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Monte Carlo Renormalization Group Study of the d=1 XXZ Model*

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Abstract

We report current progress on the synthesis of methods to alleviate two major difficulties in implementing a Monte Carlo Renormalization Group (MCRG) for quantum systems. In particular, we have utilized the loop-algorithm to reduce critical slowing down, and we have implemented an MCRG method in which the symmetries of the classical equivalent model need not be fully understood, since the Renormalization Group is given by the Monte Carlo simulation. We report preliminary results obtained when the resulting MCRG method is applied to the d=1 XXZ model. Our results are encouraging. However, since this model has a Kosterlitz-Thouless transition, it does not yet provide a full test of our MCRG method.

1 Introduction

Although the Monte Carlo method introduced by Metropolis *et al.*[1] has been a useful tool in the study of the critical behavior of classical systems, its application to the study of the critical behavior of quantum systems requires that many difficulties be circumvented. Some of these difficulties are already present in the study of classical systems, while others are present only in the study of quantum systems. In this paper we utilize present knowledge in overcoming the difficulties in such studies, and we apply the method to the study of the one-dimensional XXZ quantum spin model.

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The first difficulty to be surmounted in the study of quantum critical behavior was the problem of how to apply the Monte Carlo method to quantum systems. This difficulty was circumvented when Suzuki[2, 3, 4] proposed to use the formula of Trotter[5] to map any d-dimensional quantum system onto a d+1-dimensional classical equivalent. Convergence properties of the Suzuki-Trotter transformation[6] and of higher-order decompositions have been described[7]. Although this decomposition is applicable in general, it can lead to other difficulties not encountered in the study of most classical systems.

One of the problems often introduced by the application of the Suzuki-Trotter transformation is the minus-sign problem. The minus-sign problem occurs when the 'Boltzmann weights' of the classical equivalent of a quantum problem are not all positive. In the Monte Carlo method Boltzmann weights are interpreted as probabilities, and the minus-sign problem to date is a serious one and can only be decreased. This is done by performing a simulation with any chosen probability distribution, and reweighting to the Boltzmann weights of the classical equivalent[8, 9, 10, 11, 12, 13]. Unfortunately, this moves the difficulty from one of principle to one of acquiring adequate statistics. In general the desired quantities are ratios of two numbers, each of which come from the difference between two large numbers with statistical errors. The minus-sign problem is therefore still largely unsolved. It is interesting to note that it is possible to make some classical statistical mechanical models have a minus-sign problem. For example, the simulation of the d=2 Ising ferromagnet has a minus-sign problem in a certain representation[9, 14].

A difficulty which occurs in the study of both classical and quantum critical behavior is the critical slowing down that occurs in the standard Monte Carlo method near the critical point. The difficulty is that standard Monte Carlo algorithms employ a *local* update procedure, and consequently 'information' diffuses through the lattice slowly in a random walk fashion. This difficulty was first mastered for the ferromagnetic Potts model by Swendsen and Wang[15] where the important realization was to perform *non-local* updates on clusters closely related to the critical clusters of the model. Similar procedures have been devised for a number of systems and have recently been reviewed [16, 17]. The classical equivalent obtained from the Suzuki-Trotter transformation often maps onto a *vertex* model, and it is only recently that algorithms to alleviate critical slowing down for vertex models have been devised [18, 19, 20].

In the study of phase transitions universal quantities, such as critical exponents, are desired. However, a phase transition occurs only in the thermodynamic limit — whereas Monte Carlo simulations by necessity can be done only on finite lattices. The best ways to obtain estimates of the critical exponents from Monte Carlo studies are to use finite-size scaling methods (for reviews see [21, 22]) or renormalization group (RG) methods[23, 24]. One marriage of Monte Carlo and RG methods was given by Swendsen[25, 26, 27]. In Swendsen's implementation of the Monte Carlo Renormalization Group (MCRG) one calculates only correlation functions (not coupling constants). To successfully apply this MCRG method, it is important that the RG

chosen preserves the symmetries of the Hamiltonian[28]. However, this presents a problem for quantum MCRG calculations since typically after the application of the Suzuki-Trotter formula one does not generally know the underlying 'Hamiltonian' of the d+1-dimensional classical equivalent. If you do not know the 'Hamiltonian', how can you know its symmetries? In particular, if the minus-sign problem is present, the concept of a 'Hamiltonian' on the classical equivalent is not well defined. If the classical equivalent is a vertex model, the constraint due to the continuity of vertex loops is difficult to preserve in an RG treatment. This is the difficulty that has delayed progress on the application of MCRG procedures to quantum systems after the initial success of quantum MCRG methods to the transverse Ising model[29, 30, 31], for which the underlying classical equivalent Hamiltonian is known and has no global constraints. For a review of quantum MCRG see Sec. 8 of Ref. [32]. Similar difficulties have been encountered in applying Wilson's idea of real-space blocking[24] to exact-diagonalization studies, which has only recently been surmounted[33, 34, 35].

A method to overcome the difficulty of deciding what RG procedure to use in quantum studies was recently reported by Münger and Novotny[14]. The idea is to modify a momentum-space MCRG developed by Swendsen[27], but to let the Monte Carlo simulation itself decide which RG to use. In momentum space this leads to the RG procedure of systematically discarding the least important degrees of freedom as one renormalizes the lattice. This momentum-space MCRG procedure was successfully applied to the square lattice q-state Potts model with q not restricted to integer values. Thus the MCRG in Ref. [14] was performed on a staggered 6-vertex model which is obtained from a mapping of the q-state Potts model.

In this paper we apply this MCRG for the first time to a quantum system — the 6-vertex model, which is the classical equivalent of the d=1 spin-$\frac{1}{2}$ quantum XXZ model. The XXZ Hamiltonian is

$$\mathcal{H} = +\sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \lambda \sigma_i^z \sigma_{i+1}^z \right), \tag{1}$$

with partition function $Z = \exp(-\beta\mathcal{H})$. Periodic boundary conditions on the chain of N spins are used. Notice that $\mathcal{H}$ is invariant under ($\beta \to -\beta$, $\lambda \to -\lambda$) by rotating every second spin through an angle of π, and is thus equivalent to the Hamiltonian $\mathcal{H} = -\sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y - \lambda \sigma_i^z \sigma_{i+1}^z \right)$.

The case λ=1 corresponds to the isotropic Heisenberg antiferromagnet, while the case λ=0 corresponds to the quantum XY chain.

We have chosen this model since both the loop-algorithm of Ref. [18, 19, 20], and the MCRG program of Ref. [14] were written to study the 6-vertex model, which is the classical equivalent of the Hamiltonian in Eq. (1).

(See [42], fig. 8.2)

Figure 1: The 6 vertices which are allowed in the model are shown. For the XXZ model the weights are w_5=w_6=1 and w_1=w_2=w_3=w_4.

2 Monte Carlo Method

It is well known [2, 6, 36, 37], that the d=1 XXZ chain can be mapped to a (1+1) dimensional classical spin system by Suzuki's method. The main steps are a breakup of the Hamiltonian for an N-spin chain into pieces living on even and odd bonds, an application of the Trotter-Suzuki formula, and an insertion of complete sets of intermediate states. The result is a system of classical spins $s_{i,j} = \pm 1$ on a periodic $N \times M$ chessboard lattice with the Euclidean time (Trotter) direction having extension M, and four-spin interactions on all "black" plaquettes of the chessboard [2, 6, 36, 37]. The mapping becomes exact as $M \to \infty$.

The four spins $(s_{i,j}; s_{i+1,j}; s_{i,j+1}; s_{i+1,j+1})$ bordering an interacting plaquette obey the continuity constraint

$$s_{i,j} + s_{i+1,j} = s_{i,j+1} + s_{i+1,j+1}. \tag{2}$$

The *world lines* connecting sites with $s_{i,j} = 1$ are thus continuous.

This classical spin system is a vertex model: vertices are located at the center of interacting plaquettes; they are connected by lines. Each such line touches a lattice site (i, j). If $s_{i,j}$ =+1 (−1), then we place an arrow that points upwards (downwards) in the Trotter direction on this line. Note that the resulting lattice of arrows and vertices has lines tilted 45 degrees w.r.t. the chessboard lattice.

The constraint of Eq. (2) is that of the 6-vertex model: each vertex has two arrows pointing into the vertex and two pointing away from the vertex. The six possible vertex configurations are shown in Fig. 1. Their weights w_i in the partition function are the weights of the interacting plaquettes, namely [37]

$$\begin{array}{rclcrcl} a & = & w_1 & = & w_2 & = & e^{-\lambda\hat{\beta}}, \\ b & = & w_3 & = & w_4 & = & e^{\lambda\hat{\beta}} \sinh 2\hat{\beta}, \\ c & = & w_5 & = & w_6 & = & e^{\lambda\hat{\beta}} \cosh 2\hat{\beta}, \end{array} \tag{3}$$

with $\hat{\beta} = \beta/(2M)$. The 6-vertex model is exactly solved [42]. It is governed by the parameter [42]

$$\Delta \equiv \frac{a^2 + b^2 - c^2}{2ab} = \frac{\sinh(-2\lambda\hat{\beta})}{\sinh 2\hat{\beta}} \stackrel{\hat{\beta}\to 0}{\longrightarrow} -\lambda. \tag{4}$$

Here we use periodic boundary conditions for the vertex lattice. The normal XXZ boundary conditions would be periodic in both the spin chain direction and the

Trotter direction, and correspond to periodic boundary conditions in the 45-degree directions for the vertex lattice.

Monte Carlo simulations of constrained systems like the 6-vertex model have suffered from severe critical slowing down in the past. The situation has been drastically improved by the advent of the loop cluster algorithm [18, 19, 20], which we now sketch very briefly. In terms of arrows, the constraint of Eq. (2) is a "divergence = zero" condition. All arrows therefore lie on directed closed loops (like magnetic field lines). The loop algorithm stochastically constructs such a loop and flips the direction of all arrows on the loop in a single Monte Carlo step while maintaining detailed balance. It can therefore perform large steps in phase space, and produce statistically independent configurations within a few Monte Carlo steps even at infinite correlation length on large lattices [18]. Note that the loop algorithm also easily produces loops that wind around the lattice. At the KT transition ($\frac{a}{c} = \frac{b}{c} = \frac{1}{2}$), for example, autocorrelation times are reduced by about two orders of magnitude on a 64^2 lattice with respect to a Metropolis simulation.

3 MCRG Method

Here we use the MCRG method described in detail in Ref. [14]. The idea of this MCRG method is to let the Monte Carlo simulation itself provide the renormalization group to be used. This is done by building on the MCRG method developed by Swendsen [25, 26] to calculate critical exponents. Rather than use a block spin procedure in real space, the RG is defined in momentum space in a similar fashion as the procedure introduced by Swendsen in Ref. [27]. Rather than using the Fourier transform of the configurations [27], we use the Fourier transform of each state individually [38],

$$\hat{v}^{\alpha}_{\mathbf{k}} = \sum_{\mathbf{r}} \delta_{\alpha, v_{\mathbf{r}}} \exp\left(i\mathbf{k}\cdot\mathbf{r}\right), \tag{5}$$

where α labels the vertex state v, and the summation is over the simulated lattice. In our case, α takes the values of one through six. An inverse Fourier transform over a restricted part of the momentum-space is then performed. The same restricted part is used for all generated configurations, and the inverse transform is given by

$$v'^{\,\alpha}_{\mathbf{s}} = {\sum_{\mathbf{k}}}' \hat{v}^{\alpha}_{\mathbf{k}} \exp\Big(- i(\mathbf{k} - \mathbf{m}_{\alpha})\cdot\mathbf{s}\Big), \tag{6}$$

where $\mathbf{m}_{\alpha}$ is a shift in momentum space, and the prime on the summation indicates that the sum is over a restricted part of momentum space. Finally, on each site of the reduced lattice for each configuration the state α is chosen for which the real part, $\Re(v'^{\,\alpha}_{\mathbf{s}})$ is largest. Of course this choice is arbitrary, since for example the state with the largest modulus could have been chosen.

Both the restricted part of momentum space and the shift $\mathbf{m}_{\alpha}$ are the same for all generated configurations and are given by the Monte Carlo simulation itself. The

shift $\mathbf{m}_\alpha$ is chosen such that the important fluctuations, as determined by the peak in the momentum-space plot from the entire Monte Carlo simulation, are shifted to the center of the Brillouin zone. This transforms each state into a mainly 'ferromagnetic' state, and allows the use of normal ferromagnetic operators to obtain critical exponents from the linearized transformation matrix $\mathbf{T}^*$. The restricted region of the shifted momentum space is chosen to be the region in the center of the Brillouin zone that gives $N'=L'\times L'$ spins on transforming back to real space. Note that this MCRG procedure does not preserve the constraints of the vertex model (the continuity of loops). However, the renormalized variables should be considered to be composite variables, and the vertex constraints on the original lattice are taken into account during the RG procedure in a way dictated by the Monte Carlo simulation of the model.

In principle, one could avoid transforming back to real space, but at the expense of defining the 'majority rule' for the states in momentum space, and at the expense of defining operators for the linearized transformation matrix $\mathbf{T}^*$ in momentum space; neither of which has been attempted to the authors' knowledge. The transformation back to real space reduces the lattice size and gives the RG. However, a normalization is also required. This is done by multiplying the new real-space spins with a constant such that $\sum |v_{\mathbf{r}}|^2/N = \sum' |v'_{\mathbf{s}}|^2/N'$, where N' is the number of lattice sites on the reduced lattice, and the primed summation is over renormalized spins $v'_{\mathbf{s}}$ on the reduced lattice. Other normalization methods can be devised [14], but they should all lead to the same critical exponents from the MCRG.

The critical properties are obtained in the usual fashion from the linearized RG transformation matrix $\mathbf{T}^*$ from the elements

$$T^*_{\alpha\beta} = \frac{\partial K^{(n)}_\alpha}{\partial K^{(n+m)}_\beta}, \tag{7}$$

where $K^{(n)}_\alpha$ is the coupling constant corresponding to the operator S_α following the n^{th} RG transformation. The K_α include factors of $1/k_BT$. From the chain rule,

$$\frac{\partial \langle S^{(n)}_\gamma \rangle}{\partial K^{(n+m)}_\beta} = \sum_\alpha T^*_{\alpha\beta} \frac{\partial \langle S^{(n)}_\gamma \rangle}{\partial K^{(n+m)}_\alpha} \ , \tag{8}$$

where the angular brackets indicate the thermal average of the operator. The partial derivatives can be easily calculated from the canonical ensemble:

$$\frac{\partial \langle S^{(n)}_\gamma \rangle}{\partial K^{(n+m)}_\alpha} = \langle S^{(n)}_\gamma S^{(n+m)}_\alpha \rangle - \langle S^{(n)}_\gamma \rangle \langle S^{(n+m)}_\alpha \rangle. \tag{9}$$

The thermal averages in Eq. (9) are calculated between the renormalized lattices after n and $n+m$ RG transformations. These averages can be calculated at the simulated set of parameters, but they can also be calculated with parameters other than the simulated ones using a single reweighting method [8, 10, 11, 12], or using data from multiple simulations for different parameters [12, 13, 14].

(See [42], fig. 8.5)

Figure 2: The phase diagram for the 6-vertex model is shown. The vertex weights satisfy w_1=w_2, w_3=w_4, and w_5=w_6. The dashed line corresponds to the F-model where w_1=w_3 as well, and this line terminates at the 'infinite temperature' point where w_1=w_5 (filled circle). The open circles represent the points where we have made MCRG calculations.

The number of operators in Eq. (8) is infinite. However, the MCRG estimate for the matrix $\mathbf{T}^*$ is found from Eq. (8) by first truncating all the matrices in Eq. (8) and then multiplying Eq. (8) by the inverse of the truncated matrix that multiplies $\mathbf{T}^*$ in Eq. (8). To first order in perturbation theory, it has been shown that this procedure takes into account the operators which have not been included in the truncation procedure [39]. Since we have performed the shift $\mathbf{m}_\alpha$ for each state, we need to include only 'ferromagnetic' operators.

Once the largest eigenvalues, $\lambda_1 \geq \lambda_2 \geq \cdots$, of the linearized transformation matrix $\mathbf{T}^*_{\alpha\beta}$ are determined, the eigenvalues of the RG are given by

$$y_i = \ln(\lambda_i)/\ln(b), \tag{10}$$

where the scale factor b is given by the ratio of the lengths on the two lattice sizes used, b=L'_{large}/L'_{small}=$(N'_{large}/\ N'_{small})^{1/d}$, where d is the dimension of the model studied. The exponents y_i are irrelevant if they are less than zero, are marginal if y_i=0, and are relevant and give universal critical exponents for models associated with the fixed point if y_i>0.

For a second-order transition the two largest critical exponents of the RG (y_T from the operators in the thermal section and y_H from operators in the magnetic section) allow the critical exponents to be calculated in the normal fashion from ν=$1/y_T$ and η=$2+d-2y_H$.

Special care must be taken in the case of a model with a Kosterlitz-Thouless (KT) transition[40]. The authors in Ref. [40] show that although the magnetic exponents are given by η=$2+d-2y_H$ in the normal fashion, the values of ν for a KT transition must be obtained by fitting to the KT RG equations. We have not done such a fitting procedure, but have rather concentrated only on the magnetic exponents. In general one can also use the MCRG method to obtain the values of the critical couplings[40, 41]. However since the critical couplings for the d=1 XXZ model are known exactly, we have not tried to find them using MCRG.

4 Theoretical results for the d=1 XXZ Model

The d=1 spin-$\frac{1}{2}$ XYZ model has been studied using a wide variety of methods. These methods have ranged from exact methods[42, 43, 44], to universality

and mapping methods[45, 46], to conformal invariance methods[47, 48], to series expansion methods[49], to exact diagonalization studies[50, 51, 52], to Monte Carlo methods[4, 53, 54]. The phase diagram which has emerged from these studies is illustrated in the 6-vertex representation in Fig. 2[42]. We have performed our MCRG calculations only on the F-model (where w_1=w_2=w_3=w_4 and w_5=w_6) at points illustrated by the open circles in Fig. 2. In Fig. 2 region I corresponds to a ferroelectric region where the lowest energy state is one with all vertices equal to 1 or 2. In this region the excited states give a negligible contribution to the partition function and the system is frozen in one of the two ground states. The situation is similar for region II, where all vertices equal 3 or 4, and region IV where the two ordered states have vertices of 5 on one sublattice and 6 on the other sublattice. Region III is the disordered phase where there is no spontaneous order, nor interfacial tension, but the correlation length is infinite and correlations decay as an inverse power of distance rather than exponentially[42].

The F-model with w_1<$w_5/2$ (which corresponds to the asymmetry parameter of Eq. (1), λ>1) is in region IV. Since in this region the model is completely ordered, one expects to obtain a low-temperature discontinuity fixed point (the Nienhuis-Nauenberg criterion[55]) with the largest RG eigenvalue y=d.

There is a Kosterlitz-Thouless (KT) transition in the F-model when w_1=$w_5/2$ (where λ=1, and the model is the Heisenberg model). In the XXZ model there is a KT transition from the massless into the antiferroelectric ordered domain at λ=1. This occurs through a Kosterlitz-Thouless mechanism caused by the excitations of an umklapp process[45, 46]. At λ=1 the vortex operator (which comes from the critical exponent x_T^{8V} of the 8-vertex model) is marginal.

For the F-model in region III the critical exponents are those of the critical 8-vertex model[42] and are the same as those of the Luttinger model[45]. From conformal invariance[48] the entire operator content is known. Stringlike solutions of the Bethe-*Ansatz* equations yield excited states corresponding to operators $O_{i,j}$ with dimensions

$$x_{i,j} = i^2 x_p + j^2/4x_p \qquad i,j = 0,1,2,\cdots. \tag{11}$$

These operators are the analogs of the Gaussian-model operators composed of spin-wave excitations of index i and a "vortex" of vorticity j. In Eq. (11) x_p=$(\pi-\gamma)/2\pi$, where γ=arccos(λ). The operators $O_{1,0}$ and $O_{2,0}$ correspond respectively to the polarization and energy operators of the 8-vertex model. The operator $O_{0,1}$ is the crossover operator of the 8-vertex model, or equivalently the energy operator of the Ashkin-Teller model. From the dimensions $x_{i,j}$ the RG exponents are found through

$$y_{i,j} = d - x_{i,j}. \tag{12}$$

The exponents $\eta_{i,j}$=$2+d-2y_{i,j}$=$2x_{i,j}$ govern the behavior of correlations. For example, for $O_{0,1}$ one has $\eta_{0,1}$=$2x_{0,1}$=$2+d-2y_{0,1}$ and this critical exponent governs the correlation η_z=$\eta_{0,1}$ with

$$\langle S^z(0)S^z(r)\rangle \sim r^{-\eta_z} \tag{13}$$

where S^z=$\frac{1}{2}\sigma^z$.

(See [14], fig. 4)

Figure 3: The 11 operators used for the truncated linearized RG transformation matrix $\mathbf{T}^*$ are shown. Filled circles represent a vertex in any state, circles with numbers inside represent a δ-function for that vertex state, and the 'bull's eye' in the last operator is any vertex which is not a 5 or 6. The square lattice is drawn with light lines, while heavy lines join the interacting sites. For the operator to be nonzero all filled-circle interacting vertices must have the same vertex state. All combinations which are related by translation, rotation, and reflection to those shown were included in the calculation.

5 MCRG results

We have applied the MCRG method described in Sec. 2 to the 6-vertex model on $L\times L$ lattices with periodic boundary conditions. The 11 operators which we included in the truncated linearized RG transformation matrix $\mathbf{T}^*$ are shown in Fig. 3. Note that because the momentum-space RG does not conserve the 6-vertex constraint on the renormalized lattice, we have not included polarization-type operators in the 11 measured operators. Our calculations were done on a CRAY Y-MP432 supercomputer, and the Fourier transforms used were FFT's in the NAG library (the explicit routines used depended on the lattice sizes the FFT was applied to).

We first studied the F-model with w_1=$w_5/4$ in the ordered region IV of Fig. 2, and the results are shown in Table 1. The lattice simulated for Table 1 was 32×32 and the renormalized lattices were $L'\times L'$ with L'=27, 25, 21, 17, and 15. The RG analysis was performed using 15000 configurations which were generated skipping 250 Monte Carlo cluster updates between configurations and with 250000 cluster updates for thermalization. The exponential autocorrelation time, $\tau_{\rm exp}$ in units of 'sweeps'[20] is given by the autocorrelation time in units of cluster updates times the average cluster size divided by $2L^2$. Here $\tau_{\rm exp}$=43(5), and it is most clearly visible in the sublattice energy[20]. The average cluster size is 0.96 times $2L^2$. In principle one can obtain estimates for the statistical errors of the eigenvalues in Table 1, for example by analyzing J bins of the generated configurations. We have not yet performed such an analysis.

The values of Tables 1 and 2 should be read in a specific fashion to see the convergence of the exponents. In order to obtain good critical exponents from the MCRG one needs to be able to penetrate the *linear* region about the fixed point, since the exponents are calculated from the linearized transformation matrix $\mathbf{T}^*_{\alpha\beta}$. It may take several iterations to be able to get close enough to the fixed point that a linear approximation is reasonable. Consequently, the first iterations (the ones starting from the largest lattices, and hence on the first lines in the tables) may need to be ignored, or at least to be used only to see how the convergence toward the linear region is proceeding. For this reason we do not show the iteration between the original lattice and the next largest lattice in the tables. The exponents should then converge for

n	m 1	2	3	4
	Largest RG Exponent			
1	1.9998	1.9996	1.9981	1.9864
2	2.0003	1.9980	1.9868	
3	1.9963	1.9840		
4	1.9811			
	Second RG exponent			
1	0.6449	1.0041	1.2214	1.1063
2	0.7962	1.1325	1.0128	
3	0.9313	0.7794		
4	0.9683			
	RG scale factor b			
1	1.080	1.286	1.588	1.800
2	1.191	1.471	1.667	
3	1.235	1.400		
4	1.133			

Table 1: The two largest exponents of the linearized transformation matrix, $\mathbf{T}^*$, are listed for the simulation in the ordered phase at $w_1/w_5=\frac{1}{4}$. The lattice simulated was a 32×32 lattice, and the sizes of the renormalized $L'\times L'$ lattices were L'=27, 25, 21, 17, and 15. Listed are the exponents between renormalized lattices n and $n+m$ as well as the corresponding RG scale factors b. For example, the entry with n=2 and m=3 corresponds to an RG transformation between lattices with L'=25 and L'=15. The data should converge for large n, m, but also become susceptible to finite size effects. The expected largest eigenvalue is that of the zero-temperature fixed point since the system is ordered in Region IV of Figure 2. Consequently the largest exponent should be that of the discontinuity fixed point, y=d=2. Our data converge to this value extremely rapidly. The next largest eigenvalue would be the first analytic correction, which approaches unity.

large values of n and m.

If n, m become too large, however, there are additional difficulties. Smaller scale factors b will have the larger statistical errors[14]. Also, in MCRG studies the larger statistical errors typically occur on the smallest lattices, which correspond to the last entry in each line of the tables. The smallest lattices will also have larger finite-size effects, which are particularly disruptive for the longer-range operators included in the calculation of $\mathbf{T}^*_{\alpha\beta}$.

In Table 1 one sees extremely rapid convergence to the eigenvalue y=d=2 associated with the Nienhuis-Nauenberg criterion for a discontinuity fixed point [55]. The next-largest eigenvalue, while not having converged too well, seems to be approaching the value of unity, which would give the first analytical correction to the discontinuity fixed-point behavior.

Our other MCRG results are shown in Table 2. These are at the KT point (λ=1), the XY point (free-fermion case with $\lambda=1/\sqrt{2}$), and an intermediate point with λ=1/2. Table 2 lists the two largest eigenvalues obtained from our MCRG procedure. Each value of λ studied took approximately 23 hours of Y-MP time for the RG analysis

	$w_1/w_5 = 1/2 \quad \lambda = 1$			
n \ m	1	2	3	4
	Largest RG Exponent			
1	2.022	1.809	1.707	1.667
2	1.676	1.624	1.605	
3	1.591	1.581		
4	1.563			
	Second RG Exponent			
1	1.466	1.068	0.835	0.763
2	0.636	0.585	0.576	
3	0.436	0.500		
4	0.358			

	$w_1/w_5 = 1/\sqrt{2} \quad \lambda = 0$			
n \ m	1	2	3	4
	Largest RG Exponent			
1	1.902	1.477	1.342	1.299
2	1.098	1.145	1.165	
3	0.975	1.070		
4	0.844			
	Second RG Exponent			
1	1.185	0.493	0.175	0.198
2	−.520	−.234	−.005	
3	−.610	−.166		
4	−.931			

	$w_1/w_5 = 0.5825\cdots \quad \lambda = 1/2$			
n \ m	1	2	3	4
	Largest RG Exponent			
1	2.050	1.715	1.581	1.524
2	1.501	1.463	1.437	
3	1.397	1.391		
4	1.305			
	Second RG Exponent			
1	1.429	0.908	0.616	0.537
2	0.292	0.307	0.327	
3	0.029	0.216		
4	−.137			
n \ m	1	2	3	4
	RG scale factor b			
1	1.244	1.645	2.429	3.400
2	1.323	1.952	2.733	
3	1.476	2.067		
4	1.400			

Table 2: The two largest exponents of the linearized transformation matrix $\mathbf{T}^*$ are listed for the simulations at λ=0, $\frac{1}{2}$, and 1. The lattice simulated was 64×64, and the sizes of the renormalized $L'\times L'$ lattices were L'=51, 41, 31, 21, and 15. Listed are the exponents between renormalized lattices, n and $n+m$, as well as the corresponding RG scale factors b. For example, the entry with n=3 and m=2 corresponds to an RG transformation between lattices with L'=31 and L'=15. The data should converge for large n, m; but should also become susceptible to finite size effects. For λ=0, $\frac{1}{2}$, and 1, the largest eigenvalues y_z=2−η_z, corresponding to the operator $O_{0,1}$, are 1, $\frac{5}{4}$ and $\frac{3}{2}$, respectively.

of the generated configurations. The time required for the Monte Carlo portion of the runs depended on the value of λ since the cluster-size per volume depended on λ. For λ=0, $\frac{1}{2}$, and 1 the cluster-size was 0.15, 0.09, 0.038 times $2L^2$ and the Y-MP CPU time used corresponded to 3.9, 2.5, and 1.4 hours. The lattice simulated for Table 2 was 64×64, and the renormalized lattices were $L'\times L'$ with L'=51, 41, 31, 21, and 15. The RG analysis was again performed using 15000 configurations which were generated skipping 250 cluster updates between configurations and using 250000 cluster updates for thermalization. Consequently, a total of 4×10^6 cluster updates were generated. The exponential autocorrelation time, which is most clearly visible in the sublattice energy[20], for λ=0, $\frac{1}{2}$, and 1, is $\tau_{\rm exp}$=4.0(2), 8.1(9), and 5.7(6), respectively.

The convergence toward the linear region about the fixed point is expected to be particularly slow when a marginal eigenvalue is present, as is the case in Table 2. Consequently, in Table 2 convergence has not yet occured, but the trend toward convergence of the largest eigenvalue is evident and in agreement with the expected result.

In Table 2 we see only one nearly converged largest exponent y for each value of λ. This exponent can be associated with the operator $O_{0,1}$ corresponding to the cross-over exponent of the 8-vertex model, and the exponent η_z can be associated with the S^z correlations. The reason operators such as $O_{1,0}$ may not be found in our MCRG calculation is because such operators correspond to the polarization operator of the 8-vertex model, and such asymmetric operators are not included in the operators shown in Fig. 3. Such operators are not easily included since the momentum-space RG procedure does not preserve the local vertex constraint.

6 Discussion and Conclusions

We have implemented for the first time the marriage of a loop algorithm to alleviate critical slowing down and an MCRG procedure that does not necessitate that one know the symmetries of the underlying classical equivalent beforehand since they are given by the Monte Carlo. We have applied the resulting MCRG method to the study of the d=1 spin-$\frac{1}{2}$ quantum XXZ chain. Although this model has a Kosterlitz-Thouless transition, and consequently the convergence toward the fixed point is fairly slow, we are able to obtain the critical exponent η_z associated with the S^z correlation function reasonably well. The exponent η_z comes from the operator $O_{0,1}$, which is associated with the crossover exponent of the 8-vertex model. We have pointed out the difficulties in our study that have prevented us from obtaining the other exponents of the XXZ model. Although this is a preliminary study, our MCRG method shows a great deal of promise, since it is easily generalized to the study of many other quantum models in one and higher dimensions.

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