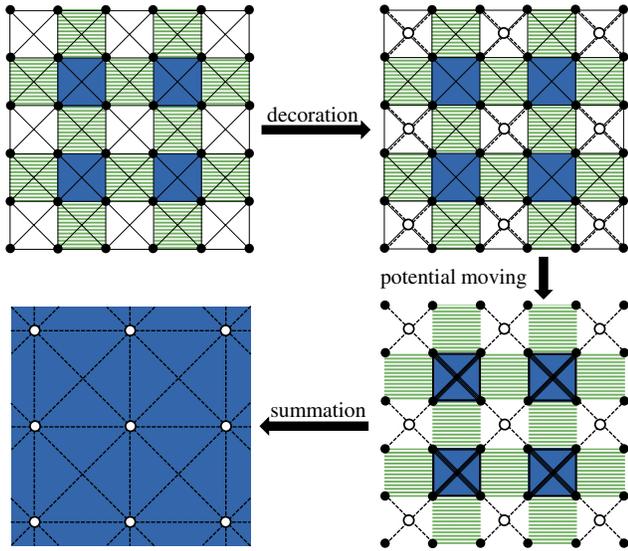


FIG. 1 (color online). The setup for a potential-moving scheme on a square lattice. The old spins (σ) are marked by solid circles located at the vertices of a square lattice. Note that each such spin belongs to four different squares. These squares form the “blocks” for our calculation. The new spins μ appear in one-quarter of the blocks and are marked as empty circles. The thick dashed lines emanating from these new spins denote coupling terms that link these to the old spins. Each such coupling connects a single old spin to a new one. The potential moving places all the interactions between old spins in one-quarter of the squares (solid colored). The old spins around every one of these squares are connected only to themselves and to the neighboring new-spin variables. They can be summed over, giving a new effective coupling between adjacent new spins. The basic blocks in the starting situation are shown as squares of different textures in the upper left panel. The blocks in the final situation are shown outlined by the dashed lines in the bottom left panel. In the course of the calculation, the lengths of the sides of the blocks have been increased by a factor of 2.⁶

the trace of a product of tensors in Eq. (10c) one replaces each of the rank four tensors by a product of rank three tensors, using a scheme derived from the SVD theorem (see Sec. II.C.1),

$$T_{ijkl} = \sum_{\alpha} S_{ij\alpha}^A S_{k\alpha}^B, \quad (12a)$$

leaving us with

$$Z = \sum_{ijkl\dots} \prod T_{mnpq} = \sum_{ijkl\dots} \sum_{\alpha\beta\gamma\dots} \prod S_{ij\alpha}^A S_{k\alpha}^B. \quad (12b)$$

2. Tracing out the original statistical variable

In the 1975 scheme the trace over the original statistical variables $\{\sigma\}$ defines a new Hamiltonian \mathcal{H}' which depends solely on the new variables $\{\mu\}$,

⁶The correspondence with the notation employed in Kadanoff (1975) is as follows: The green blocks correspond to striped block in our work, the red blocks are empty, and the blue blocks become solid shaded blocks in our work.

$$e^{-\beta\mathcal{H}'\{\mu\}} = \text{Tr}_{\{\sigma\}} e^{-\beta\tilde{\mathcal{H}}(\{\mu\},\{\sigma\})}, \quad (13)$$

so that

$$Z = \text{Tr}_{\{\mu\}} e^{-\beta\mathcal{H}'\{\mu\}}. \quad (14)$$

One can expect that some approximation will be needed in order to calculate the sum over the σ 's.

A roughly analogous procedure can be applied to the tensor sums in Eq. (12). If the positions of the S^A and S^B products and the new indices have been deftly chosen, the old indices will appear in a series of small islands in which each island is coupled only to a limited number of new indices. Following Gu and Wen (2009), we shall work with the case in which that number is four. After a rearrangement, the partition function sum in Eq. (12) can be written as

$$Z = \sum_{\alpha\beta\gamma\dots} \sum_{ijkl\dots} \prod S_{ij\alpha}^A S_{k\alpha}^B = \sum_{\alpha\beta\gamma\dots} \prod T'_{\alpha\beta\gamma\delta}, \quad (15)$$

where each of the new tensors T' was obtained via a partial summation over the old indices, for example,

$$T'_{\alpha\beta\gamma\delta} = \sum_{ijmn} S_{ij\alpha}^A S_{j\beta}^B S_{nm\gamma}^A S_{mi\delta}^B.$$

The specific tensors that enter the partial tracing (e.g., S^B vs S^A) and their connectivity depend on the details of the problem. Nonetheless, the structure of both old and new methods remains one in which one introduces new variables and then performs a summation over the old variables.

3. Obtaining a recursion relation

The new degrees of freedom μ have been defined to be identical to the variables σ , the only difference being that the μ 's are defined on a rescaled system. This identity usually permits the extraction of new coupling constants \mathbf{K}' from the new Hamiltonian. The new couplings are then connected to the old via the recursion relation $\mathbf{K}' = \mathcal{R}(\mathbf{K})$.

If the recursion relation is calculated exactly, the new set of couplings will likely contain many more terms than the old set. This proliferation of couplings reflects the additional information from several blocks of the old system that we are trying to cram into one block of the new one. An approximation is needed to limit the new couplings. This limitation usually results in a situation in which the possible couplings include only those that can be formed from spins completely within a geometrically defined block. Couplings which include spins from several blocks are excluded. One example of such a block is shown in Fig. 1.

The tensor scheme has a different approach. In order to do renormalization, the new partition function calculation of Eq. (15) must have the same structure as the old one in Eq. (10c). As discussed in detail in Sec. II.C.1, this structural identity is violated by the exact theory in which there are many more new indices than old. To obtain a recursion relation, one must use an approximation to eliminate the proliferation in the summation degree χ . As discussed in Sec. II.C.1, an approximation of this kind is automatically provided by the SVD

method. Using this approximation method, one has a renormalized problem with exactly the same structure as the original problem. The result may be expressed as a recursion relation for the rank four tensor

$$T' = S(T) \quad (16)$$

or as a recursion relation for the parameters defining those T 's, e.g., $\mathbf{K}' = \mathcal{R}(\mathbf{K})$.

There is a difficulty in using tensor components in the recursion relation of Eq. (16). Because of the gauge invariance the components of the new tensor T' are not uniquely defined. To ensure uniqueness, it would be better to define the tensors in terms of gauge-invariant parameters. While this may be done relatively easily for low χ values, identifying all independent gauge invariants for high χ value tensors may be a daunting task.

With a recursion relation at hand one can apply all the tools described in Sec. I.E and obtain a fixed-point Hamiltonian and the corresponding critical exponents.

In the remainder of this section, we describe the nuts and bolts of the real-space renormalization process, using as our example square lattice calculations based on Ising models and the version of tensor renormalization found in Gu and Wen (2009). We particularly focus on understanding the differences between the older (Kadanoff, 1975) and the newer styles (Levin and Nave, 2007; Gu and Wen, 2009) of doing renormalization work.

B. Basic statistical description

In Sec. I.H.1 we pointed out that the older calculations are based upon summations over defined stochastic variables like the Ising models $\sigma_r = \pm 1$. These calculations then use a Hamiltonian $\mathbf{H}(\{\sigma\})$ to define the statistical weight of each configuration of the variables. Consider a problem involving four spin variables $\sigma_1, \sigma_2, \sigma_3, \sigma_4$ sitting at the corners of a square (see Fig. 2), each variable taking on the values ± 1 . If this problem has the symmetry of a square, it can be described in terms of the following combinations:

$$\begin{aligned} S_0 &= 1, \\ S_1 &= \sigma_1 + \sigma_2 + \sigma_3 + \sigma_4, \\ S_{nn} &= \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1, \\ S_{nnn} &= \sigma_1\sigma_3 + \sigma_2\sigma_4, \\ S_3 &= \sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_3\sigma_4\sigma_1 + \sigma_4\sigma_1\sigma_2, \\ S_4 &= \sigma_1\sigma_2\sigma_3\sigma_4. \end{aligned} \quad (17)$$

The spin combination variables S_i form a closed algebra, i.e., any function of the spin variables of Eq. (17) may be expressed as a linear sum of these same variables with constant coefficients:

$$F(S_0, S_1, S_{nn}, S_{nnn}, S_3, S_4) = \sum a_i S_i.$$

One important example of this set of variables, denoted as $[S]$, is a Hamiltonian $\mathbf{H}^{sq}[S]$ which describes the most general

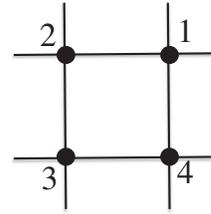


FIG. 2. Identification of the spin variables located at the vertices of a square unit cell.

isotropic interactions with the symmetries of a square unit block that can be formed from the set of σ_i 's. The basic block used in the 1975 renormalization calculation is given in terms of this Hamiltonian as

$$\text{BLOCK} = e^{-\beta \mathbf{H}^{sq}[S]} \quad \text{with} \quad -\beta \mathbf{H}^{sq}[S] = \sum_i K_i S_i. \quad (18)$$

Here the K 's are called coupling constants and their values provide a numerical description of the problems at hand.

In contrast, the host of new calculations replaces the coupling constants by tensors and uses the tensor indices as a proxy for statistical variables. To illustrate this process, we write the tensor T_{ijkl} for the cases in which each index can take on two possible values and in which there is once more the symmetry of a square. The tensors are situated on every other square and therefore capture only half of the possible four spin interaction and next nearest neighbor interaction.⁷ We use the spin notation to write the tensor as

$$T = e^{\sum K_i S_i}. \quad (19)$$

There is considerable flexibility in defining the tensor's indices. This flexibility is a feature of the gauge flexibility of the tensor-SVD method. For example, we could allow one index value (+) correspond to positive spin and the other (−) to negative spin. Then the tensor components would have the following distinct values:

$$\begin{aligned} T_{++++} &= \exp(K_0 + 4K_1 + 4K_{nn} + 2K_{nnn} + 4K_3 + K_4), \\ T_{\{++++\}} &= \exp(K_0 + 2K_1 - 2K_3 - K_4), \\ T_{\{++--\}} &= \exp(K_0 - 2K_{nnn} + K_4), \\ T_{\{+--+ \}} &= \exp(K_0 - 4K_{nn} + 2K_{nnn} + K_4), \\ T_{\{+---\}} &= \exp(K_0 - 2K_1 + 2K_3 - K_4), \\ T_{----} &= \exp(K_0 - 4K_1 + 4K_{nn} + 2K_{nnn} - 4K_3 + K_4), \end{aligned} \quad (20)$$

where curly braces stand for all cyclic index transformation, i.e.,

$$T_{\{++++\}} = T_{++++} = T_{++++} = T_{++++} = T_{++++}.$$

Alternatively, one might use the index value [1] to represent a sum over the statistical weights produced by the possible spin configurations ($\sigma = +1$) and ($\sigma = -1$) and the index [2] to

⁷We note that allowing the index four possible values allows the description of every interaction in Eq. (17). However, for simplicity we restrict our present treatment to the two valued index tensors only.

represent a difference between these two statistical weights, specifically

$$[1] = \frac{(+)+(-)}{\sqrt{2}} \quad \text{and} \quad [2] = \frac{(+)-(-)}{\sqrt{2}}. \quad (21)$$

The factor of $\sqrt{2}$ is introduced to make the index change into an orthogonal transformation. Under this definition the tensor representation would also have six distinct components, however, their values in the different representations change according to

$$\tilde{T}_{ijkl} = \sum_{mnop} O_{im} O_{jn} O_{ko} O_{lp} T_{mnop}, \quad (22)$$

where O denotes the orthogonal transformation which maps the indices $+-$ on the right to the new indices [1] and [2] that appear on the left. For example,

$$\begin{aligned} \tilde{T}_{1111} &= \frac{1}{4}(T_{++++} + 4T_{+++-} + 4T_{+--+} \\ &\quad + 2T_{+---} + 4T_{----} + T_{----}), \\ \tilde{T}_{\{1112\}} &= \frac{1}{4}(T_{++++} + 2T_{+++-} - 2T_{+---} - T_{----}). \end{aligned}$$

It is important to note that Eq. (22) gives two different descriptions of the very same tensor T in different bases. The tensors remain the same, but the coordinate system is varied.

Of course, the case described here is rather simple. The renormalization transformation develops, step by step, a succession of tensors, usually of increasing complexity. At each step, the partition function depends upon the tensor in question, but is independent of the particular representation of that tensor. When applied successively to the redefinition of indices in each step of a long calculation, the index method provides a flexibility and power not easily available through the direct manipulation of spinlike variables. We see this flexibility in the specific calculations of renormalizations described in Sec. III.

C. Tensor-SVD renormalization

In this section, we complete the discussion of renormalization as set up by Levin and Nave (2007) and Gu and Wen (2009) and then carried out by Hinczewski and Nihat Berker (2008) and Aoki, Kobayashi, and Tomita (2011). We begin by introducing the main tool of the method, singular value decomposition, and discuss its properties. We then discuss the underlying geometry of the tensor network and review the tensor gauge freedom.

1. Singular value decomposition

The new renormalization methods described in this review are based upon those of Levin and Nave (2007) and Gu and Wen (2009); [see also, for example, Zhao *et al.* (2010) and Xie *et al.* (2012)]. These make use of the singular value decomposition theorem in their analysis. The theorem states that every n by n real matrix M_{ij} can be expressed as a product of a real unitary matrix, a diagonal non-negative matrix, and another real unitary matrix:

$$M_{ij} = \sum_{\alpha=1}^n U_{i\alpha} \Lambda_{\alpha} V_{j\alpha}, \quad (23)$$

where $\sum_{\alpha} U_{i\alpha} U_{j\alpha} = \delta_{ij}$ and $\sum_{\alpha} V_{i\alpha} V_{j\alpha} = \delta_{ij}$. While the singular values Λ_{α} are uniquely determined, the normalized eigenvectors constituting the columns of U and V have a sign ambiguity. Note, however, to preserve the structure (23), the signs picked for U will determine the signs for V .⁸

Customarily, the Λ_{α} 's, called *singular values*, appear in descending order. Equation (23) can then be used to construct an approximation for M by including only the χ largest components of Λ . This approach yields an approximation of M which is optimal in the least squares sense.⁹

Finally, we fold the singular values into the matrices V and U :

$$S_{i\alpha}^A = U_{i\alpha} \Lambda_{\alpha}^{1/2} \quad \text{and} \quad S_{j\alpha}^B = V_{j\alpha} \Lambda_{\alpha}^{1/2}. \quad (24a)$$

The above matrices allow us to rewrite the approximation of M as a product¹⁰:

$$M_{ij} \approx M_{ij}^{\chi} = \sum_{\alpha=1}^{\chi} S_{i\alpha}^A S_{j\alpha}^B. \quad (24b)$$

This approximation is used throughout the discussion of rewiring methods. Notice that the approximation in Eq. (24) becomes exact when $\chi = n$.

2. SVD as an approximation method

For a square lattice, one writes down the tensor product representation of the partition function as the trace over a product of rank four tensors

$$Z = \sum_{ijklmn\dots} \prod T_{ijkl},$$

in which each index occurs precisely twice. The summation depends strongly on the topology of the network composed of the indices connecting adjacent tensors. For this reason the usual methods of describing tensor calculations make heavy use of pictures. We follow that precedent.

We show the tensor lattice in Fig. 3. Each colored box is a four-legged tensor. The tensor indices appear at the corners as solid circles. The inset shows the definition of these indices. The task at hand is to introduce new indices while isolating small groups of old indices so that these groups make no contact with other old indices. To do this we rewrite a potential term like T_{ijkl} as a matrix product in the form

⁸One can lift this ambiguity, as we do in our calculations, by setting the sign such that the first nonvanishing component of each right eigenvector is positive. Note, however, that this resolution of the sign ambiguity is not invariant under a base change.

⁹More precisely, the SVD estimate of M , called M^{χ} , serves to minimize the quantity $Q = |M - N|^2 = \text{Tr}[(M - N)(M^T - N^T)]$ within the class of N 's that are matrices with only χ nonzero eigenvalues. The minimizer is given by $N = M^{\chi}$.

¹⁰The notation S^A and S^B was introduced by Levin and Nave (2007) who then put these different matrices on different sublattices. In the case considered here the tensors in the two sublattices coincide leading to some algebraic simplification.

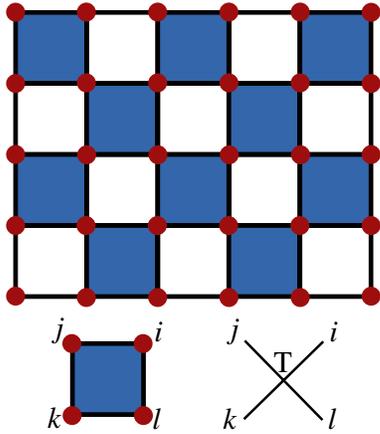


FIG. 3 (color online). The basic tensor network used here for the SVD renormalization calculations. Tensors are represented by solid shaded squares. Solid circles denote the position of the tensor's indices. Every tensor has four indices. Every index assumes integer values between 1 and χ and is shared between exactly two tensors. Four indices determine the configuration of the statistical variable, and the corresponding tensor entry gives the statistical weight of the configuration. Note that the interactions represented by the tensors occupy half the available space. The left inset shows the labeling of the indices; the right inset shows the same tensor in the stick figure usually used in the literature.

$$T^{\text{approx}}_{ijkl} = \sum_{\alpha=1}^{\chi'} S^A_{i\alpha} S^B_{j\alpha} S^A_{k\alpha} S^B_{l\alpha}, \quad (25)$$

where α is the new index. There are six ways of doing this, involving different placements of the indices $ijkl$ in S^A and S^B . Two of these are depicted in Fig. 4.

The singular value decomposition theorem points out that we can make Eq. (25) give an exact expression for the four-legged tensor by using SVD and letting $\chi' = \chi^2$. Alternatively we can use a smaller value of χ' , as, for example, $\chi' = \chi$, and use either SVD or some other method to get a good approximation involving U and V . The change suggested by Gu and Wen (2009) is shown in Fig. 4. This figure has the crucial property that blocks of four old indices are coupled to new indices but not to any other old ones. The four-index block draws its indices from four different tensors T . No interactions among these old indices are to be found in this kind of block before the renormalization process. All correlations are produced by the S^A 's and S^B 's that surround the block. The calculation of the renormalized T is then very simple. It is

$$T'_{\alpha\beta\gamma\delta} = \sum_{ilmn} S^A_{li\alpha} S^B_{in\delta} S^A_{nm\gamma} S^B_{ml\beta}. \quad (26)$$

In this way, a recursion relation is derived for any choice of S^A and S^B .¹¹ It is natural and simple to use the SVD

¹¹Note that the tensor T' is not isotropic. Moreover, it is rotated by 90° in adjacent cells. An alternative calculation resulting in rotationally invariant tensors sums either only S^A matrices or only S^B matrices for every T' . This results in two different tensors T'_1 and T'_2 placed on a bipartite lattice (Levin and Nave, 2007).

method to generate these three-legged tensors. In the remainder of this review we do that, fixing the number of indices by $\chi' = \chi$. In our numerical work, we stick with small values of χ . To get really accurate results, one squares χ several times until a large enough value is reached so that one feels one can neglect higher order indices.

3. Gauge invariance and interpretation of fixed-point tensor components

The tensorial formulation of a given statistical problem is, as previously mentioned, not unique. In particular, one can apply an orthogonal transformation to each of the legs of each of the tensors keeping the partition function obtained from their product invariant. One can naturally ask how does the fixed-point tensor behave under such transformations?

We write the renormalization step Eq. (26) for a general tensor T as $T' = \mathcal{R}(T)$. The fixed-point tensor T^* satisfies $T^* = \mathcal{R}(T^*)$. In the Appendix we prove that up to sign ambiguities any rotation of fixed-point tensor having distinct singular values yields under the renormalization step the original fixed-point tensor, i.e.,¹²

$$\mathcal{R}(O_{im} O_{jn} O_{ko} O_{lp} T^*_{nmop}) = \mathcal{R}(T^*) = T^*. \quad (27)$$

This implies that there exists one particular “preferred” base for the representation of the fixed-point tensor, picked out by the renormalization scheme. Consequently, the physical interpretation of tensor renormalization group (TRG) fixed points is complicated by the necessity for disentangling gauge-specific results from physical results. Gauge-specific terms in the tensors may also slow down and complicate the search for a physically meaningful fixed point.

D. Zeros in the response matrix

The gauge symmetry discussed previously implies that there will be many kinds of linear changes in T that will produce zero change in T' . Consequently, there will be a whole space of changes, called a *null space*, that produce zeros in the response matrix.

Another contribution to the null space comes from the loss of information in the truncation of the SVD decomposition. The number of independent components in a χ^2 by χ^2 matrix is χ^4 . If, however, the χ^2 by χ^2 matrix is known to have only χ nonvanishing eigenvalues then the number of independent components is only $2\chi^3 - \chi^2$. These two losses of information imply that the analysis of a tensor fixed point may be dominated by understanding the effects of the null space.

1. Errors

When $\chi' < \chi^2$ the approximate rewiring will generate an error. We denote the local error resulting from the approximation by

¹²This implies that a representation independent definition of the fixed-point tensor is given by $\mathcal{R}(\tilde{T}^*) = \mathcal{R}(\mathcal{R}(\tilde{T}^*))$.

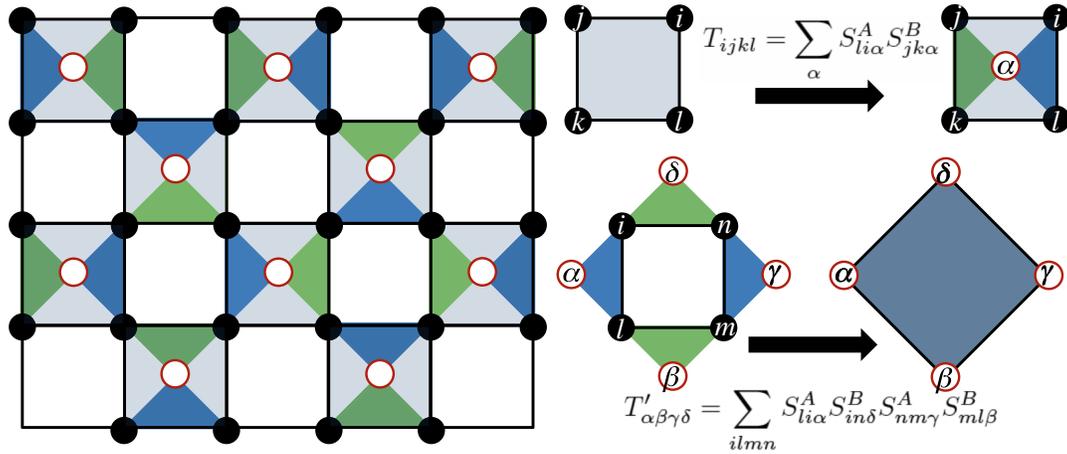


FIG. 4 (color online). The tensor network after rewiring. The old four-legged tensors are shown lightly shaded. They have disappeared and have been replaced by the three-index tensors S^A and S^B shown in darker shades. Each three-index tensor appears as a triangle with two of the old tensor indices and one new index at its vertices. These are, respectively, shown as solid circles and empty circles. Note the white squares are all empty of interactions. These squares are of two kinds: the ones flanked by colored triangles (three-legged tensors) and the one flanked by shaded triangles (the ghosts of disappeared four tensors). Each first-kind square permits the summation over the four old index variable at its corners and thereby the generation of interactions among the new indices. These white squares together with their four bounding triangles become the new tensors on the rescaled system.

$$\text{Error}_{ijkl} = \ln[T_{ijkl}/T^{\text{approx}}_{ijkl}]. \quad (28)$$

This is the error of a single tensor at a specific configuration given by its indice values. The SVD scheme yields an error for the tensor that is optimized in a mean square sense (Levin and Nave, 2007; Gu and Wen, 2009). In the analysis of Levin and Nave and Gu and Wen, the error term is then simply neglected. This method works exceptionally well for large values of χ , for which the error is quite small. In Secs. III and IV we see that this strategy does not work exceptionally well for smaller χ .

An alternative approach is to replace the error term by its maximum (minimum) over tensor indices. This yields an error of definite sign and in turn gives a lower (upper) bound on the free energy. This approach can even be used to find optimal values for S^A and S^B so as to give a best bound for the free energy.

The 1975 work employed a one parameter family of local lower-bound approximations. The value of the parameter was carefully chosen so as to minimize the *global* error of the free energy, resulting in an error term that is quadratic in the local error term. In contrast the SVD scheme yields a free-energy error that is linear in the error of Eq. (28).

This 1975 method proved to give plausible results for low χ values. We now turn to a discussion of this method.

E. Lower-bound variational renormalization

In this section, we complete the description of the lower-bound variational method. We first introduce the local conditions, formulated in terms of the symmetry of the Hamiltonian, which give rise to a lower bound on the free energy. We then construct a one-dimensional family of such lower-bound potentials characterized by a single parameter p . We finally show how to choose the parameter p to globally minimize the resulting error in the free energy.

1. Decoration

As noted in Sec. II.A the first step toward a renormalization is to introduce new statistical variables, a process known as decoration. In Eq. (12) we described the tensor analysis scheme for doing the decoration. Here we describe in more detail the 1975 scheme for decoration.

In general each of the new degrees of freedom, which we denote by μ , is coupled only to a small subset of the old spin variables σ through a coupling potential $v([\sigma], \mu)$ (where $[\sigma]$ defines the small subset of the old spin variables). For example, in Fig. 1 every new degree of freedom is placed within an interaction block and interacts only within this block with its four nearest neighboring old spin variables. We define a new Hamiltonian within the interaction block of the new variable by

$$\tilde{h}([\sigma], \mu) = h([\sigma]) + v([\sigma], \mu), \quad (29)$$

where $h[\sigma]$ is the old Hamiltonian for the block. Choosing the coupling potential to satisfy

$$\text{Tr}_{\mu} e^{-\beta v([\sigma], \mu)} = 1, \quad (30)$$

regardless of the specific value of the variables σ_i , renders the partition function, and thus the free energy, unchanged by the inclusion of the new variable. The full decoration is obtained by using

$$\tilde{V}(\{\sigma\}, \{\mu\}) = \sum_{\mathbf{R}} v([\sigma]_{\mathbf{R}}, \mu_{\mathbf{R}}),$$

where the sum over \mathbf{R} is a sum over all μ sites. With the new Hamiltonian being $\tilde{\mathcal{H}} = \mathcal{H} + \tilde{V}$, the full partition function is unchanged by the decoration as in Eq. (11).

The 1975 scheme associates one new μ spin with the group of four old σ spins in a surrounding square block. There are

multiple ways to choose a potential interaction among the spins that will satisfy Eq. (30). Following Kadanoff (1975) and Fig. 1 we define a one parameter family of such potential $v^p([\sigma], \mu)$, where the parameter p serves to vary the strength of interaction among the new and old spins. This parameter later allows us to optimize the choice of potential. The family of potentials is given explicitly by

$$\begin{aligned} -\beta v^p([\sigma], \mu) &= p\mu(\sigma_1 + \sigma_1 + \sigma_3 + \sigma_4) + c([\sigma]) \\ &= p\mu S_1 - \ln[2 \cosh(pS_1)], \end{aligned} \quad (31)$$

where S_1 is defined in Eq. (17) and $c([\sigma])$ is chosen such that the sum of $e^{-\beta v}$ over all values of μ gives unity. Because of the closed form algebra of the isotropic spin variable (17) we also know that the constant $c(\sigma)$ can be rewritten as a linear function of the isotropic invariant

$$c([\sigma]) = \sum a_i S_i.$$

As a result, the potential $v^p(\sigma, \mu)$ can be written as a linear combination of the S_i values with coefficients which depend on the variational parameter p .

2. Potential-moving theorem

The work presented by Kadanoff (1975) employed a device for making the renormalization sum tractable that goes under the name of *potential moving*. This device makes use of the following theorem: Consider the statistical sum $e^{-\beta F} = \text{Tr} e^{-\beta \mathbf{H}}$, where the trace gives a sum over a positive semidefinite set of terms involving a Hamiltonian \mathbf{H} , giving rise to a free energy F . Now assume that $-\beta \mathbf{H} = -\beta \mathbf{H}_a + \delta V$. Here we use \mathbf{H}_a to generate an approximate free energy F^a which has a value close to that of the exact free energy F . Our calculation makes use of the symmetry of $-\beta \mathbf{H}$ and δV , in which we demand that δV be odd under some exact symmetry of $-\beta \mathbf{H}$, so that

$$\text{Tr}[e^{-\beta \mathbf{H}} \delta V] = 0. \quad (32)$$

This condition yields

$$e^{-\beta F^a} = \text{Tr} e^{-\beta \mathbf{H}_a} \quad \text{implies} \quad e^{-\beta F^a} \geq e^{-\beta F}. \quad (33)$$

To derive Eq. (33) define a Hamiltonian that interpolates between the exact and the approximate Hamiltonians and a free energy that arises from this interpolation:

$$-\beta \mathbf{H}(\lambda) = -\beta \mathbf{H}_a + (1 - \lambda)\delta V \quad \text{and} \quad e^{-\beta F(\lambda)} = \text{Tr} e^{-\beta \mathbf{H}(\lambda)}.$$

These definitions imply that

$$\frac{d}{d\lambda} \beta F(\lambda) = \langle \delta V \rangle_\lambda$$

and

$$\frac{d^2}{(d\lambda)^2} \beta F(\lambda) = -\langle \delta V - \langle \delta V \rangle_\lambda \rangle_\lambda^2,$$

where the λ subscript means that the average is calculated using a Hamiltonian $\mathbf{H}(\lambda)$. It follows from Eq. (32) that the first derivative vanishes at $\lambda = 0$. The second derivative is always negative. Therefore the interpolating free energy is always larger than the true free energy. At $\lambda = 1$ the interpolating free energy reduces to our approximate free energy. Consequently,

$$\beta F^a - \beta F = -\int_0^1 d\lambda (1 - \lambda) \langle \delta V - \langle \delta V \rangle_\lambda \rangle_\lambda^2 \leq 0. \quad (34)$$

Thus, the error in the approximation is of second order in δV and the approximate free energy provides an upper bound for the real free energy.

3. Using potential moving

To construct our approximate renormalization transformation, we need to make sure that the old spins are in isolated small groups, each group coupled to the new spins, but not to any other old spins. If all the couplings obey this condition, we can calculate the new approximate Hamiltonian.

We start from a situation in which the lattice is divided into square blocks as in Fig. 1. There are three kinds of blocks: ones containing a new spin, another containing the nearest neighbor to these new-spin blocks, and another containing the next neighbors of the new-spin blocks. In figurative language, we think of δV as containing some inconvenient couplings that interfere with our calculation of the partition function in Eq. (33). What we do is then “move” the inconvenient couplings from their inconvenient positions (in the new-spin blocks and their nearest neighbors) to convenient positions in the next nearest neighbor blocks. These convenient positions are required to be completely equivalent in the exact version of the calculation to the inconvenient sites. It is only our motion that produces the distinction between these two classes of sites. Thus, Eq. (32) will be satisfied.

The geometry of our calculation is shown in Fig. 1. The original Ising spins appear as solid circles at the vertices of the squares. The new variables are the open circles in the empty squares. The new spins are linked to the old spin variables by interactions indicated by the dashed line. These bonds have interactions of the form $e^{p\sigma\mu}$. All the squares have interactions described by blocks of the form

$$\text{BLOCK} = \exp(-\beta \mathbf{H}^{sq}), \quad (35)$$

where the exponent is given by the block Hamiltonian using the stochastic variables defined by Eq. (17). In addition the empty squares have a potential in the form of $c[\sigma]$ as given by Eq. (18).

All the old interactions from the colored squares are moved into the solid colored squares. The potentials that exist at these squares define the motion. They are

$$\begin{aligned} \delta V &= -\mathbf{H}^{sq} \text{ striped squares,} \\ \delta V &= -\mathbf{H}^{sq} + c([\sigma]) \text{ empty squares,} \\ \delta V &= 3 * \mathbf{H}^{sq} - c([\sigma]) \text{ solid squares.} \end{aligned} \quad (36)$$

The value of the potential on the solid colored squares is picked so that the sum of all the potential terms is zero, allowing for the double weight of the striped squares. The new interaction between the old and new spins can be formulated as a pairwise interaction between the new spin μ and each of its surrounding old spins. It therefore can be reformulated to be centered about the solid colored squares without any approximation. After the motion of the potentials, we end up with no potential on striped or empty squares and a total potential $4 * \mathbf{H}^{sq} - c([\sigma])$ on each solid colored square.

The error generated by the potential moving is proportional to the mean variance in the δV of Eq. (36).

After that motion the spins at the four vertices of each solid colored square are linked to each other and to the surrounding new spins but to none of the other old spins. This condition permits summations to be performed over each solid colored square independently of all the others, thereby producing interactions. The result is

$$e^{-\beta \mathbf{H}^{sq}([\mu])} = \text{Tr}_{[\sigma]} \exp \left[-4\beta \mathbf{H}^{sq}([\sigma]) - c([\sigma]) + p \sum_{j=1}^4 (\sigma_j \mu_j) \right]. \quad (37)$$

The new coupling may then be projected out of the new Hamiltonian. This projection then gives us the recursion relation.

To obtain the optimal calculation in the lower-bound method being described, the parameter p was varied aiming at a p value defined so that the linear response to this change in parameter resulted in no change in the free energy at the fixed point. This resulted in one kind of optimization of the calculation. This approach is not the only reasonable one. There is a wide range of things one might do to optimize real-space calculations. The work of Knops (1977) and Van Saarloos, Van Leeuwen, and Pruisken (1978) suggested an optimization of the free energy at every stage of the renormalization calculation. This approach has the disadvantage that it cannot give any positive value to the specific heat exponent α and in general proved to be a less accurate method for determining critical exponents than the fixed-point optimization. This method gives a better (larger) free energy away from criticality, but the first goal of the renormalization calculations is to get good free-energy derivatives in the neighborhood of the fixed point. This goal appears to be best served by parameter optimization at the fixed point, followed by the use of that parameter value for derivative calculations near the fixed point. Other parameter dependent schemes are available such as by Stella *et al.* (1979).

4. Spatial vectors and tensors

This same mode of analysis enables us to discuss combinations of spin operators which behave like spatial vectors or tensors rather than the spatial scalars defined in Eq. (17). Thus, from the spin labeling shown in Fig. 2, it follows that the combination $\sigma_1 + \sigma_4 - \sigma_2 - \sigma_3$ is to leading order the derivative of the spin with respect to the horizontal coordinate x , while $\sigma_1 * \sigma_4 - \sigma_2 * \sigma_3$ is the derivative of the

energy density with respect to x . Similarly the two components T_{xx} and T_{xy} of the stress tensor¹³ operator can, respectively, be identified as the simplest operators that have the right symmetry,

$$\begin{aligned} T_{xy} &= \sigma_1 \sigma_3 - \sigma_2 \sigma_4 \quad \text{and} \\ T_{xx} &= \sigma_3 \sigma_4 - \sigma_2 \sigma_3 + \sigma_1 \sigma_2 - \sigma_1 \sigma_4. \end{aligned} \quad (38)$$

These identifications enable us to calculate the scaling properties of these operators in the lower-bound scheme. One simply calculates the scaling properties of these operator densities by putting these densities into the coupling of one particular solid colored square and then doing the recursion calculation for the lattice containing that one special square. One can retain the lower-bound property by setting up the potential moving to be symmetrical about that square. This approach then provides a recursion approximation for local operators that fit into a single block. In Sec. III we show some eigenvalues for these vector and tensor operators.

No such scheme exists within the lowest order SVD analysis. Therefore we do not show eigenvalues for any vector or tensor operators within the SVD scheme.

III. RESULTS

Both the variational lower-bound renormalization and the tensor renormalization can be realized by numerical schemes which produce fixed points and, more importantly, critical indices. The latter are expected to be a robust description of a critical point as they do not depend on the specific variables chosen to describe a given system. We next review some new numerical results, mostly in terms of critical indices, and compare them to exact results taken from the literature.

A. Results from block spin calculations

We review various systems differing in their underlying lattice structure (triangular, square, and hexagonal), spin degrees of freedom ($\chi = 2, 3, \dots$), spin coupling (Ising, three-state Potts, and tricritical Ising), and methods of approximation. We collected the results in Secs. III.A.1 and III.A.2, separating the Ising models from the other models considered. Each section begins with a brief description of the different systems and methods presented. The critical indices of the various models are collected in two tables, concluding each of the sections. Most of these results are not new. They are results from 1975 (Kadanoff, 1975; Burkhardt, 1976a; Kadanoff, Houghton, and Yalabik, 1976a), somewhat augmented by calculations done for this review. Additional results can be found in the literature (Burkhardt, 1976b; Burkhardt and Knops, 1977; Jan and Glazer, 1978; den Nijs and Knops, 1978), but the answers shown here are representative of the field.

The critical indices values x are derived from response-matrix calculations at critical fixed points. The x 's are defined by

¹³Of course, the stress tensor is a *spatial* tensor and not a gauge tensor like the T 's that appear in the rewiring scheme.

TABLE I. Ising model critical indices x_α . Note the solid agreement of observed indices with exact indices, except in the stress tensors. The final column is the exact result for the two-dimensional Ising model. All the approximate calculations were done with $\chi = 2$ except for column (D) which has $\chi = 3$. The sources for the data presented above are as follows: (A) Niemeijer and van Leeuwen (1973), (B) Southern (1978), (C) Kadanoff (1975)), new data first presented here, (D) (Burkhardt (1976a), new data first presented here, (E) Jan and Glazer (1978), (F) Jan and Glazer (1978), and (G) Di Francesco, Mathieu, and Senechal (1997).

	(A)	(B)	(C)	(D)	(E)	(F)	(G)
Lattice type	Square	Square	Square	Square	Hexagonal	Triangular	
Variational	No	Yes	Yes	Yes	Yes	Yes	
Approximation method	Error neglect	Potential moving	Exact				
x_0 free energy	0.0	0.0	0.0	0.0	0.0	0.0	0.0
x_σ spin	0.124 86	0.124 68	0.122 26	0.1173	0.1289	-0.70, -0.31	0.1250
x_T energy	1.027 74	0.999 12	0.982 473	1.0302	1.0241	0.67, 0.09	1.0
$\nabla\sigma$		1.167	1.073	1.1440			1.125
T_{xx}		1.797	1.595	2.080			2.0
T_{xy}		1.803	1.595	1.569			2.0
Φ		1.796 68	2.119 00	1.98			
∇^2 spin		2.061 67	2.116 89	1.8303			2.125
∇^2 energy		2.983 91	3.158 48	2.9389			3.0

$$x = d - \log(E)/\log(\delta L),$$

where E is the eigenvalue of the response matrix at the fixed point, d is the dimensionality, and δL is the change in length scale. Each of the critical indices is associated with an eigenvector of the response matrix which represents a scaling operator, i.e., a linear combination of the system's operators which admits a simple scaling rule under renormalization (Wegner, 1976). The distinct indices were identified by the symmetry properties of their corresponding scaling operators and their values as compared with exactly known results.

1. Block spin renormalization of Ising models

We list here different calculations using the block spin renormalization method as applied to the two-dimensional Ising model's critical fixed point. The index values are tabulated in Table I, with the columns indexed by capital letters, as described.

- (A) The first-ever block spin calculation was performed by Niemeijer and van Leeuwen (1973). In this work, studying Ising spins on a triangular lattice, they single out a subset of the triangular cells and separate the interactions into intracellular and intercellular interactions. The intracellular interactions are summed over and the intercellular interactions are recast as interactions between spins residing at the center of the chosen triangles. The "unfavorable" interactions which make the exact summation over intracellular variables intractable were simply neglected.
- (B) The original lower-bound model for Ising spins on a square lattice (Kadanoff, 1975) as described in Sec. II.E. The fixed point for which the critical exponents were computed exhibited equal nearest neighbor and next nearest neighbor couplings.
- (C) The same system as above but at a different fixed point having unequal nearest neighbor and next nearest neighbor couplings.
- (D) The $\chi = 3$ Ising model (also known as the Blum-Capel model or spin 1 model) variational potential-moving calculation which appeared in Burkhardt

(1976a) and Burkhardt, Knops, and den Nijs (1976). This calculation generates a nearby pair of fixed points: one with equal couplings between nearest neighbor and next nearest neighbor, the other with unequal couplings. Their indices are sufficiently close to one another so they are not separately reported here.

- (E) and (F) Ising spins on a hexagonal lattice studied via a variational potential-moving calculation (Jan and Glazer, 1978).
- (G) The critical indices as calculated from the exact theory for the two-dimensional Ising model (Onsager, 1944; Di Francesco, Mathieu, and Senechal, 1997).

In Table I we list the critical indices obtained. The first three indices listed in the table are for the primary operators in the theory. Their values are known from the Onsager solution to the two-dimensional Ising model (Onsager, 1944), from the calculation of that model's magnetization which appears in Yang (1952), and from the results of conformal field theory (Di Francesco, Mathieu, and Senechal, 1997). The approximate numerical results for these indices are, with one exception, very close to the exact values. The exception, the triangular lattice shown in column (F), displays indices that are considerably off the mark. It was argued by Southern (1978) that the approximate calculation on a triangular lattice resembles a situation at a dimension different from 2. However, that is an after-the-fact explanation. We do not really know why the potential-moving calculation does not work as well on the triangular lattice or indeed why it does perform so well on the other lattices.

The next three critical indices correspond to higher order operators. These operator indices were not reported in the earlier papers and are first reported here. They are obtained by calculating the critical indices for operators that do not have the full symmetry of the BLOCK in Fig. 1. For example, the index of σ_y is calculated from the recursion for the operator $\sigma_1 + \sigma_2 - \sigma_3 - \sigma_4$. Correspondingly, all of the operators beyond the primary ones are identified from their transformation properties under rotations and can further be identified with the lowest order operators with the

TABLE II. Critical indices for the three-state Potts model and the Ising model tricritical point. The numerical calculations were performed on a square lattice and employed variational potential moving. The sources for the data presented above are as follows: (A) Burkhardt (1976a) and Burkhardt and Knops (1977), (B) Burkhardt and Knops (1977), (C) Di Francesco, Mathieu, and Senechal (1997), (D) Dasgupta (1977), and (E) Di Francesco, Mathieu, and Senechal (1997).

Scaling operators	Tricritical Ising		Three-state Potts			Scaling operators
	(A) Variational potential moving	(B) Variational potential moving	(C) Exact solution	(D) Variational potential moving	(E) Exact solution	
Free energy	0.0	0.0	0.0	0.0	0.0	Free energy
Spin 1	0.0224	0.0412	0.0375	0.0896	0.0666	Spin σ
Spin 2			0.4375		0.6667	Spin Z
Energy ϵ	0.2030	0.1057	0.1		0.4	Energy ϵ
Energy ϵ'	0.8077	0.8077	0.6	1.1940	1.4	Energy X
Energy ϵ''			1.5		3	Energy Y

corresponding symmetry in the exact theory (Di Francesco, Mathieu, and Senechal, 1997).

The operator marked Φ is a scalar operator which does not fit into the above pattern. There is no operator with the corresponding index and symmetry in the exact theory. Instead it is, we believe, a redundant operator as defined by Wegner (1976). This kind of operator appears essentially as an artifact of the particular method of renormalization. A scalar operator with index close to 2.0 is a likely consequence of two nearby fixed points. The existence of two fixed points is not required by the basic theory and is itself a consequence of the particular method of constructing a renormalization. Once one has two fixed points, one expects to see an operator that powers the flow from one fixed point to the other. As a redundant operator it is extraneous to the theory and has no “correct” index value. But because it produces changes in critical behavior, it is not surprising (Kadanoff and Wegner, 1971) that it has an index close to 2.

The $\chi = 3$ result, depicted in the column (D), disappointingly shows no better index values than the ones in the $\chi = 2$ columns. In fact, one of the values, the one labeled $\nabla^2\sigma$, is substantially worse. These results tend to suggest that one will not gain advantages from going to higher values of χ with the potential-moving strategy as employed in the 1975 period. Perhaps this result should have been expected. The potentials moved may not become smaller for higher χ .

2. Block spin renormalization for other models

Additional coupling constants appear when the spin variables are allowed to take more than two values. In this case, one can find, in addition to the Ising fixed point, new fixed points displaying their own characteristic critical behavior. In Table II we give a set of indices for the fixed point corresponding to the tricritical point of the Ising model and another set for the three-state Potts model. The critical indices values, calculated by potential-moving methods on a square lattice, are compared with exact values obtained from conformal field theory (Di Francesco, Mathieu, and Senechal, 1997). As one can see, the agreement is not as good as the best obtained for the Ising model. Nonetheless, the values of the indices are good enough to be informative.

Here again a combination of the values of the critical indices and the symmetry of the corresponding operators was used to determine their identity. The free-energy exponent is exactly

zero in both the exact result and approximate models. The spin exponents describe operators that have the symmetry of the order parameters in the model. Finally the operators marked energy display the symmetry of the fixed point. Notice that the approximate calculations do not include all the indices available in the theory. There are two sources of this omission. The first is conceptual: If one starts with a limited set of operators, working with them will not necessarily produce all the operators in the theory. This limitation particularly applies to the three-state Potts model. The other limitation is calculational. The approximate calculations produce meaningful results only for a limited set of operators, those with the smallest values of the indices.

B. SVD results

We next review some fixed-point results obtained for rewiring SVD schemes at low values of χ . The main analysis included is composed of critical exponents calculated at fixed points of the tensor renormalization scheme. Most tensor renormalization calculations in the existing literature find the critical indices using extrapolation from data obtained from approximations to the free energy rather than, as we do here, by calculating a fixed point. Fixed points are usually found by a Newton’s method search, which then require derivatives of the free energy at the fixed point. The SVD analysis of this kind is then rather delicate in that it requires a careful treatment of the gauge invariance and also a careful control of which singular values will be included. These tasks, which may be trivial for small χ , become very difficult when successive iterations produce a large value of χ .

We begin with interpretations of the configurations labeled by the different index values. We then summarize the results of the tensor renormalization calculation in tables similar to Tables I and II.

1. Generation of SVD fixed point

Our first SVD fixed point was generated for the $\chi = 2$ square lattice Ising model. We put spins halfway along the bonds forming the legs of the basic SVD tensor. These spins are the filled circles in Fig. 3. For this square lattice each tensor has four legs. Each such tensor can be described by a statistical weight $\exp[-\beta\mathcal{H}^{sq}]$. We started from a tensor using two indices: (+) for up spins and (−) for down spins. We picked a tensor describing interaction strengths of the Onsager critical point of the two-dimensional Ising model. Using the

SVD recipe given in the end of Sec. II.C.1 we calculated an SVD decomposition starting from a tensor defined by

$$T_{++++} = T_{----} = e^{4K} \quad \text{and} \quad T_{\{+--+ \}} = e^{-4K} \quad (39)$$

with all the other tensor components having the value of 1. (Once again, $\{\cdot\}$ describes any cyclic permutation of indices.) This tensor represents the two-dimensional Ising model with nearest neighbor coupling K . The statistical sum is a sum over products of such tensors, each having a weight determined by values of the four spins [see Eq. (18)]. We then performed SVD recursions at $\chi = 2$, adjusting the tensor strengths until we reached a fixed point.

The first step of this process is an SVD recursion starting from the numerical data in the Ising tensor of Eq. (39). The result of an SVD renormalization is shown in Table III which gives the U matrix and the singular values, as defined in Eq. (23). Table III describes the process of rewiring one block of couplings. An essential part is going from the four configurations of two spins defined by the left-hand column of Table III to the four SVD indices [1], [2], [3], and [4]. These data enable us to construct the tensor described in Eq. (39) in the basis formed by these new indices. The interaction between spin pairs is diagonal in this base, e.g., $T_{[1],J}$ reads zero for $J = [2], [3], [4]$. This in turn allows us to eliminate the less significant index values without affecting any of the retained interaction terms.

Table III says, for example, that, in this initial rewiring calculation, the index [1] is constructed from a block with two spins and given partial weights 0.656 708 when the spins are equal but only 0.261 24 when they are unequal. These weights and the others in the table as well as the singular values Λ for the configurations are adjusted by the SVD scheme so that the

TABLE III. The U matrix. This four by four matrix describes the translation from a description that employs two spin indices to one that employs a single tensor index. This SVD translation is derived for the $\chi = 2$ Ising model calculated from a tensor representing an Ising system with coupling corresponding to the Onsager critical coupling as explained in the text. The different columns give the spin content of each index. The behaviors of the bare Ising spin variables under spin flip and site exchange imply the corresponding symmetries of the index variables noted in the first two rows of the table.

	SVD index			
	[1]	[2]	[3]	[4]
Symmetries:				
Spin flip	Even	Odd	Odd	Even
Interchange	Even	Even	Odd	Even
Spin values				
++	$\frac{1}{2}\sqrt{1+\sqrt{\frac{2}{3}}}$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{2}\sqrt{1-\sqrt{\frac{2}{3}}}$
+-	$\frac{1}{2}\sqrt{1-\sqrt{\frac{2}{3}}}$	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}\sqrt{1+\sqrt{\frac{2}{3}}}$
-+	$\frac{1}{2}\sqrt{1-\sqrt{\frac{2}{3}}}$	0	$-\frac{1}{\sqrt{2}}$	$-\frac{1}{2}\sqrt{1+\sqrt{\frac{2}{3}}}$
--	$\frac{1}{2}\sqrt{1+\sqrt{\frac{2}{3}}}$	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{2}\sqrt{1-\sqrt{\frac{2}{3}}}$
Singular value	$4+2\sqrt{3}$	$2+2\sqrt{2}$	$2\sqrt{2}-2$	$4-2\sqrt{3}$

statistical weights in a block are represented by the values of the original four-index tensors T_{ijklm} of Eq. (39). In this way, the information in the couplings K_i in the block are represented by the values of old tensors T and by the values U , V , and Λ . When all four indices are included, U , V , and Λ contain the same information as in the original interactions.

The index values each reflect a particular representation of the symmetries of the two-variable blocks of the basic problem. Here the symmetries are spin flip, $+\leftrightarrow-$, as well as the interchange of the two base spin variables. A glance at Table III shows that the configurations represented by indices [1] and [4] are even under both symmetries while that of [2] is odd under spin flip but even under interchange, with the configuration represented by [3] being odd under both symmetries.

To keep the calculation simple, we use the approximation in which we retain all tensor components with indices [1] and [2] while discarding those with the less significant indices [3] and [4]. The relative significance of the different indices is judged by the relative strength of the singular values as given in the table. Finally we complete the calculation by using Eq. (26) to give us new tensors that come out of the renormalization scheme. Since we have eliminated indices [3] and [4], the new tensors have exactly the same number of components as the old ones.

We expect that the new tensors contain the same kind of information as the starting tensors, only with different interaction strengths. Thus we can equally well represent them in terms of components that are even and odd under spin flip [1] and [2], respectively, or in terms of components described by spin values (+) and (-). This kind of correspondence between the meaning of old and new variables exists near the fixed point of any successful SVD renormalization scheme.

In this case, the mode of translation between these two representations is given in Sec. II.B, particularly in Eq. (21). One might perhaps argue that one or the other representation is more basic or more transparent. Between iterations of the renormalization transform, data can be stored in either basis, which can be equally used in fixed-point calculations.

To illustrate this point, we list in Table IV the U matrix used at the $\chi = 2$ fixed point of the two-dimensional Ising model. In this particular analysis we chose to use [1] and [2] from Table III as our indices for the representation of the tensors formed beyond the start of the renormalization process. We followed through every step of renormalization, examining the U values at every iteration. We observed that, without exception, the SVD analysis resulted in index variables possessing well-defined symmetries; specifically under spin flip the index variables follow the transformation $[1] \rightarrow [1]$ and $[2] \rightarrow -[2]$. Table IV shows that under these transformation rules all four composite variables $[1']$, $[2']$, $[3']$, and $[4']$ obtained from the U matrix are also endowed with well-defined symmetry properties for both spin flip and interchange.

Table V shows similar behavior for the $\chi = 3$ Ising case. At the fixed point, starting from three index variables [1], [2], and [3], where the first is even under spin flip and the latter two

TABLE IV. The U matrix transforming from two SVD indices to a single index calculated for the $\chi = 2$ fixed point. The spin pairs at the input (titled “old index”) use the spin variables [1] and [2] which are obtained by starting from the output of Table III and using a series of renormalizations exactly like the one described in this table. Therefore the index variables [1] and [2] at the input (left column) are, respectively, even and odd under spin flip. The first two composite variables, [1] and [2], which are the only variables retained for the $\chi = 2$ renormalization, inherit these properties directly from the structure of the U matrix.

	New index			
	[1']	[2']	[3']	[4']
SVD value	1.158	0.687	0.109	0.064
Symmetries:				
Spin flip	Even	Odd	Odd	Even
Interchange	Even	Even	Odd	Even
Old index				
[1] [1]	-0.918 32	0.0	0.0	-0.395 84
[1] [2]	0.0	-0.707 11	-0.707 11	0.0
[2] [1]	0.0	-0.707 11	0.707 11	0.0
[2] [2]	0.395 848	-0.0	0.0	-0.918 32

odd, the U matrix gives rise to composite variables with well-defined symmetries. The most relevant composite variables (associated with the largest singular values), [1'], [2'], and [3'], share the same symmetry properties under spin flip, the first being even and the latter two odd. Note that all composite variables possess well-defined symmetry also with respect to interchange.

In general, when retaining all variables after n renormalizations, every variable represents 2^n single variables and there are n additional symmetries, corresponding to the composite interchange symmetries. Because in each step we retain only two variables, [1] and [2], which are both even under interchange, at the n th step only one nontrivial interchange property survives corresponding to the interchange of the variables of the $n - 1$ step. All other interchange operations leave the system unchanged.

C. Summary of SVD numerical results

In this section we list and describe some critical indices generated by low order ($\chi = 2, 3$, or 4) SVD calculations.

1. Square $\chi = 2$

The recursion analysis gives a very simple fixed point for the case we have been discussing $\chi = 2$ with Ising variables on the square lattice. The fixed-point tensor has the following nonzero elements: $T_{1111} = 0.986 69$, $T_{\{1212\}} = 0.289 04$, $T_{\{1122\}} = 0.397 57$, and $T_{2222} = 0.2357$. The spin flip symmetry implies that any component with an odd number of [2] indices vanishes, so $T_{\{1112\}} = T_{\{1222\}} = 0$.

Because the U values in Tables III and IV indicate that this calculation has the symmetry of an Ising model, one can immediately guess that this fixed point is an approximate representation of the two-dimensional Ising model.

In the response analysis, the even-under-spin-flip elements generate four eigenvalues, which give rise to the indices $x = 0$, 0.983 31, 5.56, and $x = \infty$. The odd-under-spin-flip

elements give two more eigenvalues $x_\sigma = 0.258 48$ and $x = \infty$. These infinite indices (corresponding to vanishing eigenvalues) form the null space of the response function. Their sources are distinct: the index corresponding to the odd-under-spin-flip elements is due to the gauge symmetry whereas the index corresponding to the even-under-spin-flip elements reflects the loss of information in the SVD truncation¹⁴; see column (B) of Table VI.

The symmetry properties of the eigenvectors of the response analysis together with the values of the indices further support our identification of the fixed point as representing the two-dimensional Ising model. The first scalar index $x = 0$ is exactly right. The second index $x_T = 0.98 \dots$ is satisfyingly close to the exact value 1.0. The spin index is, however, more than a factor of 2 larger than the exact value 0.125. The index 5.56 was not identifiable and was therefore left out of Table VI. This table lists the index values obtained through different schemes alongside their interpretations and expected exact values.

2. Hexagonal $\chi = 2$

The very simplest SVD calculation is on a hexagonal lattice. The renormalization increases the lattice constant by a factor of $\sqrt{3}$. One finds the fixed point by starting out with a tensor representing a spin-flip-symmetric triangle, invariant under rotations through 120° . In the spin representation, this situation is represented by the two couplings K_0 , a normalization constant, and the nearest neighbor coupling K_m . In the SVD representation generated from this one, there are two independent tensor components T_{111} and $T_{\{122\}}$.

There are two trivial fixed points: A high temperature point in which T_{111} and $T_{\{122\}}$ both equal unity, and a low temperature fixed point in which $T_{111} = 1$ and $T_{\{122\}} = 0$.

The critical fixed point is first found by searching in the space formed by the ratio of these tensor components. After many recursions most starting points will lead to one of the trivial fixed points. However, between these two possibilities, one starting point with $T_{212}/T_{111} = 0.524 548 57$ will give a nontrivial fixed point. Two couplings means two critical indices. The exponents read $x_0 = 0$ for the free energy, and $x_T = 0.984 57$ for the temperature or energy.

To go further, one can include couplings describing configurations that are odd under spin flip. There are two groups of tensor elements of this kind $T_{\{112\}}$ and T_{222} . These four tensor components are set to zero at the fixed point. Including these components in the response analysis gives two

¹⁴In calculating the recursion relation for the odd-in-spin-flip couplings, we found a difficulty that had to be surmounted. The second index [2] could change its meaning as a result of very small perturbations. Its sign was essentially undefined. Since the tensor components with an odd number of [2]'s are all zero at the fixed point, such a sign change might be considered to be “no big deal.” However, a sign change engendered by an almost infinitesimal change in the tensor components defining the SVD transform can make a big difference in the calculation of the derivative of a recursion relation. That in turn can ruin the calculation of a response matrix. This kind of difficulty can be surmounted by defining the ambiguous signs in the U matrix *ab initio*.

TABLE V. The U matrix for the $\chi = 3$ Ising model fixed point. The transformation from two SVD indices to a single index. The $\chi = 3$ renormalization uses only columns [1]–[3]. The last three columns are not shown because they have relatively little influence on the T matrix since their singular values are 0.02, 0.003, and 0.002.

	[1']	[2']	New index		[5']	[6']
			[3']	[4']		
SVD value	1.22	0.81	0.34	0.24	0.07	0.03
Symmetries:						
Spin flip	Even	Odd	Odd	Even	Odd	Even
Interchange	Even	Even	Odd	Even	Even	Odd
Old indices						
[1] [1]	0.86	0	0	0.158	0	0
[1] [2]	0	0.69	0.43	0	0.16	0
[1] [3]	0	0.16	0.55	0	-0.69	0
[2] [1]	0	0.69	-0.43	0	0.16	0
[2] [2]	0.45	0	0	-0.56	0.16	0
[2] [3]	-0.13	0	0	-0.56	0	0.71
[3] [1]	0	0.16	-0.55	0	-0.69	0
[3] [2]	-0.13	0	0	-0.56	0	-0.71
[3] [3]	-0.16	0	0	-0.20	0	0

more eigenvalues $E = 2.5549$ and $E = 0$, which then generate the x values 0.2923 and ∞ ; see column (A) of Table VI.

All this looks surprisingly similar to the square case. Once more, we have a pretty good approximate representation of the known Ising result, marred by an unexpectedly bad x_σ .

3. Hexagonal $\chi = 3$

The $\chi = 3$ fixed point described in column (C) of Table VI has a structure determined by seven nonzero tensor components,

$$T_{111} \text{ as well as } T_{\{122\}} = T_{\{133\}}. \quad (40)$$

The structures of both of these components and of the U matrix indicate a full symmetry between the configurations represented by [2] and [3]. At the fixed point, the ratio of these tensors is $T_{\{122\}}/T_{111} = T_{\{133\}}/T_{111} = 0.57735027$. The identical behaviors of the [2] and [3] indices are reflections of the basic symmetry of this situation. A further indication of this symmetry is the singular values, which are identical for these two indices. This behavior can be expected from the

three-state Potts model, in which the system can line up in any one of the three components of its spin variable. There are then two linearly independent orderings. This degeneracy is reflected in the possibility of rotations of the indices [2] and [3] into one another.

This degeneracy of singular values made the calculation of a fixed point and the evaluations of a response matrix and eigenvalues very hard. The problem was solved in part by artificially breaking the [2]-[3] symmetry, for example, by making tensor components containing the index [3] differ from ones with the index [2] by about 1 part in 10^8 , and then seeing what response eigenvalues might arise. Two eigenvalues appeared robustly, ones with x values of zero and 1.432 274 1. The zero is, of course, the expected response of the free energy, while it seems reasonable to identify the latter values with the operator X of the three-state Potts model (Di Francesco, Mathieu, and Senechal, 1997). That operator has an x value of 1.4.

The analysis is, however, highly unstable and often shows an x value of 1.007 40. This could very likely be a reflection of the thermal index of the Ising model. The Ising model might have arisen as a consequence of our artificially added symmetry breaking.

4. Additional fixed point (hexagonal $\chi = 3$)

We found a second fixed point that, at first sight, seemed qualitatively similar to the Potts model fixed point described in Eq. (40). It looks as if we are heading once more for a fixed point of the three-state Potts model. However, in this case the one nonzero fixed-point ratio is $T_{133}/T_{111} = T_{122}/T_{111} = 0.7689453$. Thus the coupling is much stronger than in the previous case.

Furthermore, the x values are not at all the same as in the previous case. In addition to the ubiquitous $x = 0$, we find $x = 0.02669$, 0.02751 , and 2.94810 . The last x value is likely to belong to the Potts operator called Y that has the exact x value of 3.0. A possible identification of the previous two is with the Potts ordering operator with $x_\sigma = 1/15 = 0.06667$ in the exact theory. However, there are six operators in the theory (Di Francesco, Mathieu, and Senechal, 1997) that should all be generated in an algebra containing spin operators. Thus the description we have given here is not very satisfactory.

TABLE VI. Primary results from rewiring calculations using SVD. The index values are derived from fixed-point calculations that hold on to indices that have the same symmetry as the lattice. The energy, spin, etc. are defined to be the scaling operators with the appropriate symmetry and the smallest x value. We left out some of the larger response eigenvalues, which are apparently not meaningful in the SVD calculations. The sources for the data presented above are as follows: (A) (new data first presented here), (B) Aoki, Kobayashi, and Tomita (2011), (new data first presented here), (C) (D), and (E) (new data first presented here), (F) Aoki, Kobayashi, and Tomita (2011), (G) (new data first presented here).

	(A)	(B)	(C)	(D)	(E)	(F)	(G)
Lattice type	Hexagonal	Square	Square	Hexagonal	Hexagonal	Hexagonal	Square
χ	2	2	3	3	3	3	4
Fitted model	Ising	Ising	Ising	Ising $\chi = 1 + 2$	$q = 3$ Potts	$q = 3$ Potts	Ising
Free energy	0.0	0.0	0.0	0.0	0.0	0.0	0.0
x_σ spin	0.2924	0.258 48	0.275 73	-0.0018 0.306 05	0.027 52 -0.026 69	...	0.322 02
x_T energy	0.9846	0.983 30	0.985 34	0.986 85	...	1.432 27	0.983 30
Y					2.948 10		

5. And one more (hexagonal $\chi = 3$)

The nonzero fixed-point tensor values are

$$\begin{aligned} T_{111} &= 0.995\,538\,8, \\ T_{\{133\}} &= 0.521\,005\,1, \\ T_{222} &= 1.000\,489\,0. \end{aligned}$$

We interpret this situation as a direct product of a critical point of a $\chi = 2$ Ising model (indices [1] and [3]) and a trivial $\chi = 1$ situation (index [2]). It then has two indices close to zero, representing the free energies of the two uncoupled models and also indices 0.3060 and 0.9868. These indices reflect the Ising model as well as an additional uncoupled model at a trivial fixed point.

6. Square $\chi = 3$

On the square lattice, there is at least one fixed-point tensor for $\chi = 3$ that describes the two-dimensional Ising model. This tensor has ten different kinds of components, each with its own separate value. However, the outcome of the response analysis is entirely familiar. The three lowest x values are zero, for the free energy, 0.275 73 for the magnetization, and 0.985 346 for the thermal index. We notice that neither the higher χ nor the additional complexity of a four-index tensor has yielded any improvement (or change) in the response eigenvalues.

7. Square $\chi = 4$

The $\chi = 4$ fixed point on the square lattice was calculated by Aoki, Kobayashi, and Tomita (2011), getting almost exactly the same values of the free energy and thermal indices as they obtained for $\chi = 3$. They did not report a value for the magnetization index. Once again we feel disappointment to see that additional complexity did not produce improved accuracy.

8. Four-state Potts model

We found, but did not analyze, several $\chi = 4$ fixed points. One of these is especially worth mentioning. This one describes a situation that appears to be trying to represent the four-state Potts model, but does not quite get there. It has one configuration [1] that represents a scalar background situation with a tensor component tensor $T_{111} = 1.009\,378\,8$. In addition, there are three other indices [2], [3], and [4]. Our approximate numerical fixed point makes the tensor components described by these indices almost equal in value, viz.,

$$\begin{aligned} T_{\{122\}} &= 0.449\,236\,5, \\ T_{\{133\}} &= 0.449\,236\,6, \\ T_{\{144\}} &= 0.449\,236\,7. \end{aligned}$$

Finally, all six of the T_{ijk} 's that contain all three of the higher index values (e.g., T_{234}) have the value 0.351 510 6. Note that the values of three of the independent tensor entries differ from each other by less than 1 part in 10^6 . This

difference is, however, important in order to obtain a fixed point to numerical accuracy. Equating all three independent entries above does not result in a fixed point. However, adding the same small constant ($\sim 10^{-6}$) to these three independent entries (while keeping them distinct) results in an equivalent fixed point to numerical accuracy. This numerics reflects the null space of the response matrix at the fixed point. It also points to the numerical delicacy of the calculation in the presence of multiple $x = 0$ critical index values.

Note the even spacing of the numerical values of the magnitude of the T 's. The reason that three index values represent four possible values of the Potts model spin variable lies in the fact that, from the four probabilities of having one of four different values, one can form three linearly independent difference variables. In addition there is one trivial variable, the sum of these probabilities, that then has the value unity.

Unfortunately, because of the near degeneracy of this situation, we have had difficulties analyzing the consequences of this model. The near degeneracies make the eigenvalue analysis, both in the response and in the SVD, quite difficult to understand.

IV. DISCUSSION

A. Error estimates

The error in a square lattice rewiring calculation is proportional to the deviation from unity of the ratio of the exact four-index tensor to the approximate one used in the analysis. A wide variety of methods can be used to obtain the approximate tensor. In all our work, we followed previous results by employing the SVD method. In any step of the SVD analysis, the error can be set to zero by choosing the new value of χ to be the square of the old value. However, the computational complexity of the calculation will, at some point, have to be limited by demanding the cessation of the increase in χ . If this eventual value of χ is large, one can expect the calculational error to be small. Since the error terms are simply neglected in the analysis, we might expect that the inaccuracy in critical indices should be linear in the error. For this reason, we should not have been surprised when, despite the accurate calculations of free energy for large χ , low values of χ gave inaccurate results.

On the other hand, our numerical results for critical indices might suggest a different story. The magnetic index taken from the fixed point for the Ising model and its cousins is uniformly in error by about a factor of 2. In contrast, the thermal index starts out, for small χ , accurate to within a few percent and then gets worse (see Fig. 5). Might we have a situation in which the free energy derived from the fixed point converges quite well, but the indices do not show equal convergence? There are some hints in Levin and Nave (2007) and Gu and Wen (2009) that they expect a nonuniform convergence of the free energy, better convergence away from the critical point than at that point.¹⁵ The whole effort to

¹⁵Many rewiring experts believe that working with finite χ is effectively equivalent to introducing a gap in the system. The gap is expected to decrease, but not disappear, as χ gets larger.

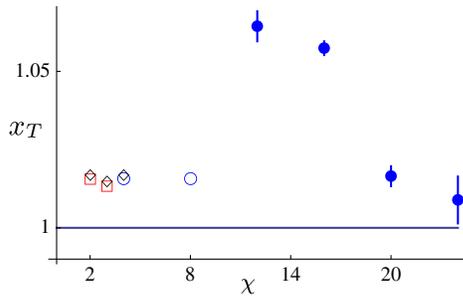


FIG. 5 (color online). The thermal exponent x_T vs χ . Empty circles denote the results that Hinczewski and Nihat Berker (2008) obtained for an hexagonal lattice tensor product. Squares denote the exponents for a square lattice obtained here, and diamonds denote the results for a hexagonal lattice obtained here. All the preceding arise from a fixed-point–response-matrix analysis. In contrast, the solid circles denote exponents obtained through the fitting of the free energy in the vicinity of the critical point.

use SVD or rewiring schemes for the calculation of fixed points might be fraught with conceptual difficulties.¹⁶

The SVD-rewiring fixed-point calculations show a wide variety of numerical difficulties. The most natural way of finding a fixed point involves a Newton’s-method search. This approach, in turn, requires that the approximation used give the parameters that determine the fixed point in differentiable form. However, there are several important impediments to such differentiability, including the following:

- (i) Crossing of singular values: The SVD method does not necessarily make the approximate matrix be analytic in the parameters of the approximated one. In particular, singular values may cross one another, producing a result containing discontinuous derivatives. This problem is likely to result in very delicate numerics for large values of χ .
- (ii) Degeneracy of singular values: In situations with higher symmetry than the Ising model, the singular values may be degenerate, making the SVD calculation very sensitive to small perturbations.
- (iii) Gauge symmetry: The tensor recursion has a gauge symmetry that makes the output tensor insensitive to some combination of components of the specific representation of input tensor. A given tensor renormalization scheme will normally employ (either explicitly or implicitly) some gauge fixing which we can interpret as selecting a particular representation of

the tensor. One can easily go between representations using an orthogonal transformation. The components of the matrix corresponding to the orthogonal transformation, however, may jump around in an unpredictable manner. This unphysical jumping could pollute the entire response-matrix calculation.

- (iv) Order parameter: The order parameter does not fit smoothly into the SVD scheme. The critical system will fluctuate among several states of order. In our calculations, and probably in all SVD calculations, some index variables had U and V values that varied discontinuously as one went from one state of order to the other. As a result we saw discontinuous derivatives of the recursion matrix.

Whatever the cause, the net result is that, for statistical mechanical problems as distinct from Hamiltonian ones,¹⁷ as far as we know, no one has calculated fixed points for χ beyond 8. Further, the one reference that has gone to large χ (Hinczewski and Nihat Berker, 2008) sees an x_T that shows little improvement as χ increases in this range¹⁸ (see Fig. 5). One promising direction of improvement of the rewiring approach is the departure from the SVD scheme in the approximation step as done, for example, by Xie *et al.* (2012) and Meurice (2013).

In contrast, the potential-moving scheme, factored into a renormalization calculation, has given remarkably accurate results for simple models of critical behavior (Kadanoff, 1975; Burkhardt, Knops, and den Nijs, 1976; Burkhardt, 1976a; Kadanoff, Houghton, and Yalabik, 1976b; Dasgupta, 1977; Katz, Droz, and Gunton, 1977; Knops, 1977; Jan and Glazer, 1978; den Nijs and Knops, 1978). See Tables I and II which lists critical indices for the two-dimensional Ising model as derived from this kind of analysis. Both thermal and magnetic critical indices derived in this manner are remarkably accurate. Several (Burkhardt, 1976b; Southern, 1978; Den Nijs, 1979) expressed surprise about this high accuracy. Additional indices, also listed in Table I are qualitatively reasonable.

There are several reasons for the increased accuracy of potential moving relative to the SVD scheme with a similar (small) value of χ . Once again the source of error may be measured as a four-index tensor, here the tensor that defines the various potentials to be moved. However, in this case, because the first order effect of the motion vanishes at $\lambda = 0$, the inaccuracy in the free energy must automatically be second order in the error source. This change is the first reason for the improvement over SVD. In addition, the parameter is adjusted to produce a minimum change in free

¹⁶In contrast, the fixed points and critical indices that arise from some other TRG schemes do not share the same difficulties. Specifically the multiscale entanglement renormalization ansatz (MERA) scheme (Evenbly and Vidal, 2009b; Vidal, 2010) to do quantum Hamiltonian renormalization gives excellent fixed points and critical indices when applied to Hamiltonian formulation of the Ising model and other standard statistical problems. Note that this method has some overlap with the 1975 scheme in that it moves elements of the quantum potential within the lattice, and it also utilizes an optimization of renormalization parameters at the fixed point.

¹⁷Excellent critical index values have been obtained for Hamiltonian approaches to renormalization, for sample via the MERA scheme of Vidal and co-workers; see, for example, Giovannetti, Montanero, and Fazio (2008), Giovannetti *et al.* (2009), Montanero *et al.* (2009) and Pfeifer, Evenbly, and Vidal (2009).

¹⁸For $\chi = 2, 3, 4$, we find that this critical index is 0.985 ± 0.0015 compared with the exact value 1.0. For higher χ , estimates in Hinczewski and Nihat Berker (2008) give the disappointing value $x_T = 0.938 \pm 0.005$ at $\chi = 12$ and the more pleasing value 0.991 ± 0.007 at $\chi = 24$. Convergence is slow and erratic.

energy. This adjustment pushes the error source to be as small as it can be.

Nonetheless, our use of the potential-moving scheme has serious flaws. The most serious one is that we do not know how accurate the method might be. Sometimes it behaves better than expected, sometimes worse. In addition, we know nothing about convergence at higher values of χ .

B. Work to be done

One can hope that the methods of analyzing the rewiring can be improved. We would argue that the advances to be considered might include the following:

- Avoid gauge degeneracy: One should calculate renormalizations and recursions using gauge-invariant quantities, built, for example, from traces of the tensors. This will eliminate the worst source of numerical instability.
- Understand gauge degeneracy: We do not understand the reason that gauge degeneracy should underlie these statistical mechanical calculations. A deeper understanding might bring us to better control of the method.
- Control index degeneracy: A physical symmetry can give a degeneracy in SVD and response functions. Learning to deal with these can be a great help.
- The magnetization: We do not understand why this index is much less accurately determined than the thermal index. We should understand that. If we can, we could design an alternative way of determining this index.
- More global analysis: Construct a variational scheme. We need a calculational scheme to replace SVD. One possibility is to replace U and V by arbitrary three-legged tensors and minimize the free-energy error they produce.¹⁹ One may achieve this goal following the principles of the variational potential moving. However, the real challenge is to design a scheme that both improves accuracy and helps convergence at higher values of χ . But we would also like our calculations to be elegant, smooth, analytic, and intelligently designed. All of that is difficult.

C. Where do we stand?

The rewiring method as put forward by [Levin and Nave \(2007\)](#) and [Gu and Wen \(2009\)](#) has a compelling elegance. The replacement of four-legged tensors by sums of three-legged ones is an excellent way of formulating the renormalization concept. The next step, the evaluation of the three-legged tensors via SVD is attractive, but not equally compelling. We follow many others in noting that this replacement depends only upon the local properties of the tensor being replaced, and not upon the global nature of the free-energy calculation. In contrast, the potential-moving calculation contains a global optimization. We hope to combine the virtues of the two methods.

¹⁹We note that alternatives to the choice of largest χ singular values, which are optimized globally rather than locally, as proposed by [Zhao *et al.* \(2010\)](#), when restricted to low χ values did not result in improved exponents.

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APPENDIX: GAUGE FREEDOM AND INVARIANCE OF THE RECURSION STEP IN ISOTROPIC TRG

Here we prove that, provided that the singular values are distinct, up to sign ambiguities, the renormalization step described in [Sec. II.C](#) is invariant under rotations, i.e., if \tilde{T} is obtained from T by isotropic rotations, or componentwise

$$\tilde{T}_{ijkl} = \mathcal{O}_{ip}\mathcal{O}_{jq}\mathcal{O}_{kr}\mathcal{O}_{ls}T_{pqrs},$$

where \mathcal{O} is an orthogonal matrix, then $\tilde{T}' = R(\tilde{T}) = R(T) = T'$ up to sign ambiguities. Again componentwise this reads

$$\tilde{T}'_{ijkl} = D_{ip}D_{jq}D_{kr}D_{ls}T'_{pqrs},$$

where $D_{ij} = \delta_{ij}f_i$, where f_i is either $+1$ or -1 . This of course can be rectified by setting the sign of $D_{11} = +1$ and then making sure that D_{1112} , D_{1113} , and D_{1114} are all positive (provided that they do not vanish). Incorporating such a sign rectifying step into the TRG scheme results in

$$\tilde{T}'_{ijkl} = T'_{ijkl}.$$

An immediate corollary of this claim is that the isotropic response matrix possesses a null space whose dimension may be greater than that of the rotation group from which \mathcal{O} was selected.

Proof

We begin with considering the uniqueness of the SVD of a given matrix T and its transformation under rotations. To avoid identity misinterpretation we denote the χ^2 valued index obtained from all the possible combinations of the χ valued indices i and j by $\{ij\}$. This makes its untangling simpler.

Let $T_{\{ij\}\{kl\}}$ be a diagonalizable matrix with distinct singular values representing a rank four tensor and let the SVD of T be given by

$$T_{\{ij\}\{kl\}} = U_{\{ij\}\alpha}\Lambda_{\alpha\beta}V_{\{kl\}\beta}, \quad (\text{A1})$$

where $\Lambda_{\alpha\beta} = \lambda_{\alpha}\delta_{\alpha\beta}$ (no summation) are the distinct principal values, and U and V are orthogonal matrices, then:

- (1) The columns of U are the normalized eigenvectors of TT^T .
- (2) The columns of V are the normalized eigenvectors of T^TT .

- (3) In this nondegenerate case the orthogonal matrices are defined up to a sign: i.e., if U and V are the orthogonal matrices obtained by some algorithm, and \tilde{U} and \tilde{V} are orthogonal matrices obtained by a different yet equivalent algorithm, then

$$U^T \tilde{U} = V^T \tilde{V} = D, \quad D_{\alpha\beta} = \delta_{\alpha\beta} f_{\beta}, \quad f_{\alpha} = \pm 1.$$

We now consider an orthogonal matrix which is the external product of two orthogonal matrices $\mathcal{O}_{\{ij\}\{kl\}} = O_{ik} O_{jl}$. The rotation by \mathcal{O} of the rank four tensor T_{ijkl} is equivalent to the rotation by \mathcal{O} of the matrix $T_{\{ij\}\{kl\}}$. By the above considerations the SVD of a rotated matrix is the rotated SVD up to sign ambiguities. If the SVD of T is given by Eq. (A1) then the SVD of the rotated matrix is given by

$$\begin{aligned} & \mathcal{O}_{\{ij\}\{mn\}} \mathcal{O}_{\{kl\}\{pq\}} T_{\{ij\}\{kl\}} \\ &= \mathcal{O}_{\{ij\}\{mn\}} U_{\{ij\}\alpha} D_{\alpha\gamma} \Lambda_{\gamma\delta} D_{\beta\delta} V_{\{kl\}\beta} \mathcal{O}_{\{kl\}\{pq\}}, \end{aligned}$$

where again $D_{ij} = \delta_{ij} f_i$, $f_i = \pm 1$, accounts for the sign ambiguity. Setting $\sqrt{\Lambda}$ to be the non-negative diagonal matrix whose square reproduces Λ , and using commutativity and symmetry of products of diagonal matrices we have

$$\begin{aligned} \mathcal{O}_{\{ij\}\{mn\}} U_{\{ij\}\alpha} D_{\alpha\gamma} \sqrt{\Lambda_{\gamma\delta}} &= O_{im} O_{jn} U_{\{ij\}\alpha} \sqrt{\Lambda_{\alpha\gamma}} D_{\gamma\delta} \\ &= O_{im} O_{jn} u_{ij\gamma} D_{\gamma\delta} = \tilde{u}_{mn\delta}. \end{aligned}$$

As the last step in the renormalization includes a product of four such u tensors, the rotations \mathcal{O} give unity and the only remnant is the sign ambiguity captured by D :

$$\tilde{u}_{ij\alpha} \tilde{u}_{jk\beta} \tilde{u}_{kl\gamma} \tilde{u}_{li\delta} = u_{ij\eta} u_{jk\mu} u_{kl\nu} u_{li\rho} D_{\alpha\eta} D_{\beta\mu} D_{\gamma\nu} D_{\delta\rho}.$$

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