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Kyoto University
Study of Quantum Spin Systems
using Real Space Renormalization Transformations

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Abstract

The spin 1/2 anisotropic Heisenberg model is studied by means of the real space renormalization transformations. Thermodynamic properties of one-dimensional systems are calculated by using an approximate decimation method. These results agree well with those obtained by Bonner and Fisher and by Katsura. Two- and three-dimensional systems are studied by generalizing the Migdal-Kadanoff renormalization transformations to quantum spin systems. For the Ising and Heisenberg models in two and three dimensions and for the X-Y model in three dimensions, the critical properties thus obtained are in qualitative agreement with those obtained from high temperature series expansions. For the two-dimensional X-Y model, our results suggest that this model undergoes some kind of phase transition and that the critical behaviour of this model is similar to that expected for the classical X-Y and planar models.

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*) 高野 宏；東大・理・物理
I. Introduction

The renormalization group approach first introduced to the study of critical phenomena by Wilson\(^1\) has turned out a very useful and powerful method in this field. This approach may be divided roughly into two classes, namely, the momentum space approach and the real space one. The momentum space renormalization approach such as the \(\epsilon\)-expansion\(^2\) deals with general reduced models and is useful to study general aspects of critical phenomena such as scaling, universality and cross-over. On the contrary, the real space approach first proposed
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by Niemeijer and van Leeuwen\textsuperscript{3)} deals with spin variables in the real space and is useful to study a specific model in specific dimensions directly.

The real space renormalization group approach was first applied to the direct study of classical spin systems. In particular, for the two-dimensional Ising-like spin systems, this approach gave very satisfactory results about their critical properties and global thermodynamic properties.\textsuperscript{4)}

In recent years, many attempts\textsuperscript{5)}\textsuperscript{−}\textsuperscript{15),46),47)} have been made to generalize the real space approach to quantum spin systems such as the Heisenberg, X-Y and transverse Ising models. Particularly many efforts\textsuperscript{5)}\textsuperscript{−}\textsuperscript{10)} have been made for the study of the two-dimensional X-Y model. However, up to now, there has been no definite result about the critical properties of this model.

In this thesis, simple real space renormalization transformations for quantum spin systems are proposed to study the spin 1/2 anisotropic Heisenberg model including the Ising, isotropic Heisenberg and X-Y models.

First, an approximate decimation method for one-dimensional systems is considered. Then, on the basis of it, the Migdal-Kadanoff approximate renormalization transformations\textsuperscript{16),17)} are generalized to quantum spin systems in higher dimensions. The Migdal-Kadanoff transformations are very simple approximate renormalization transformations in real space and can easily be applied to two- or three-dimensional systems. They are very useful to study qualitative or semi-quantitative features of the relevant system.

The outline of this thesis is as follows. In Chapter II the model is defined and previous studies on this model are briefly reviewed in connection with our calculations. In Chapter III one-dimensional models are studied by using an approximate decimation. In Chapter IV two- and three-dimensional models are studied by generalizing the Migdal-Kadanoff transformations to quantum spin systems. We summarize our conclusions in Chapter V. Appendix A gives a brief review of the formulation of the real space renormalization transformations. Appendix B deals with a derivation of the Migdal-Kadanoff transformations. Derivation of the renormalization equations of the approximate one-dimensional decimation is given in Appendix C.
II. The Spin 1/2 anisotropic Heisenberg model

In the following, the thermodynamic properties of the spin 1/2 anisotropic Heisenberg model are studied in one, two and three dimensions using renormalization transformations. The Hamiltonian $\mathcal{H}$ of this model including the factor $-\beta = -1/k_B T$, $T$ being the temperature and $k_B$ Boltzmann's constant, is given by

$$\mathcal{H} = \sum_{\langle ij \rangle} \{ K_Z \sigma_i^z \sigma_j^z + K_{XY} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \},$$

(2.1)

where $i$ denotes the lattice site of the $d$-dimensional hypercubic lattice, $\sigma_i^x$, $\sigma_i^y$ and $\sigma_i^z$ denote the Pauli spin operators on the $i$ site and $\sum$ denotes the sum over all nearest-neighbour pairs. $K_Z$ and $K_{XY}$ are written as

$$K_Z = \beta J_z$$

(2.2a)

and

$$K_{XY} = \beta J_{XY},$$

(2.2b)

where $J_z$ is an exchange coupling of $z$-components of neighbouring spins and $J_{XY}$ is that of $x$- and $y$-components.

Now, we review briefly the previous studies of this model in one, two and three dimensions in connection with our calculations.

2-1. One-dimensional systems

The exact free energy of this model in one dimension is known in special cases: The case of the Ising model (i.e., $K_{XY} = 0$) and the X-Y model\(^{19}\) (i.e., $K_Z = 0$).

In the case of $|K_Z| \geq |K_{XY}|$, Bonner and Fisher\(^{18}\) studied numerically this model with a magnetic field for finite chains. They studied both ferromagnetic and antiferromagnetic cases.

Honda\(^{12}\) studied this model in one dimension by using a renormalization transformation. He used a transformation function of the decimation type with the scale factor $\ell = 2$, and also used a finite lattice approximation: The renormalization equation was constructed for a lattice
of two cells with cyclic boundary condition. The specific heat thus calculated is in considerably good agreement with the previous results obtained by Bonner and Fisher\textsuperscript{18}) and by Katsura\textsuperscript{19}).

In Chapter III we use the same decimation type transformation function to study the model in one dimension. However, instead of the finite lattice approximation, we use another approximation, that is to say, "cluster" approximation; this approximation can be used to generalize the Migdal-Kadanoff transformations to quantum spin systems. This approximation gives results similar to those given by Honda for the specific heat.

2-2. Two-dimensional systems

For two and three dimensions, we consider only the ferromagnetic cases: $K_Z \geq 0$ and $K_{XY} \geq 0$.

Mermin and Wegner\textsuperscript{20)} proved rigorously that the spin $S$ anisotropic Heisenberg model in two dimensions with $J_Z \leq J_{XY}$ has no spontaneous magnetization at any non-zero temperature. However, it was suggested by Stanley and Kaplan\textsuperscript{21}) from the high temperature series expansion of the susceptibility that the isotropic Heisenberg model (i.e., $J_Z = J_{XY}$) with spin $S > 1/2$ in two dimensions exhibits some kind of phase transition at a finite temperature. On the contrary, Yamaji and Kondo\textsuperscript{22}) gave some evidence from the longer series to suggest that the isotropic Heisenberg model with any spin shows no phase transition. Up to now, this suggestion of Yamaji and Kondo has been generally believed to be true. For the X-Y model (i.e., $J_Z = 0$) in two dimensions, the high temperature series given by Betts et al.\textsuperscript{23}) suggests more strongly that the susceptibility diverges at a certain temperature. They estimated the values of the critical inverse temperature $K_{XYc}$ and the values of the usual power law critical exponent $\gamma$ of the susceptibility for some two-dimensional lattices. Their results are as follows: $K_{XYc} \approx 0.33$ for the triangular lattice, $K_{XYc} \approx 0.56$ for the square lattice and $\gamma \approx 1.5$ for the both lattices. The high temperature series expansion of the free energy of the same model given by Betts et al.\textsuperscript{24}) suggests that there is no singularity in the specific heat. The simulation of this model\textsuperscript{48}) also supports these critical properties.

Studies based on series expansions\textsuperscript{25),26)} and simulations\textsuperscript{49)} for the two-dimensional classical X-Y and planar models gave the evidence that these classical models have also a non-zero temperature at which the susceptibility diverges. There have been several arguments\textsuperscript{27)~31)}
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to suggest that these classical models have a line of critical points with continuously varying critical exponents. Introducing the concept of “topological order”, Kosterlitz and Thouless\textsuperscript{29}) and Kosterlitz\textsuperscript{30}) showed that the susceptibility diverges below a certain critical temperature $T_c$ and suggested that as approaching this temperature from above the susceptibility diverges exponentially

$$\chi \sim \exp \left[ B \left( \frac{T}{T_c} - 1 \right)^{-\nu} \right] \quad \text{(2.3)}$$

rather than with the usual power law

$$\chi \sim \left( \frac{T}{T_c} - 1 \right)^{-\gamma} \quad \text{(2.4)}$$

The high temperature series expansions for these classical models seem to support\textsuperscript{32,33}) this exponential divergence of the susceptibility rather than the usual power law divergence. On the contrary, for the spin 1/2 X-Y model, the result of the high temperature series\textsuperscript{23}) favours the usual power law.

There have been several attempts\textsuperscript{5,7,8,9,10}) to study the spin 1/2 X-Y model by the real space renormalization group approach. Rogiers and Dekeyser\textsuperscript{5}) and Rogiers and Betts\textsuperscript{7}) studied this model on the triangular lattice using the cells of three and seven sites respectively. For both cases, a non-trivial fixed point was found to the second order of the cumulant expansion, though no non-trivial fixed point to the first order. These calculations gave the critical inverse temperature $K_{XYc} \simeq 0.46$ and $K_{XYc} \simeq 0.51$ with an unphysical result $\delta < 0$. Betts and Plischke\textsuperscript{6}) studied the case of the square lattice in the same way with the cells of five sites. They found, however, no non-trivial fixed point to the second order. The transformation functions chosen in the above theories do not preserve some symmetries of the Hamiltonian. In other words, they do not transform a Hamiltonian of one universality class to a Hamiltonian of the same universality class. This is considered to be a serious defect of these theories.

Considering such symmetries, Stella and Toigo\textsuperscript{9}) studied the model on the triangular lattice by using a renormalization transformation. A non-trivial fixed point was found to the first order of the cumulant expansion. The critical temperature and the critical exponents derived from it were in good agreement with those estimated from the high temperature series.
expansion. However, to the second order, this non-trivial fixed point was found to vanish.

Dekeyser et al. showed that it is possible to derive results consistent with the critical properties expected for the classical models, by using the following linear transformation function

$$ T(\{\mu\}, \{\sigma\}) = \prod_i \frac{1}{2} (1 + p \mu_i \cdot \sum_{i \in j} \sigma_j) $$

where $\mu_j$ denotes the cell spin, $\sigma_i$ denotes the site spin, $\sum_{i \in j}$ denotes the summation over all the site spins within the cell $j$ and $p$ is a parameter to be determined consistently. By the critical properties of the classical models mentioned above, we mean in the sense of the renormalization group approach that there is a line of fixed points corresponding to that of the critical points. As approximate calculations of this kind cannot reproduce such a fixed line exactly, Dekeyser et al. tried to get a marginal scaling field at a non-trivial fixed point by adjusting the parameter $p$. To the first order of the cumulant expansion, they failed to get a marginal eigenvalue. Therefore, they determined the parameter $p$ from the requirement of the hyperscaling and got the results consistent with the high temperature series expansion. To the second order, they got the result with marginal eigenvalue. Since their transformation function preserves fundamental symmetries of the Hamiltonian, it can be applied to the Ising and isotropic Heisenberg models. It gave a non-trivial fixed point for the isotropic Heisenberg model. However, the position of the fixed point is considered to be out of the region where the cummulant expansion is valid.

For the case of $J_z > J_{XY}$, Fröhlich and Lieb proved rigorously that this model on the square lattice has a non-zero spontaneous magnetization at low temperatures and therefore has a phase transition at a finite temperature. Obokata et al. studied this model with $0 \leq J_{XY}/J_z < 1$ on the square and simple cubic lattices by the high temperature series expansion of the susceptibility. They suggested that the critical temperature is almost constant in the region $0 \leq J_{XY}/J_z \leq 0.7$ for the square lattice and $0 \leq J_{XY}/J_z \leq 0.8$ for the simple cubic lattice.

Brower et al. also studied this model with $0 \leq J_{XY}/J_z \leq 1$ by using the renormalization group approach. They constructed a transformation which preserves the fundamental symmetries of the Hamiltonian. They made calculations for the triangular lattice with the cummulant expansion and for the square lattice with a cluster of two cells. Though the second
order calculation for the isotropic Heisenberg model on the triangular lattice gave a non-trivial fixed point which is considered to be spurious, their calculations gave results in good agreement with the high temperature series.

In Chapter IV, we investigate the model on the square lattice with $0 \leq J_{xy}/J_z \leq 1$ and $0 \leq J_{xy}/J_z \leq 1$ by generalizing the Migdal-Kadanoff transformations to quantum spin systems. The transformation used is of the decimation type and it preserves the fundamental symmetries of the Hamiltonian. By using this transformation, the model with any anisotropy can be studied in a unified manner. A phase diagram in the parameter space which is qualitatively in agreement with the high temperature series is derived. For the X-Y model, the critical exponents thus derived are qualitatively of such a type as is expected for the classical models.

2–3. Three-dimensional systems

There have been reported some estimations of the critical temperature and the critical exponents from the high temperature series expansions for the Ising$^{37}$ isotropic Heisenberg$^{36}$ and X-Y models.$^{38}$ As mentioned in Section 2–2, Obokata et al. studied the case of $0 \leq J_{xy}/J_z < 1$.

There has been no attempt to study this model in three dimensions by using the real space renormalization group approach.

In Chapter V, we study the model on the simple cubic lattice using the generalized Migdal-Kadanoff transformation. By the help of this transformation, the two-dimensional and three-dimensional models can easily be treated in the same manner. Results thus obtained are in qualitatively good agreement with those from the high temperature series.

III. Decimation method for one-dimensional systems

3–1. Transformation function and approximation

The formulation of the real space renormalization transformations given in Appendix A can be used for quantum spin systems only by considering classical spin variables $\sigma$ and $\mu$ as Pauli spin operators. As explained in Appendix A, the transformation function $T(\{\mu\}, \{\sigma\})$ in the equation (A.2) determines the renormalization transformation. If we want to study the critical properties of a certain model by a renormalization transformation, this
transformation has to preserve the model within the same universality class as the original one. Therefore, in order to study in a unified manner the Hamiltonians with various symmetries, the transformation function should have a higher degree of symmetry than the Hamiltonians have. 11)

Below in this chapter we consider only the one-dimensional system. Then the Hamiltonian (2.1) can be written as

\[
\mathcal{H} = \sum_{i=0}^{N-1} \left[ K_Z \sigma_i^z \sigma_{i+1}^z + K_{XY} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) \right],
\]

where \( i \) denotes the lattice site of the linear chain with \( N \) sites and \( \sigma_N = \sigma_0 \).

Considering the requirements above mentioned, we use the following transformation function for the renormalization transformation with scale factor \( \xi \):

\[
T(\{ \mu \}, \{ \sigma \}) = \prod_{j=0}^{N/\xi - 1} t(\mu_j, \sigma_{\xi j}) ,
\]

where \( t(\mu_j, \sigma_{\xi j}) = \frac{1}{2} (1 + \mu_j \cdot \sigma_{\xi j}) \).

For any function \( A(\sigma) \) of the operator \( \sigma \), the relation

\[
T_{r,\sigma} [A(\sigma) t(\mu, \sigma)] = A(\mu)
\]

holds. Then the equation (A.2) with the transformation function (3.2) can be rewritten as

\[
\exp \left[ G + \mathcal{H}'(\{ \sigma_{\xi j} \}) \right] = T'_r \exp \left[ \mathcal{H}(\{ \sigma_j \}) \right],
\]

where \( j = 0, 1, \cdots, N/\xi - 1 \) and \( T'_r \) denotes the trace over all spins \( \sigma_i \) with \( i \neq \xi j \), that is,

\[
T'_r = \prod_{i \neq \xi j} T_{r,\sigma},
\]

\( (j = 0, 1, \cdots, N/\xi - 1) \).
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This means to take a partial trace over spin operators other than every \( k \)-th spin operator (See Fig. 1). This transformation is called "decimation".

For the Ising model (i.e., \( K_{XY} = 0 \)) in one dimension, this decimation can be carried out exactly. In the quantal case of general anisotropy with \( K_{XY} \neq 0 \), however, it is impossible to carry out the decimation exactly even in one dimension because of non-commutative effect of operators in the Hamiltonian. Therefore, we must make some approximation to get a renormalization equation from the equation (3.5). We propose the following simple approximation\(^{47}\) to the one-dimensional decimation. Let the Hamiltonian be a sum of nearest-neighbour interactions:

\[
\mathcal{H}(\{ \sigma_i \}) = \sum_{i=0}^{N-1} A(\sigma_i, \sigma_{i+1}),
\]

(3.7)

where \( A(\sigma_i, \sigma_{i+1}) \) denotes a nearest-neighbour interaction between \( \sigma_i \) and \( \sigma_{i+1} \). The transformed Hamiltonian \( \tilde{\mathcal{H}} \) and the constant term \( G \) are defined by the equation (3.5). We divide the Hamiltonian \( \mathcal{H} \) into clusters of the nearest-neighbour interactions as

\[
\mathcal{H}(\{ \sigma_i \}) = \sum_{k=0}^{N/2-1} \left\{ \sum_{i=0}^{q-1} A(\sigma_{k+i}, \sigma_{k+i+1}) \right\}.
\]

(3.8)

Considering only one cluster, the decimation can be carried out as

\[
\exp \left[ \tilde{G} + A'(\sigma_0, \sigma_\ell) \right] = \left( \prod_{i=1}^{q-1} T_{i-1} \sigma_i \right) \exp \left[ \sum_{i=0}^{q-1} A(\sigma_i, \sigma_{i+1}) \right],
\]

(3.9)

where \( A'(\sigma_0, \sigma_\ell) \) is a new nearest-neighbour interaction between the remaining spins \( \sigma_0 \) and \( \sigma_\ell \) and \( \tilde{G} \) is a constant term independent of \( \sigma_0 \) and \( \sigma_\ell \). Then, using \( A' \) and \( \tilde{G} \), we construct an approximate transformed Hamiltonian \( \tilde{\mathcal{H}}_A' \) and an approximate constant term \( G_A \) as follows:

\[
\tilde{\mathcal{H}}_A' \equiv \sum_{k=0}^{N/2-1} A'(\sigma_{k+1}, \sigma_{(k+1) \ell}),
\]

(3.10)

and
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\[ G_A \equiv \frac{N}{\ell} \tilde{G} \tag{3.11} \]

This process of approximation (see Fig. 2) can be written as

\[
\exp [G + \mathcal{H}'] = T'_r \exp [\mathcal{H}]
\]

\[
= T'_r \exp \left[ \sum_{i=0}^{N-1} A(\sigma_i, \sigma_{i+1}) \right]
\]

\[
\simeq T'_r \prod_{k=0}^{N/\ell-1} \exp \left[ \sum_{i=0}^{\ell-1} A(\sigma_{k+i\ell}, \sigma_{k+i\ell+1}) \right]
\]

\[
= \prod_{k=0}^{N/\ell-1} \left( \prod_{i=1}^{\ell-1} T'_r \sigma_{k+i\ell} \right) \exp \left[ \sum_{i=0}^{\ell-1} A(\sigma_{k+i\ell}, \sigma_{k+i\ell+1}) \right]
\]

\[
= \prod_{k=0}^{N/\ell-1} \exp \left[ \tilde{G} + A'(\sigma_{k\ell}, \sigma_{(k+1)\ell}) \right]
\]

\[
\simeq \exp \left[ \frac{N}{\ell} \tilde{G} + \sum_{i=0}^{N/\ell-1} A'(\sigma_{i\ell}, \sigma_{(i+1)\ell}) \right]
\]

\[
= \exp \left[ G_A + \mathcal{H}'_A \right] \tag{3.12}
\]

This approximation has the following interesting features: It takes quantum effect into account within a cluster. It preserves the form of interactions within the nearest-neighbour interactions. It becomes exact, if every \( A(\sigma_i, \sigma_{i+1}) \) commutes each other. The approximation becomes better at high temperatures, because the non-commutative effects neglected in this approximation are considered to become smaller at higher temperatures. Increase of \( \ell \) seems to improve the approximation, because it becomes exact in the limit \( \ell \to \infty \).

### 3-2. Renormalization equations for scale factor \( \ell = 2 \)

Applying the approximation explained in 3-1 to the Hamiltonian (3.1), we get the transformed Hamiltonian \( \mathcal{H}'_A \) and the constant term \( G_A \) in the following form

\[
\mathcal{H}'_A = \sum_{i=0}^{N/\ell-1} \left| K'_Z \sigma^Z_{\ell i} \sigma^Z_{\ell(i+1)} + K'_{XY} (\sigma^X_{\ell i} \sigma^X_{\ell(i+1)} + \sigma^Y_{\ell i} \sigma^Y_{\ell(i+1)}) \right| \tag{3.13}
\]
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and

\[ G_A = \frac{N}{\ell} \tilde{G} \, , \]  

(3.14)

where \( K'_Z, K'_{XY} \) and \( \tilde{G} \) are defined as

\[
\exp \left[ \tilde{G} + K'_Z \sigma_0^x \sigma_0^z + K'_{XY} (\sigma_0^x \sigma_0^x + \sigma_0^y \sigma_0^y) \right] \\
= \left( \prod_{i=1}^{\infty} T_{r_i} \right) \exp \left[ \sum_{i=0}^{\infty} \left\{ K'_Z \sigma_i^z \sigma_{i+1}^z + K'_{XY} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) \right\} \right].
\]

(3.15)

For the case of scale factor \( \ell = 2 \), we get, from Eq. (3.15), the following renormalization equations:

\[
K'_Z = \frac{1}{2} \ln \left[ e^{2K_Z} + e^{-K_Z} C_+ (K_Z, K_{XY}) \right] - \frac{1}{4} \ln \left[ 4 e^{-K_Z} C_+ (K_Z, K_{XY}) \right],
\]

(3.16)

\[
K'_{XY} = \frac{1}{4} \ln \left[ e^{-K_Z} C_+ (K_Z, K_{XY}) \right]
\]

(3.17)

and

\[
\tilde{G} = K'_Z + 2K'_{XY} + \ln 2
\]

(3.18)

with

\[
C_+ (K_Z, K_{XY}) \equiv \cosh \tilde{K} \pm \left( K_Z - \frac{K}_{XY} \right) \sinh \tilde{K},
\]

(3.19)

where

\[
\tilde{K} \equiv (K_Z^2 + 8K_{XY}^2)^{1/2}.
\]

(3.20)

Details of the derivation of these equations are given in Appendix C.
3–3. Free energy

Using the equation (A.36), we can calculate the free energy of the system from the renormalization equations (3.16) \~(3.18). The function $g$ in the equation (A.11) is given by

$$g(K_Z, K_{XY}) = \frac{1}{q} \tilde{G}(K_Z, K_{XY}),$$

(3.21)

where $\tilde{G}$ is defined by Eq. (3.15); here $q = 2$.

For the ground state (i.e., $T = 0$), it is rather easy to calculate the free energy, namely the ground state energy.

First, we consider the case of the ferromagnetic isotropic Heisenberg model (i.e., $J_z = J_{XY} > 0$). Considering the condition $K_Z, K_{XY} \gg 1$ and $K_Z = K_{XY} = K$ which means $\tilde{K} = 3K$, the renormalization equations (3.16) \~(3.18) are written to the leading order of $K$ as $K' = K'' \approx \frac{1}{2} K$ and $g = \frac{\tilde{G}}{2} \approx \frac{3}{4} K$. Hence, the equation (A.11) becomes

$$f(K) \approx \frac{3}{4} K + \frac{1}{2} f\left(\frac{1}{2} K\right).$$

The solution of this equation is

$$f(K) \approx K.$$  

(3.22)

Therefore, the ground state energy $E_0$ of the system is given by

$$E_0/NJ = -\lim_{K \to \infty} \frac{\partial}{\partial K} f = -1.$$  

(3.23)

Next, we consider the ferromagnetic case with $J_z = aJ_{XY}$, where $0 \leq a < 1$ and $K_{XY} \to \infty$. In this case, the following relation holds: $-K_Z + \tilde{K} > 2K_Z$. Using this relation, the renormalization equation are given by

$$K' \approx K'' \approx \frac{1}{4} \left(-a + \sqrt{a^2 + 8}\right) K_{XY}$$  

(3.24a)

and

\[ -419 - \]
Then, the equation (2.11) is written as

\[ f(a K_{XY}, K_{XY}) \approx \frac{3}{8} \left( -a + \sqrt{a^2 + 8} \right) K_{XY} \]

\[ + f\left( \frac{1}{4} (-a + \sqrt{a^2 + 8}) K_{XY}, \frac{1}{4} (-a + \sqrt{a^2 + 8}) K_{XY} \right) \]

for the free energy \( f(K, K) \). Using the previous result \( f(K, K) \approx K \), we get

\[ f(a K_{XY}, K_{XY}) \approx \frac{1}{2} (-a + \sqrt{a^2 + 8}) K_{XY} . \]

The ground state energy \( E_0 \) is given by

\[ \frac{E_0}{N J_{XY}} = -\lim_{K_{XY} \to \infty} \frac{\partial}{\partial K_{XY}} f \bigg|_a = -\frac{1}{2} (-a + \sqrt{a^2 + 8}) . \]

These results are shown in Fig. 3a. For the isotropic Heisenberg model (i.e., \( a = 1 \)), Eq. (3.23) gives the exact value \( \frac{E_0}{N J_{XY}} = -1 \). For the X-Y model (i.e., \( a = 0 \)), Eq. (3.27) gives \( \frac{E_0}{N J_{XY}} = -\sqrt{2} \approx -1.41 \); this value is in rough agreement with the exact value\(^{19}\) \( \frac{E_0}{N J_{XY}} = -\frac{4}{\pi} \approx -1.27 \).

For the ferromagnetic case with \( J_{XY} = b J_{Z} \), where \( 0 \leq b \leq 1 \) and \( K_{Z} \to \infty \), by using the relation \(-K_{Z} + \tilde{K} \leq 2K_{Z} \), the renormalization equations are given, to the leading order of \( K_{Z} \), by

\[ K'_{Z} \approx \left\{ 1 - \frac{1}{4} \left( -1 + \sqrt{1 + 8b^2} \right) \right\} K_{Z} , \]

\[ K'_{XY} \approx \frac{1}{4} (-1 + \sqrt{1 + 8b^2}) K_{Z} , \]

\[ g = \frac{\tilde{G}}{2} \approx \frac{1}{2} \left\{ 1 + \frac{1}{4} \left( -1 + \sqrt{1 + 8b^2} \right) \right\} K_{Z} . \]

and
Then, using Eq. (A.11), we can easily show that the free energy takes the form

\[ f \approx K_Z \]  \hspace{1cm} (3.28)

in the limit \( K_Z \to \infty \). Therefore, the ground state energy \( E_0 \) is given by

\[ \frac{E_0}{NJ_Z} = \lim_{K_Z \to \infty} \frac{\partial}{\partial K_Z} f \bigg|_{b} = -1. \]  \hspace{1cm} (3.29)

This is in accordance with the exact value \( E_0/NJ_Z = -1 \).

Finally we consider the antiferromagnetic case (i.e., \( J_Z < 0 \)) with \( J_{XY} = bJ_Z \), where \( 0 \leq b \) and \( |K_Z| \to \infty \). In the same way as above, the renormalization equations are written as

\[ K'_Z \approx K'_Z \approx \frac{1}{4} \left( 1 + \sqrt{1 + 8b^2} \right) |K_Z| \]

and

\[ g \approx \frac{3}{8} \left( 1 + \sqrt{1 + 8b^2} \right) |K_Z|. \]

Hence, the free energy \( f \) is given by

\[ f \approx \frac{1}{2} \left( 1 + \sqrt{1 + 8b^2} \right) |K_Z|, \]  \hspace{1cm} (3.30)

in the limit \( |K_Z| \to \infty \). The ground state energy \( E_0 \) is given by

\[ \frac{E_0}{NJ_Z} = -\frac{1}{2} \left( 1 + \sqrt{1 + 8b^2} \right). \]  \hspace{1cm} (3.31)

This result is shown in Fig. 3b and it is in rough agreement with the exact result.  \(^{39}\) For the Ising model (i.e., \( b = 0 \)), this gives the exact result, because the renormalization transformation
Using Eq. (A. 36), we can calculate the free energy numerically at a finite temperature for any anisotropy. The internal energy and the specific heat can be calculated as the derivatives of the free energy. Figure 4 shows the numerical results for the internal energy and Fig. 5 for the specific heat. The exact results obtained for the Ising model are not shown in these figures. The results shown in Fig. 5 are similar to those obtained by Honda in another approximation mentioned in Chapter II. At high temperatures, where the present approximation is expected to be good, these results are in good agreement with the previous results obtained by Bonner and Fisher and by Katsura. Moreover, our results are qualitatively reasonable even at low temperatures. As shown above, even at $T = 0$, the ground state energy thus obtained is in rough agreement with the exact results.

IV. The Migdal-Kadanoff transformations for two- and three-dimensional systems

In this chapter, we consider only the ferromagnetic cases in two and three dimensions.

4–1. Fixed points and critical lines

Migdal proposed simple renormalization equations for the classical spin systems. Kadanoff rederived and reinterpreted Migdal's renormalization equations in a variational method. In order to study the two- and three-dimensional models, we generalize these Migdal-Kadanoff transformations to quantum spin systems, because they are very simple and useful to study two- and three-dimensional models qualitatively or semi-quantitatively.

As explained in Appendix B, the Migdal-Kadanoff transformations are composed of the two procedures: The potential moving and the one-dimensional decimation. As shown in Appendix B, the potential moving can be carried out for the quantum spin systems in the same way for the classical systems and gives a lower bound approximation for the free energy. However, as seen in Chapter III, it is impossible to carry out the one-dimensional decimation exactly for the quantum spin systems. Therefore, we apply the same approximation as described in Chapter III to this one-dimensional decimation.

We label the direction of the axes of the $d$-dimensional hypercubic lattice as $1, 2, \cdots$.
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and \(d\); the one-dimensional decimation in each direction is to be successively performed in order of this direction number. Then, we get, in the case of \(l = 2\), the renormalization equations for the coupling constants \(K_{Z1}\) and \(K_{XY1}\) of 1-direction of the \(d\)-dimensional hypercubic lattice as

\[
K_{Z1}' = 2^{d-1} \cdot \frac{1}{2} \ln \left[ e^{2K_{Z1}} + e^{-K_{Z1}} C_+ (K_{Z1}, K_{XY1}) \right] 
\]

\[-2^{d-1} \cdot \frac{1}{4} \ln \left[ 4 e^{-K_{Z1}} C_+ (K_{Z1}, K_{XY1}) \right] \tag{4.1}\]

and

\[
K_{XY1}' = 2^{d-1} \cdot \frac{1}{4} \ln \left[ e^{-K_{Z1}} C_+ (K_{Z1}, K_{XY1}) \right], \tag{4.2}\]

where \(C_+\) are defined by Eqs. (3.19) and (3.20). For \(d = 2\), these renormalization equations have the following non-trivial fixed points:

1. an Ising fixed point at \(K^*_{Z1} \approx 0.61\) and \(K^*_{XY1} = 0\);
2. an X-Y fixed point at \(K^*_{Z1} \approx 0.58\) and \(K^*_{XY1} \approx 1.31\).

For \(d = 3\), we have the following non-trivial fixed points:

1. an Ising fixed point at \(K^*_{Z1} \approx 0.26\) and \(K^*_{XY1} = 0\);
2. an isotropic Heisenberg fixed point at \(K^*_{Z1} = K^*_{XY1} \approx 0.34\);
3. an X-Y fixed point at \(K^*_{Z1} \approx 0.02\) and \(K^*_{XY1} \approx 0.28\).

As discussed in Appendix A, the renormalization equations (4.1) and (4.2) determine the critical lines associated with these non-trivial fixed points in the parameter space. Figure 6 shows the critical lines determined from these renormalization equations for two dimensions. Figure 7 shows the critical lines for three dimensions. As discussed in Appendix A, the critical behaviour near a critical line is controled by the fixed point which the critical line is associated with. In this case, the critical behaviour for \(K_Z > K_{XY}\) is controled by the Ising fixed point and for \(K_Z < K_{XY}\) by the X-Y fixed point in both two and three dimensions. In other words, the model with \(K_Z > K_{XY}\) shows the critical behaviour of the Ising type and the model with \(K_Z < K_{XY}\) shows that of the X-Y type. In three dimensions the critical behaviour of the isotropic Heisenberg model (i. e., \(K_{XY} = K_Z\)) is controled by the isotropic Heisenberg fixed
point. That is, the isotropic Heisenberg model shows the critical behaviour of its own type. Thus, the present model is classified into three universality classes, namely, the Ising, Isotropic Heisenberg and X-Y types; this classification is very reasonable.

For the isotropic Heisenberg model, there is a non-trivial fixed point in three dimensions. On the contrary, there is no non-trivial fixed point in two dimensions. In other words, the isotropic Heisenberg model undergoes a phase transition at a finite temperature in three dimensions, but undergoes no phase transition at any non-zero temperature in two dimensions. This result agrees well with those obtained by the high temperature series expansions.\(^{22,36}\)

The critical lines for two dimensions shown in Fig. 6 and those for three dimensions shown in Fig. 7 agree very well with those suggested by the analysis of the high temperature series.\(^{35}\) That is, the critical temperature is almost constant in the region \(0 \leq J_{\text{XY}}/J_z \leq 0.7\) for the square lattice and \(0 \leq J_{\text{XY}}/J_z \leq 0.8\) for the simple cubic lattice.

### 4–2. Critical properties

In the previous section, we have determined the critical points of the present model and the types of the critical behaviour. In this section, we investigate the critical properties.

As discussed in Appendix A, critical exponents can be determined from the renormalization equation linearized around the fixed point. First, we calculate the thermal exponent \(\gamma_T\) explained in Appendix A. Linearizing the renormalization equations (4.1) and (4.2) around a non-trivial fixed point \(K_{Z1} = K^*_{Z1}\) and \(K_{\text{XY}1} = K^*_{\text{XY}1}\), we get

\[
\begin{pmatrix}
K'_{Z1} \\
K'_{\text{XY}1}
\end{pmatrix}
= \left( \begin{array}{cc}
\frac{\partial K'_{Z1}}{\partial K_{Z1}} & \frac{\partial K'_{Z1}}{\partial K_{\text{XY}1}} \\
\frac{\partial K'_{\text{XY}1}}{\partial K_{Z1}} & \frac{\partial K'_{\text{XY}1}}{\partial K_{\text{XY}1}}
\end{array} \right)
\begin{pmatrix}
K^*_{Z1} \\
K^*_{\text{XY}1}
\end{pmatrix}
\]

\[\tag{4.3}

\text{with}

\[\frac{\gamma^*_{T1}}{\gamma^*_{T1}} = \frac{\partial K'_{Z1}}{\partial K_{Z1}} \frac{\partial K'_{Z1}}{\partial K_{\text{XY}1}} \frac{\partial K'_{\text{XY}1}}{\partial K_{Z1}} \frac{\partial K'_{\text{XY}1}}{\partial K_{\text{XY}1}} \]

\[= \begin{pmatrix}
\frac{\partial K'_{Z1}}{\partial K_{Z1}} & \frac{\partial K'_{Z1}}{\partial K_{\text{XY}1}} \\
\frac{\partial K'_{\text{XY}1}}{\partial K_{Z1}} & \frac{\partial K'_{\text{XY}1}}{\partial K_{\text{XY}1}}
\end{pmatrix}
\begin{pmatrix}
K_{Z1} = K^*_{Z1} \\
K_{\text{XY}1} = K^*_{\text{XY}1}
\end{pmatrix}
\]

\[\tag{4.4}

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where $K'_{ZI}$ and $K'_{XY}$ are defined by Eqs. (4.1) and (4.2). This equation corresponds to Eq. (A.20). Then, we calculate the eigenvalues of the matrix $\tilde{T}^*_l$ for each fixed point. Only one of two eigenvalues is relevant (i.e., greater than unity) for the Ising and X-Y fixed points in two and three dimensions. The thermal exponent $\gamma_T$ is determined from this relevant eigenvalue $\lambda_T$, using Eq. (A.30); we have used the scale factor $\ell = 2$ in this case.

For the isotropic Heisenberg fixed point, two eigenvalues are both relevant in three dimensions. One of these eigenvalues is associated with a scaling field which measures the deviation from the isotropic Heisenberg axis in the parameter space. Therefore, this eigenvalue $\gamma_\text{g}$ does not enter the critical behaviour of the isotropic Heisenberg model. However, this eigenvalue $\lambda_T$ determine the cross-over behaviour from the isotropic Heisenberg model to the Ising model or the X-Y model; it determines how a point being out of the isotropic Heisenberg axis but near the isotropic Heisenberg fixed point leaves the isotropic Heisenberg fixed point and approached one of other fixed points, as the renormalization transformation goes on. Hence, we define the anisotropy exponent $\gamma_\text{g}$ as

$$\gamma_\text{g} = \ln \frac{\lambda_T}{\ln \ell} .$$  \hspace{1cm} (4.5)

On the contrary, the other relevant eigenvalue is coupled to the distance from a point on the isotropic Heisenberg axis to the isotropic Heisenberg fixed point. Therefore, this eigenvalue $\lambda_T$ determines the critical behaviour of the isotropic Heisenberg model. From this eigenvalue $\lambda_T$, the thermal exponent $\gamma_T$ is determined from Eq. (A.30). From these two exponents $\gamma_\text{g}$ and $\gamma_T$, the cross-over exponent $\phi$ \cite{40,41} is defined by

$$\phi = \frac{\gamma_\text{g}}{\gamma_T} .$$  \hspace{1cm} (4.6)

Table 1. shows the exponents thus obtained for each fixed point.

Next, we calculate the magnetic exponent $\gamma_H$. The Hamiltonian with a magnetic field is written as

$$\hat{\mathcal{H}} = \sum_{\langle ij \rangle} \left( K'_{ZI} \sigma_i^z \sigma_j^z + K'_{XY} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \right) + h_\alpha \sum_i \sigma_i^\alpha ,$$  \hspace{1cm} (4.7)
where $h_\alpha$ denotes a magnetic field coupled to $\alpha$-component of spins and $\alpha$ denotes $x$ or $z$. In order to apply the Migdal-Kadanoff transformations to this Hamiltonian, we have to generalize the one-dimensional decimation and the potential moving. These generalizations are given in Appendix C and Appendix B respectively. Using these generalizations, we can construct the renormalization equations including the magnetic field. To the first order of the magnetic field, the renormalization equations for $K_Z$ and $K_{XY}$ are unchanged. At a non-trivial fixed point $K_Z = K_Z^*$ and $K_{XY} = K_{XY}^*$, the renormalization equation for the magnetic field $h_\alpha$ takes, to the first order of it, the form

$$h'_\alpha = \lambda_\alpha h_\alpha,$$

(4.8)

where $\lambda_\alpha$ is determined from $K_Z^*$ and $K_{XY}^*$ and $\alpha$ denotes $x$ or $z$. From this eigenvalue $\lambda_\alpha$, the magnetic exponent $y_{H_\alpha}$ is given by

$$y_{H_\alpha} = \ln \lambda_\alpha / \ln \ell.$$

(4.9)

For the Ising fixed point in two and three dimensions, $y_{H_x} < 0$ and $y_{H_z} > 0$. That is, the magnetic field transverse to the Ising axis is irrelevant and the magnetic field parallel to the Ising axis is relevant. On the contrary, for the X-Y fixed point in two and three dimensions $y_{H_x} > 0$ and $y_{H_z} < 0$. That is, the magnetic field parallel to the X-Y plane is relevant and the magnetic field perpendicular to the X-Y plane is irrelevant. For the isotropic Heisenberg fixed point in three dimensions, $y_{H_x} = y_{H_z} > 0$. These results are also shown in Table 1. The above result for the Ising fixed point in two and three dimensions shows that a sufficiently small transverse magnetic field does not change the critical behaviour of the Ising model. This agrees with such result suggested from the series expansion method\textsuperscript{42) that the transverse field changes only the critical temperature without changing the critical exponents until the critical field is reached. The above result for the X-Y fixed point shows that a sufficiently small magnetic field perpendicular to the X-Y plane does not change the critical behaviour of the X-Y model. This seems to be reasonable from the analogy of the Ising model.

The renormalization equations for the coupling constants of $I$-direction are given by Eqs. (4.1) and (4.2). However, the renormalization equations for the coupling constants of 2-
direction are different from Eqs. (4.1) and (4.2). This trouble of anisotropy in the renormalization equations of the Migdal-Kadanoff transformations is explained in Appendix B. If the coupling constants \( K_m = \left( \frac{K_{zm}}{K_{Xym}} \right) \) of m-direction satisfy the condition

\[
K_1 = \ell K_2 = \cdots = \ell^{m-1} K_m = \cdots = \ell^{d-1} K_d ,
\] (4.10)

\( \ell \) being the scale factor, then the renormalized coupling constants \( K'_m \) also satisfy this condition. Hence, if we assume that the coupling constants \( \{ K_m \} \) satisfy the condition (4.10), then the renormalization equations are essentially reduced to Eqs. (4.1) and (4.2) and make no trouble. Therefore, we regard the Migdal-Kadanoff transformations as renormalization transformations for a model whose coupling constants satisfy the condition (4.10).

However, there is a new trouble in comparing these results with the results of other theories, because other theories usually studied the case of isotropic coupling constants, that is, \( K_1 = K_2 = \cdots = K_d \). To avoid this trouble, we consider the following procedure. First, we consider a model with isotropic coupling constants \( \tilde{K} \). Then, from this model, we construct a model whose coupling constants satisfy the condition (4.10) by the potential moving. According to the variational method explained in Appendix B, the potential moving must conserve the total magnitude of coupling constants of any interaction. This means the new anisotropic coupling constants \( K_m \) must satisfy the condition

\[
\sum_{m=1}^{d} K_m = \tilde{d} \tilde{K} .
\] (4.11)

From Eqs. (4.10) and (4.11), the relation between \( K_m \) and \( \tilde{K} \) is given by

\[
K_1 = \ell^{(m-1)} K_m = \frac{\ell^{d-1}(\ell-1)}{\ell^{d-1}} d \tilde{K} .
\] (4.12)

Using this relation, we can compare the results obtained by the Migdal-Kadanoff transformations with those by other theories.

Table 2 shows the results we have calculated about critical points and about exponents \( \nu_T, \nu_H \) and \( \phi \) for the Ising, isotropic Heisenberg and X-Y models in two and three dimensions.
in comparison with results by other theories.

First we examine the results for three dimensions. For the Ising, isotropic Heisenberg and X-Y models in three dimensions, the critical inverse temperature $\tilde{K}_c$ or $K_{1c}$ for each model is in rough agreement with that from the high temperature series.\textsuperscript{36,37,38} The exponents $\gamma_T$ and $\gamma_H$ are in poor agreement. However, the qualitative features are in good agreement: The relative magnitudes of the critical values $\tilde{K}_c$ or $K_{1c}$ for these three models agree with the results obtained from the high temperature series. According to them, the Ising model has the largest thermal exponent $\gamma_T$, the X-Y model has the next largest $\gamma_T$ and the isotropic Heisenberg model has the smallest $\gamma_T$. That is, the singularity of the specific heat of each model is strong in this order. Our result about the thermal exponent $\gamma_T$ for each model shows the same tendency. The high temperature series expansions suggest that the magnetic exponent $\gamma_H$, consequently the exponent $\delta$, takes the same value for the Ising, isotropic Heisenberg and X-Y models. The present magnetic exponents $\gamma_H$ for these models are also nearly the same.

Next, we examine the results for two dimensions. For the Ising model in two dimensions, the critical value $\tilde{K}_{c} \simeq 0.46$ is in very good agreement with the exact value $K_{c} \simeq 0.44$.\textsuperscript{45} Though the thermal exponent $\gamma_T \simeq 0.75$ is in poor agreement with the exact value $\gamma_T = 1.0$,\textsuperscript{45} the magnetic exponent $\gamma_H \simeq 1.81$ is in good agreement with the exact value $\gamma_H = 1.875$.\textsuperscript{46} For the X-Y model in two dimensions, the critical value $\tilde{K}_{c} \simeq 0.9$ seems too large compared with the value $K_{c} \simeq 0.55$ estimated from the high temperature series.\textsuperscript{23} Considering that the Migdal-Kadanoff transformations have the nature of high temperature approximation in this case and can give only qualitative or semi-quantitative results in general, we can only suggest that the two-dimensional X-Y model undergoes a phase transition and the critical value $K_c$ lies in the region $K_{2c} \leq K_c \leq K_{1c}$, where $K_{1c} = 2K_{2c} \approx 1.2$. The thermal exponent $\gamma_T$ obtained in our method is rather small; this means that the singularity of the specific heat is very weak. This agrees with such suggestion from the high temperature series\textsuperscript{24} that the specific heat is non-singular. The fact that $\gamma_T$ is small also means that the corresponding eigenvalue $\lambda_T$ is semi-marginal, that is, $\lambda_T \sim 1$. As discussed in Chapter II, the existence of a marginal scaling field suggests the existence of the fixed line; this fixed line is expected to appear for the classical X-Y and planar models. Therefore this semi-marginal thermal exponent $\gamma_T$ suggests that the two-dimensional spin 1/2 X-Y model shows the critical behaviour of the same type as expected for the classical models. This small $\gamma_T$ also leads to the large exponent $\gamma$ of the susceptibility
4–3. Thermodynamic properties

The free energy of the system can be calculated numerically from Eq. (A.36). The internal energy and the specific heat can be calculated as the derivatives of this free energy. Using the relation (4.12), we can compare our results with the results by other theories.

Figure 8 shows the free energy, the internal energy and the specific heat of the two-dimensional Ising model obtained from our renormalization calculation with the scale factor \( \ell = 2 \), in comparison with Onsager’s exact solution.\(^{43}\) Though the exact solution for the model with anisotropic coupling constants is available, we compare our results with the exact solution only for the isotropic model using the relation (4.12) to test how this relation works. The agreement of the two results is fairly good. For the Ising model, the approximate one-dimensional decimation gives the exact result. Therefore, the approximation used in the Migdal-Kadanoff transformation is only the potential moving. As shown in Appendix B, this potential moving gives the lower bound of the free energy. It becomes exact in the two limits of infinite and zero temperatures in this case.\(^{17}\) These features can be seen from the curves of the free energy in Fig. 8: The present free energy is always below the exact free energy and difference between the two is zero at \( K_Z = 0 \) (i.e., infinite temperature) and seems to go to zero in the limit of \( K_Z \to \infty \) (i.e., zero temperature).

For the model with \( K_{XY} \neq 0 \), the approximation for the one-dimensional decimation is employed besides the potential moving, Figure 9 shows the free energies of the two-dimensional X-Y model and the two-dimensional isotropic Heisenberg model obtained in our calculation in comparison with those from the high temperature series.\(^{24},^{36}\) Taking it into account that the additional potential moving is used to derive the relation (4.12) and that the Migdal-Kadanoff transformations give only the qualitative or semi-quantitative results, we can say that the agreement between our calculation and the result by the high temperature series is not so bad.

Figure 10 shows the specific heat of the two-dimensional model with various anisotropies
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obtained from our calculation. In Section 4-1, it is expected that the critical behaviour of the model with $0 \leq J_{XY}/J_Z < 1$ is of the Ising type and the critical behaviour of the model with $0 \leq J_Z/J_{XY} < 1$ is of the X-Y type. Moreover, as seen in Section 4-2, the singularity of the specific heat of the model with $0 \leq J_Z/J_{XY} < 1$ is expected to be weak, because the thermal exponent $\gamma_T$ of the X-Y fixed point is rather small. The features of Fig. 10 are in agreement with these expectations. The specific heat for $0 \leq J_{XY}/J_Z < 1$ has a cusp at the critical temperature. The specific heat for $0 \leq J_Z/J_{XY} < 1$ shows no distinguishable singularity even at the critical temperature; this agrees with the suggestion from the high temperature series as discussed in Section 4-2.

V. Summary and conclusions

We have proposed a simple approximate decimation method for one-dimensional quantum spin systems. The spin 1/2 anisotropic Heisenberg model in one dimension is studied by this approximation. The thermodynamic properties obtained from this approximation are in good agreement, at high temperatures, with the previous results. At low temperatures, this approximation gives qualitatively reasonable results. The ground state energies obtained from this approximation are in rough agreement with the exact results.

Using this approximation, we generalize the Migdal-Kadanoff transformations to quantum spin systems. By this generalized Migdal-Kadanoff transformation with the scale factor $\lambda = 2$, the two- and three-dimensional spin 1/2 anisotropic Heisenberg models are studied. In both two and three dimensions, the Migdal-Kadanoff transformation gives critical lines in the parameter space and divides the parameter space into some universality classes. The shape of the critical lines is in agreement with the predictions from the high temperature series. The division of the parameter space into the universality classes is also reasonable. For the Ising, isotropic Heisenberg and X-Y models in three dimensions, the critical exponents derived from the renormalization transformation are quantitatively in poor agreement with the results from the high temperature series. However, the qualitative features obtained from the renormalization transformations are in agreement with those expected from the high temperature series. That is, the thermal exponents $\{ \gamma_T \}$ for the Ising, X-Y and isotropic Heisenberg models are larger in this order, and the magnetic exponents $\{ \gamma_H \}$ are nearly the same for all three models. For the
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Ising model in two dimensions, the critical properties and the thermodynamic properties obtained from the renormalization transformation are in good agreement with the exact results. As mentioned above, this simple renormalization transformation gives qualitatively reasonable results for two- and three-dimensional models except for the two-dimensional X-Y model.

For the X-Y model in two dimensions, the critical properties obtained from the renormalization transformation suggest those expected for the classical models from other theories. That is, the thermal exponent $\gamma_T$ is close to zero. Though this small $\gamma_T$ is consistent with the suggestion from the high temperature series that the specific heat of the two-dimensional X-Y model is not singular, it is not consistent with the suggestion also from the high temperature series that the susceptibility of this model diverges with a usual power law with exponent $\gamma \approx 1.5$. In short, our results suggest that the two-dimensional X-Y model undergoes some kind of phase transition and that the critical behaviour of this model is similar to that expected for the classical models.

Finally, we point out remaining problems. For the anisotropic Heisenberg model, the calculation of the susceptibility can be done in this framework. The model with a finite magnetic field such as the transverse Ising model can also be treated in this approach.

Appendix A. Real space renormalization transformations

On the basis of the concept of length scale invariance of critical phenomena, Kadanoff\textsuperscript{45} derived scaling laws for a Ising spin system near the critical point by considering a coarse graining procedure which changes a length scale of the system. This procedure transforms the original ferromagnetic spin system whose spin variables are called site spins to a new spin system whose spin variables are called cell spins. First, the site spin system is divided into cells each containing $\ell^d$ site spins, where $d$ is the dimensionality of the lattice. The parameter $\ell$ is the factor of the change of length scale and is chosen to be much smaller than the correlation length of the site spin system measured in lattice units and larger than unity; this correlation length diverges at the critical point. Then, cell spins are assigned to each cell. Since the system is near the critical point, site spins contained in a cell are inclined to point to almost the same direction. The cell spin which is assigned to this cell is chosen to point to the same direction. The cell spin system has the same lattice structure as the site spin system has, except that the
lattice constant of the cell spin system is $\ell$ times as large. Interactions of spins of both systems are assumed to have the same form and to be characterized by coupling constants of the same kind. Coupling constants of the cell spin system are considered to be regular functions of those of the site spin system, because the singular behaviour of the site spin system comes from its fluctuations of range much longer than $\ell$. If the site spin system is at the critical point, the cell spin system is considered to be at the critical point, because critical phenomena are length scale invariant. After such considerations, relations among the critical exponents, so called scaling laws, can be derived from the scaling relation between the singular part of the site free energy and that of the corresponding cell free energy. However, critical exponents themselves cannot be determined, because the procedure which transforms the site spin system to the cell spin system is not known explicitly.

The real space renormalization group approach aims at giving microscopical procedures to transform a spin system to a new spin system which has $\ell$ times as large length scale.

Below in this appendix, we give a brief review of the formulation of the real space renormalization transformations, following Niemeijer and van Leeuwen.\footnote{Niemeijer, H. and van Leeuwen, F. (1982).}

A–1. Renormalization transformations

We consider a site spin system on a $d$-dimensional lattice. The spin variable on $i$ site of the lattice is denoted by $\sigma_i$, where $i = 1, 2, \ldots, N$. The Hamiltonian of the system including the factor $-\beta = -1/k_B T$ is denoted by $\mathcal{H}(\{\sigma\})$; this Hamiltonian $\mathcal{H}(\{\sigma\})$ is chosen to have no constant term independent of the spin variables $\{\sigma_i\}$. The free energy $F$ of the system is given by

$$F = \ln \text{Tr}_{\{\sigma\}}[\exp(\mathcal{H}(\{\sigma\}))], \quad (A.1)$$

where $\text{Tr}_{\{\sigma\}}$ denotes the trace over all spin variables $\{\sigma_i\}$. In order to construct a cell spin system, the lattice sites are divided into cells each containing $\ell^d$ sites. A cell spin variable is assigned to each cell. In the same way as the site spin system, the cell spins are denoted by $\mu_j$, where $j = 1, 2, \ldots, N/\ell^d$, and the Hamiltonian of the cell spin system is denoted by $\mathcal{H}'(\{\mu\})$; this Hamiltonian is chosen to have no constant term.

A renormalization transformation is defined by the equation
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\[
\exp(G + \mathcal{H}'(\{\mu\})) = \text{Tr}_{\{\sigma\}}[\exp(\mathcal{H}(\{\sigma\})) T(\{\mu\}, \{\sigma\})], \tag{A.2}
\]

where \(G\) denotes a constant term and \(T(\{\mu\}, \{\sigma\})\) is called a transformation function. \(T(\{\mu\}, \{\sigma\})\) is chosen to satisfy the condition

\[
\text{Tr}_{\{\mu\}} T(\{\mu\}, \{\sigma\}) = 1. \tag{A.3}
\]

This means the invariance of the free energy under this transformation:

\[
\text{Tr}_{\{\mu\}}[\exp(G + \mathcal{H}'(\{\mu\}))] = \text{Tr}_{\{\sigma\}}[\exp(\mathcal{H}(\{\sigma\}))]. \tag{A.4}
\]

\(T(\{\mu\}, \{\sigma\})\) is chosen such that the cell spin system has the same lattice structure and \(\ell\) times as large lattice constant as the site spin system has, and that \(\mathcal{H}'\) has the same symmetries as \(\mathcal{H}\) has. Then, if \(\mathcal{H}\) is characterized by interaction parameters \(K\), such as nearest-neighbour, next-nearest-neighbour and four spin coupling constants, \(\mathcal{H}'\) can also be characterized by interaction parameters \(K'\) of the same kind. Therefore, the transformation of \(\mathcal{H}\) to \(\mathcal{H}'\) can be considered as the transformation of the parameters \(K\) to the parameters \(K'\); this is expressed as

\[
K' = R(K). \tag{A.5}
\]

These equations are called the renormalization equations. The constant term \(G\) in Eq. (A.3) is also a function of \(K\) and can be written as

\[
G = G(K). \tag{A.6}
\]

The free energy \(F'\) of the cell spin system is given by

\[
F' = \ln \text{Tr}_{\{\mu\}}[\exp(\mathcal{H}'(\{\mu\}))]. \tag{A.7}
\]

Therefore, Eq. (A.4) can be written as
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\[ F' + G = F \]  \hspace{1cm} (A.8)

In the thermodynamic limit \( N \to \infty \), the free energy \( f \) per spin of the site spin system as a
function of \( K \) is written as

\[ f(K) = \frac{1}{N} F \]  \hspace{1cm} (A.9)

In the same way, the free energy per spin of the cell spin system is given by

\[ f(K') = \frac{1}{N/\rho^d} F' \]  \hspace{1cm} (A.10)

where \( f \) is the same function as is defined in Eq. (A.9). Then, using Eqs. (A.9) and (A.10), we
obtain the basic relation from Eq. (A.8):

\[ f(K) = g(K) + \rho^{-d} f(K') \]  \hspace{1cm} (A.11)

where \( g \) is defined in the thermodynamic limit by

\[ g(K) = \frac{1}{N} G(K) \]  \hspace{1cm} (A.12)

In discussion below, it is the essential assumption that \( K' = R(K) \) and \( g(K) \) are regular
functions of \( K \) even if \( K \) takes the critical value. The point of the renormalization transfor-
mations is that the singular behaviour of \( f(K) \) can be derived from the regular behaviour of \( K' \)
and \( g \). It is also assumed in the following discussion that the transformation function \( T \) can be
chosen such that the assumption of regularities holds. These assumptions are intuitively justi-
fied by the same discussion used in the scaling theory mentioned in the beginning of this appen-
dix.

In general, the transformation function \( T \) which determines the properties of the re-
normalization transformation must be chosen very carefully according to what kind of phase
transition is concerned.
A.2. Critical properties

We consider a fixed point $K^*$ of the renormalization equation (A.5) defined by

\[
K^* = R(K^*) . \tag{A.13}
\]

There are two types of trivial fixed points corresponding to the temperatures $T = \infty$ and $T = 0$. A non-trivial fixed point is assumed below to exist. Since the length scale of the cell spin system is $\ell$ times as large as that of the site spin system, the correlation length $\xi$ measured in lattice units of the system is considered to obey the scaling relation

\[
\xi(K') = \ell^{-1} \xi(K) . \tag{A.14}
\]

From Eqs. (A.13) and (A.14), we get

\[
\xi(K^*) = \ell^{-1} \xi(K^*) . \tag{A.15}
\]

The solutions of this equation are $\xi(K^*) = 0$ and $\xi(K^*) = \infty$. The former is considered to correspond to a trivial fixed point and the latter to a non-trivial fixed point. Hence, the non-trivial fixed point is considered to correspond to the critical point where the correlation length $\xi$ diverges. However, this fixed point is not the only single critical point in the parameter space. If a point $K$ in the parameter space satisfies the condition

\[
\lim_{n \to \infty} R^n(K) = K^* , \tag{A.16}
\]

where

\[
R^n(K) = R^{n-1}(R(K)) \tag{A.17}
\]

for $n \geq 2$ and

\[
R'(K) = R(K) , \tag{A.18}
\]
then the correlation length $\xi$ diverges at this point $K$:

$$\xi(K) = \infty.$$  \hfill (A.19)

Therefore, this point $K$ is also the critical point. The set of the critical points associated with the fixed point $K^*$ by the condition (A.16) is called the critical surface associated with the fixed point $K^*$. If there are more than one fixed points, each fixed point has a critical surface associated with it.

Assuming that the renormalization equation (A.5) is regular around the fixed point $K^*$, we linearize the equation (A.5) around the fixed point $K^*$ as follows:

$$K' - K^* = \hat{T}^* (K - K^*) ,$$  \hfill (A.20)

where

$$\hat{T}^* = \frac{\partial R(K)}{\partial K} \bigg|_{K = K^*} .$$  \hfill (A.21)

Let $\phi^i_i$ denotes the $i$-th left eigenvector of the matrix $\hat{T}^*$ with the eigenvalue $\lambda_i$:

$$\phi^i_i \hat{T}^* = \lambda_i \phi^i_i .$$  \hfill (A.22)

Generally, the eigenvalues of $\hat{T}^*$ are not necessarily real. Using these eigenvectors, we define the scaling field $u_i(K)$ to the first order in $(K - K^*)$ by

$$u_i(K) = \phi^i_i (K - K^*) .$$  \hfill (A.23)

Then, to the first order in $(K - K^*)$, the scaling field $u_i$ satisfies

$$u_i(K') = \lambda_i u_i(K) .$$  \hfill (A.24)
It is possible to define the scaling field \( u_i \) such that it satisfies Eq. (A.24) to any order in \( (K - K^*) \). The scaling field \( u_i \) is called relevant, irrelevant and marginal corresponding to \( |\lambda_i| \) is larger, less than and equal to unity, respectively. The fixed point corresponds to the point where all the scaling fields are zero and the critical surface corresponds to the point where all the relevant scaling fields are zero, because the scaling field \( u_i \) grows or diminishes by the renormalization transformation according to it is relevant or irrelevant.

According to the relation (A.11), the free energy \( f \) per spin as the function of the scaling fields obey the relation

\[
f(u_1, u_2, \cdots) = g(u_1, u_2, \cdots) + \xi^{-d} f(\lambda_1 u_1, \lambda_2 u_2, \cdots). \tag{A.25}
\]

In order to see how the singularities of the free energy \( f \) can be derived from the relation (A.25), we assume that there are only two relevant scaling fields \( u_T \) and \( u_H \) with real positive eigenvalues \( \lambda_T \) and \( \lambda_H \). The scaling field \( u_T \) is assumed to be coupled to the temperature and to measure the deviation of the temperature from the critical point. The scaling field \( u_H \) is assumed to be coupled to the ordering field.

Setting all the scaling fields other than \( u_T \) and \( u_H \) zero, we get from Eq. (A.25)

\[
f(u_T, u_H) = g(u_T, u_H) + \xi^{-d} f(\lambda_T u_T, \lambda_H u_H). \tag{A.26}
\]

Since it is assumed that \( g \) is a regular function of \( K \) and of \( u_i \), the singular part \( f_{\text{sing}} \) of the free energy \( f \) obeys the equation

\[
f_{\text{sing}}(u_T, u_H) \sim \xi^{-d} f_{\text{sing}}(\lambda_T u_T, \lambda_H u_H). \tag{A.27}
\]

Critical exponents \( \alpha, \beta, \gamma \) and \( \delta \) for the specific heat \( C \), the spontaneous magnetization \( M \), the susceptibility \( \chi \) and the magnetization at the critical temperature are defined by

\[
C \sim \frac{\partial^2 f}{\partial u_T^2} \bigg|_{u_H=0} \sim u_T^{-\alpha}, \tag{A.28a}
\]
From Eq. (A.27), these exponents can be expressed as

\[ \alpha = 2 - d/y_T, \]  
(A.29a)

\[ \beta = (d - y_H)/y_T, \]  
(A.29b)

\[ \gamma = (2y_H - d)/y_T. \]  
(A.29c)

and

\[ \delta = y_H/(d - y_H), \]  
(A.29d)

where the thermal exponent \( y_T \) and the magnetic exponent \( y_H \) are defined by

\[
y_T = \frac{\ln \lambda_T}{\ln \xi} \]
(A.30)

and

\[
y_H = \frac{\ln \lambda_H}{\ln \xi}. \]
(A.31)

From similar discussion for the singular part of the correlation function, the critical exponents
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\( \nu \) and \( \eta \) for the correlation length \( \xi \) and for the correlation function \( g(r) \) defined by

\[
\xi \sim u_T^{-\nu}
\]

and

\[
g(r) \big|_{u_T = u_H} = 0 \sim \gamma^{-(d-2+\eta)}
\]

are given by

\[
\nu = 1/y_T \quad \text{(A.32a)}
\]

and

\[
\eta = d + 2 - 2y_H \quad \text{(A.32b)}
\]

Thus, how the deviations from the fixed point grow determines the critical behaviour around the fixed point. Driven by the renormalization transformation, a point in the parameter space near the critical surface associated with a fixed point leaves the fixed point after it has reached in the close vicinity of the fixed point, if the relevant scaling fields are sufficiently small at the initial point. Therefore, the critical behaviour near the critical surface associated with the fixed point is of the same type as the critical behaviour near the fixed point. That is, the critical points associated with the fixed point belong to the same universality class.

A-3. Free energy

Using the renormalization transformation, we can study not only the critical properties such as the critical points and the critical exponents but also the global thermodynamic properties. Using the relation (A.11) repeatedly, we obtain a series expression for the free energy \( f(K) \):

\[
f(K) = \sum_{m=0}^{M} \xi^{-md} g(K^m) + \xi^{-(M+1)d} f(K^{M+1})
\]

(33)
where

\[ K^{(m)} = R^m (K) . \]  

(A.34)

Assuming

\[ \lim_{m \to \infty} \xi^{-m d} f(K^{(m)}) = 0 , \]  

(A.35)

we get from Eq. (A.33)

\[ f(K) = \sum_{m=0}^{\infty} \xi^{-m d} g(K^{(m)}) . \]  

(A.36)

According to this expression, the free energy and the related thermodynamic quantities can be known from the renormalization transformations.

Appendix B. The Migdal-Kadanoff transformations

In this appendix, we give a derivation of the Migdal-Kadanoff transformations, following Kadanoff.17)

First, we derive the "potential moving" by a variational method. As an example of Eq. (A.2), we consider

\[ e^{G+\mathcal{H}'} = \text{Tr}' e^{\mathcal{H}'} , \]  

(B.1)

where Tr' denotes a trace over a part of spin operators and G is a c-number. This renormalization transformation conserves the free energy:

\[ \text{Tr}'' e^{G+\mathcal{H}'} = \text{Tr}'' \text{Tr}' e^{\mathcal{H}'} = \text{Tr} e^{\mathcal{H}'} , \]  

(B.2)

where Tr'' denotes the trace over the remaining spin operators and Tr denotes the trace over all the spin operators. We also consider an approximate renormalization equation defined by
If \( \mathcal{H} \) and \( \Delta \) are hermitian, we can prove

\[
F [ \mathcal{H} + \Delta ] \leq F [ \mathcal{H} ] + \langle \Delta \rangle_{\mathcal{H}} ,
\]

where

\[
F [ A ] \equiv -\ln \left[ \text{Tr} \, e^A \right]
\]

and

\[
\langle \Delta \rangle_{\mathcal{H}} \equiv \frac{\text{Tr} \, \Delta \, e^{\mathcal{H}}}{\text{Tr} \, e^{\mathcal{H}}} .
\]

Therefore, if

\[
\langle \Delta \rangle_{\mathcal{H}} = 0 ,
\]

then

\[
G_A + F [ \mathcal{H}_A' ] = -\ln \left[ \text{Tr}'' \, e^{G_A + \mathcal{H}_A'} \right]
\]

\[
= -\ln \left[ \text{Tr}'' \, \text{Tr}' \, e^{\mathcal{H} + \Delta} \right]
\]

\[
= -\ln \left[ \text{Tr} \, e^{\mathcal{H} + \Delta} \right]
\]

\[
= F [ \mathcal{H} + \Delta ] \leq F [ \mathcal{H} ]
\]

That is, the approximate renormalization transformation gives a free energy which is smaller than the exact free energy. Let the Hamiltonian \( \mathcal{H} \) be a sum of local interactions:
\[ \mathcal{H} = \sum_{k} \sum_{i} A_{i}^{k}(\sigma), \quad (B.9) \]

where \( i \) denotes the lattice site, \( A_{i}^{k}(\sigma) \) denotes a local interaction on \( i \) site and \( k \) labels the types of local interactions. For example, \( A_{i}^{m}(\sigma) = K_{m} \sigma_{i} \cdot \sigma_{i} + \delta_{m} \), where \( m \) labels the direction of nearest-neighbour bond and \( i + \delta_{m} \) denotes the nearest-neighbour site of \( i \) site in \( m \)-direction.

From the symmetry of the Hamiltonian,

\[ \langle A_{i}^{k}(\sigma) \rangle = \frac{\text{Tr} \ e^{\mathcal{H}} A_{i}^{k} \ e^{-\mathcal{H}}}{\text{Tr} \ e^{-\mathcal{H}}} \quad (B.10) \]

is independent of \( i \). Therefore, if we choose

\[ \Delta = \sum_{i} q_{k}(i) A_{i}^{k}(\sigma) \quad (B.11) \]

with the condition

\[ \sum_{i} q_{k}(i) = 0. \quad (B.12) \]

for all \( k \), then this \( \Delta \) satisfies the condition (B.7). Using this \( \Delta \), we can construct an approximate renormalization transformation which satisfies the condition (B.8). The equations (B.11) and (B.12) are interpreted as follows: According to the variational method, we can move potential terms from one set of bonds in the lattice to equivalent bonds, but we must not increase or decrease the total amount of any type of bond. This is called “potential moving”.

Next, we derive the renormalization equations using the potential moving. We consider the following Hamiltonian on the \( d \)-dimensional hypercubic lattice:

\[ \mathcal{H} = \sum_{m} \sum_{m} <ij> \epsilon_{m} \left\{ K_{zm} \sigma_{i}^{z} \sigma_{j}^{z} + K_{xm} \sigma_{i}^{x} \sigma_{j}^{x} + K_{ym} \sigma_{i}^{y} \sigma_{j}^{y} \right\} \quad (B.13) \]

with

\[ K_{xm} = K_{ym} = K_{xy m}, \]

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where $i$ denotes the lattice site, $\sigma^x_i$, $\sigma^y_i$ and $\sigma^z_i$ denote the Pauli spin operators on $i$ site, $m = 1, 2, \cdots, d$ labels the direction of the nearest-neighbour bond and $\sum_{\langle ij\rangle \in m} \kappa$ denotes the sum over all the nearest-neighbour pairs on $m$-direction bond. First, we consider the decimation which changes the length scale of $1$-direction by a factor $\kappa$ as shown in Fig. 11(a). By the method explained above, we move the bond between the spins those which are to be eliminated by the decimation to the equivalent bonds between the spins those which are to remain after the decimation, as shown in Fig. 11(a). As a result, the spins to be eliminated are on the one dimensional chains of bonds as shown in Fig. 11(b). Therefore, if $K_{XY1} = 0$, we can carry out the decimation exactly. However, we cannot carry out the decimation exactly in the case $K_{XY1} \neq 0$. Then, using the same approximation as used in Chapter III, we carry out the decimation approximately to get a new nearest-neighbour interaction between the remaining spins. Now, we have a new lattice whose lattice constant of $1$-direction is $\kappa$ times as large as that of the original lattice; Fig. 11(c) shows this lattice. The interaction of $1$-direction in this new lattice is generated from the approximate decimation mentioned above. The coupling constants $K'_1 = \begin{pmatrix} K'_{Z1} \\ K'_{XY1} \end{pmatrix}$ of this new interaction of $1$-direction are given as the functions of the original coupling constants $K_1 = \begin{pmatrix} K_{Z1} \\ K_{XY1} \end{pmatrix}$ by

$$K'_1 = R_\kappa (K_1), \quad (B.14)$$

where $\kappa$ denotes the scale factor; the function $R_\kappa (K)$ is determined from Eq. (3.15). The interactions of the other directions, that is, $2$-, $3$-, $\cdots$ and $d$-directions, are generated from the potential moving mentioned above. The new coupling constants $K'_m = \begin{pmatrix} K'_{Zm} \\ K'_{XYm} \end{pmatrix}$ of $m$-direction bond are given by

$$K'_m = \kappa K_m, \quad (B.15)$$

where $K_m = \begin{pmatrix} K_{Zm} \\ K_{XYm} \end{pmatrix}$ denote the original coupling constants of $m$-direction bond, because $(\kappa - 1)$ bonds have been moved to one bond of $m$-direction. See Fig. 11(c). We apply this procedure which rescales the length scale of one direction by a factor of $\kappa$ to $2$-, $3$-, $\cdots$ and $d$-directions successively as shown in Figs. 11(c) and (d). Then, we have a lattice whose lattice constant of every direction is $\kappa$ times as large as that of the original lattice as shown in Fig.
11(e). The new coupling constants $K'_m$ of $m$-direction bond are given by

$$K'_m = q^{d-m} R_q (q^{m-1} K_m) .$$  \hfill (B.16)

This is the renormalization equation to be derived. This renormalization equation has a trouble: Each interaction of different direction has a different renormalization equation. Therefore, if we start with isotropic interaction $K_1 = K_2 = \cdots = K_d$, we get anisotropic interactions after this renormalization transformation. However, if the coupling constants $K_m$ satisfy the condition

$$K_1 = q K_2 = \cdots = q^{m-1} K_m = \cdots = q^{d-1} K_d ,$$  \hfill (B.17)

then the renormalized coupling constants $K'_m$ are given by

$$K'_m = q^{d-m} R_q (q^{m-1} K_m)$$
$$= q^{d-m} R_q (K_1) = q^{-(m-1)} (q^{d-1} R_q (K_1))$$
$$= q^{-(m-1)} K'_1 ,$$  \hfill (B.18)

and satisfy the same condition

$$K'_1 = q K'_2 = \cdots = q^{m-1} K'_m = \cdots = q^{d-1} K'_d .$$  \hfill (B.19)

In other words, if we assume that the coupling constants satisfy the condition (B.17), the renormalization equation (B.16) for each direction is essentially the same and can be reduced to one of them. Therefore, in order to avoid the anisotropy in the renormalization equations, we restrict ourselves to applying the renormalization equation (B.16) only to a system whose coupling constants satisfy the condition (B.17).

Finally, we apply the Migdal-Kadanoff transformation to the model with a magnetic field. There is ambiguity in moving the magnetic field term. We treat below the magnetic field term

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so that there is no anisotropy in the renormalization equations. Let $K_m = \begin{pmatrix} K_{Zm} \\ K_{Xm} \\ K_{Ym} \end{pmatrix}$ denote the nearest-neighbour coupling constants of $m$-direction bond as before, and let $h$ denote the magnetic field. We assume that the coupling constants $K_m$ satisfy the condition (B.17) in order to avoid the trouble of the anisotropy in the case $h = 0$. In order to change the length scale of 1-direction, we first move the bonds between the spins to be eliminated to the bonds between the spins to remain as shown in Fig. 12(a). Then, using the same approximation as used in Chapter III, we carry out the decimation as shown in Fig. 12(b). Then the new coupling constants of 1-direction $K'_1$ and the new magnetic field $h'$ are given as the functions of the original $K_1$ and $h$:

$$K'_1 = R_K (K_1, h) \tag{B.20}$$

and

$$h' = t_K (K_1, h) \tag{B.21}$$

where $K'_1$ and $h'$ are determined from Eq. (C.11). The new coupling constants $K'_m$ of the other directions are given by

$$K'_m = \ell K_m \tag{B.22}$$

where $m = 2, 3, 4, \cdots, d$ and $K_m$ are the original coupling constants. Next, we consider to change the length scale of 2-direction. If we move only the nearest-neighbour interactions and do not move the magnetic field, the new coupling constants $K''_2$ of 2-direction and the new magnetic field $h''$ are given by

$$K''_2 = R_K (K'_2, h') \tag{B.23}$$

and
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\[ h'' = r_\ell (K'_2, h') \]  \hspace{1cm} (B.24)

From the condition (B.17), \( K'_2 = \ell K_2 = K_1 \). However, \( h' \) is given by Eq. (B.21) and \( h' \neq h \). Therefore, the right side of Eq. (B.23) is not identical to the right side of Eq. (B.20). Hence, if we apply this procedure to 3-, 4-, \cdots and \( d \)-directions successively, the final renormalized coupling constants do not satisfy the condition (B.17). That is, this procedure causes the trouble of anisotropy. Therefore, we move the additional magnetic field \( \Delta h \equiv h' - h \) as shown in Fig. 12(c). Then, we carry out the decimation approximately as shown in Fig. 12(d) and get the new coupling constants \( K''_2 \) and the new magnetic field \( h'' \) as

\[ K''_2 = R_\ell (K'_2, h) \]

\[ = R_\ell (\ell K_2, h) = R_\ell (K_1, h) = K'_1 \]  \hspace{1cm} (B.25)

and

\[ h'' = r_\ell (K'_2, h) + \ell (h' - h) \]

\[ = r_\ell (\ell K_2, h) + \ell (h' - h) \]

\[ = r_\ell (K_1, h) + \ell (h' - h) \]

\[ = h' + \ell (h' - h) \]

\[ = (\ell + 1)h' - \ell h \]  \hspace{1cm} (B.26)

The nearest-neighbour coupling constants of other directions are given by

\[ K''_m = \ell K'_m \],  \hspace{1cm} (B.27)

where \( m = 1, 3, 4, \cdots, d \). Applying this procedure to 3-, 4-, \cdots and \( d \)-directions succes-
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sively, we get the new coupling constants $K'_m$ of $m$-direction and the new magnetic field $h'$ as

\begin{equation}
K'_m = \varphi^{d-m} R_{\varphi} (q^{m-1} K_m, h) \tag{B.28}
\end{equation}

and

\begin{equation}
h' = \frac{\varphi^{d+1} - 1}{\varphi - 1} r_{\varphi} (K_1, h) - \frac{\varphi^{d+1} - \varphi}{\varphi - 1} h, \tag{B.29}
\end{equation}

where $K_m$ and $h$ denote the original coupling constants and the original magnetic field. See Fig. 11(e). This renormalized nearest-neighbour coupling constants $K'_m$ also satisfy the condition (B.17), because

\begin{align*}
K'_m &= \varphi^{d-m} R_{\varphi} (q^{m-1} K_m, h) \\
&= \varphi^{d-m} R_{\varphi} (K_1, h) \\
&= \varphi^{-(m-1)} K'_1 \tag{B.30}
\end{align*}

Thus, we obtain the renormalization equation without the trouble of anisotropy.

Appendix C. The approximate one-dimensional decimation

In order to get the renormalization equations of the approximate one-dimensional decimation, we have to solve Eq. (3.15). From the symmetry properties, we can see that the right side of Eq. (3.15) can be expressed in the form of the left side of the equation.

We define

\begin{align*}
\phi &= Z(0,0), \tag{C.1a} \\
\pi_Z &= \frac{\partial}{\partial q} Z(p, q) \bigg|_{p=q=0} \tag{C.1b}
\end{align*}
and

\[ \pi_\ast = \frac{\partial}{\partial p} Z(p, q) \bigg|_{p=q=0}, \quad (C.1c) \]

where

\[ Z(p, q) = \left( \prod_{\ell=0}^{n} \text{Tr}_{\sigma_{\ell}} \right) \exp \left[ \tilde{\mathcal{H}}(p, q) \right], \quad (C.2) \]

with

\[ \tilde{\mathcal{H}}(p, q) = \sum_{\ell=0}^{n-1} \left\{ K_Z \sigma_{\ell}^z \sigma_{\ell+1}^z + K_{XY} \left( \sigma_{\ell}^x \sigma_{\ell+1}^x + \sigma_{\ell}^y \sigma_{\ell+1}^y \right) \right\} + p(\sigma_0^x \sigma_\xi^x + \sigma_0^y \sigma_\xi^y) + q \sigma_0^\xi \sigma_\xi^z. \quad (C.3) \]

From Eq. (3.15) and the definition (C.1), we obtain

\[ \phi = \text{Tr}_{\sigma_0} \text{Tr}_{\sigma_\xi} \exp \left[ \tilde{G} + K' \sigma_0^x \sigma_\xi^x + K' \sigma_0^y \sigma_\xi^y \right], \quad (C.4a) \]

\[ \pi_Z = \text{Tr}_{\sigma_0} \text{Tr}_{\sigma_\xi} \sigma_0^\xi \sigma_\xi^z \exp \left[ \tilde{G} + K_Z' \sigma_0^z \sigma_\xi^z + K' \sigma_0^y \sigma_\xi^y \right], \quad (C.4b) \]

and

\[ \pi_\ast = \text{Tr}_{\sigma_0} \text{Tr}_{\sigma_\xi} \left( \sigma_0^x \sigma_\xi^x + \sigma_0^y \sigma_\xi^y \right) \times \exp \left[ \tilde{G} + K_Z' \sigma_0^z \sigma_\xi^z + K' \sigma_0^y \sigma_\xi^y \right]. \quad (C.4c) \]

After simple calculation, these are written as

\[ \phi = 2 e^{\tilde{G}} (e^{K'Z} + e^{-K'Z} \cosh 2K'_{XY}'), \quad (C.5a) \]

\[ \pi_Z = 2 e^{\tilde{G}} (e^{K'Z} - e^{-K'Z} \cosh 2K'_{XY}'), \quad (C.5b) \]

and
\[ \pi_+ = 4 \varepsilon^2 e^{-K'Z} \sinh 2K_{XY}. \]  

Therefore, \( K'_Z, K'_{XY} \) and \( \tilde{G} \) can be expressed by \( \phi, \pi_z \) and \( \pi_+ \) as follows.

\[
K'_Z = \frac{1}{2} \ln (\phi + \pi_z) - \frac{1}{4} \ln \left\{ (\phi - \pi_z)^2 - \pi_z^2 \right\},
\]

\[
K'_{XY} = \frac{1}{4} \ln \left( \frac{\phi - \pi_z + \pi_+}{\phi - \pi_z - \pi_+} \right)
\]

and

\[
\tilde{G} = \frac{1}{2} \ln (\phi + \pi_z) + \frac{1}{4} \ln \left\{ (\phi - \pi_z)^2 - \pi_z^2 \right\} - \ln 4.
\]

If we know the eigenvalues \( \Lambda_i \) of \( \tilde{H}_q(p, q) \) to the first order of \( p \) and \( q \) as

\[ \Lambda_i(p, q) = \Lambda^0_i + a_i p + b_i q, \]

where \( i = 1, 2, \ldots, 2^q \), then, from the equation

\[ Z(p, q) = \sum_{i=1}^{2^q} e^{\Lambda_i(p, q)}, \]

we get

\[ \phi_z = \sum_{i=1}^{2^q} e^{\Lambda^*_i}, \]

\[ \pi_z = \sum_{i=1}^{2^q} b_i e^{\Lambda^*_i}, \]

and

\[ \pi_+ = \sum_{i=1}^{2^q} c_i e^{\Lambda^*_i}. \]

Hence, we can solve Eq. (3.15) as follows: First, we calculate the eigenvalues of \( \tilde{H}_q(p, q) \) to the first order of \( p \) and \( q \). Then, using Eqs. (C.9) and (C.6), we get \( K'_Z, K'_{XY} \) and \( \tilde{G} \) as the
functions of $K_Z$ and $K_{XY}$. For the scale factor $\ell = 2$, the result is given by Eqs. (3.16) \sim (3.20).

To generalize this approximate one-dimensional decimation to the Hamiltonian with a magnetic field, we take the nearest-neighbour interaction $A(\sigma_i, \sigma_{i+1})$ in Eq. (3.7) as follows:

$$A(\sigma_i, \sigma_{i+1}) = k_z \sigma_i^z \sigma_{i+1}^z + k_x \sigma_i^x \sigma_{i+1}^x + k_y \sigma_i^y \sigma_{i+1}^y + \frac{h}{2}(\sigma_i^2 + \sigma_{i+1}^2)$$

(C.10)

Considering the symmetry properties, we can show that the equation to be solved is given by

$$\left( \prod_{i=1}^{q-1} Tr_{\sigma_i} \right) \exp \left[ \sum_{i=0}^{q-1} A(\sigma_i, \sigma_{i+1}) \right]
\quad = \exp \left[ \tilde{G} + k'_z \sigma_0^z \sigma_k^z + k'_x \sigma_0^x \sigma_k^x + k'_y \sigma_0^y \sigma_k^y + \frac{h'}{2}(\sigma_0^2 + \sigma_k^2) \right].$$

(C.11)

In the same way as above, we can solve this equation and obtain $\tilde{G}, k'_z, k'_x, k'_y$ and $h'$ as the functions of $k_z, k_x, k_y$ and $h$. To the first order of $h$, the new parameters $\tilde{G}, k'_z, k'_x, k'_y$ are independent of $h$, and $h'$ is expressed as

$$h' = \alpha(k_x, k_y, k_z)h,$$

(C.12)

where $\alpha$ is a function of $k_z, k_x$ and $k_y$.

First, we put $k_z = K_z, k_x = k_y = K_{XY}, h = h_z$ and $h' = h'_z$, in Eq. (C.12); this corresponds to the case that the magnetic field is coupled to the $z$-component of spins in Eq. (4.7).

Then, we have

$$h'_z = \frac{A'}{A_0} h_z,$$

(C.13)

where

$$A' \equiv 2 e^{2K_z} + \frac{1}{2} e^{-K_z} \left\{ 1 - \left( \frac{K_z}{K} \right)^2 \right\} \left\{ \cosh \tilde{K} - \frac{1}{K} \sinh \tilde{K} \right\}.$$
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\[ A_0 \equiv e^{2Kz} + e^{-Kz} \left( \cosh \tilde{K} - \frac{Kz}{\tilde{K}} \sinh \tilde{K} \right) \]  

(C.15)

and \( \tilde{K} \) is defined by Eq. (3.20).

Next, we put \( k_z = k_x = K_{XY}, k_y = K_Z, h = h_x \) and \( h' = h'_x \), in Eq. (C.12); this corresponds to the case that the magnetic field is coupled to the x-component of spins in Eq. (4.7). Then, we have

\[ h'_x = \frac{\ln A - \ln B}{A - B} \quad C h_x \]  

(C.16)

where

\[ A \equiv e^{2Kz} + e^{-Kz} \left( \cosh \tilde{K} - \frac{Kz}{\tilde{K}} \sinh \tilde{K} \right) \]  

(C.17)

\[ B \equiv 2 e^{-Kz} \left( \cosh \tilde{K} + \frac{Kz}{\tilde{K}} \sinh \tilde{K} \right) \]  

(C.18)

\[ C \equiv \frac{1}{2(K_Z - K_{XY})} e^{2Kz} \]

\[ + 2 \left| \frac{K_{XY}(K_Z + 4K_{XY})}{K^2} + \frac{1}{4(K_{XY} - K_Z)} \right| e^{-Kz} \cosh \tilde{K} \]

\[ + 2 \left| \frac{K_{XY}}{K} + \frac{1}{4(K_{XY} - K_Z)} \cdot \frac{1}{K^3} \cdot (-K_Z^3 + 8K_Z^2K_{XY}) \right| e^{-Kz} \sinh \tilde{K} \]  

(C.19)

and \( \tilde{K} \) is defined by Eq. (3.20).

References


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37) C. Domb, loc. cit.
38) D. D. Betts, loc. cit.
44) C. N. Yang, Phys. Rev. 85 (1952) 808.
45) L. P. Kadanoff, Physics 6 (1966) 263.

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Table 1. Non-trivial fixed points and exponents in two and three dimensions.

<table>
<thead>
<tr>
<th>fixed point position</th>
<th>exponents</th>
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<tr>
<td>fixed point position</td>
<td>position</td>
</tr>
<tr>
<td></td>
<td>$K_{Z1}^*$</td>
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<tr>
<td>dimension type</td>
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<tr>
<td>2d</td>
<td>Ising</td>
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<td></td>
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<tr>
<td>3d</td>
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<td>X-Y</td>
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Table 2. The critical coupling and critical exponents of the Ising, isotropic Heisenberg and X-Y models in two and three dimensions.
Fig. 1. Decimation in one dimension with scale factor $l = 2$. Circles denote spin operators to be eliminated by the decimation. Dots denote spin operators to remain after the decimation. Lines denote the interactions between neighbouring spins. Crosses mean taking a trace over the spin operator marked with a cross.

Fig. 2. The approximate one-dimensional decimation. The original system is shown in (a). The decimation is carried out within one cluster shown in (b) to give a new interaction which is denoted by a wavy line in (c). From this new interaction, the renormalized system (d) is constructed.
Fig. 3. The ground state energy of the one-dimensional anisotropic Heisenberg model: in (b), "R.G." means the present result and "O." means the exact result by Orbach.39)
Fig. 4. Temperature dependence of the internal energy of the one-dimensional models. "i. H. f." and "i. H. a. f." denote the isotropic Heisenberg model with ferromagnetic and antiferromagnetic couplings, respectively. "XY" denotes the X-Y model. "R. G." means the present result. "B. F." means the result by Bonner and Fisher. 18) "K." means the exact result by Katsura. 19)

Fig. 5. Temperature dependence of the specific heat of the one-dimensional models. The notation here is the same as used in Fig. 4.
Fig. 6. Critical lines of the anisotropic Heisenberg model in two dimensions.
Fig. 7. Critical lines of the anisotropic Heisenberg model in three dimensions.
Fig. 8. The free energy (F), the internal energy (E) and the specific heat (C) of the two-dimensional Ising model. "R. G." means the present result, "O." means the exact result by Onsager.\textsuperscript{45}
Fig. 9 (a) and Fig. 9 (b)

Fig. 9. The free energy of the two-dimensional X-Y model (a) and the isotropic Heisenberg model (b). "R. G." means the present result and "H. T." means the result from the high temperature series.24,36)

Fig. 10. The specific heat of the anisotropic Heisenberg model with various anisotropies.
Fig. 11. The Migdal-Kadanoff transformation in two dimensions.
Fig. 12. The Migdal-Kadanoff transformation for the model with a magnetic field in two dimensions.