

Kramers-Wannier Approximation for the 3D Ising Model

Kouichi OKUNISHI^{*}) and Tomotoshi NISHINO^{1**)}

*Department of Applied Physics, Graduate school of Engineering, Osaka University,
Suita, Osaka 565-0781*

¹*Department of Physics, Graduate School of Science, Kobe University, Inoshishidai
657-8501*

(Received)

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 calculated transition point $K_c = 0.2184$ is only 1.5% less than the true K_c ; the result is better than that obtained by the corner transfer tensor renormalization group (CTTRG) approach. The calculated phase transition is mean-field like.

§1. Introduction

In 1941 Kramers and Wannier¹⁾ proposed a variational approximation for the two-dimensional (2D) Ising model, which is called ‘Kramers-Wannier (KW) approximation’ today. The 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 view point, their variational state can be regarded as an example of so called the matrix product state.^{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).⁵⁾⁻⁷⁾ It has been known that the variational property in both the KW approximation and Baxter’s CTM formulation has many aspects in common with that in the density matrix renormalization group (DMRG)⁸⁾⁻¹¹⁾ and the recurrent variational ansatz.^{11),12)}

The transition temperature and the specific heat of the 2D Ising model calculated by the KW approximation are more accurate than those obtained by the mean-field approximation and the Bethe approximation.²⁾ It is expected that the KW approximation is a good non-perturbative method also in higher dimensions. We therefore investigate the KW approximation for the 3D Ising model by way of the maximization of the Rayleigh ratio

$$\lambda = \frac{\langle V|T|V\rangle}{\langle V|V\rangle}, \quad (1.1)$$

where T is the ‘layer-to-layer’ transfer matrix, and $|V\rangle$ is the variational state rep-

^{*}) E-mail address: okunishi@godzilla.phys.sci.osaka-u.ac.jp

^{**}) E-mail address: nishino@phys.sci.kobe-u.ac.jp

resented 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 not been investigated so far. 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) that are partition functions of unsolvable 2D lattice models. In this paper we overcome the problem by numerically calculating λ 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⁾ Our approach shown 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 way to apply CTMRG to the variational formulation, and then show the calculated spontaneous magnetization and the internal energy. Conclusions are summarized in §4, and we discuss several possible improvements to the formulation of the KW approximation in 3D.

§2. Variational Formulation in 3D

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

$$H = -J \sum_{ijk} (\sigma_{i'j}^k \sigma_{ij}^k + \sigma_{ij}^k \sigma_{ij}^{k'} + \sigma_{ij}^{k'} \sigma_{ij}^k), \quad (2.1)$$

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

$$Z = \sum_{\{\sigma\}} \exp(-\beta H) = \text{Tr } T^L, \quad (2.2)$$

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

$$T(\sigma^{k'} | \sigma^k) = \prod_{ij} W_{ij}^k, \quad (2.3)$$

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

$$W_{ij}^k = \exp \left\{ \frac{K}{4} (\sigma_{i'j}^{k'} \sigma_{ij}^{k'} + \sigma_{ij}^{k'} \sigma_{ij}^{k'} + \sigma_{i'j}^{k'} \sigma_{i'j}^{k'} + \sigma_{i'j}^{k'} \sigma_{ij}^{k'}) \right.$$

$$\begin{aligned}
 & + \sigma_{ij}^{k'} \sigma_{ij}^k + \sigma_{ij'}^{k'} \sigma_{ij'}^k + \sigma_{ij}^{k'} \sigma_{ij'}^k + \sigma_{ij'}^{k'} \sigma_{ij}^k \\
 & + \sigma_{ij}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij'}^k + \sigma_{ij}^k \sigma_{ij'}^k + \sigma_{ij'}^k \sigma_{ij}^k \Big\}, \quad (2.4)
 \end{aligned}$$

with $K \equiv \beta J$. In the r.h.s of the eq. (2.4), the 12 terms correspond to the 12 edges of a local cube, and the coefficient $1/4$ of 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, which replaces all the Ising spins σ_{ij}^k except at the k -th spin layer σ^k by their expectation value $\langle \sigma \rangle$. The approximation draws the effective Hamiltonian for the k -th spin layer

$$\bar{H}(\sigma^k) = -J \sum_{ij} (\sigma_{ij}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij}^k + 2\langle \sigma \rangle \sigma_{ij}^k), \quad (2.5)$$

which is nothing but the Hamiltonian of the 2D Ising model under the mean field $2J\langle \sigma \rangle$ imposed from both the up and down sides of the k -th layer. In this mean-field framework, the spin profile in the k -th layer is given by the weight $P(\sigma^k) = \exp\{-\beta \bar{H}(\sigma^k)\}$. It is expected that the mean field weight $P(\sigma^k)$ well approximates the appearance probability of the layer-spin configuration, and that its square root

$$\begin{aligned}
 \sqrt{P(\sigma^k)} = \prod_{ij} \exp \Big\{ & \frac{K\langle \sigma \rangle}{4} (\sigma_{ij}^k + \sigma_{ij'}^k + \sigma_{ij}^k + \sigma_{ij'}^k) \\
 & + \frac{K}{4} (\sigma_{ij}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij}^k + \sigma_{ij}^k \sigma_{ij'}^k + \sigma_{ij'}^k \sigma_{ij'}^k) \Big\}, \quad (2.6)
 \end{aligned}$$

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

$$V(\sigma^k) = \prod_{ij} U_{ij}^k, \quad (2.7)$$

where the local factor U_{ij}^k is defined as

$$\begin{aligned}
 U_{ij}^k \equiv \exp \Big\{ & \frac{h}{4} (\sigma_{ij}^k + \sigma_{ij'}^k + \sigma_{ij}^k + \sigma_{ij'}^k) \\
 & + \frac{g}{4} (\sigma_{ij}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij}^k + \sigma_{ij}^k \sigma_{ij'}^k + \sigma_{ij'}^k \sigma_{ij'}^k) \Big\}, \quad (2.8)
 \end{aligned}$$

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 $V(\sigma^k)$ to the variational formulation in eq. (1.1), the Rayleigh ratio — the approximation partition function per layer of the size $N \times N$ — is expressed as

$$\lambda_N = \frac{\sum_{\{\sigma^{k'}\}\{\sigma^k\}} V(\sigma^{k'}) T(\sigma^{k'} | \sigma^k) V(\sigma^k)}{\sum_{\{\sigma^k\}} V(\sigma^k) V(\sigma^k)}, \quad (2.9)$$

where the denominator of the r.h.s.

$$A_N = \sum_{\{\sigma^k\}} \prod_{ij} (U_{ij}^k)^2 = \sum_{\{\sigma^k\}} \prod_{ij} \exp \left\{ \frac{h}{2} (\sigma_{ij}^k + \sigma_{ij}^k + \sigma_{ij'}^k + \sigma_{ij'}^k) \right. \\ \left. + \frac{g}{2} (\sigma_{ij'}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij}^k + \sigma_{ij'}^k \sigma_{ij}^k) \right\} \quad (2.10)$$

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

$$B_N \equiv \sum_{\{\sigma^{k'}\}\{\sigma^k\}} V(\sigma^{k'}) T(\sigma^{k'} | \sigma^k) V(\sigma^k) = \sum_{\{\sigma^{k'}\}\{\sigma^k\}} \prod_{ij} U_{ij}^k W_{ij}^k U_{ij}^{k'} \quad (2.11)$$

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 find out the pair of h and g — as functions of K — that maximizes the variational partition function per site in the thermodynamic limit:

$$z(K, h, g) = \lim_{N \rightarrow \infty} (\lambda_N)^{1/N^2} = \lim_{N \rightarrow \infty} (B_N/A_N)^{1/N^2}. \quad (3.1)$$

In order to find out 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 $N = 3, 5, 7, \dots$ up to a sufficiently large N . After that we search the maximum of $z(K, h, g)$ in the h - g plane. From the numerical point of view, it is better to use the formulation

$$z(K, h, g) = \lim_{N \rightarrow \infty} \left(\frac{B_{N+4} A_{N+2} B_N}{A_{N+4} B_{N+2} A_N} \right)^{1/8} \quad (3.2)$$

in order to accelerate the numerical convergence with respect to N , rather than just taking the limit $N \rightarrow \infty$ directly to $(B_N/A_N)^{1/N^2}$.

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 obtain A_N and B_N up to $N = 150$; the condition is sufficient for the precise determination of $z(K, g, h)$. Throughout this section we set $J = 1$ and thus $K = \beta$.

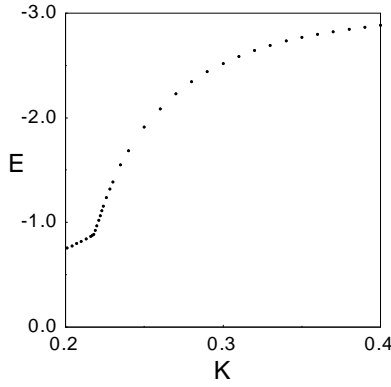


Fig. 1. The internal energy E as a function of K . The transition point is observed at $K_c = 0.2184$.

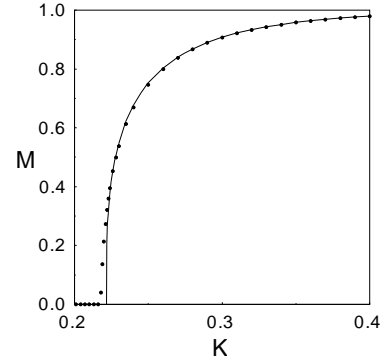


Fig. 2. The magnetization M as a function of K . The solid line denotes eq.(3.4) obtained by Monte Carlo simulations.^{22), 23)} In the very vicinity of the calculated transition point, M is proportional to $\sqrt{K - K_c}$.

First, let us see the calculated results of thermodynamic quantities. Figure 1 shows the internal energy per cube, which is given by

$$E = -\langle \sigma_{ij}^k \sigma_{i'j}^k \rangle - \langle \sigma_{ij}^k \sigma_{ij'}^k \rangle - \langle \sigma_{ij}^k \sigma_{ij}^{k'} \rangle, \quad (3.3)$$

according to the formal thermodynamic relation $E = -\frac{\partial}{\partial \beta} \ln z(K, h, g)$. We have checked that the numerically calculated $\ln z(K, h, g)$ really satisfies the relation. The plotted data 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 K_c is about 1.5% smaller than one of the reliable critical point $K_c^{\text{MC}} = 0.2216544 \pm 0.000005$ determined by Monte Carlo simulations.^{22), 23)} The discrepancy 1.5% shows 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 by the KW approximation is 6.5% smaller than the exact one $K_c = 0.4407$.²⁴⁾

In Fig. 2, we draw the spontaneous magnetization $M \equiv \langle \sigma_{ij}^k \rangle$. For comparison, we also show Tarpov and Blöte's Monte Carlo result for the cubic lattice containing up to 256^3 spins, (see eq. (10) in Ref.[22])

$$M^{\text{MC}} = t^{0.32694109} (1.6919045 - 0.34357731t^{0.50842026} - 0.42572366t), \quad (3.4)$$

where $t \equiv 1 - K_c^{\text{MC}}/K$. The KW results agrees with eq. (3.4) in almost whole the region of K . In the very vicinity of the transition point $K_c < K < K_c + 0.01$, the calculated magnetization deviates from eq. (3.4) and behaves as $5.171\sqrt{K - K_c}$ approximately. In principle, the phase transition observed by the KW approximation is mean-field like.²⁵⁾

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

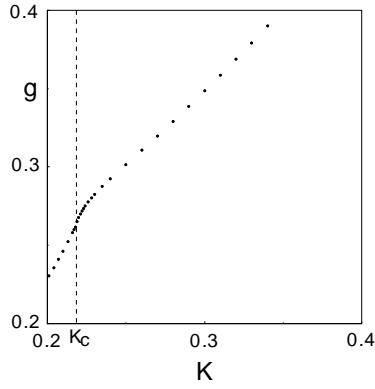


Fig. 3. The variational parameter g as a function of K .

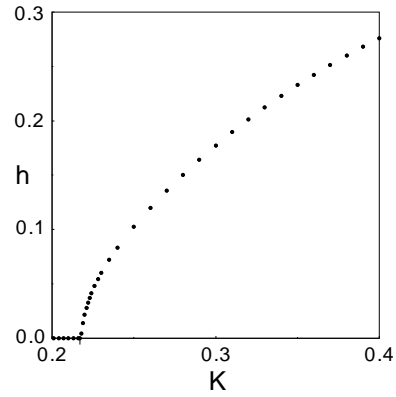


Fig. 4. The variational parameter h as a function of K . In the vicinity of the transition point, h is proportional to $\sqrt{K - K_c}$.

of the calculated K_c ; $2h \simeq KM$ is approximately satisfied in the neighborhood of K_c .

§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 CTMRG method, and maximized the function with respect to the variational parameters g and h .

The KW approximation draws the spontaneous magnetization fairly well in wide region of temperature, compared with the Monte Carlo simulations. The calculated transition point $K_c = 0.2184$ is only 1.5% smaller than one of the most reliable K_c determined by Monte Carlo simulations;^{22),23)} the K_c obtained in the KW approximation is better than that obtained by the corner tensor renormalization group (CTTRG).²⁶⁾ The critical behavior observed by the KW approximation is mean-field like in the very 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. A way is to introduce additional variational parameters into the trial state $V(\sigma^k)$. Thermal equilibrium state of arbitrary 2D classical lattice models, such as the multi-layer 2D Ising model and the Ising model with next nearest neighbor interactions, can be the 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 is limited by the numerical effort to find out optimal variational parameter sets. The other way is to introduce block spin variables into each local factors in $V(\sigma^k)$.^{15),19)} Although this approach contains much more variational parameters than the former way, we can treat the optimization problem more systematically as was done in the CTTRG.²⁶⁾ In both of these improvements, the key point is to find out 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 generalization is simply to replace the 2D tensor product state in Hieida's DMRG formulation¹⁴⁾ 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 have not been clarified yet, unlike the trivial relation in 1D.

Acknowledgments

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

References

- 1) H.A. Kramers and G.H. Wannier, *Phys. Rev.* **60** (1941), 263.
- 2) H.A. Bethe, *Proc. Roy. Soc.* **A150** (1935), 552.
- 3) I. Affleck, T. Kennedy, E.H. Lieb and H. Tasaki, *Phys.Rev. Lett.* **59** (1987), 799.
- 4) M. Fannes, B. Nachtergale and R.F. Werner, *Europhys. Lett.* **10** (1989), 633; M. Fannes, B. Nachtergale and R.F. Werner, *Commun. Math. Phys.* **144** (1992), 443; M. Fannes, B. Nachtergale and R.F. Werner, *Commun. Math. Phys.* **174** (1995), 477.
- 5) R.J. Baxter, *J. Math. Phys.* **9** (1968), 650.
- 6) R.J. Baxter, *J. Stat. Phys.* **19** (1978), 461.
- 7) R.J. Baxter: *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982), p.363.
- 8) S.R. White, *Phys. Rev. Lett.* **69** (1992), 2863.
- 9) S.R. White, *Phys. Rev.* **B48** (1993), 10345.
- 10) S. Östlund and S. Rommer, *Phys. Rev. Lett* **75** (1995), 3537; S. Rommer and S. Östlund, *Phys. Rev.* **B55** (1997), 2164.
- 11) *Density-Matrix Renormalization — A New Numerical Method in Physics*, Lecture notes in Physics, eds. I. Peschel, X. Wang, M. Kaulke, and K. Hallberg (Springer Verlag, 1999).
- 12) G. Sierra and M.A. Martín-Delgado, *Phys. Rev.* **B56** (1997), 8774.
- 13) H. Niggemann, A. Klümper and J. Zittartz, *Z. Phys.* **B104** (1997), 103.
- 14) Y. Hieida, K. Okunishi and Y. Akutsu, *New J. Phys.* **1** (1999), 7.
- 15) G. Sierra and M.A. Martín-Delgado, *cond-mat/9811170*.
- 16) T. Nishino and K. Okunishi, *J. Phys. Soc. Jpn.* **65** (1996), 891.
- 17) T. Nishino and K. Okunishi, *J. Phys. Soc. Jpn.* **66** (1997), 3040.
- 18) T. Nishino, *J. Phys. Soc. Jpn.* **64** (1995), 3598.
- 19) T. Nishino, K. Okunishi, Y. Hieida, T. Hikihara, and H. Takasaki, *Int. J. Mod. Phys.* **B13** (1999), 1.
- 20) E. Carlon and A. Drzewiński, *Phys. Rev. Lett.* **79** (1997), 1591.
- 21) The notation σ^k denotes a group of spins σ_{ij}^k for all i and j in the k -th layer in the $N \times N \times L$ simple cubic lattice.
- 22) A.L. Talapov and H.W.J. Blöte, *J. Phys. A, Math. Gen.* **29** (1996), 5727.
- 23) A.M. Ferrenberg and D.P. Landau, *Phys. Rev.* **B44** (1991), 5081.
- 24) L. Onsager, *Phys. Rev.* **65** (1944), 117.
- 25) The mean-field behavior of the CTM method or the DMRG in the very vicinity of the transition point is reported in S.K. Tsang, *J. Stat. Phys.* **20** (1978), 95; see also Šurda, *Acta Physica Slovaca* **49** (1999), 325.
- 26) T. Nishino and K. Okunishi, *J. Phys. Soc. Jpn.* **68** (1999), 3066.