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Critical Properties of an Approximant of Two-Dimensional Quantum *XYZ* Models

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It is proved that two-dimensional spin-1/2 *XYZ* models can be mapped onto generalized Ashkin–Teller models, in the first approximation of a realization of the decomposition scheme proposed by Suzuki. Consequently, it is shown that a large class of quantum spin models can be investigated analytically within the present approximation. Some analytic and numerical results are explicitly obtained with respect to thermal and critical properties in some interesting cases. It is also pointed out that the present mapping suggests a procedure to overcome the well-known negative sign problem in performing Monte Carlo calculations of frustrated quantum spin models.

KEY WORDS: Quantum *XYZ* model; Ashkin–Teller model; generalized Trotter formula; quantum Monte Carlo; negative sign problem; frustrated quantum spin system; quantum Villain model.

1. INTRODUCTION

The system studied in the present paper is the most primitive case of the path-integral formulation of quantum spin systems given by Suzuki, who presented the equivalence theorem that d-dimensional quantum systems are mapped onto $(d+1)$-dimensional classical systems, with the use of the generalized Trotter formula.[1,2] In general, the partition function Z for the relevant quantum system can be systematically approximated as

$$Z = \mathrm{Tr} \exp(-\beta \mathscr{H}) = \lim_{n \to \infty} Z(n) \tag{1.1}$$

with the nth approximant

$$Z(n) = \mathrm{Tr} \left\{ \prod_p \exp(-\beta \mathscr{H}_p / n) \right\}^n \tag{1.2}$$

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where we may use any decomposition of the hamiltonian: $\mathscr{H} = \sum_p \mathscr{H}_p$. The path-integral or classical representation of the nth approximant yields a classical system with many-spin interactions in the $(d+1)$-dimensional lattice, which consists of d-dimensional real space and a one-dimensional "time" dimension. The latter direction is introduced to express noncommutativity, namely, the quantum effect, according to the number n in Eq. (1.2).[2] We call the new direction the Trotter direction (or quantum direction) and call n the Trotter number. The analysis of the resultant classical models is of great importance in studying thermodynamic properties of quantum systems, and many investigations concerning them have been made with the use of Monte Carlo and analytic methods,[3–9,12] based upon the above equivalence theorem.[2]

In the present paper we focus upon the first (namely $n=1$) approximant $Z(1)$. For the original quantum models, $Z(1)$ is the most primitive approximation and it may give a behavior quite different from the original one at low temperatures. However, it turns out that $Z(1)$ shows an interesting ordering process and phase transitions. Thus, $Z(1)$ would be worth studying on its own. Moreover, it gives of course the reference data for the Monte Carlo simulation with $n=1$, which is a starting point to further approximations ($n>1$).

In fact, Lagendijk and De Raedt[9] first found a nontrivial closed-form solution of the two-dimensional spin-1/2 XY model for the $n=1$ approximant. They showed the existence of a phase transition characterized by the logarithmic divergence of the specific heat at a finite critical temperature, and they also showed that out-of-plane (z direction in spin space) magnetization does not appear and out-of-plane susceptibility does not diverge at any temperature. The in-plane behavior of the system was not investigated by them. In the present study an explicit realization of such a decomposition is presented, and detailed information about the two-dimensional spin-1/2 systems within the $n=1$ approximation is obtained. In particular, we investigate the in-plane magnetic properties.

The content of the present paper is as follows. In Section 2 we give an $n=1$ approximant for the two-dimensional quantum XYZ model, which forms a realization of the general decomposition scheme.[2] For this purpose, the corresponding classical representation is constructed by using the generalized Trotter formula. In Section 3 we show that the representation thus obtained can be mapped onto Ashkin–Teller models by the use of spin transformation and dual transformation. In Section 4, taking advantage of the mapping, we obtain the thermal and critical properties of the present approximant in both uniform coupling cases and frustrated ones. In Section 5 a summary of our results and a discussion are given, including prospects for future studies. Finally, we illustrate how the present

approximant can evade the so-called "negative sign problem" which occurs in Monte Carlo simulations of frustrated quantum spin models.[10]

2. APPROXIMANT AND CLASSICAL REPRESENTATION

For the two-dimensional spin-1/2 system of interest we consider the Hamiltonian described by

$$\mathscr{H} = \sum_b h_b \tag{2.1}$$

with the pair-spin interaction

$$h_b = -J_x(b)\,\sigma_i^x \sigma_j^x - J_y(b)\,\sigma_i^y \sigma_j^y - J_z(b)\,\sigma_i^z \sigma_j^z \tag{2.2}$$

where the sum runs over all the nearest neighbor bonds $b = \langle ij \rangle$ on an $L \times L$ square lattice ($L =$ even), $\{\sigma_i^x, \sigma_i^y, \sigma_i^z\}$ are Pauli matrices located at each site $i = (ix, iy)$ for $ix, iy = 1, 2, \ldots, L$, and we impose the periodic boundary conditions upon both sides of the lattice. Here note that every strength and sign of the interactions $\{J_x(b), J_y(b), J_z(b)\}$ may vary on every bond.

To define our approximant for this quantum system, we first decompose the total Hamiltonian (2.1) into the sum of sub-Hamiltonians. Our decomposition is given as follows

$$\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2 + \mathscr{H}_3 + \mathscr{H}_4 \tag{2.3}$$

where

$$\begin{aligned}
\mathscr{H}_1 &= \sum_{b \in \{1\}} h_b = \sum_{ix = \text{odd}} \sum_{iy} h_{(ix,iy)(ix+1,iy)} \\
\mathscr{H}_2 &= \sum_{b \in \{2\}} h_b = \sum_{ix} \sum_{iy = \text{odd}} h_{(ix,iy)(ix,iy+1)} \\
\mathscr{H}_3 &= \sum_{b \in \{3\}} h_b = \sum_{ix = \text{even}} \sum_{iy} h_{(ix,iy)(ix+1,iy)} \\
\mathscr{H}_4 &= \sum_{b \in \{4\}} h_b = \sum_{ix} \sum_{iy = \text{even}} h_{(ix,iy)(ix,iy+1)}
\end{aligned} \tag{2.4}$$

as is depicted in Fig. 1. This type of decomposition is the two-dimensional version of the so-called checkerboard decomposition (CBD) used for one-dimensional quantum systems,[11] and we may call this the checkercube decomposition (CCD).[12]

The general formalism immediately allows us to write formally the nth approximant as

$$\begin{aligned}
Z^{\text{CCD}}(n) = \text{Tr}\{&\exp(-\beta \mathscr{H}_1/n) \exp(-\beta \mathscr{H}_2/n) \\
&\times \exp(-\beta \mathscr{H}_3/n) \exp(-\beta \mathscr{H}_4/n)\}^n
\end{aligned} \tag{2.5}$$

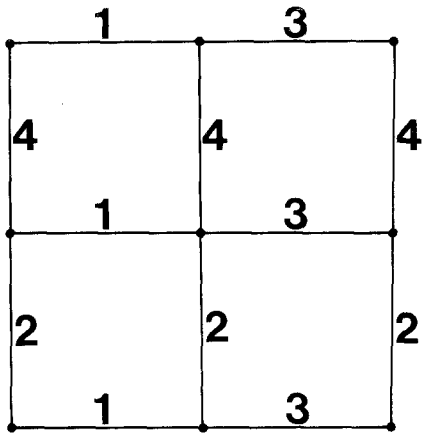

Fig. 1. Unit cell of the decomposition.

with the CCD. Here we are especially interested in the case of the $n=1$ approximant

$$Z^{\mathrm{CCD}}(1)=\mathrm{Tr}\{\exp(-\beta\mathscr{H}_1)\exp(-\beta\mathscr{H}_2)\exp(-\beta\mathscr{H}_3)\exp(-\beta\mathscr{H}_4)\} \quad (2.6)$$

Note that the pair-spin local Hamiltonians $\{h_b\}$ commute with each other within the sub-Hamiltonian $\{\mathscr{H}_i\}$ for $i=1$–4, respectively. Equation (2.6) is, then, expressed in the pair-product form

$$Z^{\mathrm{CCD}}(1)=\mathrm{Tr}\left\{\prod_{b\in\{1\}}\rho_b\prod_{b\in\{2\}}\rho_b\prod_{b\in\{3\}}\rho_b\prod_{b\in\{4\}}\rho_b\right\} \quad (2.7)$$

where $\rho_b=\exp(-\beta h_b)$. We remark here that the present approximant corresponds to the pair-product model originally introduced by Suzuki.[13]

From now on let us represent this approximant in terms of classical (Ising) spins. This is accomplished by applying the spin version of the path integral. For the case of $n=1$, we have the following primitive representation:

$$\begin{aligned}Z^{\mathrm{CCD}}(1)=\sum_{\text{states}}&\langle\alpha|\exp(-\beta\mathscr{H}_1)|\beta\rangle\langle\beta|\exp(-\beta\mathscr{H}_2)|\gamma\rangle\\&\times\langle\gamma|\exp(-\beta\mathscr{H}_3)|\delta\rangle\langle\delta|\exp(-\beta\mathscr{H}_4)|\alpha\rangle\end{aligned} \quad (2.8)$$

where the sum of states runs over four complete sets: $|\alpha\rangle$, $|\beta\rangle$, $|\gamma\rangle$, and $|\delta\rangle$. The above formula can be represented as

$$\begin{aligned}Z^{\mathrm{CCD}}(1)=\sum_{\text{states}}&\prod_{b\in\{1\}}\rho_b{}^{\alpha\beta}\prod_{b\in\{2\}}\rho_b{}^{\beta\gamma}\\&\times\prod_{b\in\{3\}}\rho_b{}^{\gamma\delta}\prod_{b\in\{4\}}\rho_b{}^{\delta\alpha}\end{aligned} \quad (2.9)$$

Table I. Local Matrix Elements

		$\|\uparrow\uparrow\rangle$	$\|\uparrow\downarrow\rangle$	$\|\downarrow\uparrow\rangle$	$\|\downarrow\downarrow\rangle$
$[\rho] =$	$\langle\uparrow\uparrow\|$	a	0	0	d
	$\langle\uparrow\downarrow\|$	0	c	b	0
	$\langle\downarrow\uparrow\|$	0	b	c	0
	$\langle\downarrow\downarrow\|$	d	0	0	a

where $a = \exp(K_x)\cosh(K_-)$, $b = \exp(-K_x)\sinh(K_+)$,
$c = \exp(-K_x)\cosh(K_+)$, $d = \exp(K_x)\sinh(K_-)$

with $K_x = \beta J_x$, etc., and $K_\pm = K_y \pm K_z$

where $\rho_b{}^{\alpha\beta}$, etc., are matrix elements of local operators:

$$\rho_b{}^{\alpha\beta} = \langle \sigma_i{}^{\alpha}\sigma_j{}^{\alpha} |\, \rho_b \,| \sigma_i{}^{\beta}\sigma_j{}^{\beta} \rangle \tag{2.10}$$

giving interactions among four spins $\sigma_i{}^{\alpha}$, $\sigma_j{}^{\alpha}$, $\sigma_i{}^{\beta}$, and $\sigma_j{}^{\beta}$. Here the sum is taken over all states of $4N$ ($N = L^2$) Ising spins $\{\sigma_i{}^{\alpha}, \sigma_i{}^{\beta}, \sigma_i{}^{\gamma}, \sigma_i{}^{\delta}\}$. In the present paper we take the σ^x-representation ($\sigma^x |\sigma\rangle = \sigma |\sigma\rangle$, $\sigma = \pm 1$) for the states. The matrix elements of (2.10) evaluated in this representation are summarized in Table I.

Next, the above procedure is applied to construct an effective lattice of the Ising system represented by (2.9). In Fig. 2a we show the $L \times L \times 4$ lattice (checkercube lattice), where the vertical dimension corresponds to the Trotter direction and the shaded squares stand for the four-spin interactions with the Boltzmann weights a, b, c, or d shown in Table I. This is the standard way of drawing it, but we can have a more tractable description for the effective lattice by a suitable lattice-folding. The resultant lattice structure is a $2L \times 2L$ checkerboard lattice, as shown in Fig. 2b. It should be noted that the bold arrows in the Fig. 2b, which denote the local transfer direction, come from those of the lattice in Fig. 2a. From now on we refer to this lattice as a σ-lattice.

3. MAPPED ISING REPRESENTATION

The effective lattice or σ-lattice has many redundant spin configurations that contribute nothing to the partition sum, because of the symmetry of the pair-spin interaction. Our purpose in the present section is to eliminate these redundant degrees of freedom in order to find an Ising representation without any restriction. It should be remarked that our procedure here is complementary to the eight-vertex formulation by Lagendijk and De Raedt.[9]

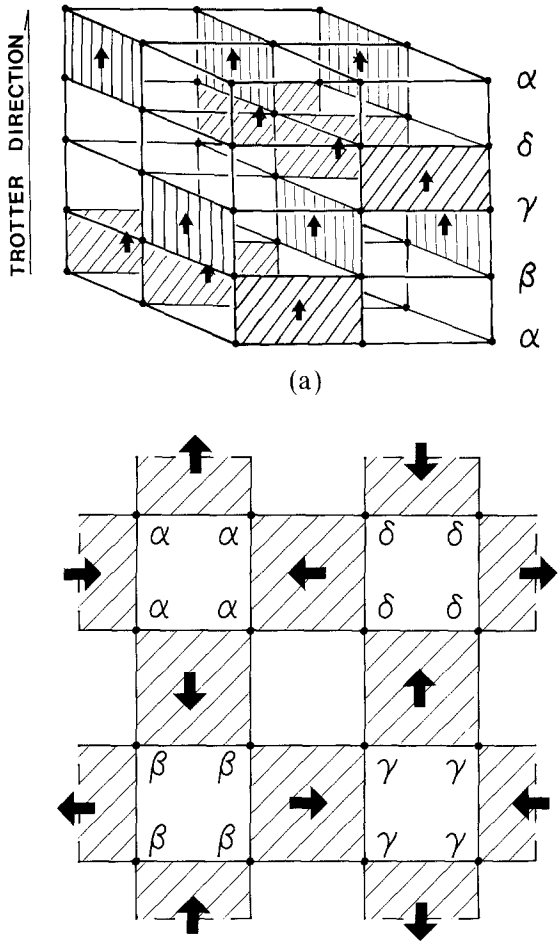

Fig. 2. (a) Unit cell of the effective lattice: checkercube lattice. (b) Unit cell of the folded effective lattice: σ-lattice.

We make use of a sort of spin transformation.[14,15] Let us prepare two $L \times L$ lattices, dual to each other, with Ising spins τ and μ on each lattice, as is shown in Fig. 3. Next we consider such a local spin transformation between the old σ-lattice and the two new lattices as

$$\sigma = \tau \cdot \mu \tag{3.1}$$

where τ and μ are two nearest neighbor spins adjacent to σ, as shown in Fig. 3. Because of the restriction on the σ-lattice, this transformation can

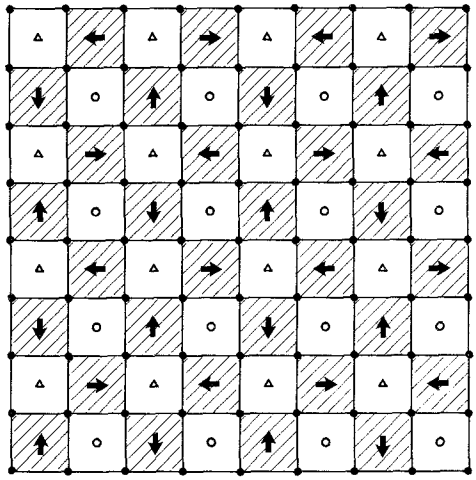

Fig. 3. The τ, μ-lattice, together with the σ-lattice. The τ-spins and the μ-spins are denoted by the open circles and the triangles, respectively.

be performed consistently all over the lattice. Through the transformation, a σ-spin configuration corresponds to a twofold-degenerate τ-spin and μ-spin configuration. Any four-spin interaction of the σ-lattice is transformed to the sum of two kinds of nearest neighbor interactions of the form $K_2\tau_k\tau_1$ and $K_2'\mu_m\mu_n$ and a four-spin interaction of the form $K_4\tau_k\tau_l\mu_m\mu_n$. We thus obtain the first Ising representation for our approximant as follows:

$$[\mathrm{I}] \quad Z^{\mathrm{CCD}}(1)=\frac{1}{2}\sum_{\{\tau\}}\sum_{\{\mu\}} C\exp\left[\sum_b K_2(b)\,\tau_k\tau_l + \sum_{b^*} K_2'(b^*)\,\mu_m\mu_n + \sum_p K_4(p)\,\tau_k\tau_l\mu_m\mu_n\right] \tag{3.2}$$

where $\sum_b$ ($\sum_{b^*}$) denotes the sum over nearest neighbor bonds b (b^*) of the $\tau(\mu)$-lattice, and $\sum_p$ denotes the sum over plaquettes with b and b^* as diagonals. Here the corresponding interactions are given by

$$K_2(b)=K_x(b)+\frac{1}{4}\ln\frac{\cosh K_-(b)\sinh|K_-(b)|}{\cosh K_+(b)\sinh|K_+(b)|} + \frac{\pi i}{4}\left[\theta(-K_-(b))-\theta(-K_+(b))\right]$$

$$K_2'(b^*)=-\frac{1}{4}\ln[\tanh|K_+(b)|\tanh|K_-(b)|] - \frac{\pi i}{4}\left\{\theta(-K_+(b))+\theta(-K_-(b))\right\}$$

$$K_4(b)=\frac{1}{4}\ln\frac{\tanh|K_+(b)|}{\tanh|K_-(b)|}$$

$$-\frac{\pi i}{4}[\theta(-K_+(b))-\theta(-K_-(b))]$$

$$C=\prod_b[\cosh K_+(b)\cosh K_-(b)\sinh K_+(b)\sinh K_-(b)]^{1/4} \quad (3.3)$$

where $\theta(x)=1$ for $x\geqslant 0$ and $\theta(x)=0$ for $x<0$.

Finally we perform the dual transformation[16,17] only for the μ-lattice, which yields the second Ising representation as follows:

$$[\mathrm{II}]\quad Z^{\mathrm{CCD}}(1)=\frac{1}{2}\sum_{\{\tau\}}\sum_{\{\mu^*\}}\exp\left[\sum_b L_2(b)\,\tau_k\tau_l + \sum_b L_2'(b)\,\mu_k^*\mu_l^* + \sum_b L_4(b)\,\tau_k\tau_l\mu_k^*u_l^*\right] \quad (3.4)$$

where the corresponding interaction parameters are given by

$$L_2(b)=K_x(b),\qquad L_2'(b)=K_y(b),\qquad L_4(b)=-K_z(b) \quad (3.5)$$

Consequently, the $n=1$ CCD approximant is expressed as an Ashkin–Teller model[18] in which the strength and sign of the interactions may vary from bond to bond.

4. THERMODYNAMIC PROPERTIES OF THE $n=1$ APPROXIMANT

By making use of the Ising representation [I] or [II], we discuss here the thermal and critical properties of the $n=1$ approximant for the XYZ model defined by Eq. (2.6). We confine ourselves to some interesting cases.

4.1. Uniform XY Case: $J_x(b)=J_x>0$, $J_y(b)=J_y$, and $J_z(b)=0$

We find from (3.4) that

$$K_2=K_x$$

$$K_2'=-\frac{1}{2}\ln(\tanh K_y) \quad (4.1)$$

$$K_4=0$$

This relationship clearly reveals that the present approximant for the XY model is decoupled into two independent 2D Ising models, one with nearest neighbor coupling constant K_x and the other with K_2^* [$= -\frac{1}{2}\ln(\tanh K_y)$] dual to K_y. Therefore we can obtain an exact free energy of this system from that of the ordinary 2D Ising model.[19] Consequently, the logarithmic divergence of the specific heat appears at $K_x = K_c$ and $K_y = K_c$ [$\sinh(2K_c) = 1$], which is in agreement with the result for the isotropic case ($J_x = J_y$) by Lagendijk and De Raedt, who studied the model in the σ^z (out-of-plane) representation.[9] Furthermore, our formulation allows us to find an in-plane (xy plane) behavior of the approximant, namely a two-spin in-plane correlation function defined by

$$G(r) = \mathrm{Tr}[\sigma_0^x \sigma_r^x \exp(-\beta\mathscr{H}_1)\exp(-\beta\mathscr{H}_2) \times \exp(-\beta\mathscr{H}_3)\exp(-\beta\mathscr{H}_4)]/Z^{\mathrm{CCD}}(1) \tag{4.2}$$

It is easy to show, from the decoupling property (4.1), that

$$\begin{aligned} G(r) &= \langle \sigma_0 \sigma_r \rangle_{\sigma\text{-lattice}} \\ &= \langle \tau_0 \mu_0 \tau_r \mu_r \rangle_{\tau,\mu\text{-lattice}} \\ &= g(r; K_x) \cdot g(r; K_y^*) \end{aligned} \tag{4.3}$$

where $g(r; K)$ is the correlation function of two spins separated by a distance r for the ordinary 2D Ising model with coupling constant K. From (4.3) we can deduce the following in-plane critical property. We first consider the isotropic case ($J_x = J_y$). It is well known that $g(r; K)$ approaches m_s^2 (m_s is the spontaneous magnetization) as r goes to infinity when $T < T_c$, while it shows a power decay with a critical exponent 1/4 at $T = T_c$ and an exponential decay when $T > T_c$. This property, with the relation (4.3), leads to the behavior of $G(r)$ as follows:

$$G(r) \xrightarrow[r \gg 1]{} \begin{cases} A \exp(-r/\xi) & \text{when } T \gtrless T_c \\ B r^{-1/2} & \text{when } T = T_c \end{cases} \tag{4.4}$$

where A and B are constant factors and ξ denotes the correlation length. One then find that the present approximant always shows only short-range order (SRO) in in-plane behavior, except for the critical temperature T_c. Therefore, we find that the present approximant exhibits a sort of reentrant phenomenon, and it seems to show a transition without long-range order (LRO). We thus obtain the values of in-plane critical exponents as follows:

$$\eta = \frac{1}{2}\left(\text{not } \frac{1}{4}\right) \qquad \text{and} \qquad \nu = 1 \tag{4.5}$$

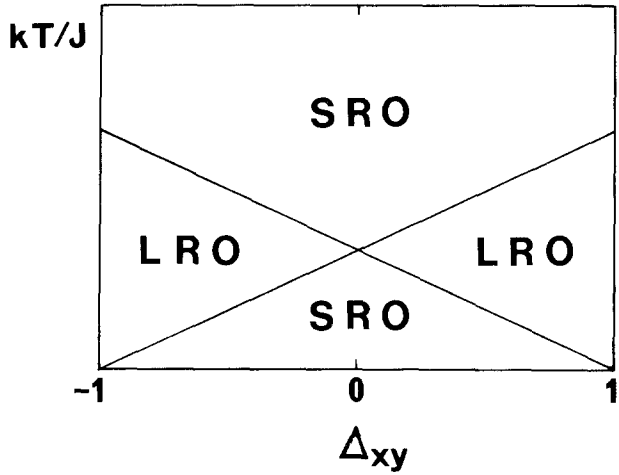

Fig. 4. Phase diagram in the XY case: $J_x = J(1+\Delta_{xy})$, $J_y = J(1-\Delta_{xy})$, where Δ_{xy} denotes the anisotropy parameter of the coupling in the xy plane of the spin space.

where the exponents η and ν are defined by $G(r) \sim r^{-\eta}$ at $T = T_c$ and $\xi \sim |T - T_c|^{-\nu}$ near the critical point. Furthermore, assuming the scaling relation that $\gamma = (2-\eta)\nu$, we also obtain the critical exponent for the in-plane susceptibility

$$\gamma = \frac{3}{2} \tag{4.6}$$

These exponents (4.5) and (4.6) concerning the in-plane behavior are the important new results obtained here. Next, in the anisotropic case ($J_x \neq J_y$), the present approximant shows a typical reentrant-type of transitions SRO → LRO → SRO as the temperature is varied. The individual transition is characterized by the same critical exponents as those of the 2D Ising model. The phase diagram including the isotropic case is shown in Fig. 4. Such a mechanism of reentrant transition in the present case might suggest an idea for quantum reentrant phenomena, e.g., a successive phase transition liquid → solid → liquid.[20],[2]

4.2. Uniform *XXZ* Case: $J_x(b) = J_y(b) = J_{xy}(>0)$ and $J_z(b) = J_z$

We find from (3.5) that

$$L_2 = L_2' = K_{xy} \qquad \text{and} \qquad L_4 = -K_z \tag{4.7}$$

[2] For the mechanism of classical reentrant transition due to frustrated bond structure see Ref. 21.

This Ising representation corresponds to the isotropic AT model. As a result, by using the known phase boundaries of the AT model, we can express the phase boundaries for the present approximant of the *XXZ* case.[12,15,22] This is shown in Fig. 5a. In this figure, the solid line denotes an exact phase boundary or critical line

$$K_z = \frac{1}{2} \ln[\sinh(2K_{xy})] \qquad K_{xy} > -K_z \tag{4.8}$$

(see Appendix A), while those shown by dashed lines are not known exactly, except for some special points, which are critical points of the 2D Ising model. The critical exponents are also known to vary continuously on the exact line.[23] Hence it is of interest to explore concretely how the in-plane correlation exponent η varies along the critical line in the present case. With this motivation we have performed a Monte Carlo simulation. Our numerical results are shown in Fig. 5b. Our data show that the so-called weak universality[24] is broken along the critical line (4.8) for the $n=1$ approximant of the *XXZ* case. For our Monte Carlo simulation, see Appendix B.

4.3. Frustrated Case

First we consider the *XY* case: $K_z(b)=0$ for any bond, and $\{K_x(b), K_y(b)\}$ are set as in Fig. 6. This is a quantum Villain *XY* model. According to the corresponding Ising representation [II], the approximant of this case is decoupled into two independent 2D Ising models with the coupling constants $\{L_2 = K_x(b)\}$ and $\{L_2'(b) = K_y(b)\}$. It thus follows that our problem is reduced to that for frustrated Ising systems. As a result we find that no phase transition occurs for the $n=1$ approximant of the quantum Villain *XY* model.

More attention shall be directed to the frustrated *XXZ* (including isotropic Heisenberg) cases. From the Ising representation [II], the approximant is characterized not only by frustrated two-spin interactions $\{L_2(b) = K_x(b)\}$ and $\{L_2'(b) = K_x(b)\}$, but also by the four-spin interactions $\{L_4(p) = K_z(b)\}$, which take positive or negative coupling at each plaquette. Although the effect of the latter interactions is interesting to study, this class of AT models has not been solved yet. This should be investigated exactly or at least numerically in the future. It should be noted here that one of the great merits of our AT representation consists in the fact that Monte Carlo calculations can be performed without facing to "negative sign problem," the key point of which will be mentioned in the next section. The Monte Carlo simulation along this line is now in progress.

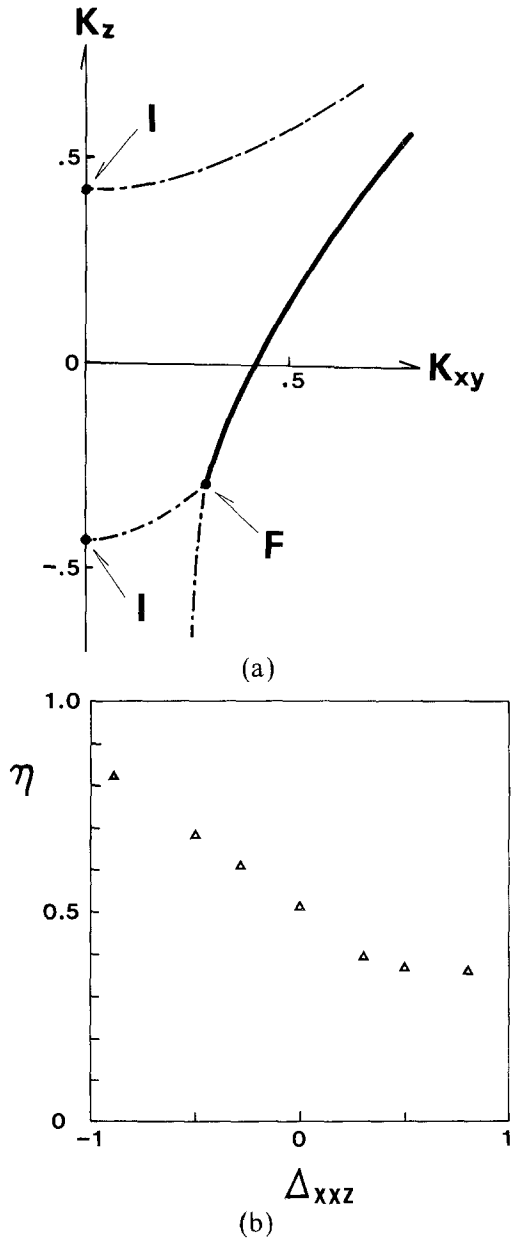

Fig. 5. (a) Phase boundaries in the XXZ case. The bold line denotes the exact critical line, and the broken lines denote other phase boundaries. Here I indicates the Ising critical point, and F the critical point of the F-model. (b) Critical exponent η versus anisotropy, $\Delta_{xxz} \equiv J_z/J_{xy}$.

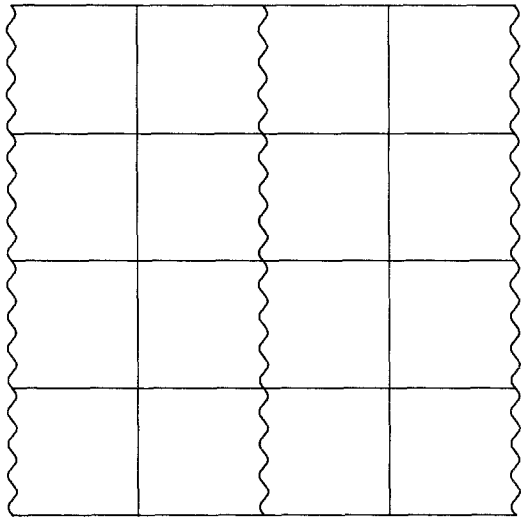

Fig. 6. Bond structure of a quantum Villain XY model. The straight line denotes a ferromagnetic bond with $J_x = J_y = J > 0$, while the wavy line denotes an antiferromagnetic bond with $J_x = J_y = -J < 0$.

5. SUMMARY, DISCUSSION, AND FUTURE PROBLEMS

We have shown that the two-dimensional spin-1/2 XYZ models can be mapped onto Ashkin–Teller models for the $n = 1$ approximant with the checkercube decomposition. Within the present approximant $Z(1)$, in particular, for the case corresponding to the XY model, we have studied the in-plane reentrant behavior and obtained some in-plane critical exponents, in addition to the result on the out-of-plane property given by Lagendijk and De Raedt. For the case corresponding to the XXZ model we have shown the phase boundaries, including an exact critical line on which the weak universality is broken. In the frustrated cases it also has been shown that the fully frustrated quantum XY model can be exactly solved within the $n = 1$ approximant, by transforming them into frustrated 2D Ising models.

Let us discuss the nature of the phase transition of the original quantum XY model, which should be of final interest. The high-temperature expansion method (HTEM) strongly suggests the existence of a phase transition at a finite temperature.[25] If we extend the concept of universality between "classical" and "quantal" systems, we would expect the occurrence of the Kosterlitz–Thouless transition,[26,27] associated with the dissociation of vortices, even for the quantum XY systems. The HTEM

result, however, does not seem to support the KT transition strongly. Although Monte Carlo simulations have been performed by several groups,[3,7,8] they have found no clear answer to questions concerning the values of critical exponents for the quantum XY model. In Table II we show critical exponents obtained so far, along with our results as a reference. To obtain more conclusive data, we should study systems with $n \geqslant 2$, for which only the Monte Carlo method is available at the present stage.

Monte Carlo simulations for the higher ($n \geqslant 2$) approximant in our checkercube decomposition scheme are now in progress.[32] It should be remarked that the following convergence property for the general nth approximant

$$|Z - Z(n)| = O(1/n^2) \tag{5.1}$$

was proved very recently in general.[6,28] The size dependence of physical quantities such as the specific heat should be investigated after each $1/n^2$ plot. Thus we can investigate the properties of a singularity quantitatively.

Next we give some considerations on the frustrated cases. Generally we meet with a difficulty, namely, the negative sign problem[10] in studying frustrated quantum spin systems by applying Monte Carlo methods following the equivalence theorem given by Suzuki. This problem comes from the negative Boltzmann factors of the classical approximant. The existence of negative Boltzmann factors causes the seriously poor precision of the measured quantities at low temperatures[30] because pathological cancellation occurs between positive and negative contributions to the par-

Table II. Values of Critical Exponents Investigated for Quantum *XY* Model

Exponent	HTEM[a]	$n=1$ (exact)[b]	MC[c,d]	Classical[e]
			$\leqslant 0$[c]	
a	<0	0	<0[d]	$-\infty$
ν	1.43 ± 0.10	1	—	∞
γ	2.50 ± 0.3	3/2	—	∞
η	$0 \leqslant \eta \leqslant 0.7$	1/2	—	1/4

[a] Ref. 25.
[b] The present result, in addition to Ref. 9.
[c] Ref. 7.
[d] Ref. 8.
[e] Ref. 26.

tition sum. Keeping this in mind, let us consider again carefully our approximate mapping. The negative sign problem surely occurs for the σ-lattice representation of the $n=1$ approximant. However the finally mapped Ising representation [II] or AT representation (3.5) with variables (τ, μ^*) has only positive weights, and therefore the $n=1$ approximant is fortunately free of the negative sign problem. This fact shows a hopeful route to overcome the problem. Our next work will be to construct a mapped representation only with positive weights for higher approximants $(n \geqslant 2)$. It also should be noted that the mapping $\sigma \to (\tau, \mu)$ in Section 3 eliminates the redundant configurations, so that the problem of ergodicity in the Monte Carlo simulation is removed. Consequently, Monte Carlo simulations can be performed very efficiently by adopting an appropriate mapping. The present paper is the first version of such a construction. Further development along this line is expected to investigate various thermodynamic problems of frustrated quantum systems, e.g., the Anderson problem in the quantum Heisenberg antiferromagnet on the triangular lattice.[29–31]

APPENDIX A

In this appendix we briefly show that Eq. (4.8) gives an exact critical line for the $n=1$ approximant in the uniform XXZ case, by utilizing the same technique as for the AT model. Some details of the explanation have been given previously.[12]

Starting with the σ-lattice, we can map it onto a staggered eight-vertex model on a square lattice in the same way as shown by Lagendijk and De Raedt.[9] Denoting the vertex weights by $\{\omega_1, \omega_2, ..., \omega_8\}$ on one sublattice and $\{\omega_1', \omega_2', ..., \omega_8'\}$ on the other sublattice, we have

$$\begin{aligned} &\omega_1 = \omega_2 = \omega_1' = \omega_2' = a \\ &\omega_3 = \omega_4 = \omega_3' = \omega_4' = b \\ &\omega_5 = \omega_6 = \omega_7' = \omega_8' = c \\ &\omega_7 = \omega_8 = \omega_5' = \omega_6' = d \end{aligned} \tag{A.1}$$

where a, b, c, and d are equal to those given in Table I. Just on the line defined by (4.8), it follows that $c=d$ in (A.1), and consequently our approximant is reduced to the symmetric eight-vertex model or Baxter model. Then we have the following w weights

$$\begin{aligned} w_1 &\equiv (a+b)/2 \\ w_2 &\equiv (a-b)/2 \\ w_3 &\equiv (c+d)/2 \\ w_4 &\equiv (c-d)/2 = 0 \end{aligned} \tag{A.2}$$

By interchanging w_2 and w_4, which does not change the partition function $Z[w_1, w_2, w_3, w_4]$,[15] we define new vertex weights by $\tilde{a} = w_1 + w_4$, $\tilde{b} = w_1 - w_4$, $\tilde{c} = w_3 + w_2$, and $\tilde{d} = w_3 - w_2$. Concretely we have that $\tilde{a} = \tilde{b}$, $\tilde{d} = 0$. Thus our approximant is furthermore reduced to the F-model. As is well known, the F-model has two phases: one is an ordered phase when $\tilde{a}/\tilde{b} = \tilde{b}/\tilde{c} < 1/2$, and the other is a "disordered" phase for $\tilde{a}/\tilde{c} = \tilde{b}/\tilde{c} > 1/2$, where the correlation length is infinite. The latter phase is always critical in the ordinary sense. Therefore it is concluded that the approximant is critical on (4.8) for $K_{xy} \geqslant (\ln 3)/4$.

Finally, we remark that the $\sigma^x\sigma^x$ correlation for the approximant in the general case, which becomes equivalent to the $\sigma\sigma$ correlation on the σ-lattice, is reduced to an arrow–arrow correlation on the corresponding vertex lattice.

APPENDIX B

A kind of finite size scaling has been used to calculate values of the in-plane critical exponent η on the exact critical line (4.8) by the standard Monte Carlo method. It is, in general, stated that the thermal average of the squared magnetization for two-dimensional systems has a size dependence of the form[27]

$$\ln(\langle M^2 \rangle / N) \cong (2-\eta) \ln L + \text{const} \tag{B.1}$$

on the critical point, for large linear dimension L ($N = L^2$). Here, for the present system, M implies the in-plane magnetization of the $n = 1$ approximant.

In order to investigate how η varies on the critical line, we first chose seven critical points on the critical line with $J_Z/J_{xy} = -0.9$, -0.5, -0.3, 0.0, 0.3, 0.5, 0.8. At each critical point we carried out simulations according to the Metropolis rule for the τ, μ-lattice whose size is $2 \times (L \times L)$ with $L = 6$, 8, 12, 16 (note that L denotes the linear size of the original quantum system). In each run, the first 5000 MCS were discarded to make the system reach equilibrium, and the next 50,000 MCS were used to obtain thermal properties. Finally, the value of η was determined at each of the critical points by log–log plot of $\langle M^2 \rangle / N$ versus L.

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