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A NEW RENORMALIZATION APPROACH TO THE GROUND STATE OF THE ANISOTROPIC XY MODEL[1]

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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). A flow diagram, critical exponents and energies have been calculated. It is found that this scheme is a distinct improvement over the standard technique as far as the computation of the ground state is concerned. The accuracy increases rapidly, when we keep more states in each renormalization step, but the errors in the ground state energy are always the largest in the neighborhood of the phase transitions. Comparing with the Ising model in a transverse field, on account of more complicated symmetries, the AXY demands more precautions during constructing a renormalization group transformation.

1. Introduction.

The determination of the nature of the ground state and its energy is 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 systems and used by many authors to study spin and fermionic systems[2, 3, 4, 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 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

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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 calculated iteratively by accumulating the energies of the blocks.

For the Ising model in a transverse field (ITF) and the XY model in a transverse field (XYTF)[2, 3, 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 the accuracy of the energy was considered, the situation was definitely poorer. What is more, Iglói[6] has recently argued that the success for the ITF is accidental and that in general the truncation method mixes bulk and surface properties in an unacceptable way.

Therefore a series of recent papers by White[7], where he criticizes the standard technique and proposes a new scheme, has aroused a significant interest. 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 surrounding. Suppose that $|i\rangle$ is a complete set of states of a block and $|j\rangle$ are the states of the rest of the lattice. In practice, we will usually be restricted to the ground state of some finite section of the lattice, the so-called superblock. Then we can write $|\psi_0\rangle = \sum_{i,j} \psi_{ij}|i\rangle|j\rangle$. The density matrix[8] is defined as:

$$\rho_{mn} \equiv \sum_j \overline{\psi_{mj}}\psi_{nj}. \tag{1}$$

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

White has shown that for the Heisenberg spin chain his method gives amazingly accurate results for the energy. We have decided to test White's proposal for the anisotropic XY model in a transverse field (AXY) [9, 10], which shows continuous phase transitions and it is a credible probe in situations with large fluctuations.

2. The two-level case.

In one dimension the AXY has been introduced by Lieb *et. al.*[11] ($h = 0$) and by Katsura[12]. They considered a chain of N spins governed by the Hamiltonian:

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

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.

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

x / γ	1	0.5	0
0	−1	−0.770982	−0.636620
0.1	−1.002502	−0.773836	−0.639806
0.2	−1.010025	−0.782422	−0.649395
0.3	−1.022630	−0.796819	−0.665489
0.5	−1.063544	−0.843657	−0.717996
0.7	−1.126829	−0.916481	−0.800181
0.9	−1.216001	−1.020211	−0.919077
1	−1.273240	−1.088110	−1
1.1	−1.342864	−1.172393	−1.1
1.2	−1.419619	−1.262806	−1.2
1.3	−1.500823	−1.355913	−1.3
1.5	−1.671926	−1.546324	−1.5
2	−2.127089	−2.033024	−2

Table 1. The exact ground state energies per site for the AXY.

ground state. Furthermore for a strong field the system reduces to a set of noninteracting sites, which leads to a singlet ground state. This shows that the AXY ($\gamma \neq 0$) should exhibit a critical line for finite values $x_c(\gamma)$. For the XYTF ($\gamma = 0$) the end point of the critical line is connected with a phase transition between a singlet ground state (a strong magnetic field region) and a low magnetic field phase without long-range order. For the value $\gamma = 0$ 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.

The formula for ground state free energy has the form[11, 12, 13]:

$$\epsilon_0 \equiv E_0/NJ = -\frac{1}{2\pi}\int_{-\pi}^{\pi} dk\ \lambda(k), \tag{3}$$

where $\lambda(k) = \sqrt{(x+\cos k)^2 + \gamma^2 \sin^2 k}$. The exact ground state energies per site are collected in Table 1. for the AXY with $\gamma = 1, 0.5$ and 0, respectively. For the ITF Pfeuty has found that the phase transition appears for $x_c^I = 1$. For the XYTF Austen *et. al.*[15] have proved that $x_c^{XY} = 1$.

In order to construct the effective states in a proper way, we have taken the symmetry of the Hamiltonian under careful consideration. The eigenvectors $S_i^z = |S_{i1}^z\rangle \otimes \ldots \otimes |S_{iN}^z\rangle$ 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: $\mathrm{sign}\left(\prod_{p=1}^N \epsilon_{ip}\right) = \pm 1$. It means that the Hilbert space of the AXY for $0 < \gamma \leq 1$ is the direct sum of two invariant subspaces (even and odd). 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 constructing the effective states we ought to conserve these symmetries.

Let us first consider the case where we keep two states. For a 2-site block the

fixed point	3sa	34	36	4sa	46
I	1.155	1.360	1.295	0.936	0.918
XY	0.943	1	1	0.926	1

Table 2. The values of the critical points for different blocks and superblocks.

effective states in the two new subspaces should be written as a linear combination of the original states belonging to the adequate subspaces:

$$|\Uparrow\rangle = |\uparrow\uparrow\uparrow\rangle + e_1\,|\downarrow\downarrow\rangle, \qquad |\Downarrow\rangle = |\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle, \tag{4}$$

where e_1 is a coefficient depending on γ and x. Since the original states building up the $|\Downarrow\rangle$ state are equivalent through particle exchange, their contributions are equal.

For a 3-site block the new states are obtained in a similar way:

$$\begin{aligned} |\Uparrow\rangle &= |\uparrow\uparrow\uparrow\uparrow\rangle + e_1\,|\uparrow\downarrow\downarrow\rangle + e_2\,|\downarrow\uparrow\downarrow\rangle + e_1\,|\downarrow\downarrow\uparrow\rangle, \\ |\Downarrow\rangle &= |\downarrow\downarrow\downarrow\rangle + o_1\,|\downarrow\uparrow\uparrow\rangle + o_2\,|\uparrow\downarrow\uparrow\rangle + o_1\,|\uparrow\uparrow\downarrow\rangle. \end{aligned} \tag{5}$$

As we have checked there is an important difference between both cases. For example, for the 3-site block, as we can see in Figure 1, when the starting Hamiltonian lies on the axis 0γ ($x = 0$), the effective Hamiltonian stays always on this line. For the 2-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 ($\gamma = 1, x = 0$) as for the 3-site case (for more details see [10]). It shows that for the 2-site cases with $0 \leq \gamma < 1$ 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 $|\uparrow\uparrow\uparrow\rangle$ with one with a maximal number of sites down $|\downarrow\downarrow\downarrow\rangle$. As a result *e.g.*, the RG transformation for the 2-site case is not invariant under sign reversal of the magnetic field. It is worth noticing that this does not depend on the superblock idea. So, it is simply a failure of even blocks and in the truncation method with two states kept for the AXY only odd blocks give a proper result. The only exception is the ITF region [9]. For this reason, we have presented results only for the 3-site block cases. Since at the zero-field XY fixed point ($\gamma = 0, x = 0$) the ground state of an odd superblock is a doublet, we have used here the even superblocks with four and six sites (34,36). In this way we avoid a breaking of the superblock Hamiltonian symmetry. We compare superblock results with results for the standard case (3sa).

As Figure 1 shows for these cases flow diagrams are in qualitative agreement with the exact results, which we have described. 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. As we reach the axis $0x$ (for $0 \leq x < x_c^{XY}$) we start to observe a behavior which has been described by Jullien *et al.* [4]. Because 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. In an intermediate region the effective Hamiltonian jumps from one

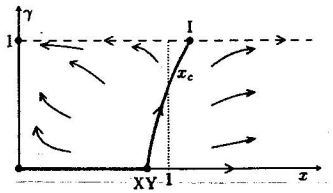

Fig. 1. Flow diagram of the AXY

position to another and usually it finally ends up in the infinite fixed point. Sometimes we can observe some cyclic fixed points. As we can see in Table 2. the suggestion by White makes the I fixed point value worse than for the standard approach, but improves the position of the XY fixed point.

Next we complete the energies in Tables 3.-5. As we can see White's approach yields definitively better energies than the standard one. The least progress was obtained around the lines of the phase transitions: $x_c(\gamma)$ and the axis $0x$. The deficiencies are likely to be connected with the increase of the quantum fluctuations.

The energy differences: $\Delta\epsilon_0 \times 10^6$					
x	3sa	34	36	4sa	46
0	0	0	0	0	0
0.1	1664	2	1	1002	2
0.2	6563	25	9	3779	6
0.3	14154	129	47	7970	31
0.5	31821	980	459	19269	254
0.7	44671	3568	2541	32402	1151
0.9	50876	9554	9181	43782	3663
1	52821	15868	16033	42110	1804
1.1	56914	27721	28222	38901	719
1.2	56725	39202	39320	36379	391
1.3	54059	46708	44462	34171	239
1.5	48436	45317	41531	30450	108
2	37598	34631	32778	23877	25

Table 3. The energies for different blocks and superblocks; $\gamma = 1$. Here and in the following tables: $\Delta\epsilon_0 = E(\text{calculated}) - E(\text{exact})$.

For both fixed points we have collected the eigenvalues of the RG transformation and the critical exponents in Tables 6 and 7 (for details see [5]). The critical exponent α connected with the specific heat was calculated from the relation [16]: $2 - \alpha = d^*\nu$, where $d^* = d + z$ (with d the dimension of the space). The critical exponent ν describes the behavior of the correlation length $\nu = \log(b)/\log(\lambda_1)$ and z is the dynamical exponent $b^{-z} = J'/J = h'/h$, where b is the scaling factor. As we can see White's approach gives usually worse results than the standard one. The only exception

The energy differences: $\Delta\epsilon_0 \times 10^6$					
x	3sa	34	36	4sa	46
0	18936	18936	8167	11355	4259
0.1	18082	18760	7963	11413	4242
0.2	16959	18144	7358	16185	4175
0.3	20197	16840	6049	18914	4461
0.5	39984	12773	4526	22147	2810
0.7	41694	3865	1641	27544	1634
0.9	32964	144	178	29376	72
1	26408	3407	3631	19936	396
1.1	22345	13804	13477	15047	49
1.2	19396	19194	15873	12715	18
1.3	17269	17449	14527	11197	10
1.5	14319	14061	12264	9226	3
2	10242	9515	8888	6630	1

Table 4. The energies for different blocks and superblocks; $\gamma = 0.5$.

The energy differences: $\Delta\epsilon_0 \times 10^6$					
x	3sa	34	36	4sa	46
0	70935	70935	70935	24610	8239
0.1	73036	72928	72145	30129	11426
0.2	77201	76557	71857	40210	21013
0.3	79605	79773	62032	48126	46987
0.5	78896	92996	47873	35351	29992
0.7	50668	48306	63391	33250	10265
0.9	16847	13313	14988	17077	10265
≥ 1	0	0	0	0	0

Table 5. The energies for different blocks and superblocks; $\gamma = 0$.

is the critical exponent α at the ITF fixed point where a significant progress has been obtained. It semms to be important, that contrary to ν and z, the specific heat exponent α is connected with the free energy.

The values for the critical exponents (calculated at the left hand side) of the XY fixed point are rather erratic. Since the two lines of phase transitions join each other at this point, the quantum fluctuations seem to be responsible for this deficiency. The full accuracy of the energies for $x \geq 1$ is accidental in some sense. It comes from the fact that at the right hand side of the XYTF fixed point the XYTF model is known[17] to be equivalent to the classical $d = 2$ Ising model. In this region the ground state energy per site is always proportional to the magnetic field $\epsilon_0 = -x$ and due to the fact that we retain the lowest energy states (there equivalent to the highest states of the density matrix), the errors of the energies are zero for the truncation method in any approach.

	Exact	3sa	34	36
λ_1	-	2.313	2.153	2.266
λ_2	-	0.25	0.355	0.373
ν	1	1.311	1.433	1.343
z	1	0.631	0.397	0.443
α	0	−0.137	−0.002	0.062

Table 6. Eigenvalues and critical exponents at the I fixed point.

	Exact	3sa	34	36
λ_1	-	4	3	3
λ_2	-	2.2	3	3
ν	0.5	0.793	1	1
z	2	1.262	1	1
α	0.5	0.207	0	0

Table 7. Eigenvalues and critical exponents at the XY fixed point.

3. The four-level case.

Since White has found that the accuracy of the representation of the ground state increases roughly exponentially with the number of states kept, we have decided to check this also for the AXY model. 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 2 sites into groups. These multi-sites (the spin operators in fact) are now represented as 4×4 matrices. We then bring together the multi-sites into blocks and diagonalize them exactly. Retaining only 4 states, we reconstruct the effective multi-sites with their interactions. At the same time we obtain the effective multi-site Hamiltonian, which enables us to accumulate the energy during the iteration. For White's approach we build a superblock by adding one more multi-site. This case is compared with the standard approach (4sa), where also the four states are kept.

Because the effective states should conserve the Hamiltonian symmetry, there are only 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 multi-site and the two lowest states from an odd block subspace rebuild two states of an odd multi-site subspace.

$$|\uparrow\uparrow\uparrow\uparrow\rangle + e\,|\downarrow\downarrow\downarrow\downarrow\rangle + \ldots \quad \rightarrow \quad |\Uparrow\Uparrow\rangle + e'|\Downarrow\Downarrow\rangle\,; \quad |\Uparrow\Uparrow\rangle - e''|\Downarrow\Downarrow\rangle,$$
$$|\uparrow\uparrow\uparrow\downarrow\rangle + o\,|\downarrow\downarrow\downarrow\uparrow\rangle + \ldots \quad \rightarrow \quad |\Uparrow\Downarrow\rangle + o'|\Downarrow\Uparrow\rangle\,; \quad |\Uparrow\Downarrow\rangle - o''|\Downarrow\Uparrow\rangle. \qquad (6)$$

In the second case the assignment is opposite. But, as we have checked, both assignments yield RG transformations which are identical up to a unitary transformation.

As we can see in Table 2., just as for retaining 2 states, White's approach gives the exact value for the XY fixed point and comparing with the standard approach the worse position for the I fixed point. Tables 3.-5. present as before differences of the energy with respect to the exact values. As we can see for the case with the four states kept, White's approach gives a strong improvement over the standard technique, however, as usual the least progress is along the lines of phase transitions.

4. Conclusion.

We have tested White's proposal for a model with two lines of phase transitions in the ground state (the $d = 1$ AXY) and have confirmed his statement about a greater accuracy of the energy. This accuracy increases rapidly when we keep more states in each renormalization step. So, in order to improve results we should increase the number of states kept rather than enlarge a superblock. The least progress is always obtained close to the lines of phase transitions.

In this paper we presented the eigenvalues of the RG transformation and critical exponents for the method with 2 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 Ising 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 higher accuracy of the ground state energy around the Ising fixed point. As it was discussed [9], using the multi-sites we are not able to calculate critical exponents. We see this as an open problem.

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