Suzuki-Trotter decomposition and renormalization of a transverse-field Ising model in two dimensions

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(Received 19 September 1996; revised manuscript received 8 January 1997)

The combined Suzuki-Trotter decomposition and Niemeijer–van Leuween real-space renormalization-group techniques are used to study the critical properties of a two-dimensional Ising system with a transverse field. The inverse critical temperature as a function of the external field and the temperature dependence of the transverse component of the magnetization are found. It is also shown that any real-space renormalization-group procedure based on the simple generalization of the Niemeijer–van Leeuwen majority rule for one of the components of the total-cell spin does not preserve the symmetry of the quantum spin space.
[S0163-1829(97)04422-6]

I. INTRODUCTION

Since developing real-space renormalization (RSRG) of Ising spins on a lattice,[1] many attempts have been made to generalize this method to two-dimensional (2D) quantum spin systems such as the anisotropic Heisenberg[2–5] or transverse field Ising[6] (ITF) models. Unfortunately, up to now, for the quantum spins the RSRG studies have not given fully satisfactory results. The main problems appear to be the difficulties in the choice of the proper transformation which allocate original site-spin configurations among effective cell-spin states and decomposition of exponential operators for noncommutable terms of Hamiltonians.

It is true that contrary to the first procedures[2,3] the rotationally invariant RSRG transformations[4,5] confirm univocally[7] the existence of the critical points in 2D quantum XY models at temperatures close to those found from high-temperature expansions;[8] however concerning the character of the critical behavior the results are rather inconclusive.[5] Furthermore the rotationally invariant transformation leads to rather bad results for an Ising system with a transverse field. In this latter case Stella and Toigo[6] proposed simple generalization of the Niemeijer–van Leeuwen (NvL) majority rule for the z component of the spin operators. The authors considered the $s=1/2$ ITF model on the triangular lattice and the method was essentially as follows: the lattice was divided into cells of three spins $(\mathbf{s_i})$; a new effective cell spin operator $(\mathbf{S}_\alpha)$ was assigned to each cell; in the basis of the product eigenstates $|s_1^z s_2^z s_3^z\rangle$ the eight states of the cell were divided into two groups $|+,\tau\rangle$ and $|-,\tau\rangle$ $(\tau=1,2,3,4)$ and associated with two states of the effective spin $|+\rangle'$ and $|-\rangle'$; the renormalization transformation leading from a site Hamiltonian $\mathcal{H}$ to cell Hamiltonian $\mathcal{H}'$ was defined by

$$'\langle\alpha|e^{\mathcal{H}'}|\beta\rangle' = \sum_{\tau=1}^{4} \langle\alpha,\tau|e^{\mathcal{H}}|\beta,\tau\rangle, \quad \alpha,\beta=+,-. \tag{1}$$

According to the NvL majority rule Stella and Toigo[6] associated the following four states of the cell:

$$|+++\rangle,\ |++-\rangle,\ |+-+\rangle,\ |-++\rangle, \tag{2}$$

with the effective spin state $|+\rangle'$ and the other four states with $|-\rangle'$. The same division of the cell states was also used to study the critical behavior of the quantum XY model.[2]

It is obvious that the transformation proposed by Stella and Toigo, similarly as any transformation based on the division of the states with respect to a given component of the total cell spin, distinguishes this component from others. At first glance this kind of procedure is fully justifiable for the systems with axial symmetry like ITF or XY models. However, it can be seen that the above-mentioned transformations *violate* also the symmetry in the xy plane.

Let us consider a rotation through angle ϕ about the z axis; then the states of the spin 1/2 become transformed as follows:

$$|+\rangle \rightarrow e^{i\phi/2}|+\rangle, \quad |-\rangle \rightarrow e^{-i\phi/2}|-\rangle. \tag{3}$$

According to the transformation (1) any operator in the cell-spin space $\mathbf{A}'$ can be expressed in the following form:

$$'\langle\alpha|\mathbf{A}'|\beta\rangle' = \sum_{\tau=1}^{4} \langle\alpha,\tau|\mathbf{A}|\beta,\tau\rangle, \tag{4}$$

where $\mathbf{A}$ is the operator in the site-spin space. It is easy to see that if the diagonal elements of the operator $\mathbf{A}'$, for example,

$$'\langle+|\mathbf{A}'|+\rangle' = \langle+++|\mathbf{A}|+++\rangle + \langle++-|\mathbf{A}|++-\rangle + \cdots, \tag{5}$$

are invariant with respect to the rotation (3) because the phase factors cancel out, the off-diagonal elements are not invariant because the phase factors of the elements $\langle\alpha\alpha\alpha|\mathbf{A}|\beta\beta\beta\rangle$ with $\alpha\neq\beta$ differ from others. As an obvious consequence of this fact, for the ITF model, is dependence of the results found by using the transformation (4) on the direction of the field in the xy plane. The results are different for the fields directed along the x or y axis and if originally the field is directed between the x and y axes then its direction is not preserved in the method outlined above.[6] The same problem of the spin-space symmetry violation appears if one uses, as it has been proposed by Stella *et al.*,[9] the

eigenstates of the cell Hamiltonian with the z component of the total spin fixed, instead of the states (2). In conclusion, it seems that any RSRG procedure based on the simple generalization of the NvL majority rule for one of the components of the total spin of the cell does not preserve the symmetry of the spin space for the quantum models, even in the case of the uniaxial symmetry. Thus, use of procedures of this kind can lead to uncontrolled spurious results.

As mentioned above a second problem in using the RSRG approach to study quantum spin systems is the necessity to make some approximation to decompose the exponential operator

$$e^{\mathcal{H}}=e^{\mathcal{H}_0+V} \quad \text{for } [\mathcal{H}_0,V]\neq 0, \tag{6}$$

where as usual $\mathcal{H}_0$ and V denote the intercell and intracell terms of the Hamiltonian, respectively. Up to now two different schemes of approximation have been used: first based on the Baker-Campbell-Hausdorf (BCH) formula or some of its symmetric versions, and second based on the Feynman identity. Unfortunately, in some cases, especially for systems with single-ion interactions,[10] there are difficulties in estimation of the errors connected with several decomposition formulas and the results depend on the kind of chosen formula. Thus, the main purpose of this paper is to show how a different scheme based on the Suzuki-Trotter (ST) decomposition formula,[11] used mainly in the Monte Carlo simulations, can be applied as a starting point for the RSRG studies of the Ising model in a transverse field.

II. ST DECOMPOSITION

The following Trotter formula

$$e^{A+B}=\lim_{N\to\infty}(e^{A/N}e^{B/N})^N, \tag{7}$$

allows us to transform a d-dimensional quantum system into the corresponding $(d+1)$-dimensional classical system (Suzuki-Trotter transformation).[11] For any finite value of N formula (6) can be treated as an approximation and the found classical counterpart of the considered quantum systems will be composed of the finite number of d-dimensional ''layers'' in the $d+1$ direction. The convergence of Eq. (6) is rather slow[10] thus, if one decomposes the exponential operator $e^{\mathcal{H}/kT}$, the approximation based on formula (6) is a high-temperature approximation. In this paper we are interested in the phase transitions of the 2D Ising model in a transverse field, so for small field $H/kT<1$ we need a reasonable approximation for relatively high temperatures $K\equiv J/kT\sim 0.5$, where J is an interaction constant. The quality of the finite-N ST approximation has been tested for spin chains. It has been found that for the above-mentioned range of the temperature ($J/kT\sim 0.5$) even the lowest orders of the approximation ($N=1,2,3$) lead to almost the exact results.[12] Considering the noncommutability of several terms of a Hamiltonian in this temperature region the ST formula seems to be a better approximation than the BCH formula or Feynman identity. However, the main point is that it is much more intuitively obvious in which way one should construct the RSRG transformation for the effective classical system than for an original quantum one.

We consider an ITF model defined by

$$-\beta\mathcal{H}=K\sum_{\langle i,j\rangle}s_i^z s_j^z+h\sum_i\,(s_i^x\cos\phi+s_i^y\sin\phi) \tag{8}$$

where $\mathbf{s}_i$ is the spin-1/2 operator associated with the ith site of the triangular lattice. Because of the system symmetry the angle ϕ defining the direction of the magnetic field is, of course, irrelevant for the problem. It is obvious that the proper calculation procedure should not violate the symmetry of the system and preserve the independence of the results on ϕ.

After setting

$$A\equiv K\sum_{\langle i,j\rangle}s_i^z s_j^z \quad \text{and} \quad B\equiv h\sum_i\,(s_i^x\cos\phi+s_i^y\sin\phi), \tag{9}$$

and using formula (6) one finds the N-order classical approximation of the original model.[11] The new effective model is composed of N layers of Ising spins $s=\pm 1$ with interaction $K_x=K/N$ between the nearest neighbors in each layer. The nearest neighbors of neighboring layers $(n-1)$ and (n) are coupled by the interaction

$$H_{12}=K_z s^{(n-1)}s^{(n)}-\frac{1}{2}\,i\phi(s^{(n-1)}-s^{(n)}),$$

where $K_z=\frac{1}{2}\ln\coth(h/N)$. This interaction contains the imaginary fields dependent on ϕ. However, the effective classical system is periodic in the Trotter direction and as it is easy to see the imaginary fields cancel out. It means that for any angle ϕ the ST decomposition leads to the same classical model described by two interaction parameters K_x and K_z. Thus, contrary to the method proposed in Ref. 6 the present method does not introduce the spurious dependence of the results on the field direction.

The obtained classical model can be understood as a model on the two-dimensional lattice with some objects, more complicated than single Ising spins, associated with each site. In the Nth order approximation a quantum spin of the ITF model is replaced by the column of N classical spins. It is easy to see that the ST approximative mapping cannot be used in the limit of high magnetic fields for any finite value of N. For, in this case, the original quantum model is transformed into the 2D classical Ising model with the interaction K/N, which leads to the wrong result that an ITF system with infinite field undergoes a phase transition at finite temperature.

III. RSRG TRANSFORMATION

Let us start with the lowest nontrivial order of the ST transformation, i.e., $N=2$. In this case the corresponding effective Hamiltonian

$$\mathcal{H}_{\text{eff}}=K_x\sum_{\langle i,j\rangle}\,(s_i^1 s_j^1+s_i^2 s_j^2)+K_z\sum_i\,s_i^1 s_i^2\,, \tag{10}$$

describes the classical system with a two-Ising-spin column associated with each site of the triangular lattice (Fig. 1). Now we apply to this model the NvL RSRG defined by the transformation:

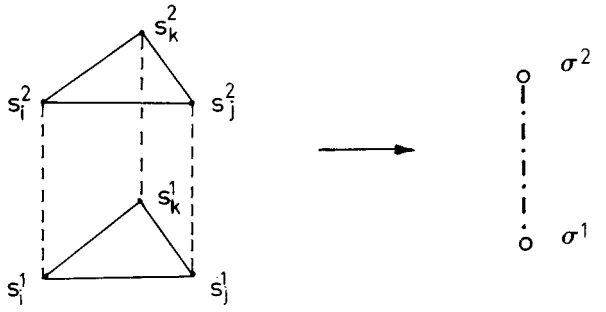

FIG. 1. Two cells-to-two sites transformation on the triangular lattice.

$$e^{\mathcal{H}'(\sigma)}=\sum_s P(\sigma,s)e^{\mathcal{H}(s)}, \tag{11}$$

where $P(\sigma,s)$ denotes the weight operator which couples the cell (σ) and site (s) spins. The mapping to the effective classical system and the character of the phase transition in the ITF model connected with the appearance of the magnetization $\langle s^z\rangle$ allows us to use a simple and intuitively obvious generalization of the NvL majority rule. Namely, we can formulate the NvL majority rule for each layer independently, it means we transform three two-spin columns into one two-cell-spin column (Fig. 1), with the weight function in the form

$$P=P_1P_2,$$

where

$$P_n=\frac{1}{2}\,[1+\sigma^n\mathrm{sgn}(s_i^n+s_j^n+s_k^n)]. \tag{12}$$

We may now use the standard cumulant expansion for classical spins.[1] In the first-order calculation an interaction

$$K_p\sum_{\langle i,j\rangle}(s_i^1s_j^2+s_i^2s_j^1) \tag{13}$$

comes into play and the only fixed point is located at

$$K_x^*=K_p^*\approx 0.084, \quad K_z=\infty.$$

Now we are able to find the critical line of the ITF model separating two regions in the (K,h) plane which correspond to a low-temperature, ordered phase ($\langle s^z\rangle\neq 0$) with the flow of the coupling constants under the RSRG transformation toward the $T=0$ fixed point and a high-temperature, disordered phase ($\langle s^z\rangle=0$) with the flow toward the $T=\infty$ fixed point. It is easy to see that for $K_z=\infty$ the two interactions K_x and K_p are identical and as one would expect we reveal the NvL fixed-point value of the interaction

$$K^*=2K_x^*+2K_p^*\approx 0.3356.$$

In the outlined procedure we make two approximations. The first one is connected with using small Trotter number N and the second one with truncation of the cumulant expansion. In order to examine the quality of these approximations we have performed the calculations for $N=3$ in the first- and second-order cumulant expansion. In this case the classical model is composed of three layers and the RSRG transforms three columns of three spins into one column of the three cell spins. Now in the first order calculation three new interactions arise:

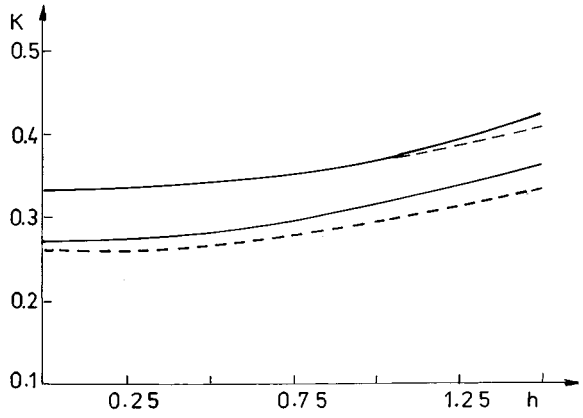

FIG. 2. The field dependence of the critical temperature for ITF model on the triangular lattice. The dashed and solid lines denote the results for the Trotter number $N=2$ and 3, respectively, in the first- (upper curves) and second-order cumulant expansions.

$$K_p\sum_{\alpha\neq\beta,\alpha,\beta=1}^{3}\sum_{\langle i,j\rangle}s_i^\alpha s_j^\beta, \tag{14}$$

$$K_4\sum_{\langle i,j\rangle}[(s_i^1+s_i^2+s_i^3)s_j^1s_j^2s_j^3+s_i^1s_i^2s_i^3(s_j^1+s_j^2+s_j^3)], \tag{15}$$

$$K_6\sum_{\langle i,j\rangle}(s_i^1s_i^2s_i^3s_j^1s_j^2s_j^3), \tag{16}$$

and the fixed-point values of the interactions are

$$K_x=K_p=K_4=K_6\approx\frac{1}{16}\,0.3356, \quad K_z=\infty. \tag{17}$$

It is seen in Fig. 2 that for a small enough field in the first-order calculation the results for $N=3$ are only slightly different from that for $N=2$.

In the second-order calculation 14 and 36 various interactions come into play for $N=2$ and $N=3$, respectively. The appropriate results for the variation of the critical temperature with strength of the transverse field are shown in Fig. 2 (upper curves). Because of a slightly different truncation of the cumulant expansion, we have used for the studied model the zero-field value of the critical temperature that is not exactly the same as in the NvL approximation. Namely, we find $K_c(h=0)=0.2620$ and 0.2735 for $N=2$ and 3, respectively, while the NvL result is 0.2575,[1] and the exact value $K_c=\ln\frac{3}{4}\approx 0.2744$.

IV. CONCLUSIONS

The quantum versions of the RSRG method suffer from the difficulties of choosing an optimal weight operator and suitable approximation. On the other hand, as we have shown in the Introduction, the methods based on the simple

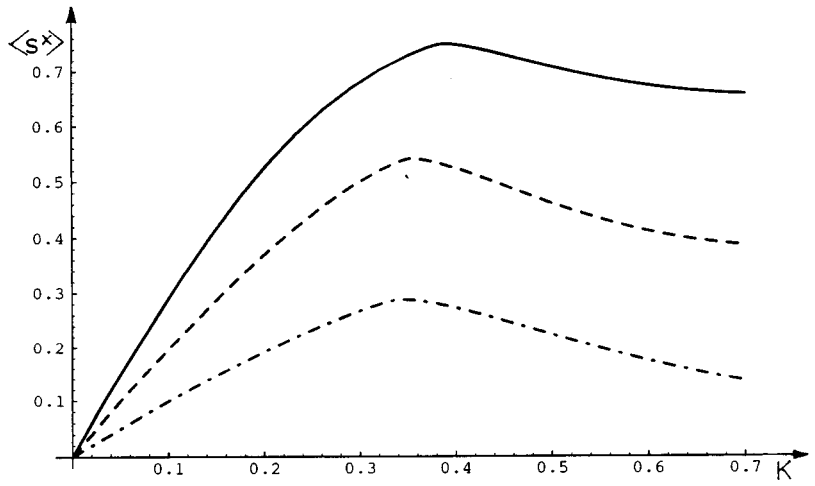

FIG. 3. The temperature dependence of the transverse component of the magnetization for $\gamma/J=3$ (solid line); 2 (dashed line); and 1 (dot-dashed line).

generalization of the NvL majority rule for one of the spin components violate the symmetry of the spin space. For these reasons we have used the Suzuki-Trotter transformation to map the original quantum model onto the corresponding classical one and then applied the intuitively obvious extension of the NvL majority rule. Unfortunately, similarly as a choice of the weight operator the ST transformation is not unique and one can find several classical models corresponding to an original quantum one. However, in the case of the ITF model, decomposition proposed by Suzuki[11] seems to be the most natural and leads to the effective Ising system with the order parameter $\langle s\rangle$, which corresponds directly with the quantum model order parameter $\langle s^z\rangle$. Such a simple relation between physical quantities of the quantum model and its classical counterpart is not generally true, and for example, the transverse component of the ITF magnetization $\langle s^x\rangle$ can be expressed by the correlation of the effective Ising spins of the same column

$$\langle s^x\rangle=\frac{1}{2}\left(\tanh\frac{h}{N}+\coth\frac{h}{N}\right)+\frac{1}{2}\left(\tanh\frac{h}{N}-\coth\frac{h}{N}\right)\times\langle s_i^1 s_i^2\rangle. \tag{18}$$

The temperature dependence of the magnetization transverse component for several values of $\Gamma/J=h/K$ is shown in Fig. 3.

Of course, the critical singularities of the ITF model are the same as those appropriate to the free-field Ising model ($h=0$). As one has expected the transverse field is an irrelevant parameter of the RSRG transformation.[6] However, the purpose of the present paper has been to show how combined ST decomposition and NvL RSRG techniques can be applied to study the spin-1/2 Ising model with transverse field at finite temperature and find for this model the dependence of the transition temperature on the field strength. Such a procedure seems to be reasonable because both methods, as it was shown in many cases, lead to qualitatively and quantitatively good results.

Our approximation is only reliable for small values of K and h and for this reason we are not able to find the critical value of the external strength for $T\to 0$. But the approximation is expected to be valid for the temperature range close to the zero-field critical point which has allowed us to draw the critical line $K_c(h)$ vs h for small enough values of the external field (Fig. 2). As shown in Fig. 4 the critical line found in this paper for $N=3$ in the second-order calculation (full line) essentially differs from that obtained by Stella and Toigo[6] (dashed line). Unfortunately, we have not found any other results for the ITF model on the triangular lattice to compare with ours. For this reason we have performed the calculation for the same model on the square lattice using the five-spin cells in the first order of the cumulant expansion to compare with the results of the high-temperature series expansions (HTSE's).[13] The appropriate critical lines are presented also in Fig. 4. Of course, the results of the RSRG in the lowest approximation (top curve) are as usual not very accurate and rather far from the HTSE result (dot-dashed line). However, the slopes of both curves are close to each

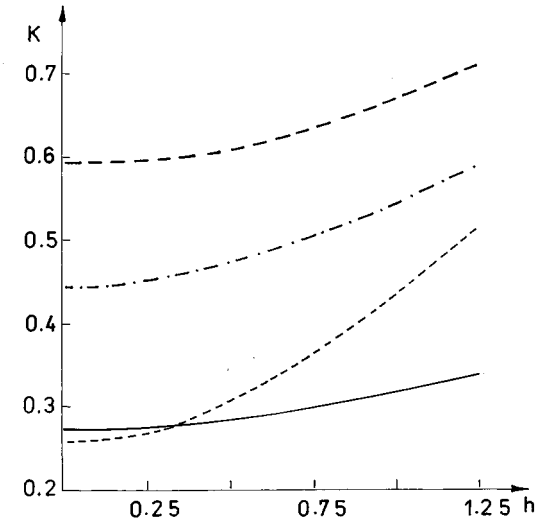

FIG. 4. The critical temperature as a function of field strength for the ITF model: on the triangular lattice, solid line (this paper), dashed line (Stella-Toigo, Ref. 6); on the square lattice, upper dashed line (this paper), dot-dashed line (Elliot-Wood, Ref. 13).

other and the dependence of the critical temperature on the field strength is much weaker than that obtained by Stella and Toigo,[6] similarly as the dependence found in the present paper.

One can fit the critical line found in this paper to the form $K_c(h)-K_c(0)\sim h^{\omega}$. The fit for the field range $0<h<0.2$ is very good and gives only small deviation from the parabolic dependence, $\omega=2.03$. Of course, this deviation increases for higher field strength. We have also obtained the temperature dependence of the transverse magnetization component $\langle s^x\rangle$ (Fig. 3) which may be compared with the molecular field approximation results.[14] However, in this latter case we have had to confine ourselves to the first-order cumulant expansion and results are much less accurate than that for the critical line.

The approach proposed in this paper seems to be rather promising for some class of the quantum spin models. The method can be easily generalized for Ising models with higher values of spin with nondiagonal single ion terms (e.g., the Blume-Capel model in a transverse field). However, there are no general rules how to decompose a Hamiltonian of the original quantum model and then how to choose an appropriate RSRG scheme. So we are not able to find an effective classical Hamiltonian corresponding to quantum XY or Heisenberg models suitable for the NvL RSRG procedure. The point is that in the effective models that we can find by applying the ST procedure to the XY or Heisenberg models, some of the spin configurations are forbidden.[11] It means that in these cases it is impossible to construct appropriate spin Hamiltonians with finite interaction parameters.

ACKNOWLEDGMENT

The authors are indebted to Professor Jan Klamut for his interest in this work.

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