Renormalization of the anisotropic linear XY model

A. Drzewiński
Institute for Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 937, 50-950 Wroclaw 2, Poland

R. Dekeyser
Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium
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The renormalization scheme recently proposed by White is applied to the $d = 1$ anisotropic XY model in a transverse field (AXY). It is found that this scheme offers a distinct improvement over standard techniques as far as the computation of the ground state is concerned. However, compared to the Ising model in a transverse field, on account of more complicated symmetries the AXY demands more precautions during the construction of a renormalization-group transformation. The new method predicts definitely better the location of the phase transition in the XY-like region than in the Ising-like region, but only in the Ising-like region is there any progress for the critical exponent α.

I. INTRODUCTION

The quantum aspect of many models is quite important for the theory of phase transitions. This is particularly true at zero temperature where, due to the quantum fluctuations in the ground state, phase transitions may demonstrate a different character from the corresponding classical systems. The determination of the nature of the ground state and its energy is therefore a central point of quantum many-body problems and few methods exist which can work with strongly interacting systems. One of the techniques is the truncation method, introduced by Drell *et al.*[1] for lattice models and used by many authors to study spin and fermionic systems.[2–4] A comparison of the various approaches was made by Stella *et al.*[5]

The truncation method is a block-spin method, which makes use of the ground-state properties of the systems at $T = 0$, where the low-lying states are the most important. In a standard approach (sa) the lattice is divided into blocks inside which the Hamiltonian is exactly diagonalized. By selecting a number of low-lying eigenstates of the block and projecting the full Hamiltonian on these eigenstates, a renormalized Hamiltonian is constructed for the blocks as new units. The interactions between adjacent blocks are also reconstructed. By repeating the operation, the ground state is formed in a hierarchical way and its energy is calculated iteratively by accumulating the energies of the blocks. Since the method constructs an approximate wave function for the whole system, the ground-state energy so found is necessarily bounded from below by the exact one. The accuracy of the method is determined by the number of states retained in the calculation.

The method is best suited for a number of problems where the character of the ground state changes dramatically at a critical value of some parameter. As a renormalization scheme, the truncation method can handle fluctuations around a continuous phase transition. It remains to be seen whether a specific scheme does indeed do this adequately.

The quality of the procedure has usually been judged on its accuracy in the analysis of such a phase transition. The systems to which the method has been applied are the Ising model in a transverse field (ITF) and the XY model in a transverse field ($XYTF$).[2–4] The positions of the phase transition, the critical indices, and the behavior of the correlation functions were calculated in satisfactory agreement with the exact results (for $d = 1$). Unfortunately, if we consider the accuracy of the energy, the situation is definitely poorer. For the ITF we find an energy larger than the exact one by up to 7%, 4%, 1% and for the $XYTF$ by 20%, 8%, 4% for the method with two, four, and eight states kept, respectively. It is important that the energies do not seem to be sufficiently improved by any reasonable increase in the number of states kept. Although modifications have been proposed,[6] the results for other systems (especially fermionic ones) are usually even more discouraging.[7] This strongly suggests that the origin of the problems lies elsewhere.

In a series of recent papers White[8] has criticized the standard technique and proposed a scheme that for the Heisenberg spin-chain gives amazingly accurate answers for the energy. He argues that for the standard truncation method the neglect of all connections to neighboring blocks during the diagonalization of the block Hamiltonian introduces such large errors that they cannot be corrected by any reasonable number of states kept. White's idea is to embed the block in a superblock of which the lowest state is determined. From this state the density matrix for the block is then constructed. The eigenvalues of the density matrix determine the importance of the corresponding states for the truncation.

In a previous paper[9] White's proposal has been tested on the ITF. We now consider a more general model:

the anisotropic XY model in a transverse field (AXY), which besides the ITF also includes in an opposite limit the $XYTF$. In a large region of the parameter space the AXY shows a continuous phase transition and it is a credible probe in situations with large fluctuations. Our results concern the $d = 1$ case where a comparison with exact results is possible and where also the ideal superblock (the infinite system) can be handled. We believe that the conclusions resulting from the $d = 1$ case are to be useful for calculating the AXY in $d = 2$. In Sec. II we collect some relevant information about the exact solution. In Sec. III we give a description and a discussion of the renormalization procedure that will be applied. In Sec. IV we present the results for various truncations with two states kept and in Sec. V we extend the calculation to the cases with four states kept. The paper ends with a conclusion on the trends of the results.

II. THE EXACT SOLUTION OF THE AXY

In one dimension the AXY has been introduced by Lieb *et al.*[10] ($h = 0$) and by Katsura.[11] They considered a chain of N spins governed by the Hamiltonian

$$\mathcal{H} = -J\sum_i [\tfrac{1}{2}(1+\gamma)S_i^x S_{i+1}^x + \tfrac{1}{2}(1-\gamma)S_i^y S_{i+1}^y] - h\sum_i S_i^z \ , \tag{1}$$

where the operators S_i^x, S_i^y, and S_i^z are spin-1/2 operators represented by Pauli matrices and γ is a parameter characterizing the degree of anisotropy of the interactions in the xy plane. The $\gamma = 1$ case corresponds to the ITF, while the $\gamma = 0$ case gives the $XYTF$. To facilitate the following considerations, we recall the main facts.

The $\gamma \neq 0$ case belongs to the universality class $\gamma = 1$ (the ITF) for any ratio $x = h/J$. Therefore, for a weak field the system behaves as the doubly degenerate Ising-like ground state. Furthermore for a strong field the system reduces to a set of noninteracting sites, which leads to a singlet ground state. This means that the AXY ($\gamma \neq 0$) should exhibit a critical line for finite values $x_c(\gamma)$ (see Fig. 1). For the $XYTF$ ($\gamma = 0$), the end point of the critical line is connected with a phase transition between a strong magnetic-field region with a singlet ground state and a low magnetic-field phase without long-range order. On the x axis the system has an additional line of a phase transition for $0 \leq x < x_c^{XY}$ connected with a rapid change of the Hamiltonian symmetry from an Ising-like behavior to an XY-like one. To demonstrate these facts exactly, we first make the transformation

$$S_i^x = b_i^\dagger + b_i \ , \quad S_i^y = -i(b_i^\dagger - b_i) \ , \quad S_i^z = 2b_i^\dagger b_i - 1 \ , \tag{2}$$

which produces a so called *hard-core* boson representation (at each site the b_i behaves as a fermion operator).

$$\mathcal{H} = Nh - J\sum_i (b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger + \gamma b_i^\dagger b_{i+1}^\dagger + \gamma b_i b_{i+1}) - 2h\sum_i b_i^\dagger b_i \ , \tag{3}$$

where N is the number of sites. Next, using the Jordan-Wigner transformation,[12]

$$b_i = \exp\left[-i\pi\sum_l^{i-1} c_l^\dagger c_l\right] c_i, \qquad b_i^\dagger = c_i^\dagger \exp\left[i\pi\sum_l^{i-1} c_l^\dagger c_l\right] \ , \tag{4}$$

we go over to a quadratic form in the Fermi operators c_i. Neclecting for $N \to \infty$ the boundary term, we obtain

$$\mathcal{H} = Nh - J\sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + \gamma c_i^\dagger c_{i+1}^\dagger + \gamma c_{i+1} c_i) - 2h\sum_i c_i^\dagger c_i \ . \tag{5}$$

It is worth remembering that such a transformation is possible due to the fact that we have a one-dimensional system with only nearest-neighbor interactions. In order to diagonalize the Hamiltonian we carry out the Bogoliubov canonical transformation with k numbering the elementary plane waves:

$$c_j = \sum_k \left[A_k \eta_k e^{ikr_j} - iB_k \eta_k^\dagger e^{-ikr_j}\right] \tag{6}$$

with

$$|A_k|^2 = \frac{1}{2N}\left(1 - \frac{x + \cos k}{\lambda(k)}\right), \tag{7a}$$

$$|B_k|^2 = \frac{1}{2N}\left(1 + \frac{x + \cos k}{\lambda(k)}\right), \tag{7b}$$

where $\lambda(k) = \sqrt{(x + \cos k)^2 + \gamma^2 \sin^2 k}$. In this way we have obtained a system of noninteracting fermions:

$$\mathcal{H} = E_0 + 2J\sum_k \lambda(k)\eta_k^\dagger \eta_k \ , \tag{8}$$

with the ground state defined as $\eta_k|\mathbf{0}\rangle = 0$. The ground-state free energy has the form

$$\epsilon_0 \equiv E_0/NJ = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\ \lambda(k) \ . \tag{9}$$

This formula has been presented[10,11,13] by several authors. In limiting cases it can be transformed to a more useful form. For the ITF Pfeuty has found the energy as[14]

$$\epsilon_0 \equiv E_0/NJ = \frac{2(1+x)}{\pi}\,\mathcal{E}\left(\frac{4x}{(1+x)^2}\right) \ , \tag{10}$$

where the symbol $\mathcal{E}$ means the elliptic integral of the second order.[15] He has also shown that the phase transition appears for $x_c^I = 1$. For the $XYTF$ ($x \leq 1$) the ground-state energy can be presented in the analytical form[16]

$$\epsilon_0 = -\frac{2}{\pi}\left(\sqrt{1-x^2} + x \arcsin x\right). \tag{11}$$

Austen and Plischke[17] have proved (for all d) that $x_c^{XY} = \frac{1}{2}z$, where z is the number of nearest neighbors. Hence, for a chain $x_c^{XY} = 1$. It is worth noticing that in the region $0 \leq x < 1$ the ground-state energy (9) for small γ behaves as $\epsilon_0 \sim \gamma^2 \ln\gamma$ which implies a singularity of its second derivative with respect to γ and the presence of a line of phase transitions. Besides, the critical point at the end of this line ($\gamma = 0$, $x = 1$) has also a singular behavior of the second derivative of ϵ_0 with respect to x.

III. THE SUPERBLOCK IDEA

Both the standard approach and White's approach are based on a truncation of the energy spectrum and they are therefore sensitive to the choice of the states that are used for this truncating in each step of the RG transformation. In the former case, for the formation of the effective Hamiltonian, the low-lying eigenstates of blocks are used. White has proposed a new choice of the states, which is more appropiate for calculating the ground-state energy. In this paper we are following his idea, but we would like to throw some more light on it by presenting a different mechanism that leads to the same result.

Let us assume that we know the state of the entire chain, for example, the ground state $|\psi_0\rangle$. In practice, we will usually be restricted to the ground state of some finite section of the chain, the so-called superblock. If we want to generate for a part of the chain a set of states, which are especially appropriate for representing its properties when the whole chain has the state $|\psi_0\rangle$, we can use the density matrix.[18] Suppose that $|i\rangle$ is a complete set of states of a block and $|j\rangle$ are the states of the rest of the chain. Then we can write $|\psi_0\rangle = \sum_{i,j} \psi_{ij}|i\rangle|j\rangle$. The density matrix is defined as

$$\rho_{mn} \equiv \sum_j \overline{\psi_{mj}}\psi_{nj} \ . \tag{12}$$

White has argued that the eigenvectors of ρ_{mn} with the largest eigenvalues are the optimal states to be kept in the truncation method.

Before we present some details, let us first take the symmetry of the Hamiltonian under careful consideration. The eigenvectors $S_i^z = |S_{i1}^z\rangle \otimes \cdots \otimes |S_{iN}^z\rangle$ with $i = 1, \ldots, 2^N$, which span the Hilbert space of the Hamiltonian, can be represented by the eigenvalues of the S_{ip}^z ($p = 1, \ldots, N$), as $|\epsilon_{i1}, \ldots, \epsilon_{iN}\rangle$, where $\epsilon_{ip} = \pm 1$ or with the symbols $\uparrow$ and $\downarrow$. One can observe that the AXY Hamiltonian acting on a basis vector does not change its parity: $\mathrm{sign}\left(\prod_{p=1}^N \epsilon_{ip}\right) = \pm 1$. This means that the Hilbert space of the AXY for $0 < \gamma \leq 1$ is the direct sum of two invariant subspaces (even and odd). In constructing the effective states we ought to conserve this symmetry. For $\gamma = 0$ (the $XYTF$) both subspaces undergo an additional splitting according to the value of the total z spin projection: $S^z = \sum_{p=1}^N \epsilon_{ip}$.

In order to present our interpretation of White's ideas, we can limit our considerations to the ITF case, when two states are kept. For simplification we divide the chain into two-site blocks and the Hamiltonian into an intrablock part $\mathcal{H}_0$ and an interblock coupling $\mathcal{V}$: $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}$. The intrablock Hamiltonian can be written as a sum of decoupled block Hamiltonians: $\mathcal{H}_0 = J\sum_i[-S_{i1}^x S_{i2}^x - x(S_{i1}^z + S_{i2}^z)]$, where i labels the blocks. In the truncation method, we use some states only (low-lying states of a block in the standard approach or high-lying states of the density matrix in White's approach) for constructing the renormalized Hamiltonian. For both cases, independently of the size of the superblock, the effective states in the two new subspaces are written as a linear combination of the original states belonging to the subspaces with opposite parities.

$$|\Uparrow\rangle = |\uparrow\uparrow\rangle + q\,|\downarrow\downarrow\rangle \ , \qquad |\Downarrow\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \ , \tag{13}$$

where q is a coefficient depending on x. Since the original states building up the $|\Downarrow\rangle$ state are equivalent through particle exchange, their contributions are equal. So, all approximations keeping two states can be characterized by a function $q(x)$ (see Ref. 9).

Since White's approach takes into account the interactions of a block with its surroundings, the natural question can be raised whether or not it is not possible to obtain the same results in the standard approach, but with a new, effective magnetic field in the blocks. This suggests a modification of the perturbation scheme by introducing a different separation of $\mathcal{H}$ into unperturbed and perturbed parts.[5] Indicating by $\mathcal{H}_0$ and $\mathcal{V}$ the previous terms, we might replace them by $\tilde{\mathcal{H}}_0 = \mathcal{H}_0 + \mathcal{H}_1$ and $\tilde{\mathcal{V}} = \mathcal{V} - \mathcal{H}_1$, where $\mathcal{H}_1$ is defined as $\mathcal{H}_1 = -\mathcal{H}_0 + \tilde{J}\sum_i[-S_{i1}^x S_{i2}^x - \tilde{x}(S_{i1}^z + S_{i2}^z)]$. If the effective magnetic field $\tilde{x}$ really expresses the influence of the neglected surroundings, we may expect that the lowest-energy states of a block with this new $\tilde{\mathcal{H}}_0$ correspond indeed to the eigenstates of White's density matrix with the largest eigenvalues. Therefore, $\tilde{x}$ may be determined by imposing the condition that the eigenstates used in White's approach become identical to the states (13), used in the standard approach with an effective field. This requirement gives the equation $q_{\mathrm{st.app.}}(\tilde{x}) = q_{\mathrm{Wh.app.}}(x)$, which defines the effective field $\tilde{x}(x)$. For ground-state calculations, the overall scale of the total energy is irrelevant, so that we can simply assume $\tilde{J} = J$. The recursion relations then take the form

$$J' = \frac{J}{2}\left(1 + \frac{1}{\sqrt{1+4\tilde{x}}}\right), \tag{14}$$

$$x' = \frac{-1 - 2x\tilde{x} - 2\tilde{x}^2 + (1+2x\tilde{x})\sqrt{1+4\tilde{x}}}{2\tilde{x}^2}, \tag{15}$$

and the contribution to the ground-state energy takes the form

$$\Delta\epsilon_0 = -\frac{J}{2}\left(1+\frac{1+4x\tilde{x}}{\sqrt{1+4\tilde{x}}}\right). \tag{16}$$

Our calculations have shown that in this way we obtain exactly the same results (e.g., the flow diagram or energies) as for White's approach. It is interesting to notice that for the ITF model White's approach works exactly as the standard one, but with an effective magnetic field. A shortcoming of this conclusion is the fact that we are not able to find $\tilde{x}$, when we do not know the function $q_{\mathrm{Wh.app.}}(x)$. It is likely that also for other cases we can find untypical separations of $\mathcal{H}$, which may reconstruct the results coming from White's approach. Furthermore, it may be possible that, for determining the effective fields that are added to the block Hamiltonian, other arguments can be found besides the diagonalization of a superblock: symmetry considerations, self-consistency conditions, series expansions, etc. are possible techniques that may lead to interesting approximations for the effective block Hamiltonian and for the corresponding renormalization method.

In the rest of this paper, however, we will use White's method in its simplest version with the density matrix (12), determined through the diagonalization of the original Hamiltonian on a superblock. Since we will report on a large class of calculations, let us introduce a simple abbreviation for the applied methods: "$[nz]$" will refer to a calculation on a block with n sites and a superblock with z sites. If $z = \mathrm{sa}$, it means that we have applied the standard approach (sa), which means no superblock. [Examples: [35] means a calculation on a three-site block in a five-site superblock, [2∞] is on a two-site block in an infinite superblock, and [2sa] represents the standard approach on a two-site block. If we want to make a distinction between this approach with a single density matrix and the method with a double density matrix [see Eq. (18) below], we will add the suffix "s" or "d" (e.g., [35s] and [35d]).]

IV. THE TWO-LEVEL CASE

A. An infinite superblock

For the AXY, let us first consider the case where we keep two states. The advantage is that the Hamiltonian can again be written as a spin Hamiltonian at each iteration (see Ref. 2). It is obvious that in building a suitable superblock we should add spins symmetrically with regard to the block. However, as it was shown,[9] if we choose periodic boundary conditions for the superblock, this will not be important. Moreover, in this section we consider the best superblock, e.g., the whole chain. In this way we want to leave out effects connected with the finite size of a superblock. In the Appendix we calculate the equivalent form of the density matrix based on the exact solution, considering the whole chain as a superblock. Because, due to the Hamiltonian symmetry, it is very likely that the results depend on the number (even or odd) of sites in a block, we have calculated both cases. For the two-site block we consider the standard approach [2sa] and White's approach with the infinite superblock [2∞]. The states kept for the two-site cases have been presented in a previous section (13). For the three-site block we consider also the standard case [3sa] and White's case with the infinite superblock [3∞].

For a three-site block the states kept are again linear combinations of the original states belonging to the adequate subspaces:

$$|\Uparrow\rangle = |\uparrow\uparrow\uparrow\rangle + e_1|\uparrow\downarrow\downarrow\rangle + e_2|\downarrow\uparrow\downarrow\rangle + e_1|\downarrow\downarrow\uparrow\rangle\,, \tag{17a}$$

$$|\Downarrow\rangle = |\downarrow\downarrow\downarrow\rangle + o_1|\downarrow\uparrow\uparrow\rangle + o_2|\uparrow\downarrow\uparrow\rangle + o_1|\uparrow\uparrow\downarrow\rangle\,, \tag{17b}$$

where the e_j and o_j are parameters depending on the approximation.

For all cases the flow diagrams are in qualitative agreement with the exact results, which we have described in Sec. II. As far as the critical behavior is concerned, we have found a finite value of $x_c(\gamma)$, where the system undergoes a phase transition. Figure 1 shows that, when the starting Hamiltonian lies on the critical line x_c ($\gamma > 0$), the effective Hamiltonian flows under consecutive steps of the RG transformation to the I fixed point. If we would be exactly at the XY fixed point, we would always remain there. As we can see in Table I, the suggestion by White makes the I fixed point value for x_c worse than in the standard approach, but it improves the position of the XY fixed point. For $\gamma > 0$ the points in Fig. 1 on the left of x_c go to the fixed point connected with the zero-field Ising fixed point ($\gamma = 1$, $x = 0$), but on the right of x_c they go to the "infinite" line of the fixed points ($\gamma = \mathrm{const}$, $x = \infty$). As we reach the x axis (for $0 \le x < x_c^{XY}$) we start to observe a behavior which has been described by Jullien *et al.*[4] Since the RG transformation is not able to find a whole line of phase transitions, we reveal only the XY fixed point and the zero-field XY fixed point ($\gamma = 0$, $x = 0$) for the three-site block. In an intermediate region the effective Hamiltonian jumps from one position to another and usually it finally ends up in the infinite fixed point. Sometimes we can observe some cyclic fixed points.

For both fixed points (I and XY) we have collected the eigenvalues of the RG transformation and the critical exponents in Tables II and III (for details see Ref. 3). The critical exponent α connected with the specific heat was calculated from the relation[22] $2 - \alpha = d^*\nu$, where $d^* = d + z$ (with d the dimension of the space). The critical exponent ν describes the behavior of the correlation length $\nu = \ln(b)/\ln(\lambda_1)$ and z is the dynamical exponent $b^{-z} = J'/J = h'/h$, where b is the scaling fac-

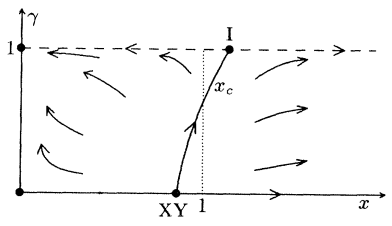

FIG. 1. The flow diagram for the AXY model.

TABLE I. The x values of the critical points for different blocks and superblocks with two states kept. The abbreviations $[\cdots]$ are explained in the text.

Fixed point	[2sa]	[3sa]	[2∞]	[3∞]	[34s]	[34d]	[35s]	[35d]
I	1.277	1.155	1.328	1.243	1.360	1.459	1.316	1.405
XY	1	0.943	1	1	1	1	1	1

tor. As we can see, White's approach gives usually worse results than the standard approach. The only exception is the critical exponent α at the ITF fixed point, where significant progress has been obtained.

Now we devote more attention to the differences between even and odd blocks. For the three-site block, when the starting Hamiltonian lies on the γ axis ($x = 0$), the effective Hamiltonian stays always on this line. For the two-site block, the RG transformation produces an effective magnetic field ($x' \neq 0$) and the effective Hamiltonian leaves the axis, although at the end it reaches the same zero-field Ising fixed point as for the three-site case. It affects strongly the flow diagram. The result is that energies for the two-site cases are worse than for the three-site cases. What is more, they have a nonphysical maximum around $x = 0.1$ (for $0 < \gamma \lesssim 0.7$). The three-site block ([3sa], [3∞]) is free from such an abnormality.

We are convinced that for the two-site cases the new states have been built incorrectly. In constructing $|\Uparrow\rangle$ we are forced, in order to conserve parity, to combine an original state with a maximal number of sites up $|\uparrow\uparrow\rangle$ with one with a maximal number of sites down $|\downarrow\downarrow\rangle$. As a result, e.g., the RG transformation for the two-site case is not invariant under sign reversal of the magnetic field. Likewise, if we look at the formula (13) we can see that only the effective state $|\Uparrow\rangle$ depends on γ (because of the coefficient q) while the state $|\Downarrow\rangle$ remains always the same. In this way we obtain an incorrect flow diagram and an erroneous energy from the iterative construction. It is worth noticing that this does not depend on the superblock idea. The [2sa] case as well as the [2∞] case use the same assignment (13); only the form of the coefficient q is different. So, it is simply a failure of even blocks, and in the truncation method with two states kept only odd blocks give the proper result for the AXY. That is why we do not present energies for the two-site cases.

In order to test White's scheme for the spin-spin correlations we have investigated the following functions describing the short-range order: $G_{xx} = \langle S_i^x S_{i+1}^x \rangle$ and $G_{zz} = \langle S_i^z S_{i+1}^z \rangle$. Because for simplicity we consider them only at zero magnetic field, they are functions of the degree of anisotropy γ. We have calculated them for the [3sa] and the [3∞] cases. These spin-spin correlations can be obtained from a scheme proposed by Sznajd and Zittartz,[19] where we accumulate contributions to the correlation functions at each step of the RG procedure averaging over all possible distributions of the bonds. The results can be compared with exact values calculated by Lieb *et al.*[10] for the antiferromagnetic chain, which, due to the symmetries of the Hamiltonian,[20] is equivalent to the ferromagnetic one, up to a unitary transformation. It is worth noticing that having the G_{xx} and G_{yy} we can obtain the ground-state energy immediately from the relation $\epsilon_0 = -\frac{1}{2}(1+\gamma)G_{xx} - \frac{1}{2}(1-\gamma)G_{yy}$. The G_{zz} function is independent from them because of the absence of $S_i^z S_{i+1}^z$ terms in the Hamiltonian. This seems to explain why White's approach, which produces the best results for the energies, gives also better values for G_{xx} than the standard approach (see Fig. 2). For G_{zz} the standard approach seems to be a better approximation.

We show the energies for the three-site cases in Figs. 3–5 for the ITF, the "intermediate" AXY, and $XYTF$ with $\gamma = 1$, 0.5, and 0, respectively. As a point of reference we have taken the values for the exact energy coming from Eq. (9), and we present in our figures only the differences. As we can see, White's approach yields definitely better energies than the standard one. The worst progress was obtained around the lines of the phase transitions: $x_c(\gamma)$ and the x axis. The deficiencies are likely to be connected with an increase of the quantum fluctuations. In these regions even an infinite superblock is not able to provide the correct results. Because the $XYTF$ is known to be equivalent[21] to the classical $d = 2$ Ising model for $x \geq 1$, here the ground-state energy (per site) is always equal to the magnetic field $\epsilon_o = -x$. In this region, due to the fact that we retain the lowest-energy states (equivalent to the highest states of the density matrix), the errors of the energies are zero for the truncation method in any approach. This fact corresponds with the generally better accuracy of the XY fixed point than that of the I fixed point.

At the end of this section we would like to discuss the relation of the discarded weight of the density matrix to the accuracy of the method. Since each eigenvalue λ_i of the density matrix represents the probability of a block being in the state $|\lambda_i\rangle$, the following relation is ful-

TABLE II. Eigenvalues and critical exponents at the I fixed point.

	Exact	[2sa]	[3sa]	[2∞]	[3∞]	[34s]	[34d]	[35s]	[35d]
λ_1	-	1.596	2.313	1.659	2.243	2.153	2.234	2.227	2.280
λ_2	-	0.466	0.25	0.446	0.393	0.355	0.289	0.367	0.304
ν	1	1.482	1.311	1.369	1.36	1.433	1.367	1.372	1.333
z	1	0.552	0.631	0.532	0.464	0.397	0.465	0.423	0.476
α	0	−0.299	−0.137	−0.098	0.009	−0.002	−0.002	0.040	0.032

TABLE III. Eigenvalues and critical exponents at the XY fixed point (calculated on the left-hand side).

	Exact	[2sa]	[3sa]	[2∞]	[3∞]	[34s]	[34d]	[35s]	[35d]
λ_1	-	2	4	2	3	3	3	3	3
λ_2	-	1.5	2.2	2	3	3	3	3	3
ν	0.5	1	0.793	1	1	1	1	1	1
z	2	1	1.262	1	1	1	1	1	1
α	0.5	0	0.207	0	0	0	0	0	0

filled: $\sum_i^{\text{all}} \lambda_i = 1$. If we keep m states, the deviation of $P_m = \sum_i^m \lambda_i$ from unity measures the accuracy of the truncation to m states. White has shown that P_m is an excellent estimator of the accuracy for the Heisenberg chain.[8] In our case, the AXY model behavior is more complicated, due to the anisotropy and the magnetic field. During the RG transformation, the effective Hamiltonian flows in the parameter space (x,γ) and P_m may vary substantially under this flow. Nevertheless P_m seems to be still a good estimator for the errors in the results. The closer P_m remains to unity, the smaller are the errors of the energy. For the ITF, the "intermediate," and the $XYTF$ regions, the minimal $P_m(x,\gamma)$ is around 0.97, 0.99, and 0.8, respectively. In fact, as we have already mentioned (see Figs. 3–5), the errors for the $XYTF$ case are in general the largest. We can also notice that P_m decreases around the critical line $x_c(\gamma)$.

B. Finite superblocks

Let us now consider finite superblocks, which are certainly more easy to realize. In order to observe superblock size effects, we use an odd (three-site) block with even (four-site) and odd (five-site) superblocks.

It is worth noticing that in the $x = 0$ region the ground state of the odd superblock is a doublet. If we should choose only one state, we would immediately break the system symmetry. This suggests that we may assume that the superblock is in a mixed state which is made up of the lowest states from both parities. Because this assumption is in agreement with the global Hamiltonian symmetry, it is interesting to check how it affects the results in the whole region of parameter space. According to White's proposal,[8] we can build a double density matrix in the following way:

$$\rho = W_e \rho_e + W_o \rho_o, \tag{18}$$

where ρ_e (ρ_o) comes from Eq. (12) with $|\psi_0\rangle$ equal to the lowest state of an even (odd) subspace of the superblock Hamiltonian. When $\Delta E = |E_e - E_o|/J$ is the dimensionless difference between both energies and $E_e \leq E_o$ ($E_e > E_o$), the coefficients have the form $W_e = \frac{1}{1+\exp(-\Delta)}$ and $W_o = \frac{\exp(-\Delta)}{1+\exp(-\Delta)}$ (or opposite). This simple choice satisfies the normalization condition and seems to be reasonable.

The calculations have been performed both for single density matrices ([34s], [35s]) and for double density matrices ([34d], [35d]). As we can see in Table I, the positions of the I fixed points are always worse than for the standard approach and for White's approach with an infinite superblock. Contrary to this, for the XY

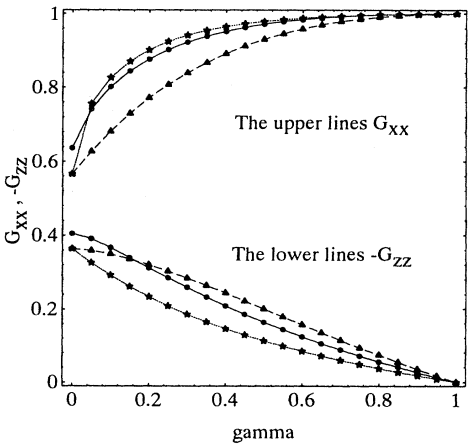

FIG. 2. The spin-spin correlations for zero magnetic field. The triangles represent the [3sa] results, the stars represent the [3∞] results, and the solid circles correspond to the exact results.

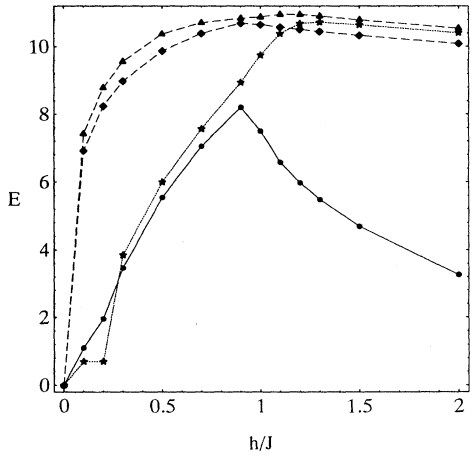

FIG. 3. The energy differences for $\gamma = 1$. Here and in the following figures $E = \ln[(\epsilon_{\text{calculated}} - \epsilon_{\text{exact}}) \times 10^6 + 1]$. We add the unity to avoid (eventually large) negative values of E, when the difference is smaller than 10^{-6}. The triangles represent the [3sa] case, the stars the [3∞] case, the diamonds the [4sa] case, and the solid circles represent the [46s] case. These last two cases were obtained with the multisite approach, reported in Sec. V.

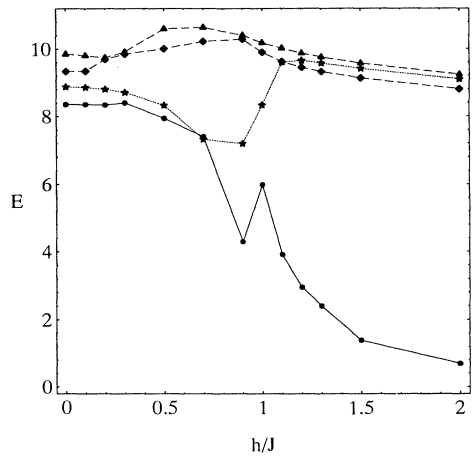

FIG. 4. The energy differences for $\gamma = 0.5$. See Fig. 3 for the meaning of E and of the symbols in the figure.

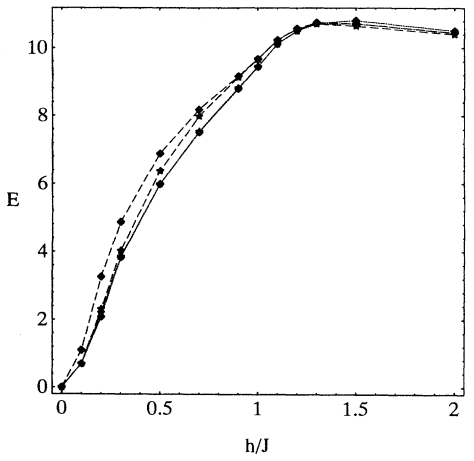

FIG. 6. The energy differences for $\gamma = 1$. The diamonds represent the results for the four-site superblock and the stars those for the five-site superblock. The results on the dashed lines were obtained with the single density matrix and those on the dotted lines were obtained with the double density matrix.

fixed point each superblock gives the exact position of the phase transition. Looking at the critical exponents for the I fixed point (Table II) we see no progress for z and ν, but again some progress for α. The values of the critical exponents for the XY fixed point collected in Table III are identical to those of an infinite superblock [3∞] and they are in bad agreement with exact results. As we can see by taking both the positions of the phase transitions and their critical exponents into account, there is no difference between singlet and doublet cases.

The situation is different for the energies. They are presented in Figs. 6–8. For the ITF case double density matrices give a distinct progress in the energies around the I fixed point compared with the single density matrices. Figure 7 shows that this tendency takes place along the whole line x_c. This suggests that for the Ising-like phase transition region it is more profitable to build a density matrix from Eq. (18), where we take both parities of a superblock into consideration. Notice that these states are always the lowest states of the Hamiltonian. At the I fixed point it gives also a high accuracy for the critical exponent α.

For $x \simeq 0$, our assumption about the advantage of a double density matrix seems to be partially confirmed. For the "intermediate" case the energies coming from the [35d] approximation are decidedly better than for the [34s] case. The absence of critical lines causes the RG scheme to work without problems and our assumption is confirmed. For the $XYTF$ case the energies coming from the odd superblock with a double density matrix ([35d]) are close to the energies obtained from the even superblock with a single density matrix ([34s]) but both are not in good agreement with the exact results. For a small magnetic field ($x \leq 0.5$) our energies are always worse than for the standard approach [3sa]. An even superblock with a double density matrix [34d] gives here poor results because, although its ground-state is a singlet, the second state is a doublet and we are forced to

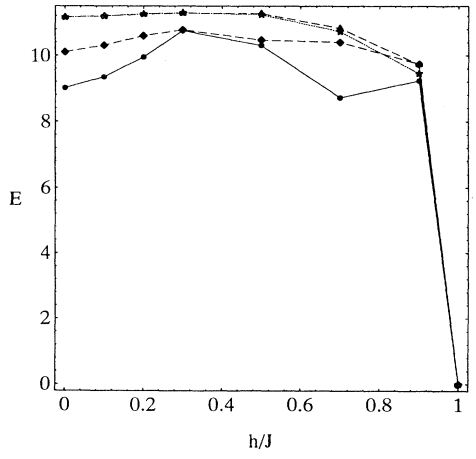

FIG. 5. The energy differences for $\gamma = 0$. See Fig. 3 for the meaning of E and of the symbols in the figure.

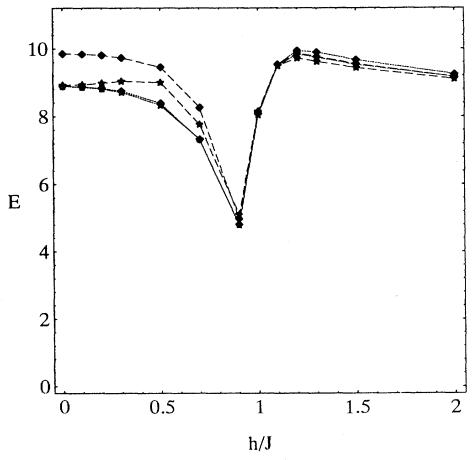

FIG. 7. The energy differences for $\gamma = 0.5$. The meaning of the symbols is the same as for Fig. 6.

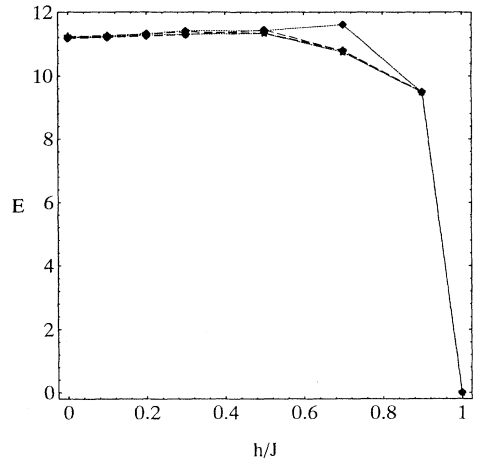

FIG. 8. The energy differences for $\gamma = 0$. The meaning of the symbols is the same as for Fig. 6.

break its symmetry. We have also checked that taking three states of an even superblock into account does not improve the results. This suggests that if we want to reconstruct the ground-state energy we should not consider too many higher states of a superblock simultaneously. This evidence seems to indicate that the character of the low magnetic-field phase of the $XYTF$ is too complicated to be improved with too small a superblock.

Summing up, we would like to emphasize that there is no approximation that is clearly the best over the whole space of the parameters. Because of the small number of states kept and a small size of the superblocks, all approximations are sensitive to the position in the parameter space. Especially the regions around the critical lines are noteworthy, because there the symmetry of the system changes dramatically. Nevertheless, the [35d] approximation seems to be the most recommended.

As we have mentioned in the preceding section, the estimator P_m is able to predict the regions where the errors of the ground-state energy are the largest. Unfortunatelly, the estimator is not enough good to compare and judge different approximations. Their reciprocal relations may alter considerably during succeeding steps of the RG transformation. We can also come across situations, such as for the [34s] case, where P_m is everywhere equal to unity. It does not automatically lead to a high accuracy of the results and this seems to prove that for approximations with two states kept, P_m can be helpful only to some extent.

V. THE FOUR-LEVEL CASE

White has found that the accuracy of the representation of the ground state increases roughly exponentially with the number of states kept. As has been shown for the ITF case,[9] the results for the standard approach demonstrate only a weak progress, contrary to the superblock results, which become more rapidly accurate for a larger number of states. So, we have decided to check this also for the AXY model considering single as well as double density matrices. We calculated the four-level case in the spirit of Jullien's paper.[2] In that way we do not reconstruct the new Hamiltonian as a spin Hamiltonian at each iterative step. Instead of it, we first combine the two sites into groups called multisites. They are now represented as 4×4 matrices. We then bring together the multisites into blocks and diagonalize them exactly. Retaining only four states, we reconstruct the effective multisites (Fig. 9) with their interactions. At the same time we obtain the effective multisite Hamiltonian, which enables us to accumulate the energy during the iteration. For White's approach we build a superblock by adding one more multisite.

Because the effective states should conserve the Hamiltonian symmetry, let us consider two possible assignments. In the first case the two lowest states from an even subspace of a block rebuild two states of an even subspace of a multisite and the two lowest states from an odd block subspace rebuild two states of an odd multisite subspace:

$$|\uparrow\uparrow\uparrow\uparrow\rangle + e\,|\downarrow\downarrow\downarrow\downarrow\rangle + \cdots \rightarrow \quad |\Uparrow\Uparrow\rangle + e'|\Downarrow\Downarrow\rangle\,; \quad |\Uparrow\Uparrow\rangle - e''|\Downarrow\Downarrow\rangle\,, \tag{19a}$$

$$|\uparrow\uparrow\uparrow\downarrow\rangle + o\,|\downarrow\downarrow\downarrow\uparrow\rangle + \cdots \rightarrow \quad |\Uparrow\Downarrow\rangle + o'|\Downarrow\Uparrow\rangle\,; \quad |\Uparrow\Downarrow\rangle - o''|\Downarrow\Uparrow\rangle\,. \tag{19b}$$

In the second case the assignment is opposite. As we can see, the situation is different from the case with two states. Now the states with the maximal number of sites up or down belong always to the same parity.

The first assignment seems to be optimal for a strong magnetic field, since there both the lowest state of a block $|\uparrow\uparrow\uparrow\uparrow\rangle$ and the lowest state of a multisite $|\Uparrow\Uparrow\rangle$ have even parity. For a small magnetic field the relation is different. The ground state of a block ($S^z = 0$) has even parity whereas the ground state of a multisite ($S^z = 0$) has odd parity. So, the second assignment is optimal. As we have checked, both assignments yield RG transformations which are identical up to a unitary transformation. The effect is that both give identical results and both are optimal for small as well as for strong magnetic fields. Nevertheless, they are likely to be not optimal for "intermediate" magnetic fields.

Since for the four-level case the multisite is equivalent to two original sites, we cannot build an odd superblock. This is why we have performed calculations only for an even superblock, both with single and double density matrices ([46s], [46d]). They are compared with results for the standard approach ([4sa]).

Table IV collects the values of the critical points. Just

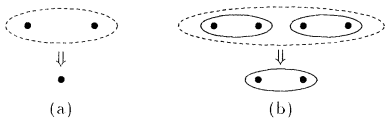

FIG. 9. The construction of an effective site (a) and an effective multisite (b) during the RG transformation. A dashed line shows blocks, whereas a solid line presents multisites.

TABLE IV. The x values of the critical points for the cases with four states kept.

Fixed point	[4sa]	[46s]	[46d]
x_c^I	0.936	0.918	0.998
x_c^{XY}	0.926	1	1

as for retaining two states, White's approach gives the exact value for the XY fixed point. For the [46d] case the position of the I fixed point is in excellent agreement with the exact result. Because a double density matrix seems always to shift the position of the I fixed point to the right (see Table I), it is not clear if this accuracy is now accidental or not.

The results of this calculation were included in Figs. 3–5, where we presented the differences of the energy with respect to the exact values. As we can see for the case with four states kept, White's approach gives a strong improvement over the standard technique, however, as usual the worst progress is along the lines of phase transitions. As in the preceding section for the ITF region (below the critical field), a double density matrix is again more appropriate, but now the differences in energy are definitely smaller. In almost the whole remaining space the [46s] approximation gives better energies than the [46d] one. This shows that for the case with more states kept there is no special virtue in taking a double density matrix.

In general around $x = 0.25$ all calculations suffer from a nonphysical maximum in the energy in the $XYTF$ region. In our opinion the reason is that there the above assignments are unsuitable for intermediate magnetic fields. This discrepancy comes from the relation between block states and multisite states and is independent of the superblock idea.

If we consider P_m, for the [46s] approximation the condition $P_m = 1$ is again fulfilled, as it was for the [34s] case. It means that for the density matrix only four states have nonzero (positive) eigenvalues and all of them are taken into account. As a consequence, the results obtained seem to be in satisfactory agreement with the exact ones. However, we should remember that for the [34s] the same condition did not guarantee a high accuracy. This shows that P_m is a better estimator for the approximations with a larger number of states kept.

It is worth stressing that for White's approach with four states kept the behavior of the energy for the ITF agrees with the exact expansion in the neighborhood of the trivial fixed points: $x \to 0$ and $x \to \infty$,

$$\epsilon_o(x) \begin{cases} \simeq -1 - x^2/4 & \text{for } x \to 0 \\ \simeq -x - 1/4x & \text{for } x \to \infty \ . \end{cases} \tag{20}$$

The standard approach ([4sa]) fails for both limits, whereas for the approach with two states kept only the $x \to 0$ limit is appropriate.

VI. CONCLUSION

The origin of the shortcoming of the standard method is due to the fact that eigenstates of an isolated block are chosen to be kept in the truncation. In this way all connections to neighboring blocks are neglected during the diagonalization. We have tested White's proposal for a model with two lines of phase transitions in the ground state (the $d = 1$ AXY) and we have confirmed his statement about a greater accuracy of the energy. This accuracy increases rapidly when we keep more states in each renormalization step. The least progress is obtained close to the lines of phase transitions.

For the ITF model with two states kept we have argued the equivalence of White's approach to the standard approach with an effective field. This equivalence can be generalized to other models. It may lead to the application of alternative criteria for determining an effective field and for performing an efficient truncation renormalization procedure. It can certainly be seen to be a promising method for extending White's procedure to nonzero temperature applications.

However, on account of complicated symmetries, the AXY model demands more precautions during the construction of a RG transformation. We have shown that for the method with two states kept there is no distinctly best approximation for the whole AXY model. The most optimal approximation seems to be obtained when the numbers of spins in a block and in a superblock are odd and when we build a density matrix from the lowest two states of a superblock belonging to opposite parities. At the same time we have found that using a double density matrix does not lead to appreciable improvements in the case when a larger number of states is kept.

We did not discuss cases in which more than four states are kept. One knows that keeping more states automatically needs larger blocks and this leads obviously to more accurate results. (For example solving with an infinite block gives an exact result.) In our opinion, RG methods are the most interesting if good results can be obtained from small blocks, which means here that a small number of states are kept. That is why we presented results only for the cases with two and four states kept. For more complex applications, it will be worthwhile to remember that the best choice will depend on the particular relation between the lowest states of a block and the lowest states of a multisite. As we have shown, if we are able to match these lower states, the accuracy of the energy will be very high.

In this paper we have presented the eigenvalues of the RG transformation and critical exponents for the method with two states kept. We have checked that White's approach does not improve the critical exponents in comparison with the standard approach. The only exception is the value of the critical exponent α at the I fixed point. Since α is connected with the specific heat, which is proportional to the second derivative of the free energy with respect to a magnetic field, its significant progress is likely to come from the high accuracy of the ground-state energy around the I fixed point. As it was discussed,[9] we are not able to calculate critical exponents by using multisites, but we still consider this to be an open problem.

After this study, there is some hope to obtain new reasonable results by applying White's approach to quantum systems where exact results are unknown. For example,

it seems to be promising for calculating the ground-state energy in the $d = 2$ AXY model.[23] Contrary to the original White method, where the treatment of a two-dimensional system is currently a nontrivial problem in the development of the density-matrix method,[24] for our algorithm we need not introduce any essential modification. We merely have to decide on two-dimensional blocks and superblocks, which can fulfill the lattice symmetries. For planar systems also calculating the spin-spin correlations seems to be more interesting and fruitful. Although the size of the matrices is here a substantial inconvenience, the calculations are now in progress.

ACKNOWLEDGMENTS

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APPENDIX

From the exact solution for the entire chain (the infinite superblock), we know the ground state. Then, in order to calculate all elements of the density matrix, it is more convenient to use expectation values of the Fermi operators c_i and occupation number operators n_i, which is equivalent to using formula (12).[9] First we present it for the two-site block, where we have four states labeled by $(\uparrow\uparrow)$, $(\uparrow\downarrow)$, $(\downarrow\uparrow)$, $(\downarrow\downarrow)$ or 1, 2, 3, and 4. Due to the Hermiticity and parity symmetry of the Hamiltonian only five different elements of the density matrix ρ_{mn} are nonzero. $|\mathbf{0}\rangle$ is the true ground state of the AXY in $d = 1$,

$$\rho_{11} \equiv \langle \mathbf{0}|n_1 n_2|\mathbf{0}\rangle \ , \tag{A1a}$$
$$\rho_{22} = \rho_{33} \equiv \langle \mathbf{0}|(1-n_1)n_2|\mathbf{0}\rangle \ , \tag{A1b}$$
$$\rho_{44} \equiv \langle \mathbf{0}|(1-n_1)(1-n_2)|\mathbf{0}\rangle \ , \tag{A1c}$$
$$\rho_{41} = \rho_{14} \equiv \langle \mathbf{0}|b_1^\dagger b_2^\dagger|\mathbf{0}\rangle \ , \tag{A1d}$$
$$\rho_{32} = \rho_{23} \equiv \langle \mathbf{0}|b_1^\dagger b_2|\mathbf{0}\rangle \ , \tag{A1e}$$
$$\rho_{m,n} \equiv 0 \quad \text{for the rest.} \tag{A1f}$$

These elements can be expressed as combinations of integrals:

$$L_1 = \frac{1}{2\pi}\int_0^\pi dk \left(1 + \frac{x+\cos k}{\lambda(k)}\right), \tag{A2a}$$
$$L_2 = \frac{1}{2\pi}\int_0^\pi dk \cos k \left(1 - \frac{x+\cos k}{\lambda(k)}\right) \ , \tag{A2b}$$
$$L_3 = \frac{1}{2\pi}\int_0^\pi dk \cos k \left(1 + \frac{x+\cos k}{\lambda(k)}\right), \tag{A2c}$$
$$L_4 = \frac{\gamma}{2\pi}\int_0^\pi dk \frac{\sin^2 k}{\lambda(k)} \ . \tag{A2d}$$

We then obtain

$$\rho_{11} = L_1^2 + L_2 L_3 + L_4 \ , \tag{A3a}$$
$$\rho_{33} = L_1 - L_1^2 - L_2 L_3 - L_4^2 \ , \tag{A3b}$$
$$\rho_{44} = (1-L_1)^2 + L_4^2 + L_2 L_3 \ , \tag{A3c}$$
$$\rho_{14} = L_4 \ , \qquad \rho_{23} = L_3 \ . \tag{A3d}$$

For the three-site block we have eight states labeled by $(\uparrow\uparrow\uparrow)$, $(\uparrow\uparrow\downarrow)$, $(\uparrow\downarrow\uparrow)$, ..., $(\downarrow\downarrow\downarrow)$ or 1, 2, 3, ..., 8. Due to the Hermiticity and parity symmetry of the Hamiltonian only 14 different elements of the density matrix ρ_{mn} are nonzero:

$$\rho_{11} \equiv \langle \mathbf{0}|n_1 n_2 n_3|\mathbf{0}\rangle \ , \tag{A4a}$$
$$\rho_{77} = \rho_{44} \equiv \langle \mathbf{0}|n_1(1-n_2)(1-n_3)|\mathbf{0}\rangle \ , \tag{A4b}$$
$$\rho_{66} \equiv \langle \mathbf{0}|(1-n_1)n_2(1-n_3)|\mathbf{0}\rangle \ , \tag{A4c}$$
$$\rho_{88} \equiv \langle \mathbf{0}|(1-n_1)(1-n_2)(1-n_3)|\mathbf{0}\rangle \ , \tag{A4d}$$
$$\rho_{55} = \rho_{22} \equiv \langle \mathbf{0}|(1-n_1)n_2 n_3|\mathbf{0}\rangle \ , \tag{A4e}$$
$$\rho_{33} \equiv \langle \mathbf{0}|n_1(1-n_2)n_3|\mathbf{0}\rangle \ , \tag{A4f}$$
$$\rho_{17} = \rho_{71} = \rho_{41} = \rho_{14} \equiv \langle \mathbf{0}|n_1 b_2^\dagger b_3^\dagger|\mathbf{0}\rangle \ , \tag{A4g}$$
$$\rho_{61} = \rho_{16} \equiv \langle \mathbf{0}|b_1^\dagger n_2 b_3^\dagger|\mathbf{0}\rangle \ , \tag{A4h}$$
$$\rho_{76} = \rho_{67} = \rho_{64} = \rho_{46} \equiv \langle \mathbf{0}|b_1^\dagger b_2(1-n_3)|\mathbf{0}\rangle \ , \tag{A4i}$$
$$\rho_{74} = \rho_{47} \equiv \langle \mathbf{0}|b_1^\dagger(1-n_2)b_3|\mathbf{0}\rangle \ , \tag{A4j}$$
$$\rho_{82} = \rho_{28} = \rho_{85} = \rho_{58} \equiv \langle \mathbf{0}|(1-n_1)b_2 b_3|\mathbf{0}\rangle \ , \tag{A4k}$$
$$\rho_{32} = \rho_{23} = \rho_{53} = \rho_{35} \equiv \langle \mathbf{0}|b_1 b_2^\dagger n_3|\mathbf{0}\rangle \ , \tag{A4l}$$
$$\rho_{83} = \rho_{38} \equiv \langle \mathbf{0}|b_1(1-n_2)b_3|\mathbf{0}\rangle \ , \tag{A4m}$$
$$\rho_{52} = \rho_{25} \equiv \langle \mathbf{0}|b_1 n_2 b_3^\dagger|\mathbf{0}\rangle \ , \tag{A4n}$$
$$\rho_{m,n} \equiv 0 \ \text{ for the rest.} \tag{A4o}$$

These elements can be expressed as combinations of integrals from formulas (A2) and

$$L_5 = \frac{1}{2\pi}\int_0^\pi dk \left(1 - \frac{x+\cos k}{\lambda(k)}\right), \tag{A5a}$$
$$L_6 = \frac{\gamma}{2\pi}\int_0^\pi dk \frac{\sin k \sin 2k}{\lambda(k)} \ , \tag{A5b}$$
$$L_7 = \frac{1}{2\pi}\int_0^\pi dk \cos 2k \left(1 + \frac{x+\cos k}{\lambda(k)}\right), \tag{A5c}$$
$$L_8 = \frac{1}{2\pi}\int_0^\pi dk \cos 2k \left(1 - \frac{x+\cos k}{\lambda(k)}\right). \tag{A5d}$$

We then obtain

$$\rho_{11} = L_1 L_7 L_8 - 2L_3 L_4 L_6 + L_1 L_6^2 + L_4^2(2L_1 + L_7 - L_8) - L_3^2 L_8 + 2L_1 L_2 L_3 + L_1^3 + L_2^2 L_7 + 2L_2 L_4 L_6 \ , \tag{A6a}$$
$$\rho_{33} = L_1^2 + L_7 L_8 + L_6^2 - \rho_{11} \ , \tag{A6b}$$
$$\rho_{44} = L_1 - 2L_1^2 - L_2 L_3 - L_7 L_8 - L_4^2 - L_6^2 + \rho_{11} \ , \tag{A6c}$$
$$\rho_{55} = L_1^2 + L_2 L_3 + L_4^2 - \rho_{11} \ , \tag{A6d}$$
$$\rho_{66} = L_1 - 2L_1^2 - 2L_2 L_3 - 2L_4^2 + \rho_{11} \ , \tag{A6e}$$
$$\rho_{88} = 1 - 3L_1(1-L_1) + 2L_2 L_3 + L_7 L_8 + 2L_4^2 + L_6^2 - \rho_{11} \ , \tag{A6f}$$

$$\rho_{14} = L_4(L_1 - L_8) + L_2L_6 \ , \tag{A6g}$$
$$\rho_{16} = L_3L_4 - L_1L_6 - L_2L_4 \ , \tag{A6h}$$
$$\rho_{25} = L_1L_8 + L_2^2 + L_4^2 \ , \tag{A6i}$$
$$\rho_{35} = L_4L_6 - L_1L_2 + L_3L_8 \ , \tag{A6j}$$
$$\rho_{38} = L_6(1 - L_1) - L_2L_4 + L_3L_4 \ , \tag{A6k}$$
$$\rho_{46} = L_3(1 - L_1) - L_4L_6 - L_2L_7 \ , \tag{A6l}$$
$$\rho_{47} = L_7(1 - L_1) + L_3^2 + L_4^2 \ , \tag{A6m}$$
$$\rho_{58} = L_4(1 - L_7) - L_1L_4 + L_3L_6 \ . \tag{A6n}$$

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