Kramers-Wannier Approximation for the 3D Ising Model

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(Received September 6, 1999)

We investigate the Kramers-Wannier approximation for the three-dimensional (3D) Ising model. The variational state is represented by an effective 2D Ising model, which contains two variational parameters. We numerically calculate the variational partition function using the corner transfer matrix renormalization group (CTMRG) method, and find its maximum with respect to the variational parameters. The value of the calculated transition point, $K_c = 0.2184$, is only 1.5\% less than the true $K_c$. This result is better than that obtained using the corner transfer tensor renormalization group (CTTRG) approach. The calculated phase transition is mean-field like.

§1. Introduction

In 1941 Kramers and Wannier\textsuperscript{1} proposed a variational approximation for the two-dimensional (2D) Ising model, which is now called the ‘Kramers-Wannier (KW) approximation’. The important feature of the approximation is that the variational state is constructed as the thermal equilibrium state of the 1D Ising model in an effective magnetic field. From the modern viewpoint, their variational state can be regarded as an example of the so-called matrix product state.\textsuperscript{3,4} More than 20 years later, Baxter improved the KW approximation by introducing additional degrees of freedom into the variational state; he reformulated the variational principle of the KW approximation using the corner transfer matrix (CTM).\textsuperscript{5-7} It is known that the variational properties of both the KW approximation and Baxter’s CTM formulation have many aspects in common with those of the density matrix renormalization group (DMRG)\textsuperscript{8-11} and the recurrent variational ansatz.\textsuperscript{11,12}

The transition temperature and the specific heat of the 2D Ising model calculated with the KW approximation are more accurate than those obtained with the mean-field approximation and the Bethe approximation.\textsuperscript{2} It is expected that the KW approximation is also a good non-perturbative method in higher dimensions. For this reason, we investigate the KW approximation for the 3D Ising model employing the maximization of the Rayleigh ratio

$$\lambda = \frac{\langle V | T | V \rangle}{\langle V | V \rangle},$$

where $T$ is the ‘layer-to-layer’ transfer matrix, and $| V \rangle$ is the variational state rep-
presented as a 2D generalization of the matrix product state. Though the variational formulation is quite simple, such a generalization of the KW approximation to 3D systems has to this time not been investigated. This is partially because there is no analytical tool to calculate \( \langle V | T | V \rangle \) and \( \langle V | V \rangle \) in Eq. (1.1), which are partition functions of unsolvable 2D lattice models. In this paper we overcome this problem by numerically calculating \( \lambda \) using the corner transfer matrix renormalization group (CTMRG),\(^{16},^{17}\) which is a variant of the DMRG for 2D classical systems\(^ {11},^{18}-^{20}\) formulated via Baxter’s CTM.\(^ {5}-^{7}\) The approach we present in the following can be regarded as the DMRG applied to 3D classical systems. It should be noted that the formulation of the KW approximation in Eq. (1.1) is related to the tensor product variational formulation for 2D quantum systems.\(^ {13}-^{15}\)

In the next section, we introduce the KW variational state \(| V \rangle\) for the 3D Ising model and present the concrete definition of Eq. (1.1). In §3, we explain the method of applying CTMRG to the variational formulation, and then calculate the spontaneous magnetization and the internal energy. Conclusions are given in §4, and we discuss several possible improvements to the present formulation of the KW approximation in 3D.

§2. Variational formulation in 3D

We consider the 3D Ising model on a simple cubic lattice of size \( N \times N \times L \) in the \( X, Y, \) and \( Z \) directions, respectively, where on each lattice point \((i, j, k)\) — the position \((i, j)\) in the \( k\)-th spin layer — there is an Ising spin \( \sigma^k_{ij} = \pm 1 \). We use open boundary conditions in both \( X \) and \( Y \) directions and periodic boundary conditions in the \( Z \) direction. The Hamiltonian of the 3D Ising model is

\[
H = -J \sum_{ijk} (\sigma^k_{ij} \sigma^k_{ij}' + \sigma^k_{i'j} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{i'j}) ,
\]

where we have used the notation \( i' \equiv i + 1, j' \equiv j + 1, \) and \( k' \equiv k + 1 \) for bookkeeping. Throughout this paper we consider the ferromagnetic case \( J > 0 \). The partition function of the system is expressed as

\[
Z = \sum_{\{\sigma\}} \exp(-\beta H) = \text{Tr} T^L ,
\]

where \( T \) is the layer-to-layer transfer matrix, and the sum is taken over all the spin configurations. In the following, we consider the symmetrized transfer matrix \( T (= T^T) \) constructed as a product of local Boltzmann weights

\[
T(\sigma^k | \sigma^k) = \prod_{ij} W^k_{ij} ,
\]

where \( \sigma^k \) and \( \sigma^{k'} \) represent spin configurations in the \( k\)-th and the \( k+1\)-th layer, respectively,\(^ {21}\) and \( W^k_{ij} \) is the local Boltzmann weight defined by

\[
W^k_{ij} = \exp \left\{ \frac{K}{4} (\sigma^k_{ij} \sigma^k_{ij}' + \sigma^k_{i'j} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{i'j} + \sigma^k_{ij} \sigma^k_{i'j}') \right\}
\]
with $K \equiv \beta J$. On the r.h.s of Eq. (2.4), the 12 terms correspond to the 12 edges of a local cube, and the coefficient 1/4 on $K$ denotes that each bond between the nearest-neighbor spins is shared by 4 adjacent cubes.

As an introduction to the KW approximation for the 3D Ising model, let us consider a special mean-field approximation, in which all the Ising spins $\sigma_{ij}$, except at the $k$-th spin layer $\sigma^k$, are replaced by their expectation value $\langle \sigma \rangle$. This approximation has the effective Hamiltonian for the $k$-th spin layer

$$H(\sigma^k) = -J \sum_{ij} (\sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij} + 2\langle \sigma \rangle \sigma^k_{ij}) ,$$  

(2.5)

which is identical to the Hamiltonian of the 2D Ising model under a mean field $2J \langle \sigma \rangle$ imposed from both above and below the $k$-th layer. In this mean-field framework, the spin profile in the $k$-th layer is given by the weight $P(\sigma^k) = \exp\{-\beta H(\sigma^k)\}$. It is expected that the mean field weight $P(\sigma^k)$ accurately approximates the appearance probability of the layer-spin configuration, and that its square root,

$$\sqrt{P(\sigma^k)} = \prod_{ij} \exp \left\{ \frac{K}{4} (\sigma^k_{ij} + \sigma^k_{ij} + \sigma^k_{ij} + \sigma^k_{ij}) + \frac{K}{4} (\sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij}) \right\} ,$$  

(2.6)

which is proportional to $T(\sigma^k|\langle \sigma \rangle)$, can be used for the variational state in Eq. (1.1).

Such a direct usage of $\sqrt{P(\sigma^k)}$ as the variational state, however, has a shortcoming in the paramagnetic region, where $\langle \sigma \rangle$ is zero and $\sqrt{P(\sigma^k)}$ has no adjustable parameter. Following Kramers and Wannier, we introduce an additional parameter to the nearest-neighbor coupling term in Eq. (2.6). The variational state (in the product form) is then given by

$$V(\sigma^k) = \prod_{ij} U^k_{ij} ,$$  

(2.7)

where the local factor $U^k_{ij}$ is defined as

$$U^k_{ij} = \exp \left\{ \frac{h}{4} (\sigma^k_{ij} + \sigma^k_{ij} + \sigma^k_{ij} + \sigma^k_{ij}) + \frac{q}{4} (\sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij}) \right\} ,$$  

(2.8)

with two variational parameters $h$ (= effective magnetic field) and $g$ (= effective nearest-neighbor coupling). The variational state $V(\sigma^k)$ in Eq. (2.7) has at least one
variational parameter $g$ even when the system is paramagnetic ($h = 0$). Substituting $T(\sigma^k|\sigma^k)$ and $V(\sigma^k)$ into the variational formulation in Eq. (1.1), the Rayleigh ratio — the approximate partition function per layer of size $N \times N$ — is expressed as

$$\lambda_N = \frac{\sum_{\{\sigma^k\}} V(\sigma^k) T(\sigma^k|\sigma^k) V(\sigma^k)}{\sum_{\{\sigma^k\}} V(\sigma^k) V(\sigma^k)},$$

(2.9)

where the denominator of the r.h.s.,

$$A_N = \sum_{\{\sigma^k\}} \prod_{ij} (U^k_{ij})^2 = \sum_{\{\sigma^k\}} \prod_{ij} \exp\left\{ \frac{\hbar}{2} (\sigma^k_{ij} + \sigma^k_{ij} + \sigma^k_{ij}) + \frac{g}{2} (\sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij} + \sigma^k_{ij} \sigma^k_{ij}) \right\}$$

(2.10)

is a partition function of an effective 2D Ising model parameterized by $h$ and $g$. Similarly, the numerator

$$B_N = \sum_{\{\sigma^k\}} V(\sigma^k) T(\sigma^k|\sigma^k) V(\sigma^k) = \sum_{\{\sigma^k\}} \prod_{ij} U^k_{ij} W^k_{ij} U^k_{ij}$$

(2.11)

is a partition function of a two-layer Ising model parameterized by $h$, $g$, and $K$.

§3. Numerical result

The goal of the KW approximation is to determine the pair of $h$ and $g$ — as functions of $K$ — that maximizes the variational partition function per site in the thermodynamic limit:

$$z(K, h, g) = \lim_{N \to \infty} (\lambda_N)^{1/N^2} = \lim_{N \to \infty} \left( \frac{B_N}{A_N} \right)^{1/N^2}.$$  

(3.1)

In order to determine the maximum of $z(K, h, g)$ in the $h$-$g$ parameter space, we calculate $z(K, h, g)$ for various values of $h$ and $g$ via the numerical calculation of $A_N$ and $B_N$ for $N = 3, 5, 7, \cdots$, up to a sufficiently large $N$. When $N$ is sufficiently large, $B_N/A_N$ is nearly equal to $\exp(fN^2 + aN + b)$, where $f = \ln z(K, h, g)$, and where $a$ and $b$ represent the finite size effect. We can cancel the finite size effect to obtain $\exp(f) = z(K, h, g)$ by using the formulation

$$z(K, h, g) = \lim_{N \to \infty} \left( \frac{B_{N+4}A_{N+2}A_{N+2}B_N}{A_{N+4}B_{N+2}B_{N+2}A_N} \right)^{1/8},$$

(3.2)

where the convergence of the r.h.s. with respect to $N$ is faster than $(B_N/A_N)^{1/N^2}$. After we obtain $z(K, h, g)$, we search for its maximum in the $h$-$g$ plane.

We use the CTMRG method$^{16,17}$ for the calculation of $A_N$ and $B_N$, since the method enables us to obtain $A_N$ and $B_N$ very rapidly and accurately. We keep $m = 32$ states in the CTMRG calculations, and we obtain $A_N$ and $B_N$ up to
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Fig. 1. The internal energy $E$ as a function of $K$. The transition point is observed at $K_c = 0.2184$.

Fig. 2. The magnetization $M$ as a function of $K$. The solid line denotes $M^{\text{MC}}$ in Eq. (3.4) obtained from Monte Carlo simulations. $^{22,23}$ In the vicinity of the calculated transition point, $M$ is proportional to $\sqrt{K - K_c}$.

$N = 150$: this condition is sufficient for the precise determination of $z(K,h,g)$. We used the Alpha 21164 station for several hours to obtain all the results shown below. Roughly speaking, the computational time is proportional to $m^3$. Throughout this section we set $J = 1$, and thus $K = \beta$.

First, let us consider the calculated results for thermodynamic quantities. Figure 1 plots the internal energy per cube, which is given by

$$E = -\langle \sigma^k_{ij} \sigma^k_{ij'} \rangle - \langle \sigma^k_{ij} \sigma^{k'}_{ij'} \rangle - \langle \sigma^{k}_i \sigma^{k'}_{ij} \rangle,$$

according to the formal thermodynamic relation $E = -\frac{\partial}{\partial \beta} \ln z(K,h,g)$. We have checked that the numerically calculated $\ln z(K,h,g)$ actually satisfies this relation. The data plotted in Fig. 1 has a kink at $K_c = 0.2184$, which is the transition point from the paramagnetic state to the ferromagnetic state. The calculated value of $K_c$ is about 1.5% smaller than one of the reliable critical points $K^{\text{MC}}_c = 0.2216544 \pm 0.000005$ determined with Monte Carlo simulations. $^{22,23}$ This relatively small discrepancy of 1.5% indicates that the KW approximation for the 3D Ising model is more accurate than that for the 2D Ising model; for the latter, the critical point $K_c = 0.4122$ calculated with the KW approximation is 6.5% smaller than the exact one, $K_c = 0.4407$. $^{24}$

In Fig. 2, we display the spontaneous magnetization $M \equiv \langle \sigma^k_i \rangle$. For comparison, we also show Tarpov and Blöte’s Monte Carlo result for a cubic lattice containing up to $256^3$ spins, (see Eq. (10) in Ref. 22)),

$$M^{\text{MC}} = 0.32694109(1.6919045 - 0.34357731t^0.50842026 - 0.42572366t),$$

where $t = 1 - K^{\text{MC}}_c/K$. This expression is very accurate for $t < 0.26$. The KW results agree with Eq. (3.4) in almost the entire region of $K$. In the vicinity of the transition point, $K_c < K < K_c + 0.01$, the calculated magnetization deviates
from Eq. (3-4) and behaves approximately as $5.171 \sqrt{K - K_c}$. In principle, the phase transition observed with the KW approximation is mean-field like.\textsuperscript{25}

Let us now consider the properties of the variational parameters $g$ and $h$, since they are closely related to $E$ and $M$. Like the internal energy $E$ in Fig. 1, the parameter $g$ shown in Fig. 3 has a kink at the calculated $K_c$, and it is always larger than $K$. The parameter $h$ shown in Fig. 4 is approximately $0.5516 \sqrt{K - K_c}$ in the vicinity of the calculated $K_c$, and $2h \simeq KM$ is approximately satisfied in the neighborhood of $K_c$.

\section{4. Conclusion and discussion}

We have applied the KW approximation to the 3D Ising model, representing the variational state as the thermal equilibrium state of an effective 2D Ising model. We have calculated the variational partition function numerically using the CTMRG method and maximized the function with respect to the variational parameters $g$ and $h$.

The KW approximation produces the spontaneous magnetization fairly well in a wide region of temperature, compared with the Monte Carlo simulations. The calculated value of transition point $K_c = 0.2184$ is only 1.5\% smaller than one of the most reliable $K_c$ determined by Monte Carlo simulations.\textsuperscript{22,23} In particular the value of $K_c$ obtained in the KW approximation is better than that obtained using the corner tensor renormalization group (CTTRG).\textsuperscript{26} The critical behavior observed with the KW approximation is mean-field like in the vicinity of the transition point.

There are at least two ways to improve the variational state used in the KW approximation for the 3D Ising model. One way is to introduce additional variational parameters into the trial state $V(\sigma^k)$. The thermal equilibrium states of arbitrary 2D classical lattice models, such as the multi-layer 2D Ising model and the Ising model with next-nearest-neighbor interactions, are candidates for $V(\sigma^k)$. It is straightforward to apply the CTMRG to such a variational state to evaluate...
the variational partition function. However, the number of variational parameters
we can use is limited by the computational time necessary to determine the optimal
variational parameter sets. The second way is to introduce block spin variables into
each local factor in $V(\sigma^k)$.\(^{15,19}\) Although this approach contains many more vari-
ational parameters than the former, with it we can treat the optimization problem
more systematically, as was done in the CTTRG.\(^{20}\) For both of these improvements,
the key point is to determine the best variational parameter set quickly.

We finally comment that the formulation of the KW approximation for the 3D
Ising model presented here can be applied to various 2D quantum spin systems. The
necessary generalization is simply to replace the 2D tensor product state in Hieida’s
DMRG formulation\(^ {14}\) by the thermal equilibrium state of 2D classical lattice models.
This is not a trivial simplification, since the relation between the 2D KW variational
state and the 2D tensor product state has not yet been clarified, in contrast to the
trivial relation in 1D.

Acknowledgements
The authors thank Y. Akutsu and Y. Hieida and N. Maeshima for valuable
discussions. The present work was partially supported by a Grant-in-Aid from the
Ministry of Education, Science, Sports and Culture of Japan. K. O. is supported by
the Japan Society for the Promotion of Science.

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