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ESTIMATION OF THE MAGNETIC CRITICAL EXPONENT BY TENSOR PRODUCT VARIATIONAL APPROACH

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A variational problem for three-dimensional (3D) classical lattice models is considered with trial state given by two-dimensional (2D) uniform product of local variational weights. This approach, the tensor product variational approach (TPVA), has been applied to 3D classical models (the Ising and the Potts models). We consider a way of estimating the magnetic critical exponent β for the simple 3D Ising model assuming a functional form of the spontaneous magnetization in the off critical region, where the TPVA provides reliable data.

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1 Introduction

Extension of Density Matrix Renormalization Group (DMRG) [1–4] to higher dimensions is still of main interest because a very slow decay in the density matrix eigenvalue spectrum prevents the creation of efficient renormalization group transformation [5].

The numerical efficiency of the DMRG for the low-dimensional systems can be explained from the variational background [6–8]. In DMRG, the variational state is constructed by the product of orthogonal matrices. This type of the variational state can be defined in any dimension. In the three-dimensional case, Nishino *et al.* proposed the tensor product variational approach (TPVA) [9]. It is possible to regard the TPVA as an extension of the DMRG to 3D classical (or 2D quantum) systems.

The TPVA has been mostly applied to 3D classical spin models such as the Ising and the Potts models [9–12], where we considered the spatially uniform spin systems. We have also applied it to the 2D quantum Heisenberg model [13]. The TPVA is of use for the spin models which exhibit ordered magnetic structures such as in the 3D Axial-Next-Nearest-Neighbor Ising model, where the trial state is constructed from the position dependent tensors [14]. Such a position dependence is also considered by Verstraete *et al.* for 2D quantum systems [15–17].

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For the models which exhibit the second-order phase transition, the TPVA tends to overestimate the critical temperature. For example, the error in $T_{\rm c}$ is about 1% or less for the 3D Ising model compared with the Monte Carlo (MC) result [18]. This is partially because the correlation length diverges at the criticality and the TPVA cannot treat this divergence properly due to a finite number of variational parameters. As a result, the thermodynamic functions obtained by the TPVA show mean-field-like behavior around $T_{\rm c}$. Thus, in order to obtain critical indices from the numerical data by the TPVA, one has to calculate the thermodynamic functions in off critical region, where the TPVA is more accurate.

The main purpose of this paper is to obtain the magnetic critical exponent β for the 3D lattice models using the spontaneous magnetization calculated in the off critical region. We assume a scaling form for the numerical fitting of β with respected to the calculated data.

The paper is organized as follows: in Section 2, we define the model and discuss the variational background of the numerical method. We propose four types of tensor product states (TPS) which are used to calculate the variational state. By increasing the total number of variational parameters in the TPS, we obtain more precise numerical results. We calculate the critical temperature and the magnetic critical exponent for these four types of TPS in Section 3. A brief summary of the results obtained is summarized in Section 4.

2 Model and variational background

We consider the 3D Ising model on a simple cubic lattice of infinite size along all the x, y, and z axis coordinates. The model studied is described by the spin Hamiltonian

$$\mathcal{H} = -J \sum_{i,j,k} \sigma_{i,j,k} \left(\sigma_{i+1,j,k} \, + \, \sigma_{i,j+1,k} \, + \, \sigma_{i,j,k+1} \right) \tag{1}$$

with the nearest-neighbor spins $\sigma = \pm 1$ interacting via coupling constant J. The transfer matrix $\mathcal{T}$ connects two adjacent spin layers $[\sigma_k]$ and $[\sigma_{k+1}]$. It can be expressed by product of the Boltzmann weights

$$\mathcal{T}[\sigma_k|\sigma_{k+1}] = \prod_{i,j} W^{\rm B}_{i,j}\{\sigma_k|\sigma_{k+1}\} \, , \tag{2}$$

where we abbreviated the notation gathering four spins into one

$$\{\sigma_k\} \equiv (\sigma_{i,j,k} \; \sigma_{i+1,j,k} \; \sigma_{i,j+1,k} \; \sigma_{i+1,j+1,k}) \, . \tag{3}$$

We have employed the local Boltzmann weight of the interaction round-a-face (IRF) type which is defined as

$$\begin{aligned} W^{\rm B}_{i,j}\{\sigma_k|\sigma_{k+1}\} = \exp \Bigg[\frac{J}{4k_{\rm B}T} (& \sigma_{i,j,k}\sigma_{i,j,k+1} + \sigma_{i+1,j,k}\sigma_{i+1,j,k+1} \\ & + \sigma_{i,j+1,k}\sigma_{i,j+1,k+1} + \sigma_{i+1,j+1,k}\sigma_{i+1,j+1,k+1} + \sigma_{i,j,k}\sigma_{i+1,j,k} + \sigma_{i+1,j,k}\sigma_{i+1,j+1,k} \\ & + \sigma_{i+1,j+1,k}\sigma_{i,j+1,k} + \sigma_{i,j+1,k}\sigma_{i,j,k} + \sigma_{i,j,k+1}\sigma_{i+1,j,k+1} + \sigma_{i+1,j,k+1}\sigma_{i+1,j+1,k+1} \\ & + \sigma_{i+1,j+1,k+1}\sigma_{i,j+1,k+1} + \sigma_{i,j+1,k+1}\sigma_{i,j,k+1}) \Bigg] \, , \end{aligned} \tag{4}$$

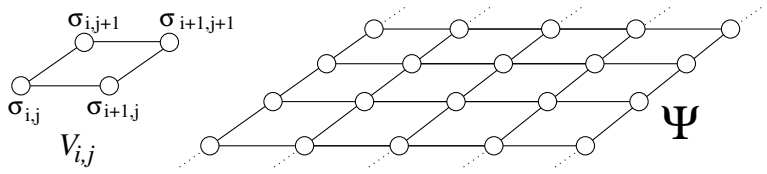

Fig. 1. Graphical representation of the four-spin local variational weight $V_{i,j}$ (left) which is used to construct the trial state Ψ (right). Notice that we have dropped the subscript k from the spins for simplicity.

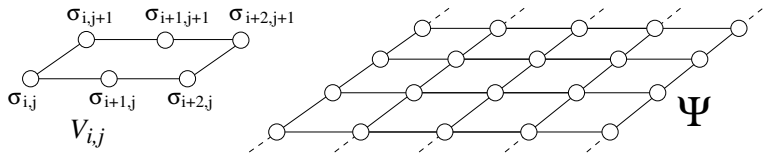

Fig. 2. The six-spin local variational weight $V_{i,j}$ (left) and the trial state Ψ (right). The weights $V_{i,j}$ overlap one another only in the x axis direction (denoted by the subscript i).

where $k_{\rm B}$ is the Boltzmann constant and T is temperature. Due to simplicity, we set $J/k_{\rm B} = 1$ in what follows on.

The variational partition function per layer for the given transfer matrix $\mathcal{T}$ has the form

$$\lambda_{\rm var}(\Psi) = \frac{\langle\Psi|\mathcal{T}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum\limits_{[\sigma_k],[\sigma_{k+1}]} \Psi[\sigma_k]\mathcal{T}[\sigma_k|\sigma_{k+1}]\Psi[\sigma_{k+1}]}{\sum\limits_{[\sigma_k]} (\Psi[\sigma_k])^2}. \tag{5}$$

Purpose of the TPVA is to maximize Eq. (5) by a proper approximation of the trial state Ψ. We assume that Ψ can be written by the product of identical local variational weights V. This approximation is often referred to as the tensor product state [12, 13, 15–17].

In the following, we consider four candidates of Ψ, where the difference is in the definition of the local weights V and their connection.

(i) In the lowest approximation, the single local weight V consists of four spins. Hence, we have $2^4 = 16$ adjustable parameters and V graphically represents a square-shaped object as shown in Fig. 1. Taking product over all the uniformly given local weights V, the trial state yields

$$\Psi[\sigma_k] = \prod_{i,j} V_{i,j}(\sigma_{i,j,k}, \sigma_{i+1,j,k}, \sigma_{i,j+1,k}\sigma_{i+1,j+1,k}). \tag{6}$$

(ii) A way to increase precision of the variational calculations is to enlarge the size of the local weight V up to six spins, see Fig. 2. Then, we let the weights V partially overlap one another defining the trial state as follows

$$\Psi[\sigma_k] = \prod_{i,j} V_{i,j}(\sigma_{i,j,k}, \sigma_{i+1,j,k}, \sigma_{i+2,j,k}\sigma_{i,j+1,k}, \sigma_{i+1,j+1,k}, \sigma_{i+2,j+1,k}). \tag{7}$$

The number of the adjustable parameters is $2^6 = 64$.

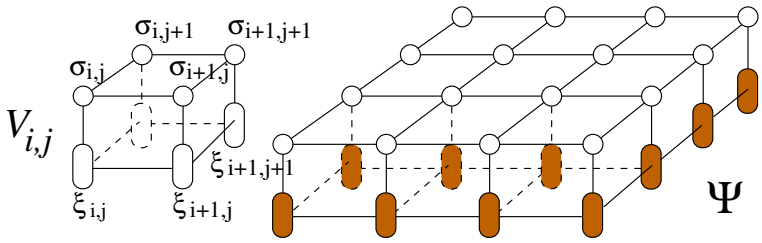

Fig. 3. The local variational weight $V_{i,j}$ of the IRF type with the auxiliary variables ξ (left) and the trial state Ψ (right). The dark ovals represents the auxiliary variables to be summed up.

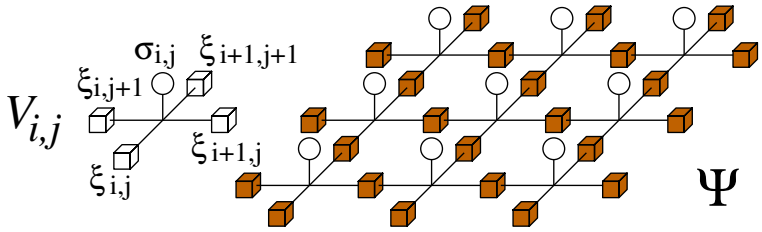

Fig. 4. The local variational weight $V_{i,j}$ of the vertex type with the auxiliary variables ξ (left) and the trial state Ψ (right). The dark cubes are the summed up auxiliary variables.

(iii) Further increase of the free parameters leads to a better approximation of the trial state (for details, see Ref. [12]). Therefore, we introduce the so-called auxiliary variables which are included in the local weight V

$$\Psi\left[\sigma_k\right] = \sum_{[\xi]} \prod_{i,j} V \begin{pmatrix} \sigma_{i,j,k} & \sigma_{i+1,j,k} & \sigma_{i,j+1,k} & \sigma_{i+1,j+1,k} \\ \xi_{i,j,k} & \xi_{i+1,j,k} & \xi_{i,j+1,k} & \xi_{i+1,j+1,k} \end{pmatrix}, \tag{8}$$

where ξ denotes the auxiliary variable which can be in one of n states $(1, 2, ..., n)$. The sum runs over all the auxiliary variables as depicted in Fig. 3. Thus, there are $(2n)^4$ adjustable parameters in total. By setting $n = 1$, the case (i) is satisfied.

(iv) Finally, we consider the vertex-type representation [19] of the 3D Ising model where the auxiliary variables ξ can be naturally included. The trial state is then given by

$$\Psi\left[\sigma_k\right] = \sum_{[\xi]} \prod_{i,j} V \begin{pmatrix} & \sigma_{i,j,k} & \\ \xi_{i,j,k} & \xi_{i+1,j,k} & \xi_{i,j+1,k} & \xi_{i+1,j+1,k} \end{pmatrix} \tag{9}$$

and is graphically represented in Fig. 4. There are $2n^4$ parameters in total.

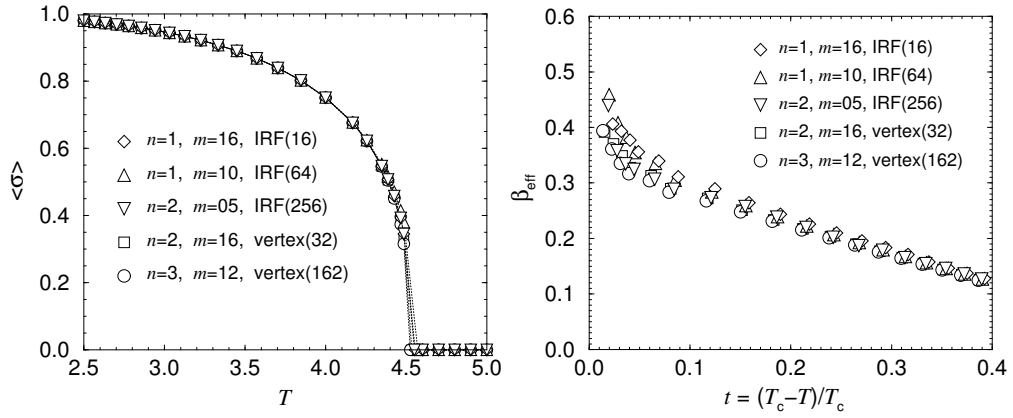

Fig. 5. Left: dependence of the spontaneous magnetization $\langle\sigma\rangle$ on temperature T for selected variables n and m as listed in Table 1. Right: the plot of the effective critical exponent $\beta_{\rm eff}$ versus relative temperature t for the same variables as shown on the left graph. The total number of the adjustable parameters is shown in the parenthesis.

We treat the local variational weights V with different number of adjustable parameters (up to 256) by the TPVA. In fact, not all of them are independent due to the symmetries of the model. The main advantage of the numerical algorithm TPVA is that we have derived a self-consistent equation (based on the a generalized eigenvalue problem) which iteratively tunes all the adjustable parameters regardless of initial choice. Numerical details of the self-consistent improvement for the trial state Ψ with explanation of the TPVA are reviewed in Refs. [9–14].

Having written the trial state Ψ and the transfer matrix $\mathcal{T}$ in the product forms, we can accurately calculate the numerator of Eq. (5)

$$\langle\Psi|\mathcal{T}|\Psi\rangle = \sum_{[\sigma_k],[\sigma_{k+1}]} \prod_{i,j} V_{i,j}\{\sigma_k\} W^{\rm B}_{i,j}\{\sigma_k|\sigma_{k+1}\} V_{i,j}\{\sigma_{k+1}\} \tag{10}$$

and also the denominator

$$\langle\Psi|\Psi\rangle = \sum_{[\sigma_k]} \prod_{i,j} \left(V_{i,j}\{\sigma_k\}\right)^2 \tag{11}$$

using the renormalization techniques. In particular, we use both the DMRG and its variant the Corner Transfer Matrix Renormalization Group [4, 19, 20].

3 Results

We calculate the spontaneous magnetization per spin site using the relation

$$\langle\sigma\rangle \equiv \langle\sigma_{i,j}\rangle = \frac{\langle\Psi|\sigma_{i,j}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{12}$$

n	m	type of TPS	lattice type	$T_{\rm c}$	$\mathcal{E}_{\rm T}$ / [%]	β	$\mathcal{E}_{\beta}$ / [%]
1	16	(i)	IRF	4.570	1.30	0.357	9.58
1	10	(ii)	IRF	4.554	0.94	0.348	6.81
2	5	(iii)	IRF	4.550	0.85	0.338	3.74
2	16	(iv)	vertex	4.533	0.47	0.332	1.90
3	12	(iv)	vertex	4.525	0.30	0.327	0.37

Tab. 1. List of the critical temperatures $T_{\rm c}$ and the magnetic critical exponents β computed for the 3D Ising model for various kinds of approximation. The relative errors $\mathcal{E}_{\rm T}$ and $\mathcal{E}_{\beta}$ are computed with respect to the results of the MC simulations [18].

for all the four kinds of approximation discussed above. The corresponding graph is shown in Fig. 5 on the left. The number of the states kept in the DMRG's block-spin variable is denoted by the letter m. Details which concern the meaning of this m-state variable can be found in Ref. [1–4]. The Table 1 summarizes the critical temperatures $T_{\rm c}$ obtained by the TPVA for the several selected variables n and m. The MC result ($T_{\rm MC} = 4.5116$) is used as a reference to evaluate the corresponding relative error $\mathcal{E}_{\rm T} = (T_{\rm c} - T_{\rm MC})/T_{\rm MC}$. Precision of our results improves with the increasing number of the adjustable parameters in V (for both the IRF and the vertex type lattice models).

We calculate the magnetic critical exponent β which describes the vanishing of the spontaneous magnetization

$$\langle\sigma\rangle \propto \left(\frac{T_{\rm c}-T}{T_{\rm c}}\right)^{\beta} \equiv t^{\beta} \tag{13}$$

when approaching the critical temperature $T_{\rm c}$ from the ferromagnetic phase. We analyze the effective critical exponent $\beta_{\rm eff}$ as a function of the relative temperature t [21, 22]

$$\beta_{\rm eff}(t) = \frac{\rm d}{{\rm d}\log(t)}\log\langle\sigma(t)\rangle. \tag{14}$$

Figure 5 (on the right) displays dependence of the effective exponent $\beta_{\rm eff}$ on the reduced temperature t. It is evident that for $t < 0.1$ the linear dependence of the exponent $\beta_{\rm eff}$ is broken and $\beta_{\rm eff}$ tends to the mean-field value equal to 1/2.

In order to calculate β, we assume dependence of the spontaneous magnetization $\langle\sigma\rangle$ on the relative temperature t in the series

$$\langle\sigma(t)\rangle = \gamma t^{\beta_{\rm eff}(t)} = \gamma t^{(\beta+\alpha_1 t+\alpha_2 t^2+\alpha_3 t^3+\cdots)} \tag{15}$$

with unknown constants γ, β, and α_i for $i = 1, 2, \ldots$. Neglecting the terms of the second-order and higher in the effective exponent $\beta_{\rm eff}$, we have a linear dependence. The linear dependence is well satisfied in the case of the 2D Ising model [22]. For simplicity, we also assume the same linear dependence for the 3D Ising model [21], in particular,

$$\langle\sigma(t')\rangle = \gamma {t'}^{\,\beta_{\rm eff}(t')} = \gamma {t'}^{\,\beta+\alpha_1 t'} \tag{16}$$

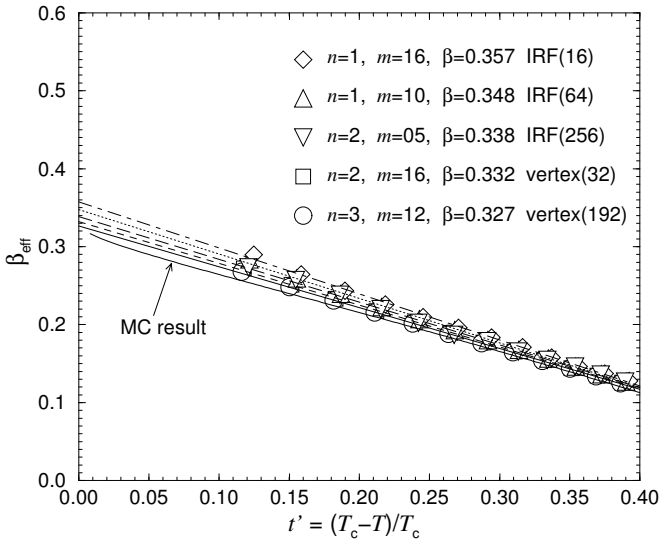

Fig. 6. The extrapolation of the effective critical exponent $\beta_{\rm eff}(t')$ down to $t' = 0$ using Eq. (16). The plotted numerical data are not affected by the mean-field effect. The lowest full line is obtained from the fit of the MC simulation [23].

with $t' = (T_{\rm c} - T)/T_{\rm c}$ where $T_{\rm c}$ is obtained by the TPVA as listed in Table 1. Note, that $\beta_{\rm eff}(t' = 0) = 1/2$ is the consequence of the mean-field behavior. Therefore, we use the linear extrapolation of the effective critical exponent $\beta_{\rm eff}(t') = \beta + \alpha_1 t'$ for $t' \gg 0$ within the off-critical region in order to find the constants β and α_1. We identify the constant β with the critical exponent after taking the limit $t' \to 0$ from the linear fit. The results are depicted in Fig. 6. Justification to carry out the linear extrapolation is supported by the plotting of the MC result [23] in the same graph which gives the nearly linear behavior. The critical exponents β obtained for various variables n and m are listed in Table 1 and compared with the MC result $\beta_{\rm MC} = 0.3258(14)$ [24].

The error in determining β from the extrapolation procedure is deduced from the following consideration. Assume a small deviation ε from the critical temperature $T_{\rm c}$ obtained by the TPVA, i. .e, $T_{\rm c}' = T_{\rm c} + \varepsilon$. Table 2 shows that for a given ε, the relative error in $T_{\rm c}$ affects the relative error in β of about ten times.

4 Conclusion

We have applied the TPVA to the simple 3D Ising model and calculated the critical temperature from the spontaneous magnetization. Using the scaling form, we obtained the magnetic critical exponent β from the spontaneous magnetization in the off critical region. The way of estimation of the critical index is of use for future applications of the TPVA to various 3D classical lattice models.

ε	$T_{\rm c}'(\varepsilon)$	$\mathcal{E}_{\rm T'}$ / [%]	β	$\mathcal{E}_{\beta(\varepsilon)}$ / [%]
-0.010	4.515	0.22	0.320	2.1
-0.005	4.520	0.11	0.323	1.1
0.000	4.525	—	0.327	—
+0.005	4.530	0.11	0.330	1.1
+0.010	4.535	0.22	0.334	2.2

Tab. 2. The relative errors $\mathcal{E}_{\rm T'}$ and $\mathcal{E}_{\beta(\varepsilon)}$ calculated for given deviations ε from the $T_{\rm c}$. This example is demonstrated on the data with the variables $n = 3$ and $m = 12$.

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