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EFFECTIVE-FIELD APPROXIMATIONS, INCLUDING DMRG METHOD, FOR CLASSICAL INHOMOGENEOUS 2D SPIN LATTICE MODELS*

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A new approach to derivation of various effective-field approximations for lattice spin models in a unique way is presented. It is shown that it can give a number of methods, including the DMRG method, that can be used to find generally inhomogeneous solutions of 2D classical lattice problems. A method, closely related to the DMRG method but without necessity to perform spin renormalization, is derived, yielding results practically not different from the DMRG ones. The matrix-product wave function of Rommer and Östlund can be constructed from the output of the method. The computational costs of all the derived methods are smaller than those of the DMRG. Most of the results are applicable to the 1D quantum systems, as well.

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1 Introduction

The rapid development of computational technique is accompanied by an increasing interest in numerical treatments of the problems of statistical mechanics. Besides Monte Carlo techniques, which simulate finite systems, the effective-field methods, which, in principle, treat infinite systems, became recently extremely popular.

After traditional effective-field approaches, as molecular-field approximation and quasichemical (Bethe) approximation, the first sophisticated effective-field approach was Baxter's Corner-Matrix Method [1], which gave the possibility of systematic improvements of the approximation. This was also the feature of the cluster transfer-matrix method of the author [2], [7–9], which was used for an effective description of the incommensurate structures. Finally, Density Matrix Renormalization Group (DMRG) Method for calculation of the ground state of one-dimensional quantum models was developed by White [3, 4]. A little later it was applied also to the 2D classical lattice models by Nishino and its relation to the Baxter's method was pointed out [5, 6].

All these works are closely linked to Kramers-Wannier [10] suggestion of factorizing the wave function.

*Dedicated to Doc. Eva Majerníková, DrSc. on the anniversary of her birthday.
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The DMRG method started from the real-space renormalization approaches, where, calculating the trace of the Hamiltonian or summing up the partition function, spin degrees of freedom where reduced by discarding eigenstates of the Hamiltonian corresponding to the highest energy level (lowest eigenvalues of the transfer matrix). It was shown by White that, instead of the Hamiltonian, the density matrix of the target state is more appropriate for this purpose. In this paper we show that if the summation of the partition function is done in a proper way no further spin reduction is necessary, and the renormalization process by discarding the eigenstates of the density matrix can be eliminated from the DMRG method at all.

It is shown that DMRG method is, in fact, not based on repeated reduction, renormalization, and addition of new spin variables as in the real-space renormalization group methods, but on a subsequent summation of spin variables in presence of effective fields when calculating the partition function (energy of the ground state in quantum case).

The paper is organized as follows: In Section 2 a general method for derivation of various of effective-field approximation in a unique way is developed. It is used, in Section 3, for re-derivation of the cluster transfer-matrix method and DMRG method, and derivation a new effective-field method closely related to DMRG, but working more effectively. In section 4 the links between our and Rommer-Östlund's [11, 12, 13] approach are shown, and the correct choice of the density matrix in the case of non-symmetric or non-Hermitian Hamiltonian of kinetic or quantum models is elucidated.

2 Method

The main task of statistical treatment of a classical system of spins σ_i described by a Hamiltonian $H(\sigma_i)$ is calculation of the partition function

$$Z = \sum_{\{\sigma_i\}} \exp[-\beta H(\sigma_i)].$$

For short-range interactions the Boltzmann's weight $\exp[-\beta H(\sigma_i)]$ can be rewritten in the form of a product of functions $\mathcal{T}_i$ which depend on spin variables of few rows. The number of rows is given by the range of the interactions.

$$\exp[-\beta H(\sigma_i)] =$$

$$\dots \mathcal{T}_{i-1}(\Lambda_{i-1}, \dots, \Lambda_{i-1+k})\mathcal{T}_i(\Lambda_i, \dots, \Lambda_{i+k})\mathcal{T}_{i+1}(\Lambda_{i+1}, \dots, \Lambda_{i+1+k}) \dots, \tag{1}$$

where $\Lambda_i \equiv \dots \sigma_{i,j-1}, \sigma_{i,j}, \sigma_{i,j+1} \dots$ are row spin variables and k is the interaction range. Usually the functions $\mathcal{T}$ are written in a matrix form and called transfer matrices. We shall treat $\mathcal{T}$ as a function, but using the common phraseology we shall call it transfer matrix (T-matrix).

For the case of nearest-neighbour interactions the elements of the matrix

$$\mathcal{T}(\sigma_{i,1}, \dots, \sigma_{i,n}; \sigma_{i+1,1}, \dots, \sigma_{i+1,n})$$

are equal to the values of the function

$$\mathcal{T}(\sigma_{i,1}, \dots, \sigma_{i,n}, \sigma_{i+1,1}, \dots, \sigma_{i+1,n}).$$

If the summation of the Boltzmann's weight for a 2D system is performed row by row, the calculation of the partition function can be reformulated in a series of consecutive steps

$$\sum_{\Lambda_{i+k}} \mathcal{T}_i(\Lambda_i, \Lambda_{i+1} \ldots, \Lambda_{i+k-1}, \Lambda_{i+k}) \Phi^{\mathrm{U}}_{i+k}(\Lambda_{i+1}, \ldots, \Lambda_{i+k}) = \lambda_i \Phi^{\mathrm{U}}_{i+k-1}(\Lambda_i, \ldots, \Lambda_{i+k-1})$$

$$\sum_{\Lambda_i} \Phi^{\mathrm{D}}_i(\Lambda_i, \ldots, \Lambda_{i+k-1}) \mathcal{T}_i(\Lambda_i, \Lambda_{i+1} \ldots, \Lambda_{i+k-1}, \Lambda_{i+k}) = \lambda_i \Phi^{\mathrm{D}}_{i+1}(\Lambda_{i+1}, \ldots, \Lambda_{i+k}) \quad (2)$$

or the same in the presence of the functions Φ from the opposite half-plane

$$\begin{aligned} \textstyle\sum_{\Lambda_{i+k}} \Phi^{\mathrm{D}}_i \mathcal{T}_i \Phi^{\mathrm{U}}_{i+k} &= \lambda_i \Phi^{\mathrm{D}}_i \Phi^{\mathrm{U}}_{i+k-1} \\ \textstyle\sum_{\Lambda_i} \Phi^{\mathrm{D}}_i \mathcal{T}_i \Phi^{\mathrm{U}}_{i+k} &= \lambda_i \Phi^{\mathrm{D}}_{i+1} \Phi^{\mathrm{U}}_{i+k}, \end{aligned} \quad (3a)$$

where $i = 1, \ldots, N$, and the Φ's at the left-hand sides of the equations are results of previous summations. 'U' and 'D' are for 'up' and 'down', respectively, to distinguish from the next step where the summation will be performed in the horizontal directions.

Eqns. (2) and (3) are equivalent, but in the effective-field treatment they yield different results, as the functions Φ provide effective fields only from below in the first case or from below and above in the second one.

The functions Φ_i are eigenfunctions of the T-matrices only for the homogeneous solutions deeply in the bulk; for inhomogeneous ones all the functions are spatially dependent and the upper and lower functions $\Phi^{\mathrm{U(D)}}_i$ are different from each other (also for symmetric T-matrices). They represent Boltzmann's weights of effective fields by which one half of the lattice acts onto the other one. Similarly, $\Phi^{\mathrm{D}}_i \mathcal{T}_i$ and $\Phi^{\mathrm{D}}_i \mathcal{T}_i \Phi^{\mathrm{U}}_{i+k}$ can be considered as Boltzmann's weights of one dimensional problems, and, assuming that the functions can be factorized, they may be again treated by the T-matrix technique; e.g. $\Phi^{\mathrm{D}}_i \mathcal{T}_i = \prod_j T_{i,j}$, where $T_{i,j} = \Phi^{\mathrm{D}}_{i,j} \mathcal{T}_{i,j}$.

Let us study a general one-dimensional problem with n row of spins. Then, the T-matrices and "eigenfunctions" Ψ are defined on finite clusters for finite-range interaction problems. Further, for the sake of simplicity, we shall consider only models with interactions within a square plaquette.

$$\sum_{\{\sigma_{i,j}\}} T(\sigma_{1,j-1}, \ldots, \sigma_{n,j-1}; \sigma_{1,j}, \ldots, \sigma_{n,j}) \Psi^{\mathrm{R}}_j(\sigma_{1,j}, \ldots, \sigma_{n,j}) = \lambda_j \Psi^{\mathrm{R}}_{j-1}(\sigma_{1,j-1}, \ldots, \sigma_{n,j-1})$$

$$\sum_{\{\sigma_{i,j-1}\}} \Psi^{\mathrm{L}}_{j-1}(\sigma_{1,j-1}, \ldots, \sigma_{n,j-1}) T(\sigma_{1,j-1}, \ldots, \sigma_{n,j-1}; \sigma_{1,j}, \ldots, \sigma_{n,j}) = \lambda_j \Psi^{\mathrm{L}}_j(\sigma_{1,j}, \ldots, \sigma_{n,j})$$

(4)

Having in mind that we have to perform summation in (2) and (3), we try, in an effective way, to reduce the number of rows, n, in the one-dimensional model by one. For that reason we double each column and insert between them new columns with $n-1$ spins, as shown in Fig. 1.

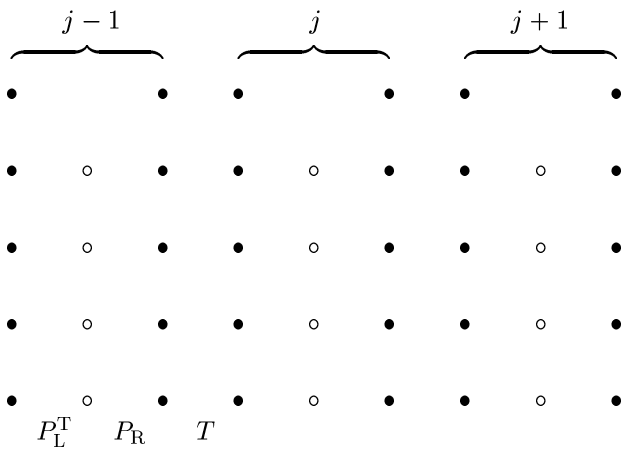


Fig. 1. Decorated one-dimensional lattice. • – old spins $\sigma_{i,j}$, ∘ – new spins $\pi_{i,j}$.

The Boltzmann's weight of the whole 1D lattice instead of

$$\ldots T_{j-1} T_j T_{j+1} \ldots$$

would be

$$\ldots T_{j-1} P^{\mathrm{T}}_{j-1,\mathrm{L}} P_{j-1,\mathrm{R}} T_j P^{\mathrm{T}}_{j,\mathrm{L}} P_{j,\mathrm{R}} T_{j+1} \ldots$$

where the functions P are the transfer matrices between the original columns of spins, whose number is doubled, and the new ones

$$\begin{aligned}
P^{\mathrm{T}}_{j,\mathrm{L}} &\equiv P^{\mathrm{T}}(\sigma_{1,j}, \ldots, \sigma_{n-1,j}, \sigma_{n,j}; \pi_{1,j}, \ldots, \pi_{n-1,j}) \\
P_{j,\mathrm{R}} &\equiv P(\pi_{1,j}, \ldots, \pi_{n-1,j}; \sigma'_{1,j}, \ldots, \sigma'_{n-1,j}, \sigma'_{n,j}) \\
T_j &\equiv T(\sigma'_{1,j}, \ldots, \sigma'_{n-1,j}, \sigma'_{n,j}; \sigma_{1,j+1}, \ldots, \sigma_{n-1,j+1}, \sigma_{n,j+1})
\end{aligned}$$

The newly introduced spins π (∘) divide the lattice into isolated blocks so that it can be easily summed up over the original spins σ and σ' (•). After the summation the number of new spins is one less per column and the number of spin degrees of freedom is reduced, i.e. the right-hand sides of Eqns. (2, 3) are found.

Since all the statistical properties of the 1D lattice can be determined from the functions Φ_j, they will remain unchanged after introduction of the new spin variables if the following equalities are satisfied:

$$\boxed{P^{\mathrm{T}}_{j,\mathrm{L}} P_{j,\mathrm{R}} \Psi^{\mathrm{R}}_j = \Psi^{\mathrm{R}}_j \qquad \Psi^{\mathrm{L}}_j P^{\mathrm{T}}_{j,\mathrm{L}} P_{j,\mathrm{R}} = \Psi^{\mathrm{L}}_j} \tag{5}$$

All our further considerations are based on this requirement.

Clearly, the functions P should be constructed from the known values of the function Ψ. There are many possibilities how to satisfy (5). Here, we discuss two choices of P:

(i)

$$P^{\mathrm{T}}_{j,\mathrm{L}}(\sigma_{1,j},\ldots,\sigma_{n-1,j},\sigma_{n,j};\pi_{1,j},\ldots,\pi_{n-1,j}) =$$

$$= \Psi^{\mathrm{R}}_j(\sigma_{1,j},\ldots,\sigma_{n,j})(\rho(\sigma_{1,j},\ldots,\sigma_{n-1,j}))^{-\frac{1}{2}}\delta_{\sigma_{1,j},\pi_{1,j}}\ldots\delta_{\sigma_{n-1,j},\pi_{n-1,j}} \qquad (6)$$

where

$$\rho(\sigma_{1,j},\ldots,\sigma_{n-1,j}) == \sum_{\sigma_{n,j}} \Psi^{\mathrm{L}}_j(\sigma_{1,j},\ldots,\sigma_{n-1,j},\sigma_{n,j})\Psi^{\mathrm{R}}_j(\sigma_{1,j},\ldots,\sigma_{n-1,j},\sigma_{n,j})$$

This choice of P leads to the cluster transfer-matrix method [2].

(ii)

$$P^{\mathrm{T}}_{j,\mathrm{L}}(\sigma_{1,j},\ldots,\sigma_{n,j},\sigma_{n,j};\pi_{1,j},\ldots,\pi_{n-k,j}) =$$

$$= \sum_{\{\tau\}} \Psi^{\mathrm{R}}_j(\tau_{1,j},\ldots,\tau_{l,j},\sigma_{l+1,j},\ldots\sigma_{n,j})\hat{\rho}^{-\frac{1}{2}}(\tau_{1,j},\ldots,\tau_{l,j};\pi_{l+1,j}\ldots\pi_{2l,j})\cdot$$

$$\cdot\delta_{\sigma_{1,j},\pi_{1,j}}\ldots\delta_{\sigma_{l,j},\pi_{l,j}}, \qquad n-k=2l \qquad (7)$$

where $\hat{\rho}^{-\frac{1}{2}}$ is the square root of the inverse to the matrix

$$\hat{\rho}(\tau_{1,j},\ldots,\tau_{l,j};\pi_{l+1,j}\ldots\pi_{2l,j}) =$$

$$= \sum_{\{\omega\}} \Psi^{\mathrm{L}}_j(\tau_{1,j},\ldots,\tau_{l,j},\omega_{l+1,j}\ldots\omega_{n,j})\Psi^{\mathrm{R}}_j(\pi_{l+1,j},\ldots,\pi_{2l,j},\omega_{l+1,j}\ldots\omega_{n,j}).$$

$\hat{\rho}$ is the density matrix corresponding to the functions $\Psi^{\mathrm{L(R)}}_j$. In the formulas for P_{R}, in both cases, the indices R and L should be interchanged.

The construction of both P's are based on the idea that Ψ in (5) meets another Ψ from the neighbouring P, forms the density function ρ or density matrix $\hat{\rho}$, which are canceled by the inverse in P, and finally, it replaced by the same Ψ from the second P in (5).

The choice (ii) of the function P reduces the number of spins by $k = n - 2l$. k can be equal to 1 only if n is odd.

If $k = 0$, the choice (ii) gives the Density Matrix Renormalization Group (DMRG) method. Now, no reduction of spin variables takes place and it must be done artificially by discarding the spin degrees of freedom corresponding to one-half of the density matrix eigenvalues (the smallest ones). In this case the requirement (5) is not satisfied for low-order approximations.

In the DMRG, one-half of eigenvectors of the density matrix, play the rôle of P. Their sign may be chosen arbitrarily, what sometimes leads to irregularities in the convergence of the iteration process. The choice (ii) this problems removes. (Note that P corresponds to the eigenvectors of the density matrix, which, in distinction to Eqn. 7, is summed up over first half of the spins in the argument of Ψ's.)

3 Some methods derived from the requirement (5)

3.1 Cluster transfer-matrix method

The choice (i) of P can be successfully applied to the Eqns. (2) if the possibility of factorization of the functions

$$\Phi^{\mathrm{U}}_{i+k} = \prod_j \Phi^{\mathrm{U}}_{i+k,j}(\sigma_{i+1,j}, \ldots, \sigma_{i+k,j}; \sigma_{i+1,j+1}, \ldots, \sigma_{i+k,j+1})$$

is assumed. From the fact that the interactions are of short range, the same factorization follows for the transfer matrix

$$\mathcal{T}_i = \prod_j \mathcal{T}_{i,j}(\sigma_{i,j}, \ldots, \sigma_{i+k,j}; \sigma_{i,j+1}, \ldots, \sigma_{i+k,j+1}).$$

Then, the left-hand side of (2) can be expressed as a product $\prod_j \Phi^{\mathrm{U}}_{i+k,j}\mathcal{T}_{i,j} \equiv \prod_j T_{i,j}$. Inserting $P_{\mathrm{L}}^{\mathrm{T}} P_{\mathrm{R}}$ (choice (i)) between every pair of T, and summing up over all original spins σ, we obtain a function on $n-1$ rows of spins π, i.e. the function $\lambda\Phi^{U}_{i+k-1}$

$$\Phi^{\mathrm{U}}_{i+k-1} = \prod_j \Phi^{\mathrm{U}}_{i+k-1,j}$$

$$\Phi^{\mathrm{U}}_{i+k-1,j}(\pi_{i,j}, \ldots, \pi_{i+k-1,j}; \pi_{i,j+1}, \ldots, \pi_{i+k-1,j+1}) =$$

$$\sum_{\substack{\sigma_{i+k,j}\\ \sigma_{i+k,j+1}}} \Psi^{\mathrm{L}}_j(\pi_{i,j}, \ldots, \pi_{i+k-1,j}, \sigma_{i+k,j})(\rho(\pi_{i,j}, \ldots, \pi_{i+k-1,j}))^{-\frac{1}{2}}\cdot$$

$$\cdot\Phi^{\mathrm{U}}_{i+k,j}(\pi_{i+1,j}, \ldots, \pi_{i+k-1,j}, \sigma_{i+k,j}; \pi_{i+1,j+1}, \ldots, \pi_{i+k-1,j+1}, \sigma_{i+k,j+1})\cdot$$

$$\cdot\mathcal{T}_{i,j}(\pi_{i,j}, \ldots, \pi_{i+k-1,j}, \sigma_{i+k,j}; \pi_{i,j+1}, \ldots, \pi_{i+k-1,j+1}, \sigma_{i+k,j+1})\cdot$$

$$\cdot\Psi^{\mathrm{R}}_{j+1}(\pi_{i,j+1}, \ldots, \pi_{i+k-1,j+1}, \sigma_{i+k,j+1}) \cdot (\rho(\pi_{i,j+1}, \ldots, \pi_{i+k-1,j+1}))^{-\frac{1}{2}} \tag{8}$$

where the functions Ψ are calculated from the Eqns. (4).

The accuracy of the method is given by the number of rows k that have to be as large as possible, despite of the fact that, for our short-range interactions, the function $\mathcal{T}$ and Φ may, in principle, be defined only on a two and one row of spins, respectively.

The cluster transfer-matrix method can be used for calculation of spatially dependent properties of inhomogeneous solutions of lattice models. If the inhomogeneities are controlled by the boundary conditions, the method 'sees' only three of them, e.g. the lower, right, and left boundaries, as it is based on one of Eqns. (2) and Eqns. (4). If the boundary conditions are given on sides of a rectangle, information from one of the sides is missing, i.e. the cluster transfer matrix method can be used only to a somewhat limited class of inhomogeneous situations. For homogeneous solutions all the quantities in (8) are independent of their indices and after necessary number of iterations the bulk value of Φ is obtained.

The cluster transfer-matrix method is much less time consuming than the DMRG method as no matrix diagonalization is necessary. Nevertheless, the value of the critical temperature of the 2D Ising model is only slightly worse than the DMRG one for the same size of Φ as shown in Table 1.

On the other hand, if the cluster transfer matrix method is applied to Eq. (3), it can describe an arbitrary inhomogeneous situation, but the resulting critical temperature is for low-order approximations distinctly higher then the exact one and converges with increasing k to the exact value rather slowly.

The method can be generalized to long-, but finite, range of interactions and modified in several ways. This is described in more details in [2], [7-9].

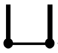
3.2 Modified DMRG method

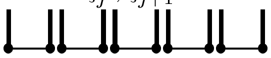
To derive the standard DMRG method, we have to factorize the function Φ (for nearest-neighbour interactions defined on one row of spins), according to Baxter [1], by a matrix product of matrices $\phi_{\sigma_j,\sigma_{j+1}}(\xi_j;\xi_{j+1})$, indexed by the lattice spins to which they belong:

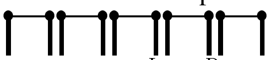
$$\Phi_i = \sum_{\{\xi\}} \prod_j \phi_{\sigma_{i,j},\sigma_{i,j+1}}(\xi_{i,j};\xi_{i,j+1}).$$

The multi-value variables ξ acquire m values, which control the order of the approximation.

To provide a deeper insight in the further formulas we shall depict the resulting equations in a graphical way.

Let us denote the matrix $\phi^{\mathrm{U}}_{\sigma_j,\sigma_{j+1}}(\xi^{\mathrm{U}}_j;\xi^{\mathrm{U}}_{j+1})$ graphically by . The black dots denote the spins σ_j, σ_{j+1} and thick vertical lines the multi-value variables $\xi^{\mathrm{U}}_j, \xi^{\mathrm{U}}_{j+1}$.

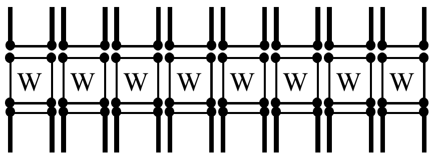
Then, Φ^{U} can be expressed as a matrix product ...  .... A summation is expected over the neighbouring thick lines, which describe the same variable ξ. Similarly, the close-to-each-other dots denote the same spin σ.

Analogously, Φ^{D} is ...  ...

Then, the left-hand side of Eq. (3a) $\Phi^{\mathrm{L}}_i \mathcal{T}_i \Phi^{\mathrm{R}}_{i+1}$ can be depicted as

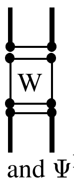
$i+1$

i



(3b)

where $\mathcal{T}_i$ is written as a product of plaquette Boltzmann's weights W: $\mathcal{T}_i = \prod_j W^i_{j,j+1}$.

Inserting between each two T-matrices $T =$  functions $P^{\mathrm{T}}_{\mathrm{L}}$ and P_{R} of the type (ii)

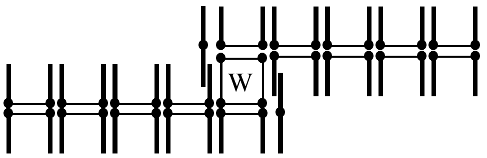
constructed from the T-matrix eigenfunctions Ψ^{R} and Ψ^{L}, reducing the number of the rows and columns in the density matrix by one-half, summing up over all the spin variables σ and ξ in the row i, the standard DMRG method is obtained. Nevertheless, our approach, comparing with the standard one, shows more clearly how to to construct the density matrix in the case of non-homogeneous solution or non-symmetric T-matrix.

In the one-dimensional system (3) even number of spins in each column is used: 2 original spins of the model used in the Boltzmann's weight W and two m-valued spins ξ. To get odd number of spins, we must omit one of the original spins, i.e. also the weight W. This step would seemingly lead to omission of the whole information about the Hamiltonian of the system. To avoid this, we discard all W's but one.

j $j{+}1$

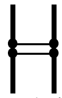
$i+1$

i

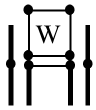


(9)

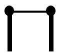
In the diagram there appeared two new symbols  which, as it will be seen, denote $P_{\mathrm{R}}(i+1,j)$ and $P_{\mathrm{L}}^{\mathrm{T}}(i,j+1)$.

Summing over sites $k<j$ in the row i, we get $\Psi^{\mathrm{L}}_{i,j}(\xi^{\mathrm{D}}_{i,j},\sigma_{i,j},\xi^{\mathrm{U}}_{i,j})$, and over the site $j+1$ in the row i and all sites in the row $i+1$, we get $\Psi^{\mathrm{R}}_{i,j}(\xi^{\mathrm{D}}_{i,j},\sigma_{i,j},\xi^{\mathrm{U}}_{i,j})$. From this two functions the density matrix is constructed according to the rule (ii), and the functions $P_{\mathrm{L}}^{\mathrm{T}}(i,j)$ and $P_{\mathrm{R}}(i,j)$ are calculated. The density matrix is generally non-symmetric. For the homogeneous phases Ψ^{R} and Ψ^{L} are the eigenvectors of the transfer matrix $T=$  , they are equal to each other, and the density matrix is symmetric. The number of spins in Ψ's is three, and, after inserting $P_{\mathrm{R}}(i,j)$ and $P_{\mathrm{L}}^{\mathrm{T}}(i,j)$ between the matrices at the site (i,j), their number will be reduced.

The function $P_{\mathrm{L}}^{\mathrm{T}}(i,j)$ should be remembered for the calculation at the site $i,j-1$ and $P_{\mathrm{R}}(i,j)$, together with $P_{\mathrm{L}}^{\mathrm{T}}(i,j+1)$ from the previous step, is used for calculation of the new value of $\phi^{\mathrm{D}}_{i+1,j;i+1,j+1}$



$\longrightarrow$



(10a)

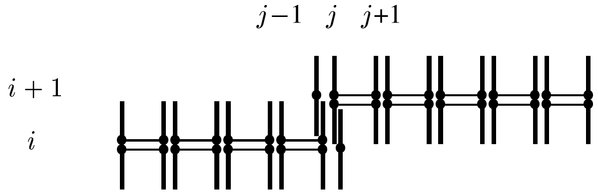
or

$$\phi^{\mathrm{D}}_{\sigma_{i+1,j},\sigma_{i+1,j+1}}(\xi^{\mathrm{U}}_{i+1,j};\xi^{\mathrm{U}}_{i+1,j+1}) =$$

$$\sum_{\substack{\sigma_{i,j},\sigma_{i,j+1}\\ \xi^{\mathrm{D}}_{i,j},\xi^{\mathrm{D}}_{i,j+1}}} P_{\mathrm{R}}(\xi^{\mathrm{D}}_{i,j},\sigma_{i,j},\xi^{\mathrm{U}}_{i,j})\phi^{\mathrm{D}}_{\sigma_{i,j},\sigma_{i,j+1}}(\xi^{\mathrm{D}}_{i,j};\xi^{\mathrm{D}}_{i,j+1})P_{\mathrm{L}}^{\mathrm{T}}(\xi^{\mathrm{D}}_{i,j+1},\sigma_{i,j+1},\xi^{\mathrm{U}}_{i,j+1})\cdot \\ \cdot W(\sigma_{i,j},\sigma_{i,j+1},\sigma_{i+1,j},\sigma_{i+1,j+1})$$

$$\xi^{\mathrm{U}}_{i+1,j}\to\xi^{\mathrm{D}}_{i+1,j} \quad \xi^{\mathrm{U}}_{i+1,j+1}\to\xi^{\mathrm{D}}_{i+1,j+1} \tag{10b}$$

The result of this summation is

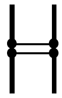
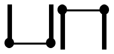


(11)

In the next step a new Boltzmann's weight W can be created from $\phi^{\mathrm{R}}_{i,j-1;i,j}$ between the columns $j-1$ and j by a procedure inverse to (10), and the sweep to the left can be continued. The sweep to the right is performed analogously.

When the steady state (fixed point) is reached, the sweeps leave the functions $\Psi_{\mathrm{L}}^{\mathrm{T}}$ and Ψ_{R} unchanged at any site of the lattice, and the calculations, in the framework of the approximation given by the number m of values of the variable ξ in the matrices ϕ, are exact. The Boltzmann's weights can be created between two arbitrary rows so that the sweeps can be performed in the horizontal and vertical directions. Finally, after sufficient number of sweeps, the values of Boltzmann's weights of effective fields $P_{\mathrm{L(R)}}$ and $\phi^{\mathrm{L(R)}}$ are obtained at all the sites of the finite lattice, from which all interesting average quantities can be calculated.

The calculation for homogeneous case is very simple. It consists of three steps iteratively performed until the fixed point is reached.

1. The ground state eigenfunction Ψ of the transfer matrix $T =$  , is calculated. The functions Φ  are assumed to be known from the previous step.
2. Knowing Ψ, the function P is found from (7).
3. The new value of Φ for the step 1 is calculated from Eqn. (10).

As for the homogeneous case it is no need to distinguish between right, left upper, and lower functions, the indices R, L, U, D are ommited.

In the effective-field methods spontaneous symmetry-breaking occurs, as a rule. Thus, the critical temperature is given by the onset of non-zero magnetization. Actually, no calculation of magnetization is needed, e.g. the difference $\Phi_{\uparrow\uparrow}(\xi,\xi') - \Phi_{\downarrow\downarrow}(\xi,\xi')$ also shows if the system is in ferromagnetic or paramagnetic state.

The described method is much faster than the standard DMRG method, as for the same accuracy the functions Ψ acquire only one-half of the values of Ψ in DMRG and the density matrix has one-quarter of elements. This statement applies for the improved DMRG algorithms [14], as well, as it can be used for calculation of the superblock (T) wave function also in our case.

However, far faster than the DMRG is the cluster transfer-matrix method, where instead of density matrix $\hat{\rho}$ a density function ρ is used, and the matrix inversion or matrix diagonalization is replaced by division.

For comparison, the values of critical interaction constants (inverse of the temperatures) for all the above-mentioned methods in the case of the homogeneous 2D Ising model are given in Table 1.

Method	Number of spin-degrees of freedom in Ψ	K_c
Cluster matrix method applied to Eq. (3) (fastest)	$2^{10} = 1024$ (no diagonalization)	0.4347
Cluster matrix method applied to Eq. (2) (fastest)	2^{10}=1024 (no diagonalization)	0.44111
Our modification of DMRG	$m = 16 \quad 2m^2 = 512$	0.44050
Our modification of DMRG	$m = 22 \quad 2m^2 = 968$	0.44052
Standard DMRG (slowest)	$m = 16 \quad 4m^2 = 1024$	0.44050
Exact value		0.44068

Table 1. Critical values of the interaction constant K_c of the Ising model on the 2D square lattice.

Since the methods are based on an approximate summation of the partition function all interesting thermally averaged physical quantities can be found as functions of coordinates. It was found that the simplified DMRG without renormalization yields practically the same values as standard DMRG also for other relevant physical quantities.

4 Discussion and conclusion

For re-derivation of DMRG and derivation of the modified DMRG, the Baxter approximate expression in the form of matrix product for the wave function was used. Similar factorization was applied by Rommer and Östlund (RO) [11] for derivation of their variational approach. Nevertheless, the matrices in both approaches are different. Baxter's matrices are indexed by two site spins while Rommer and Östlund's only by one spin. They represent the functions P in our approach. In formula (9) they appear as vertical lines with one dot. It is easily seen that if the step in (9) is high of several rows the wave function Ψ in the vertical direction would be a product of RO matrices. The step from (9) to (11) may be taken not only as a calculation of $\phi^{\mathrm{D}}_{i+1,j;i+1,j+1}$ from $\phi^{\mathrm{D}}_{i,j;i,j+1}$ but also as of $P^{\mathrm{T}}_{\mathrm{L}}(i,j)$ from $P^{\mathrm{T}}_{\mathrm{L}}(i,j+1)$ or iterative calculation of RO eigenfunctions in horizontal directions. This procedure would lead to the minimum of the free energy. As formation of arbitrary steps is, in our approach, exact at fixed point, we see that we have to obtain the same results as RO method, if treated exactly for arbitrary m as it was done here. Our method and Rommer-Östlund variational approach are complementary, but their results slightly differs from the standard DMRG ones, what can be seen, e.g. from the fact that $\sum_{\sigma,\xi^{\mathrm{D}}} P_{\mathrm{R}}(\xi^{\mathrm{D}},\sigma,\xi^{\mathrm{U}}) P^{\mathrm{T}}_{\mathrm{L}}(\xi^{\mathrm{D}},\sigma,\xi'^{\mathrm{U}}) = \delta_{\xi^{\mathrm{U}}\xi'^{\mathrm{U}}}$ is satisfied only for two first methods and not for DMRG.

A direct application of RO factorization in the general approach described in Section 2 would lead to necessity of singular decomposition of matrices, what we want to avoid in this paper. We established a connection between Baxter's and RO factorization. The possibility of wave-function factorization in Baxter's way was assumed and RO factorization derived from it.

We claim that our method avoids the renormalization of the spin variables. Here, the notion of renormalization is taken in the sense of real-space quantum renormalization group, where the states corresponding to some eigenvalues of certain matrix are discarded and the spin variables are mixed together and lose their identity. This is not done in this paper. In both choices of P (i,ii) many δ-functions appear so that most of the new and old spins are really identical. However, the new spins $\pi_{l+1,j} \ldots \pi_{2l,j}$ in (7) are different from the old ones and may be considered in another sense as renormalized.

The requirement (5) applies also to one-dimensional quantum and kinetic problems. The matrices $P_{\mathrm{L}}^{\mathrm{T}}$ and P_{R} have to be inserted between Ψ and H in the expression $\Psi^{+}H\Psi$, where H is the Hamiltonian of the superblock in the White's approach [2]. Now, from (5) it is clear that, for non-hermitian H, the left and right reduction matrices (here P's) should be both equal and non-symmetric, or different and symmetric, constructed from the left and right eigenvectors, respectively. The fact that the standard derivation of DMRG does not give transparent prescription for constructing the density matrix in non-symmetric case is seen in [15], where instead of the correct choice [16, 17] of the non-symmetric density matrix, the second possibility of right and left density matrix at the left- and right-hand side of the superblock operator, respectively, suggested by us, is not used, but the incorrect average of the left and right density matrices, or only the right density matrix, or the density matrix with mixed terms.

This approach enables effective numerical treatment of one-dimensional non-equilibrium kinetic models and quantum systems approximatively solved by analytical methods [18].

It was proposed a new method for derivation of different types of effective-field approximate methods for calculation of thermal averages of physical quantities and thermodynamic functions of inhomogeneous classical 2D spin lattices and zero-temperature properties of 1D quantum lattice system.

The effective fields appear after summation over all spins except a square plaquette. In (10) they are applied from below, left, and right and are represented by ϕ^{D}, $P_{\mathrm{L}}^{\mathrm{T}}$, and P_{R}, respectively. The effective field from above affects the calculation indirectly, through Ψ, and consequently P. The effective fields should be really perceived in a generalized sense – while in the cluster transfer matrix method their Boltzmann's weights are positive in the DMRG method, they may be negative.

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