

## Relationship between $d$ -Dimensional Quantal Spin Systems and $(d+1)$ -Dimensional Ising Systems

—*Equivalence, Critical Exponents and Systematic Approximants of the Partition Function and Spin Correlations*—

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The partition function of a quantal spin system is expressed by that of the Ising model, on the basis of the generalized Trotter formula. Thereby the ground state of the  $d$ -dimensional Ising model with a transverse field is proven to be equivalent to the  $(d+1)$ -dimensional Ising model at finite temperatures. A general relationship is established between the two partition functions of a general quantal spin system and the corresponding Ising model with many-spin interactions, which yields some rigorous results on quantum systems. Some applications are given.

### § 1. Introduction

Critical phenomena in classical systems (whose Hamiltonians are described by scalar variables such as Ising spins) have been studied by many people since Onsager found the exact solution of the two-dimensional Ising model. It seems, however, very difficult to investigate critical phenomena in quantum systems such as the Heisenberg model. Although there are many perturbational calculations based on high temperature expansions,<sup>1)</sup> no rigorously soluble model of quantum systems which show a phase transition at finite temperatures has been found except for extremely long-range interaction models.<sup>2), 3)</sup>

Recently, Elliott, Pfeuty and Wood<sup>4)</sup> found numerically the equivalence of the ground state singularities of the  $d$ -dimensional Ising model with a transverse field<sup>5), 6)</sup> (which is the simplest quantal model) to the singularities of the  $(d+1)$ -dimensional Ising model. Quite recently Yanase, Takeshige and Suzuki<sup>7)</sup> have also confirmed numerically the above equivalence conjecture by calculating a power series expansion of the susceptibility up to a few more terms.

On the other hand, the present author<sup>8)</sup> proved rigorously the equivalence of the two-dimensional Ising model to the ground state of the linear XY-model, which is described by the following Hamiltonians:

$$\mathcal{H}_I = -J_1 \sum_{n=1}^N \sum_{m=1}^M \sigma_{n,m}^z \sigma_{n+1,m}^z - J_2 \sum \sigma_{n,m}^z \sigma_{n,m+1}^z \quad (1 \cdot 1)$$

and

$$\mathcal{H}_{XY} = - \sum_{j=1}^M (J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y - \mu H \sigma_j^z), \quad (1.2)$$

respectively, where  $\{\sigma_r^x, \sigma_r^y, \sigma_r^z\}$  are Pauli operators associated with a lattice point  $\mathbf{r}$ . The equivalence of the above two models holds<sup>8)</sup> under the relations that

$$J_y/J_x = \exp(-4K_1) \quad \text{and} \quad \mu H/J_x = 2 \exp(-2K_1) \coth(2K_2) \quad (1.3)$$

with  $K_j = J_j/kT$ . This equivalence was proven<sup>8)</sup> by showing that  $\mathcal{H}_{XY}$  commutes with the transfer matrix of  $\mathcal{H}_I$  under the relations (1.3). This leads to the following correspondences<sup>8)</sup> of the singularities for the two systems:

$$\begin{array}{ll} \text{Ising model } (d=2) & XY\text{-model } (d=2, T=0) \\ \left\{ \begin{array}{l} M_s \propto (T_c - T)^{1/8} \\ C_v \propto \log|T - T_c| \\ \chi_0 \propto (T - T_c)^{-7/4} \end{array} \right. & \iff \left\{ \begin{array}{l} M_s^{XY} \propto (H_c - H)^{1/8}, \\ \chi_{\parallel}^{XY} \propto \log|H - H_c|, \\ \chi_{\perp}^{XY} \propto (H - H_c)^{-7/4}. \end{array} \right. \end{array} \quad (1.4)$$

Here  $M_s^{XY}$  has already been calculated explicitly by Barouch and McCoy.<sup>9)</sup> In the above equivalence, the magnetic field  $H$  of the  $XY$ -model plays the role of the temperature in the Ising model. Recently Ferrell<sup>10)</sup> has also discussed asymptotically the equivalence of  $\mathcal{H}_I$  and the one-dimensional Dirac particle.

One of our purposes in the present paper is to investigate generally the relationship between  $d$ -dimensional quantal spin systems and the  $(d+1)$ -dimensional Ising model and particularly to prove the equivalence of the ground state of the  $d$ -dimensional Ising model with a transverse field to the  $(d+1)$ -dimensional Ising model, which was conjectured by Elliott et al.<sup>4)</sup> and by Yanase et al.<sup>7)</sup> The Ising model with a transverse field is described by the Hamiltonian

$$\mathcal{H}_{(Q)}^{(d)} = - \sum_{i,j \in R^d} J_{ij} \sigma_i^z \sigma_j^z - \mu H \sum_j \sigma_j^z - \Gamma \sum_j \sigma_j^x, \quad (1.5)$$

where  $R^d$  denotes a lattice space in  $d$  dimensions.

In § 2, main results are stated as theorems, whose proofs are given in the succeeding sections. In § 3, the generalized Trotter formula is reviewed, which is our keystone to prove the theorems in § 2. A proof is given in § 4 for the equivalence of the ground state of the  $d$ -dimensional Ising model with a transverse field, (1.5), to the  $(d+1)$ -dimensional Ising model by the help of the generalized Trotter formula. A general formulation is presented in § 5, concerning Trotter's representation for the partition function of some quantal spin systems. Some examples are shown in § 6. A crossover effect is discussed in § 7 for the critical exponent of (1.5).

## § 2. Statements and discussion

In this section we summarize our main results. We first state Theorems 1 and 2, which lead to Theorem 3 as a direct consequence of Theorem 1 and the

renormalization group theory.<sup>11)</sup> We then present Theorems 4, 5 and 6 on the relationship between the partition functions and spin-correlations of  $d$ -dimensional quantal spin systems and those of the  $(d+1)$ -dimensional Ising model. Theorems 7 and 8 are derived from Theorem 4.

**Theorem 1:** *The ground state of the  $d$ -dimensional quantal system described by (1.5) is equivalent to the  $(d+1)$ -dimensional Ising model. Consequently we have*

$$\alpha^{(Q)}(d) = \alpha^{(I)}(d+1), \quad \beta^{(Q)}(d) = \beta^{(I)}(d+1), \quad \gamma^{(Q)}(d) = \gamma^{(I)}(d+1), \quad \text{etc.}, \quad (2.1)$$

where  $\alpha^{(Q)}(d)$ ,  $\beta^{(Q)}(d)$  and  $\gamma^{(Q)}(d)$  denote the critical exponents of energy derivative spontaneous magnetization and susceptibility of (1.5) in  $d$  dimensions, respectively, and  $\{\alpha^{(I)}(d)\}$  denote those of the Ising model.

This yields a proof of the conjecture by Elliott et al.<sup>4),7)</sup> This theorem is easily extended to the following more general case.

**Theorem 2:** *The ground state of a  $d$ -dimensional quantal spin system is equivalent to a certain  $(d+1)$ -dimensional Ising model with many-body interactions.*

It should be noted that if the interaction of the relevant quantal spin system is of finite-range, then the corresponding Ising model is expressed by finite-range interactions, as will be shown in §§ 4 and 5.

Theorem 1 leads to the following result if we accept the renormalization group theory<sup>11)</sup> and the equivalence<sup>11)</sup> between the  $\phi^4$ -theory and Ising model.

**Theorem 3:** *The critical exponents of the ground state of (1.5) in dimensions higher than three ( $d > 3$ ) assume classical values, namely we have*

$$M_s \propto (\Gamma_c - \Gamma)^{1/2}, \quad \chi_{\perp} \propto (\Gamma - \Gamma_c)^{-1}, \quad \text{etc.}, \quad (2.2)$$

for  $d > 3$  at the zero temperature.

For finite temperatures, the following relationship exists:

**Theorem 4:** *The partition function of the  $d$ -dimensional quantal spin system (1.5),  $Z_Q^{(d)}(\{K_{ij}\}, h, \gamma)$ , is expressed by*

$$Z_Q^{(d)} = \lim_{n \rightarrow \infty} \left( \frac{1}{2} \sinh \frac{2\gamma}{n} \right)^{Nn/2} Z_I^{(d+1)} \left( \left\{ \frac{1}{n} K_{ij} \right\}, \frac{1}{2} \log \coth \frac{\gamma}{n}, \frac{h}{n} \right), \quad (2.3)$$

where  $K_{ij} = \beta J_{ij}$ ,  $h = \beta \mu H$  and  $\gamma = \beta \Gamma$ ,  $N$  denotes the number of the original lattice points and  $Z_I^{(d+1)}$  is the partition function of the  $(d+1)$ -dimensional Ising model with the interaction  $J_{ij}/n$  in the  $d$ -dimensional hyper plane and with the nearest-neighbour interaction  $(1/2) \log(\coth \gamma/n)$  in the  $(d+1)$ -th direction of the lattice thickness  $n$ . More explicitly we have

$$Z_Q^{(d)} = \lim_{n \rightarrow \infty} \sum_{\{\sigma_{i,k} = \pm 1\}} \exp \left\{ \sum_{i,j \in R^d} \sum_{k=1}^n \frac{1}{n} K_{ij} \sigma_{i,k} \sigma_{j,k} \right\}$$

$$+ \sum_i \sum_{k=1}^n \left[ -\frac{1}{2} \left( \log \frac{n}{\gamma} \right) (1 - \sigma_{i,k} \sigma_{i,k+1}) + \frac{h}{n} \sigma_{i,k} \right]. \quad (2.4)$$

It should be remarked here that this theorem does not necessarily insist that the critical behavior of (1.5) at finite temperatures be the same as that of the  $(d+1)$ -dimensional Ising model, because a part of interaction vanishes and the other part diverges as the lattice thickness  $n$  goes to infinity. Furthermore, the above series (2.3) with respect to  $n$  converges uniformly and the critical behavior of the system for all finite  $n$  and for a finite  $\gamma (T > 0)$  shows the  $d$ -dimensional character according to the universality<sup>(12)~(14)</sup> of critical exponents. Thus, we may assert the following statement:

**Proposition:** *The critical behavior of (1.5) in  $d$  dimensions at finite temperatures may be the same as that of the  $d$ -dimensional Ising model.*

This yields a plausible explanation of the numerical results obtained by Yanase et al.<sup>7)</sup> at finite temperatures.

Theorem 4 is easily extended to the following more general case:

**Theorem 5:** *The partition function of a  $d$ -dimensional quantal spin system is expressed by that of a certain appropriate  $(d+1)$ -dimensional Ising model with many-spin interactions. If the interaction of the relevant quantal spin system is of finite-range, then the corresponding Ising model is described by finite-range interaction.*

The last half part of this theorem is very useful in applying the Monte Carlo method to quantal spin systems on the basis of Theorem 5, as will be discussed later again. How to find the corresponding Ising model of finite-range interactions will be explained in detail in § 5.

Spin correlations  $\{\langle \sigma_A^z \sigma_B^z \rangle\}$  are also calculated from the corresponding Ising model as shown in the following theorem:

**Theorem 6:** *Spin correlations  $\{\langle \sigma_A^z \sigma_B^z \rangle\}$  are calculated as those of the corresponding  $(d+1)$ -dimensional Ising model, by newly re-interpreting  $\sigma_A^z \sigma_B^z$  as an spin operator located in a  $d$ -dimensional hyper-plane in  $(d+1)$  dimensions:*

$$\langle \sigma_A^z \sigma_B^z \rangle = Z_{d+1}^{-1} \lim_{n \rightarrow \infty} \sum_{\{\sigma_j = \pm 1\}} \{ \sigma_A \sigma_B \exp \mathcal{H}_{\text{eff}}^{(d+1)}(\{\sigma_j\}) \}, \quad (2.5)$$

where  $\mathcal{H}_{\text{eff}}^{(d+1)}(\{\sigma_j\})$  is the effective Hamiltonian of the corresponding  $(d+1)$ -dimensional Ising model and  $Z_{d+1}$  denotes the partition function of it.

Theorem 4 together with the Lee-Yang theorem<sup>(15)~(18)</sup> on the ordinary Ising model leads to the following result:

**Theorem 7 (Circle theorem):** *All the zeros of the partition function of (1.5) for ferromagnetic interactions ( $J_{ij} \geq 0$ ) and for  $T > 0$  lie on the imaginary axis of the complex magnetic field  $H$ .*

This theorem is a special anisotropic limit of the more general case proven by Suzuki and Fisher,<sup>(19)</sup> but the present proof of Theorem 5 is slightly different

from the previous one, as was mentioned above. This theorem yields the analyticity of the limiting free energy of (1.5) with ferromagnetic interactions for all (real) nonzero magnetic field  $H$ . Therefore, a phase transition occurs only at  $H=0$  in such a system, if possible.

For the quantal spin system (1.5), we obtain the following result with the compact notations:

$$\sigma_A^z = \prod_{j \in A} \sigma_j^z \quad \text{and} \quad \sigma_A^x = \prod_{j \in A} \sigma_j^x. \quad (2.6)$$

**Theorem 8 (correlation inequalities):** *If  $J_{ij} \geq 0$ ,  $H \geq 0$  and  $\Gamma \geq 0$ , then we have*

$$\begin{aligned} \langle \sigma_A^z \rangle &\geq 0, \quad \langle \sigma_A^z \sigma_B^z \rangle \geq \langle \sigma_A^z \rangle \langle \sigma_B^z \rangle, \\ \frac{\partial \langle \sigma_A^z \rangle}{\partial J_{ij}} &\geq 0 \quad \text{and} \quad \frac{\partial \langle \sigma_A^z \rangle}{\partial \Gamma} \leq 0. \end{aligned} \quad (2.7)$$

This has already been proven in a previous paper<sup>20)</sup> for more general situations. The case  $H=0$  of (1.5) was proven by Gallavotti.<sup>21)</sup> It should be, however, instructive to remark that Theorem 8 is derived immediately from Theorem 4 and Griffiths inequalities<sup>22)</sup> on the ordinary Ising model. As discussed in Ref. 20), the above inequalities are useful in proving nonexistence of long-range order in (1.5) for all nonzero temperatures in one dimension under the condition

$$\lim_{N \rightarrow \infty} \{\log(\log N)\}^{-1} \sum_{n=1}^N n J_{i, i+n} = 0, \quad (2.8)$$

by the help of Dyson's results on the Ising model.

### § 3. The generalized Trotter formula

It is convenient to summarize here the generalized Trotter formula.<sup>24), 16), 19), 25)</sup> Namely, for bounded operators  $\{A_j\}$ , we have

$$\exp\left(\sum_{j=1}^p A_j\right) = \lim_{n \rightarrow \infty} f_n(\{A_j\}), \quad (3.1)$$

where the  $n$ -th approximant<sup>25)</sup>  $f_n(\{A_j\})$  is defined by

$$f_n(\{A_j\}) = \left[ \exp\left(\frac{1}{n} A_1\right) \exp\left(\frac{1}{n} A_2\right) \cdots \exp\left(\frac{1}{n} A_p\right) \right]^n. \quad (3.2)$$

Matrix elements of  $\exp(\sum_{j=1}^p A_j)$  are expressed in terms of a certain representation as follows:

$$\begin{aligned} \langle \alpha | \exp\left(\sum A_j\right) | \alpha' \rangle &= \lim_{n \rightarrow \infty} \sum_{\{\alpha_{ij}\}} \langle \alpha | Q_1 | \alpha_{11} \rangle \langle \alpha_{11} | Q_2 | \alpha_{12} \rangle \times \cdots \\ &\times \langle \alpha_{1, p-1} | Q_p | \alpha_{1, p} \rangle \langle \alpha_{1, p} | Q_1 | \alpha_{21} \rangle \langle \alpha_{21} | Q_2 | \alpha_{22} \rangle \times \cdots \\ &\times \langle \alpha_{n-1, p-1} | Q_p | \alpha_{n-1, p} \rangle \langle \alpha_{n-1, p} | Q_1 | \alpha_{n, 1} \rangle \cdots \langle \alpha_{n, p-1} | Q_p | \alpha' \rangle, \end{aligned} \quad (3.3)$$

where  $Q_j \equiv \exp((1/n)A_j)$ . We may call (3.3) *Trotter's representation* of the exponential operator (3.1). This representation is particularly useful when the partial exponential matrix elements  $\{\langle \alpha_{ik} | Q_j | \alpha'_{ik} \rangle\}$  can be evaluated explicitly, as shown in the succeeding sections.

The above Trotter formula is easily extended to the following bounded exponential *hyper-operators*<sup>25)</sup>  $\{\mathcal{F}_j\}$ :

$$\exp\left(\sum_{j=1}^p \mathcal{F}_j\right) = \lim_{n \rightarrow \infty} \left[ \exp\left(\frac{1}{n} \mathcal{F}_1\right) \exp\left(\frac{1}{n} \mathcal{F}_2\right) \cdots \exp\left(\frac{1}{n} \mathcal{F}_p\right) \right]^n. \quad (3.4)$$

In particular, for  $\mathcal{H}^\times$  with Kubo's notation<sup>26)</sup> we have

$$\exp(\mathcal{H}_1^\times + \mathcal{H}_2^\times) = \lim_{n \rightarrow \infty} \left[ \exp\left(\frac{1}{n} \mathcal{H}_1^\times\right) \exp\left(\frac{1}{n} \mathcal{H}_2^\times\right) \right]^n, \quad (3.5)$$

where  $\mathcal{H}_j^\times A = [\mathcal{H}_j, A] = \mathcal{H}_j A - A \mathcal{H}_j$ , as was proven by the present author,<sup>25)</sup> with the use of a *hyper-operator norm*.

It should also be remarked that Trotter's representation (3.3) above is quite analogous to a path integral in statistical mechanics.

#### § 4. Proof of Theorems 1, 2 and 3 (equivalence)

First we prove Theorem 1. The ground state energy  $E_g$  of (1.5) is expressed by

$$E_g = \lim_{T \rightarrow 0} [-kT \log \text{Tr} \exp(-\mathcal{H}_{(Q)}^{(d)}/kT)]. \quad (4.1)$$

It is convenient to introduce here a dimensionless parameter  $n$  defined by

$$n = \Gamma/kT. \quad (4.2)$$

In taking the limit  $T \rightarrow 0$ , we consider a subset  $T = T_n = \Gamma/(kn)$ , where  $n$  is an integer. Thus, we have

$$\begin{aligned} E_g &= -\Gamma \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp \left[ n \left\{ \sum \left( \frac{J_{ij}}{\Gamma} \right) \sigma_i^z \sigma_j^z + \sum \left( \frac{\mu H}{\Gamma} \right) \sigma_j^z + \sum \sigma_j^x \right\} \right] \\ &= -\Gamma \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \left[ \exp \left\{ \sum \left( \frac{J_{ij}}{\Gamma} \right) \sigma_i^z \sigma_j^z + \sum \left( \frac{\mu H}{\Gamma} \right) \sigma_j^z + \sum \sigma_j^x \right\} \right]^n \\ &= -\Gamma \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \frac{1}{n} \log \left[ \left( \frac{1}{2} \sinh \frac{2}{m} \right)^{Nmn/2} \sum_{\{\sigma_{ij} = \pm 1\}} \exp \mathcal{H}_{\text{eff}}^{(n, m)} \right] \end{aligned} \quad (4.3)$$

and

$$\begin{aligned} \mathcal{H}_{\text{eff}}^{(n, m)} &= \frac{1}{m\Gamma} \sum_{i, j \in \mathbb{R}^d} \sum_{k=1}^{mn} J_{ij} \sigma_{i, k} \sigma_{j, k} + \frac{1}{2} \left( \log \coth \frac{1}{m} \right) \sum_{i \in \mathbb{R}^d} \sum_{k=1}^{mn} \sigma_{i, k} \sigma_{i, k+1} \\ &\quad + \frac{\mu H}{m\Gamma} \sum_{i \in \mathbb{R}^d} \sum_{k=1}^{mn} \sigma_{i, k}, \end{aligned} \quad (4.4)$$

where we have used Trotter's formula (3.2) and the following simple relation:

$$\langle \sigma | e^{\tau \sigma^z} | \sigma' \rangle = \left( \frac{1}{2} \sinh 2\tau \right)^{1/2} \exp \left( \frac{1}{2} \sigma \sigma' \log \coth \tau \right) \quad (4.5)$$

with  $\sigma = \pm 1$ ,  $\sigma' = \pm 1$  and  $\sigma_{i,k} = \pm 1$ . Thus, the ground state energy of (1.5) in  $d$  dimensions is expressed by the partition function of the effective  $(d+1)$ -dimensional Ising model  $\mathcal{H}_{\text{eff}}^{(\infty, m)}$ , in which  $\Gamma$  plays the role of temperature. Therefore, if  $\Gamma > \Gamma_c$  (critical point), the system is paramagnetic and if  $\Gamma < \Gamma_c$ , the system becomes ferromagnetic in the  $z$ -direction. This correspondence is valid for all finite values of  $m$ . It should be remarked that the limit  $n \rightarrow \infty$  can be taken for  $m$  fixed. Furthermore, spin correlations  $\{\langle \sigma_1^z \sigma_2^z \cdots \sigma_p^z \rangle_Q\}$  in the ground state of (1.5) are expressed by those of the corresponding  $(d+1)$ -dimensional Ising model as follows:

$$\langle \sigma_1^z \sigma_2^z \cdots \sigma_p^z \rangle_{Q, T=0} = \langle \sigma_1 \sigma_2 \cdots \sigma_p \rangle_I, \quad (4.6)$$

where the right-hand side of (4.6) is a spin correlation on a  $d$ -dimensional hyper-plane vertical to the “ $n$ -direction”. Thus we obtain Theorem 1.

The above procedure is easily extended to a more general quantal spin system which is described by the Hamiltonian  $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ ,  $\mathcal{H}_0$  being diagonal. The ground state energy  $E_g$  of such a system is expressed by

$$\begin{aligned} E_g &= \lim_{T \rightarrow 0} [-kT \log \text{Tr} \exp(-\mathcal{H}/kT)] \\ &= -\Gamma \lim_{n \rightarrow \infty} \left\{ -\frac{1}{n} \log \text{Tr} \left[ \exp \left( -\frac{\mathcal{H}_0}{\Gamma} - \frac{\mathcal{H}_1}{\Gamma} \right) \right]^n \right\}, \end{aligned} \quad (4.7)$$

where  $\Gamma$  is a typical strength of off-diagonal interactions. Using Trotter's formula (3.2), we obtain

$$E_g = -\Gamma \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \left\{ \frac{1}{n} \log \sum_{\{\alpha\}} \exp(\mathcal{H}_{\text{eff}}^{(n, m)}) \right\}, \quad (4.8)$$

where

$$-\mathcal{H}_{\text{eff}}^{(n, m)} = \frac{1}{m\Gamma} \sum_{j=1}^{mn} \mathcal{H}_0(\alpha_j) + \sum_{j=1}^{mn} \hat{\mathcal{H}}_1(\alpha_j, \alpha_{j+1}) \quad (4.9)$$

and

$$\hat{\mathcal{H}}_1(\alpha, \alpha') = \log \langle \alpha | \exp \left( -\frac{1}{m\Gamma} \mathcal{H}_1 \right) | \alpha' \rangle. \quad (4.10)$$

Here  $\alpha_j$  denotes a state in a  $d$ -dimensional hyper-plane, and it diagonalizes  $\mathcal{H}_0$ . Thus, (4.7) denotes the Ising model on the  $(d+1)$ -dimensional lattice. The equivalence of all spin correlations is also proven as before. This yields Theorem 2.

An alternative formulation is given by applying the generalized Trotter formula (3.2) to the Hamiltonian  $\mathcal{H} = \sum \mathcal{H}(j)$ , where  $\mathcal{H}(j)$  denotes a local interaction such as nearest-neighbour interactions, as follows:

$$E_g = -\lim_{T \rightarrow 0} kT \log \text{Tr} e^{-\mathcal{H}/kT} = -T \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \frac{1}{n} \log \text{Tr} \left[ \prod_j \exp \left( -\frac{\mathcal{H}(j)}{mT} \right) \right]^{mn}. \quad (4.11)$$

For more details, see the next section.

Theorem 3 is almost evident from Theorem 1 and the renormalization group theory.<sup>11)</sup>

## § 5. General formulations for partition functions of quantal spin systems

### —Proof of Theorems 4, 5 and 6—

As has been seen in §§ 3 and 4, it is very useful to transform quantal spin systems into classical (or Ising) representations. In this section we formulate partition functions and spin correlations of quantal spin systems in terms of Ising spins, on the basis of the generalized Trotter formula (3.2). Such transformations make it possible to find rigorous results of quantal systems with the use of properties already known on the Ising model.

#### (i) The first formulation

We start with the following Hamiltonian composed of two parts:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1; \quad \mathcal{H}_0|\alpha\rangle = \mathcal{H}_0(\alpha)|\alpha\rangle. \quad (5.1)$$

In terms of the representation  $|\alpha\rangle$  diagonalizing  $\mathcal{H}_0$ , the partition function is expressed as

$$\begin{aligned} Z &= \text{Tr} e^{-\beta\mathcal{H}} = \lim_{n \rightarrow \infty} \text{Tr} \left[ \exp \left( -\frac{1}{n} \beta \mathcal{H}_0 \right) \exp \left( -\frac{1}{n} \beta \mathcal{H}_1 \right) \right]^n \\ &= \lim_{n \rightarrow \infty} \sum_{\{\alpha_j\}} \exp [\hat{\mathcal{H}}_0(\alpha_1) + \hat{\mathcal{H}}_1(\alpha_1, \alpha_2) + \cdots + \hat{\mathcal{H}}_0(\alpha_n) + \hat{\mathcal{H}}_1(\alpha_n, \alpha_1)] \\ &\equiv \sum_{\{\alpha_j\}} \exp \mathcal{H}_{\text{eff}}, \end{aligned} \quad (5.2)$$

where we have used Trotter's formula (3.2) and

$$\mathcal{H}_{\text{eff}} = \lim_{n \rightarrow \infty} \sum_{j=1}^n \{ \hat{\mathcal{H}}_0(\alpha_j) + \hat{\mathcal{H}}_1(\alpha_j, \alpha_{j+1}) \} \quad (5.3)$$

with

$$\hat{\mathcal{H}}_0(\alpha) = -\frac{1}{n} \beta \mathcal{H}_0(\alpha) \quad \text{and} \quad \hat{\mathcal{H}}_1(\alpha, \alpha') = \log \langle \alpha | \exp \left( -\frac{1}{n} \beta \mathcal{H}_1 \right) | \alpha' \rangle. \quad (5.4)$$

This formulation is particularly useful for the case that  $\mathcal{H}_1$  is a sum of commutable local operators:

$$\mathcal{H}_1 = \sum_{\mathbf{r}} \mathcal{H}_1(\mathbf{r}); \quad [\mathcal{H}_1(\mathbf{r}), \mathcal{H}_1(\mathbf{r}')] = 0. \quad (5.5)$$

In this case  $\mathcal{H}_1(\alpha, \alpha')$  is easily found to be of finite range. That is, we have



$$\hat{\mathcal{H}}_1(\alpha, \alpha') = \log \langle \alpha | \prod_{\mathbf{r}} Q_{\mathbf{r}} | \alpha' \rangle; \quad Q_{\mathbf{r}} = \exp \left[ -\frac{1}{n} \beta \mathcal{H}_1(\mathbf{r}) \right] \quad (5.6)$$

and then

$$\langle \alpha | \prod_{\mathbf{r}}^M Q_{\mathbf{r}} | \alpha' \rangle = \langle \alpha | Q_1 | \alpha_1 \rangle \langle \alpha_1 | Q_2 | \alpha_2 \rangle \cdots \langle \alpha_{M-1} | Q_M | \alpha' \rangle. \quad (5.7)$$

When  $\mathcal{H}_1(\mathbf{r})$  is of finite range, the matrix elements of  $\{Q_{\mathbf{r}}\}$  are simplified as follows:

$$\langle \{\alpha_j\} | Q_{\mathbf{r}} | \{\alpha'_j\} \rangle = Q(\{\alpha_j\}, \{\alpha'_j\}; j \in I_{\mathbf{r}}) \prod_{j \in I_{\mathbf{r}}} \delta(\alpha_j, \alpha'_j), \quad (5.8)$$

where  $I_{\mathbf{r}}$  denotes a relevant lattice region of  $Q_{\mathbf{r}}$ , and  $\delta(\alpha, \alpha')$  is a Kronecker  $\delta$  function. Since  $Q(\{\alpha_j\}, \{\alpha'_j\}; j \in I_{\mathbf{r}})$  is a partial Boltzmann factor with finite-range interaction,  $\hat{\mathcal{H}}_1(\alpha, \alpha')$  is thus expressed by finite-range interactions, as is seen from (5.6) and (5.7).

This formulation is easily extended to a Hamiltonian composed of many parts:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \cdots + \mathcal{H}_m, \quad (5.9)$$

where  $\mathcal{H}_j$  is a sum of commutable local operators. For example, the Heisenberg model can be separated into such three parts:

$$\mathcal{H}_H = -\sum J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = \sum_{k=0}^2 \mathcal{H}_k; \quad \mathcal{H}_0 = -\sum J_{ij} S_i^z S_j^z, \quad \mathcal{H}_1 = -\sum J_{ij} S_i^x S_j^x, \quad \text{etc.} \quad (5.10)$$

Then, using the generalized Trotter formula, we have

$$Z = \text{Tr } e^{-\beta \mathcal{H}} = \sum_{\{\alpha_j, k\}} \exp \mathcal{H}_{\text{eff}}, \quad (5.11)$$

where

$$\mathcal{H}_{\text{eff}} = \lim_{n \rightarrow \infty} \sum_{j=1}^n \left\{ -\frac{1}{n} \beta \mathcal{H}_0(\alpha_j) + \sum_{k=0}^{m-1} \hat{\mathcal{H}}_k(\alpha_j, k, \alpha_{j,k+1}) \right\}, \quad (5.12)$$

with  $\alpha_{j,0} = \alpha_j$ ,  $\alpha_{j,m} = \alpha_{j+1}$  and

$$\hat{\mathcal{H}}_k(\alpha, \alpha') = \log \langle \alpha | \exp \left( -\frac{1}{n} \beta \mathcal{H}_k \right) | \alpha' \rangle. \quad (5.13)$$

As before, this becomes of finite range, if  $\mathcal{H}_k$  is a sum of commutable local operators.

In particular, the partition function of the Hamiltonian (1.5) is reduced as follows:

$$\begin{aligned} Z &= \text{Tr } e^{-\beta \mathcal{H}} = \text{Tr } \exp \left\{ \sum K_{ij} \sigma_i^z \sigma_j^z + h \sum \sigma_j^z + \gamma \sum \sigma_j^x \right\} \\ &\equiv \text{Tr } \exp \{ \mathcal{H}_0(\{\sigma_j^z\}) + \gamma \sum \sigma_j^x \} \\ &= \lim_{n \rightarrow \infty} \text{Tr} \left[ \exp \left( \frac{1}{n} \mathcal{H}_0 \right) \exp \left( \frac{1}{n} \gamma \sum \sigma_j^x \right) \right]^n \end{aligned}$$

$$\begin{aligned}
 &= \lim_{n \rightarrow \infty} \sum_{\{\sigma_{j,k} = \pm 1\}} \left( \frac{1}{2} \sinh \frac{2\gamma}{n} \right)^{nN/2} \exp \left[ \frac{1}{n} \sum_{k=1}^n \mathcal{H}_0(\{\sigma_{j,k}\}) + \frac{1}{2} \left( \log \coth \frac{\gamma}{n} \right) \right. \\
 &\quad \left. \times \sum \sigma_{j,k} \sigma_{j,k+1} \right], \quad (5.14)
 \end{aligned}$$

where we have used the relation (4.5) and  $N$  denotes the number of the original lattice points in  $d$  dimensions. This yields Theorem 4. As is seen from the above derivation,  $\mathcal{H}_0(\{\sigma_j^z\})$  may be an arbitrary Ising Hamiltonian with many-spin interaction. The above representation (5.14) is a special case of more general situations previously discussed.<sup>20)</sup>

(ii) *The second formulation*

Another slightly different formulation is given by regarding, from the beginning, the Hamiltonian as a sum of (local) Hamiltonians  $\mathcal{H}(\mathbf{r})$ ;  $\mathcal{H} = \sum_{\mathbf{r}} \mathcal{H}(\mathbf{r})$ , and by applying the generalized Trotter formula (3.2) as follows:

$$\begin{aligned}
 Z &= \text{Tr } e^{-\beta \mathcal{H}} = \lim_{n \rightarrow \infty} \text{Tr} \left\{ \prod_{\mathbf{r}} \exp \left[ -\frac{1}{n} \beta \mathcal{H}(\mathbf{r}) \right] \right\}^n \\
 &= \lim_{n \rightarrow \infty} \sum_{\{\alpha_j\}} \exp \mathcal{H}_{\text{eff}}, \quad (5.15)
 \end{aligned}$$

where

$$\mathcal{H}_{\text{eff}} = \sum_{\mathbf{r}} \sum_{j=1}^n \hat{\mathcal{H}}(\alpha_{\mathbf{r},j}, \alpha_{\mathbf{r},j+1}) \quad (5.16)$$

and

$$\begin{aligned}
 \exp \hat{\mathcal{H}}(\alpha, \alpha') &= \langle \alpha | \exp \left[ -\frac{1}{n} \beta \mathcal{H}(\mathbf{r}) \right] | \alpha' \rangle \\
 &= Q(\{\alpha_j, \alpha'_j\}; j \in I_{\mathbf{r}}) \prod_{j \in I_{\mathbf{r}}} \delta(\alpha_j, \alpha'_j), \quad (5.17)
 \end{aligned}$$

as in (5.8). Thus, the quantal spin system is reduced to the  $(d+1)$ -dimensional Ising model. Furthermore, if the interaction of  $\mathcal{H}$  is of finite range, the corresponding Ising model is also of finite range, as is seen from (5.17). This yields a proof of Theorem 5.

More explicitly we study here the lattice structure of the corresponding Ising model  $\mathcal{H}_{\text{eff}}$ . For simplicity, we consider a quantal spin Hamiltonian with nearest neighbour pair interaction:

$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathcal{H}_{i,j}. \quad (5.18)$$

Correspondingly, the effective Hamiltonian  $\mathcal{H}_{\text{eff}}$  or partial Boltzmann factor  $Q$  defined by (5.17) becomes such a four-spin interaction (including pair interactions) as

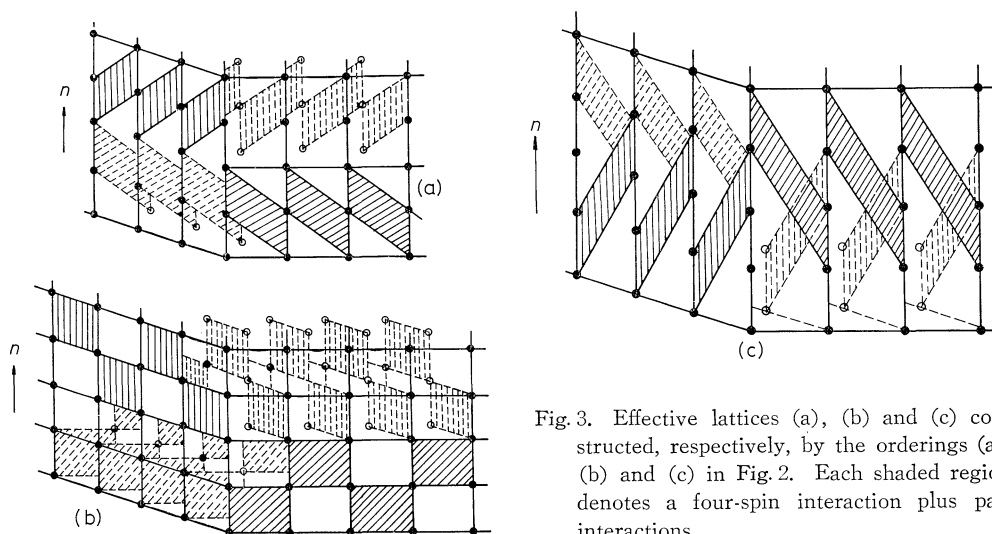
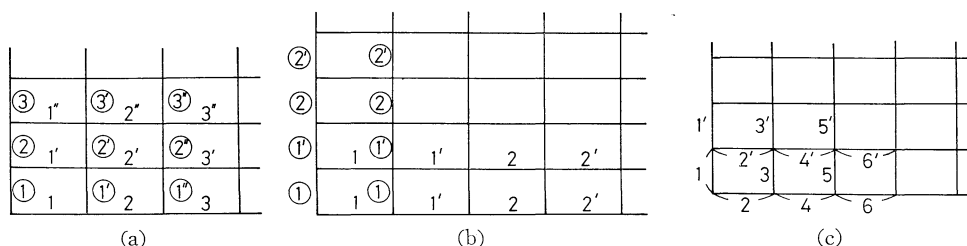
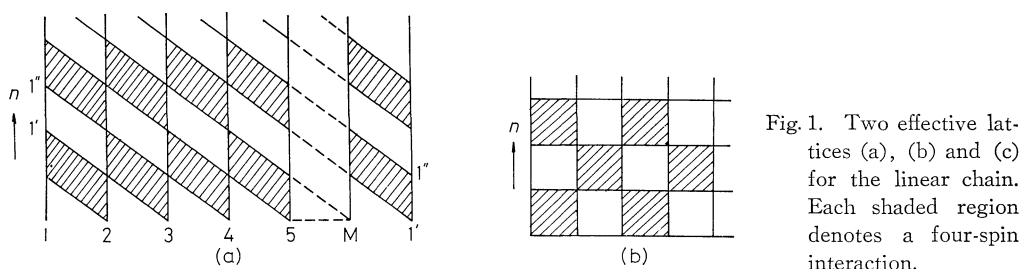
$$Q = Q_{i,j;i',j'}(\sigma_i, \sigma_j; \sigma_{i'}, \sigma_{j'}). \quad (5.19)$$

The partition function is expressed by

$$Z = \sum_{\{\sigma_j = \pm 1\}} \prod_{[\text{effective lattice}]} Q_{i,j;i',j'}(\sigma_i, \sigma_j; \sigma_{i'}, \sigma_{j'}). \quad (5.20)$$

1. An effective lattice of the linear chain with periodic boundary conditions is represented by a checker board lattice as shown in Fig. 1. Each shaded region indicates a four-spin interaction or partial Boltzmann factor  $Q_{i,j;i',j'}$ . Clearly, the interaction of this effective Ising system is of finite range.

2. An effective lattice of the two-dimensional (square) quantal spin system with periodic boundary conditions is constructed, for example, following the procedures shown in Fig. 2, in which the order of partial Boltzmann factor exp



$((-1/n)\beta\mathcal{H}_{i,j})$  of (5.15) is indicated, namely  $1, 2, 3, \dots; 1', 2', 3', \dots; 1'', 2'', 3'', \dots; \dots$ . The effective lattices thus constructed are shown in Fig. 3. Each shaded region indicates a four-spin interaction or partial Boltzmann factor. That is, the effective Ising system is also described by finite-range interactions, at most, of finite range.

In general, an effective Ising system is described by finite-range interactions, *at most, with range  $z$* , where  $z$  is the number of the nearest neighbours of the original quantal system. More generally, the above statement is valid *for any quantal spin with finite-range interactions of range  $b$* , if  $z$  is replaced by  $\max(b, \hat{z})$ , where  $\hat{z}$  is the frequency of how many times each spin operator appears in the original Hamiltonian. Thus, it is concluded in general that an effective Ising system is described by finite-range interactions. Hence results Theorem 5. Theorem 6 is also easily proven by repeating the above procedure for spin correlations.

The following formulae on matrix elements will be useful for practical applications:

1.  $\langle \sigma | e^{r\sigma^x} | \sigma' \rangle = \left( \frac{1}{2} \sinh 2r \right)^{1/2} \exp \left[ \frac{1}{2} (\log \coth r) \sigma \sigma' \right],$
2.  $\langle \sigma | e^{h\sigma^y} | \sigma' \rangle = \left( \frac{1}{2} \sinh 2h \right)^{1/2} \exp \left[ \frac{1}{2} (\log \coth h) \sigma \sigma' + \frac{\pi i}{4} (\sigma - \sigma') \right],$
3.  $\langle \sigma | e^{h\sigma^z} | \sigma' \rangle = e^{h\sigma} \delta(\sigma, \sigma') = e^{h\sigma} \cdot (1 + \sigma \sigma') / 2,$
4.  $\langle \sigma_i, \sigma_j | \exp(K_x \sigma_i^x \sigma_j^x + K_y \sigma_i^y \sigma_j^y + K_z \sigma_i^z \sigma_j^z) | \sigma_i', \sigma_j' \rangle$   
 $= \tilde{a} \left\{ (1 + X_3 \sigma_i \sigma_j) \delta(\sigma_i, \sigma_i') \delta(\sigma_j, \sigma_j') \right.$   
 $\left. + X_1 \frac{(1 - \sigma_i \sigma_i') (1 - \sigma_j \sigma_j')}{4} - X_2 \frac{(\sigma_i - \sigma_i') (\sigma_j - \sigma_j')}{4} \right\}, \quad (5.21)$

where

$$\begin{cases} \tilde{a} = \cosh K_x \cosh K_y \cosh K_z - \sinh K_x \sinh K_y \sinh K_z, \\ X_1 = (\tanh K_x - \tanh K_y \tanh K_z) / (1 - \tanh K_x \tanh K_y \tanh K_z), \\ X_2 \text{ and } X_3 \text{ are cyclic with respect to } x, y \text{ and } z. \end{cases} \quad (5.22)$$

As is seen from Theorem 5 and (5.21), the partition function of the Heisenberg model is reduced to the Ising model with four-spin interactions.<sup>10), 19) ~ 21)</sup>

## § 6. Examples

In this section we discuss some illustrative examples.

### (i) One-dimensional Ising model with a transverse field

The Hamiltonian of this system is described by

$$\mathcal{H} = -J \sum_{j=1}^M \sigma_j^z \sigma_{j+1}^z - \Gamma \sum_{j=1}^M \sigma_j^x; \quad \sigma_{M+1} = \sigma_1. \quad (6.1)$$

From Theorem 4, the partition function of this system is written in the form

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \mathcal{H}} = \text{Tr} \exp \left\{ K \sum_{j=1}^M \sigma_j^z \sigma_{j+1}^z + \gamma \sum_{j=1}^M \sigma_j^x \right\} \\ &= \lim_{n \rightarrow \infty} A_n^{Mn} \text{Tr} \exp \left\{ \sum_{j=1}^M \sum_{k=1}^n \left( \frac{1}{n} K \sigma_{j,k} \sigma_{j+1,k} + K_n \sigma_{j,k} \sigma_{j,k+1} \right) \right\}, \end{aligned} \quad (6.2)$$

where  $K = J/kT$ ,  $\gamma = \Gamma/kT$  and

$$A_n = \left[ \frac{1}{2} \sinh \left( \frac{2\gamma}{n} \right) \right]^{1/2} \quad \text{and} \quad K_n = \frac{1}{2} \log \coth \left( \frac{\gamma}{n} \right). \quad (6.3)$$

This is nothing but the Onsager problem *in two dimensions*. Consequently, we can make use of the celebrated exact solution by Onsager and Kaufman.<sup>28)</sup> Thus, we obtain

$$\begin{aligned} Z &= \lim_{n \rightarrow \infty} A_n^{Mn} \times \frac{1}{2} (2 \sinh 2K_n)^{Mn/2} \\ &\quad \times \left\{ \prod_{k=1}^M \left( 2 \cosh \frac{n}{2} \gamma_{2k} \right) + \prod_{k=1}^M \left( 2 \sinh \frac{n}{2} \gamma_{2k} \right) \right. \\ &\quad \left. + \prod_{k=1}^M \left( 2 \cosh \frac{n}{2} \gamma_{2k-1} \right) + \prod_{k=1}^M \left( 2 \sinh \frac{n}{2} \gamma_{2k-1} \right) \right\}, \end{aligned} \quad (6.4)$$

where  $\gamma_k$  is given by

$$\cosh \gamma_k = \cosh \left( \frac{2\gamma}{n} \right) \cosh \left( \frac{2K}{n} \right) - \sinh \left( \frac{2\gamma}{n} \right) \sinh \left( \frac{2K}{n} \right) \cos \left( \frac{\pi k}{M} \right). \quad (6.5)$$

For a large  $n$ ,  $\gamma_k$  is simplified as follows:

$$\gamma_k = \frac{2}{n} \beta \varepsilon_k + O \left( \frac{1}{n^2} \right); \quad \varepsilon_k = \left\{ (\Gamma^2 + J^2) - 2\Gamma J \cos \frac{\pi k}{M} \right\}^{1/2}. \quad (6.6)$$

Substituting this  $\gamma_k$  into (6.4) and taking the limit  $n \rightarrow \infty$ , we arrive at a new type of expression for the partition function of (6.1):

$$\begin{aligned} Z &= \frac{1}{2} \left[ \prod_{k=1}^M (2 \cosh \beta \varepsilon_{2k}) + \prod_{k=1}^M (2 \sinh \beta \varepsilon_{2k}) \right. \\ &\quad \left. + \prod_{k=1}^M (2 \cosh \beta \varepsilon_{2k-1}) + \prod_{k=1}^M (2 \sinh \beta \varepsilon_{2k-1}) \right] \end{aligned} \quad (6.7)$$

with  $\varepsilon_k$  defined by (6.6). In the thermodynamic limit, we obtain

$$\lim_{M \rightarrow \infty} \frac{1}{M} \log Z = \frac{1}{2\pi} \int_0^{2\pi} \log (2 \cosh \beta \varepsilon(q)) dq, \quad (6.8)$$

where

$$\varepsilon(q) = (J^2 + I^2 - 2JI \cos q)^{1/2}. \quad (6.9)$$

This agrees with the well-known result obtained by Katsura<sup>29)</sup> and also with the solution for a special limit ( $m=1$ ) of the generalized XY-model investigated by the present author.<sup>8)</sup> The above derivation of (6.7) or (6.8) is quite interesting in that the partition function of a *quantal* system is obtained in classical methods such as Pfaffian, combinatorial technique, or quaternion algebra, *without diagonalizing the relevant Hamiltonian*.

## (ii) Linear Heisenberg model

In general, we study the following anisotropic Hamiltonian

$$\mathcal{H} = - \sum_{j=1}^N (J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z) - \mu H \sum \sigma_j^z \quad (6.10)$$

with a cyclic boundary condition  $\sigma_{N+1} = \sigma_1$ . Following the general procedure presented in § 5, the partition function  $Z$  is expressed by

$$Z \equiv \text{Tr} e^{-\beta \mathcal{H}} = \lim_{n \rightarrow \infty} Z_n(\{J\}, H), \quad (6.11)$$

where the  $n$ -th approximant  $Z_n$  is

$$Z_n = \text{Tr} \left[ \prod_{j=1}^N \exp \left\{ \frac{1}{n} K_x \sigma_j^x \sigma_{j+1}^x + \frac{1}{n} K_y \sigma_j^y \sigma_{j+1}^y + \frac{1}{n} K_z \sigma_j^z \sigma_{j+1}^z \right\} \exp \left( \frac{h}{n} \sigma_j^z \right) \right]^n. \quad (6.12)$$

The first approximant  $Z_1$  corresponds to the “Pair-Product Model” introduced by the present author<sup>27)</sup> as the zeroth approximation of Kubo’s systematic expansions<sup>30)</sup> quite different from the present systematic approximants. As was already calculated in Ref. 27),  $Z_1(\{J\}, 0)$ , for example, is given by

$$Z_1(\{J\}, 0) = (2\tilde{\alpha})^N (1 + X_1^N + X_2^N + X_3^N) \quad (6.13)$$

with (5.19). This represents well the thermodynamic properties in the temperature region  $T \gtrsim 2J (\sim J_x \sim J_y \sim J_z)$ , as was discussed in Ref. 27). It is possible to proceed with these approximants up to higher order. An effective Ising lattice is shown in Fig. 1.

## (iii) Other examples

It will be quite interesting to study the two-dimensional Heisenberg model and XY-model even in the first approximant  $Z_1$  (or Pair-Product Model), because it is expected that the essential singular behavior is manifested even in the first approximant.<sup>31)</sup> These investigations are suggested to be performed in future.

## § 7. Crossover effect

As was proven in § 4 (Theorem 1), the critical exponents of (1.5) at  $T=0$  are expressed by those of the  $(d+1)$ -dimensional Ising model. On the other hand, the critical behavior of (1.5) for  $T>0$  may be described by those of the  $d$ -dimensional Ising model, as was stated in the Proposition of § 2.

Consequently, it is expected that a crossover effect occurs near  $T=0$  and  $\Gamma=\Gamma_c$ . That is, there exists a crossover parameter  $\gamma^* \sim T^{1/\phi}$  whose critical behavior is  $d$ -dimensional in the region  $|\Gamma-\Gamma_c(T)| \lesssim \gamma^*$ , and  $(d+1)$ -dimensional in the region  $|\Gamma-\Gamma_c(T)| \gtrsim \gamma^*$  near  $T=0$ , as shown in Fig. 4, similarly to the ordinary crossover theory.<sup>32)~36)</sup>

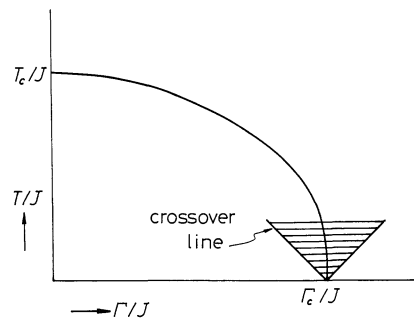


Fig. 4. Critical line and crossover line.

### § 8. Concluding remarks

All the present arguments are easily extended to systems of higher spin, although much more complications appear. Our systematic approximants (3.2) and (3.4) will be convenient for numerical calculations by a high speed computer. Theorem 5 and the general formulation of § 5 based on Trotter's formula *make it possible to perform the Monte Carlo calculation of quantal spin systems such as the Heisenberg model and XY-model*, which is now in progress. They are also of great use in applying the renormalization group technique, particularly the block spin method<sup>37)~40)</sup> to quantal spin systems, as will be reported in a separate paper.

Using Theorem 5 and the generalized Trotter formula (3.2) or (3.4), it is possible to prove the existence of the thermodynamic limit of the generating function  $\mathcal{V}(\lambda, t)$  in non-equilibrium quantal spin systems *for operators bounded in the sense of a norm* and consequently to prove the extensivity<sup>41), 42)</sup> of a macrovariable under more explicit conditions than before.<sup>43)</sup> This proof will be given elsewhere. Time correlation functions of quantal spin systems will be also studied in a forthcoming paper by extending the present method and using the formula (3.4) on exponential hyper-operators.

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