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STUDIES ON MEAN-FIELD APPROACH TO RENORMALIZATION GROUP RECURSION

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ABSTRACT

The combination of mean field theory and renormalization group theory is studied under the conjecture of finite size scaling. We derive an equation of state scaling invariance, then reduce to a small size by a mean field approximation, and use it to analyse the critical surfaces of an Ising Model on square lattice with nearest- and next-nearest-neighbours interactions for the ferro-, anti-ferro-, layered I-, and layered II-ground states. The results are reasonable good in high-temperature region, and, with some modification, able to recover a qualitative feature of the low-temperature region.

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0. Introduction.

Most of Statistical Mechanics calculations deal with some approximation. The main stream is perturbation theory, basically a series expansion in some parameters like temperature, density, dimensionality, etc.. The problem of a divergency of any source may arise, and the perturbation theory is breakdown. The ways to avoid such divergency are mostly heuristic, except the exact solution approach. Such calculations are usually called non-perturbative approach or renormalized approximations. The aim is just to absorb all singularities that make the problems in the reference part, which of course must be solvable.

One of the most successful non-perturbative approach is the mean field theory. It gives good quantitative results for first order phase-transitions, and qualitatively shows the critical point behavior. It has been proved rigorously that the three most important phenomenological theories of phase-transition and critical phenomena (the van der Waals-Maxwell, the Curie-Weiss, and the Bragg-William theory) can be recovered by mean field theory for the infinitely-weak-long-range interaction system.¹ The physical assumption of the theory consists in neglecting the local fluctuations. Therefore, for any short range interaction systems, in which statistical information can only propagate step wise through a short distance, the mean field theory is not expected to be valid.

Near the critical point, it is known that fluctuations of all range playing an important role.

Another line of thought, which at least in principle fully takes care of the fluctuations, is the renormalization group theory. The aim of this theory is well described in Wilson's first paper on the subject;² it consists of keeping track of the singularity, that must appear at thermodynamic limit if there is a phase-transition, through a semi-group structure. The critical point singularities are generally power law singularities which can be described in terms of scaling laws. One can generally define a renormalization group theory as a way of taking self-consistently the scaling laws.

Both mean field and renormalization group theory have important advantages: the first one is generally more easy to apply, and is of much help in complicated problems, even if it can not give a correct description of critical singularities; the later approach, on the other hand, is in principle able to give a correct description of the singularity and scaling, but has of course the disadvantages of being much less easily applicable in most cases.

One could certainly expect that a "marriage" of both theory could lead to an approach with the advantages of them.³

In the present work we show how mean field-like renormalization methods can be adapted to the study of critical surfaces of Ising-like system with nearest- and next-nearest interactions.

A model with many interaction parameters has been recently studied in mean field approximation for understanding thermodynamic properties of Ammonium Halide.⁴ We believe that the methods presented in this thesis

will probably allow a more realistic study of the phase-diagram of this models.

In this thesis; chapter I contain an argument that arrives to an equation of state invariance, which we use under a mean field theory in chapter II and obtain an important equation (II.10). In chapter III we apply (II.10) to the Ising Model with nearest- and next-nearest interaction in 2-dimension, and also discussion some feature that appears. At last we present the numerical results and conclusion in chapter IV.

I. A Finite Size Scaling Law.⁵

Conventionally, a scaling law means an assumption that the thermodynamic energy function is a generalized homogeneous function of the deviation of the independent thermodynamic variables from their critical values.⁶ Of course, the critical point to be considered is at thermodynamic limit, the only case where a phase transition can appear. Any large but finite sized system can be in a state very close to the critical point. It is expected to follow a scaling law, with an additional independent thermodynamic variable, the inverse volume of the system, $1/\Omega$. This parameter has the dimension of inverse volume.

This allow us to write the scaling law in term of free energy per unit volume:

$$f(u, h, 1/\Omega) = g_{\lambda}(u, h, 1/\Omega) + \lambda^{-d} f(\lambda^y u, \lambda^z h, \lambda^d / \Omega) \quad (1)^{5,7}$$

Here λ is the scaling length; u , y are the usual scaling fields and their exponents; z is the exponent of the external field h , usually denoted by y_h ; d is the dimensionality of the system.

Considering a spin lattice system with a symmetry breaking corresponding to a chosen ground state S_i^0 , the partition function at finite volume $\Omega = Z^d$ is

$$Q = \sum_{\{S_i\}} e^{-H - h \sum_{i \in \Omega} S_i^0 S_i} \quad (2)$$

and the free energy density is given by

$$f = - \frac{1}{\Omega} \ln Q \quad (3)$$

Consequently the average local magnetization per unit volume is given by

$$m = \frac{\partial f}{\partial h} = \frac{1}{\Omega} \sum_{i \in \Omega} S_i^0 S_i \quad (4)$$

thus, the total magnetization:

$$M = \sum_{i \in \Omega} S_i^0 S_i \quad (5)$$

If we except the conjecture of finite size scaling as our starting point, we will easily verify that

$$m(u, h, l/\Omega) = \lambda^{y_h - d} m(\lambda^{y_u} u, \lambda^{y_h} h, \lambda^d / \Omega) \quad (6)$$

subjected to a condition that the derivative with respect to h of the regular part is zero. Consequently, we have the total magnetization transform as

$$M(u, h, l/\Omega) = \lambda^{y_h} M(\lambda^{y_u} u, \lambda^{y_h} h, \lambda^d / \Omega) \quad (7)$$

At last, we found an equation of state invariance:

$$hM(u, h, l/\Omega) = (\lambda^{y_h} h) M(\lambda^{y_u} u, \lambda^{y_h} h, \lambda^d / \Omega) \quad (8)$$

Using (5), we can rewrite the equation of state invariance under the symmetry breaking condition as

$$h \sum_{i \in \Omega} S_i^0 S_i = (\lambda^{y_h} h) \sum_{i \in \Omega_\lambda} S_i^{A0} S_i^A \quad (9)$$

In Indekeu, et.al.'s paper, the way of embodying mean field concepts (namely the idea of the effective field) into a strategy for obtaining implicit recursion relation from the scaling (6) of the finite system magnetization was based mainly on intuitive arguments.³ Only in one very specific example ($\text{---} \text{+} \text{---}$, $\text{---} \text{+}$), it was possible to show that the recipe given is consistent with the real-space-renormalization group strategies. It is one of the aims of the present work to try to embed the formulas of the above reference into a more consistent mean field theory. The detail of this trial is in the next chapter.

II. A Mean Field Approximation.

A confidence can be given to the finite size scaling law only for the very large sizes, and there is no a priori reason to trust any small size calculation.⁵ Any advantage we can gain from such strategy is in question. In fact, it seems more difficult than the usual scaling law, or renormalization group theory. However, the application by considering the law as implicit definition of a renormalization group recursion relation under the mean field approximation for an infinite system is extremely simple, and as we will show below, gives rather good estimate of the location of the critical surfaces.

Let us consider a special case in which the hamiltonian H in (I.2) is given by the bi-linear form:

$$H = \sum_{i,j \in \Omega} S_i K^{ij} S_j \quad (1)$$

If we partition Ω into N disjoint cell ω_α :

$$\Omega = \bigcup_{\alpha=1}^N \omega_\alpha \quad ; \quad \omega_\alpha \cap \omega_\beta = \emptyset \quad \alpha, \beta = 1, 2, \dots, N \quad ,$$

we have

$$H + h \sum_{i \in \Omega} S_i^0 S_i = H' + V \quad , \quad (2.a)$$

where

$$H' = \sum_{\alpha=1}^N H'_\alpha \quad ; \quad H'_\alpha = \sum_{\substack{i \in \omega_\alpha \\ j \in \omega_\alpha}} S_i K^{iaja} S_{ja} + h \sum_{i \in \omega_\alpha} S_i^0 S_i \quad (2.b)$$

$$V = \sum_{\alpha \neq \beta} V_{\alpha\beta} \quad ; \quad V_{\alpha\beta} = \sum_{\substack{i \in \omega_\alpha \\ j \in \omega_\beta}} S_i K^{iaj\beta} S_{j\beta} \quad (2.c)$$

Notice that V can also be expressed as

$$V = \sum_{\alpha=1}^N V_{\alpha\alpha} \quad ; \quad V_{\alpha\alpha} = \sum_{\beta=1}^N \sum_{\substack{i \in \omega_\alpha \\ j \in \omega_\beta}} S_i K^{ij} (1 - \delta^{\alpha\beta}) S_j, \quad (2.d)$$

which is more convenient for some calculations.

In the mean field theory, any island ω_α notices its surrounding as a permanent magnetic sea $\bar{\omega}_\alpha$ which effectively act as a field. Iteratively considering the island and sea, we obtain an homogeneous magnetization, i.e. no distinction between the island and sea, as the final result.

In order to have a rigorous mean field theory, we prefer to approach it from a variational point of view. It is the well known Gibbs-Bogolyubov Inequality⁹, deriving from the Jensen Inequality for a convex function that we are going to use.

Any hamiltonian that was separated into two parts like (2.a) has the free energy bounded by the first cumulant approximation. If we have any free parameters or functions, we can minimize the bound, and get the best approximation to the exact value. Notice that it is a non-perturbative calculation, in which there is no need to have any small parameters in the theory. Unfortunately, the direct application to (2.a) has no free parameter. To insert parameters is an art of the variational method; we put a zero effect by adding and subtracting $\sum_{i \in \Omega} J_i S_i^0 S_i$ to H and V , respectively:

$$H + h \sum_{i \in \Omega} S_i^0 S_i = \tilde{H} + \tilde{V} \quad (3.a)$$

$$\tilde{H} = H' + \sum_{\alpha=1}^N \sum_{i \in \omega_{\alpha}} J_{i\alpha} S_{i\alpha}^0 S_{i\alpha} ; \quad \tilde{V} = V - \sum_{\alpha=1}^N \sum_{i \in \omega_{\alpha}} J_{i\alpha} S_{i\alpha}^0 S_{i\alpha} \quad (3.b)$$

The Gibbs-Bogolyubov Inequality reads

$$F \leq F^U(J) = \tilde{F} + \langle \tilde{V} \rangle_{H: \Omega} \quad (4)$$

Note that F^U depends on J , while F must not. the minimum of F^U is the solution of

$$0 = \frac{\partial F^U}{\partial J_{i\alpha}} = \sum_{\beta=1}^N \sum_{\substack{j \in \omega_{\beta} \\ \alpha' \neq i}} \left\{ 2K^{i\alpha'j\beta} (1 - \delta^{\alpha\beta}) \langle S_{j\beta} \rangle_H - J_{i\alpha'} S_{i\alpha'}^0 \right\} \frac{\partial \langle S_{i\alpha'} \rangle_H}{\partial J_{i\alpha}} \quad (5)$$

Since the partial derivative of the local magnetization by the field J is just a correlation function which is not identically zero, we have

$$J_{i\alpha} S_{i\alpha}^0 = 2 \sum_{\beta=1}^N \sum_{j \in \omega_{\beta}} K^{i\alpha j\beta} (1 - \delta^{\alpha\beta}) \langle S_{j\beta} \rangle_H \quad (6)$$

A way to obtain the solution of (6) is to define an iterative map:

$$J_{i\alpha}^{n+1} S_{i\alpha}^0 = 2 \sum_{\beta=1}^N \sum_{j \in \omega_{\beta}} K^{i\alpha j\beta} (1 - \delta^{\alpha\beta}) m_{j\beta}^n \quad (7.n+1)$$

Here $m_{j\beta}^n$ denote the local magnetization of the mean field $\{J_{i\beta}^n\}$. The fixed point of the map are the solution of (6).

From the previous discussion we know that the equation of state is scaling invariant even for a finite sized, but large, system near a critical point. In order to recover such invariance, we assume the invariance at each iterative step that close to the solution:

$$h \sum_{\alpha=1}^N \sum_{i \in \omega_{\alpha}} S_{i\alpha}^0 m_{i\alpha}^n = h^{\Lambda} \sum_{\xi=1}^N \sum_{p \in \omega_{\xi}^{\Lambda}} S_{p\xi}^{\Lambda 0} m_{p\xi}^{\Lambda n} \quad (8.n)$$

Since we are interested in only the critical point solution, $J_i = 0$ for all i when $h = 0$, which is equivalent to keep the power series expansion in $h+J_i$ up to first order, thus,

$$\begin{aligned} h \sum_{\alpha=1}^N \sum_{i \in \omega_{\alpha}} S_{i\alpha}^0 m_{i\alpha}^{n+1} &= h \sum_{\alpha=1}^N \sum_{\substack{i, k \in \omega_{\alpha} \\ j \in \omega_{\beta}}} S_{i\alpha}^0 \left\{ G_{i\alpha k\alpha} (h+J_{k\alpha}^{n+1}) + O(h+J_{k\alpha}^{n+1})^3 \right\} \\ &= 2h \sum_{\alpha, \beta=1}^N \sum_{\substack{i, k \in \omega_{\alpha} \\ j \in \omega_{\beta}}} S_{i\alpha}^0 G_{i\alpha k\alpha} K^{k\alpha j\beta} (1-\delta^{\alpha\beta}) m_{j\beta}^n S_{j\beta}^0, \quad (9.n+1) \end{aligned}$$

where we use (7.n+1), and

$$G_{i\alpha k\alpha} = \langle S_{i\alpha} S_{k\alpha} \rangle_{H: h=0},$$

the correlation function in the cell ω_{α} with out external field.

According to the chosen symmetry breaking condition (in chapter I) the local magnetization must be of the form

$$m_i = \tilde{m} S_i^0$$

for all $i \in \Omega_{\alpha}$ as the final result.

If we start by assuming that all ω_{α} are equivalent, and initiating the iteration by an homogeneous local magnetization, $m_{i\beta} = m^0 S_{i\beta}^0$ for all i we have (8.0) read

$$hN_{\omega_{\alpha}^{\Lambda} m^{\Lambda} 0} = h^{\Lambda} N_{\omega_{\xi}^{\Lambda} m^{\Lambda} 0}$$

and (9.1):

$$hN \sum_{i \in \omega_{\alpha}} S_{i\alpha}^0 m_{i\alpha}^1 = 2hNm^0 \sum_{\beta=1}^N \sum_{\substack{i, k \in \omega_{\alpha} \\ j \in \omega_{\beta}}} S_{i\alpha}^0 G_{i\alpha k\alpha} K^{k\alpha j\beta} (1 - \delta^{\alpha\beta}) S_{j\beta}^0$$

so that (8.1)/(8.0) give us an important invariance relation:

$$\frac{1}{\omega_{\alpha}} \sum_{\beta=1}^N \sum_{\substack{i, k \in \omega_{\alpha} \\ j \in \omega_{\beta}}} S_{i\alpha}^0 G_{i\alpha k\alpha} K^{k\alpha j\beta} (1 - \delta^{\alpha\beta}) S_{j\beta}^0 = \frac{1}{\omega_{\xi}^{\Lambda}} \sum_{\xi=1}^N \sum_{\substack{p, r \in \omega_{\xi} \\ q \in \omega_{\xi}}} S_{p\xi}^{\Lambda 0} G_{p\xi r\xi}^{\Lambda} K^{Ar\xi q\xi} \cdot (1 - \delta^{\xi\xi}) S_{q\xi}^{\Lambda 0} \quad (10)$$

This is a big reduction of the calculation since we need to consider only a small sized cell $\omega_{\alpha}, \omega_{\xi}^{\Lambda}$ statistics.

This equation defines the critical surfaces on the zero external field $h = 0$ plane, where the fixed point lay on.

III An Ising Model

To show the strategy in a very clear manner, a specific simple, but not trivial, must be worked out. It is the Ising Model on the square lattice with nearest- and next-nearest-neighbours interactions that simple enough to be studied.

Since the interaction are always assumed to be translational invariance, and symmetric, for the case, thus, there are only three distinct interactions, K_1, K_2, L that play the role in our calculation.

Let the cell of interest denote by $\omega_{n,n'} := \{x / n_1 \in x_1 \in n_1', n_2 = x_2 = n_2'; x, n, n' \in Z^2\}$. Because of the interaction range, we need to consider at most $\omega_{n-1, n'+1}$ if the ω_n is chosen to $\omega_{n,n}$ while Ω is infinitely large.

There are four interesting ground state for this model on the square lattice: ferromagnetic, anti-ferromagnetic, layered I, layered II. We would like to define a unique form of the ground states:

$$S_i^0 := \begin{matrix} i_1 & i_2 \\ \mu_1 & \mu_2 \end{matrix} \quad (1)$$

correspondingly, $\mu = (1,1), (-1,-1), (-1,1), (1,-1)$.

Consequently, either side of (II.10) can be written in the same form as

$$\frac{1}{\omega_{\alpha}} \sum_{\beta=1}^N \sum_{i, k \in \omega_{\alpha}} S_{ia}^{\circ} G_{ik\alpha} K^{k\alpha j\beta} (1 - \delta^{\alpha\beta}) S_{j\beta}^{\circ} := I_{n, n'} = K_1 \mu_1 \Sigma_{n, n'}^1 + K_2 \mu_2 \Sigma_{n, n'}^2 + L \mu_1 \mu_2 \left\{ 2(\Sigma_{n, n'}^1 + \Sigma_{n, n'}^2) - \Sigma_{n, n'}^{\circ} \right\}, \quad (2)$$

where

$$\Sigma_{n, n'}^{\circ} = \sigma(n_1, n_2) + \sigma(n_1, n_2') + \sigma(n_1', n_2) + \sigma(n_1', n_2') \quad , \quad (3.a)$$

$$\Sigma_{n, n'}^1 = \sum_{y_2=n_2}^{n_2'} \left\{ \sigma(n_1, y_2) + \sigma(n_1', y_2) \right\} \quad , \quad (3.b)$$

$$\Sigma_{n, n'}^2 = \sum_{y_1=n_1}^{n_1'} \left\{ \sigma(y_1, n_2) + \sigma(y_1, n_2') \right\} \quad , \quad (3.c)$$

$$\text{and} \quad \sigma(y) = \frac{1}{\omega_{n, n'}} \sum_{x=n}^{n'} S_{xy}^{\circ} G_{xy} S_y^{\circ} \quad . \quad (4)$$

It is clear that the most basic quantity to be calculated is the correlation function G_{xy} of a finite size $\omega_{n, n'}$ system. There are several techniques to calculate a finite size statistics, but the computing may consume enormous time.

The evaluation of (2) for various sizes are calculated analytically only for the cell of size 1×1 , and 2×2 and given in the appendix. For the higher size can be done on the same footing and lead to a polynomial fraction of the hyperbolic tangent of K_1, K_2, L , denote by $\bar{K}_1, \bar{K}_2, \bar{L}$.

At fixed point solution of the equation (II.10), using (2), rearranging, we obtain

$$K_1^* \mu_1 (\Sigma_{\lambda}^{1*} - \Sigma_{\lambda}^{1*}) + K_2^* \mu_2 (\Sigma_{\lambda}^{2*} - \Sigma_{\lambda}^{2*}) + L^* \mu_1 \mu_2 \left\{ 2 \left[(\Sigma_{\lambda}^{2*} - \Sigma_{\lambda}^{2*}) + (\Sigma_{\lambda}^{1*} - \Sigma_{\lambda}^{1*}) \right] - (\Sigma_{\lambda}^{0*} - \Sigma_{\lambda}^{0*}) \right\} = 0 \quad , \quad (5)$$

where Σ , Σ_A denote the $\Sigma_{n,n}$, and $\Sigma_{n/A, n/A}$, respectively.

When the temperature is very low, i.e. $\|K\| \gg 1$ while $\|\tilde{K}\| \sim 1$, so that all Σ is slowly varying. Consequently, we must have the asymptotic solution of (5) laid on the plane that all Σ assumed the zero temperature, or ground state, i.e. $G_{xy} = S_x^0 S_y^0$:

$$K_1^* \mu_1 C + K_2^* \mu_2 + 2L^* \mu_1 \mu_2 (1 + C) = 0 \quad , \quad (6)$$

where

$$C = \frac{n_2' - n_2 + 1}{n_1' - n_1 + 1} \quad ,$$

the deviation from a square. Here we found that the asymptotic solution of (5) is depend on the shape of the cell.

Let us put the isotropic condition that $K_1 = K_2 := K$ into (6), then differentiating with respected to K , we have

$$\frac{dL}{dK} = -\frac{1}{2} \frac{\mu_1 + \mu_2 C}{1 + C} \quad (7)$$

The asymptotic solution for the ferro- and anti-ferro-magnetic ground states is the line passing the origin, having the slope $-\frac{1}{2}, +\frac{1}{2}$, respectively, while for the layered I, and II having slope zero. A way out is suggested by the formular (7): limiting C to infinity, the slope is $-\frac{1}{2}\mu_2$, it is the correct asymptotic solution to all ground states. Accordingly, the infinitely long strip in vertical direction is hope to give a good results for the low temperature region.

The statistic of the strip is algebraically solvable. Unfortunately, a direct computer calculation is impossible since the machine is finite. Since the limit $C \rightarrow \infty$ does not request any exact results, so that a convenient cell would be an infinitely long strip with a periodic condition of finite period, P :

$$S_{x_1, x_2} = S_{x_1, x_2 + aP} \quad ; \quad a = 0, 1, 2, \dots \quad (8)$$

For a short range interaction, like the model we concern, the limit $P \rightarrow \infty$ gives the same result as a rigid wall boundary condition.

At fixed point, the same argument we have given to obtain (5) is recalled, thus, we have

$$(K_1^* \mu_1 + 2L^* \mu_1 \mu_2)(\Sigma^{1*} - \Sigma^{1*}) = 0 \quad (9.a)$$

so that there are two possible solution:

$$L^* = -\frac{1}{2} K_1^* \mu_2 \quad , \quad (9.b)$$

$$\text{and} \quad \Sigma^{1*} - \Sigma^{1*} = 0 \quad . \quad (9.c)$$

At $T \rightarrow 0$, $\Sigma^{1*} - \Sigma_{\lambda}^{1*} = 2(n_2' - n_2 + 1)(1 - 1/\lambda)$ which is non-zero, thus, the only solution is (9.b). At arbitrary T , $\Sigma^{1*} - \Sigma_{\lambda}^{1*}$ may or may not give the real root, however, we always have (9.b) as a solution.

For the isotropic case, at $T \rightarrow \infty$, (9.b) gives a trivial solution $(0, 0)$, thus the physical solution must come from (9.c). To check whether (9.c) can give any non-trivial solution or not, we consider the cell $2 \times 2P$ and $1 \times P$ with the period $2P$, and P respectively. It is very easy to verify that at $K = 0$:

$$\Sigma_{2 \times 2P}^1 = \frac{1 - \tilde{L}^{2P}}{1 + \tilde{L}^{2P}} \frac{1 + \tilde{L} \mu_1 \mu_2}{1 - \tilde{L} \mu_1 \mu_2}$$

and $\Sigma_{1 \times P}^1 = 2$

We found that $\tilde{L}^* = \frac{1}{3} \mu_1 \mu_2$, at $P \rightarrow \infty$, which is reasonably good, while at $P = 1$ there is no solution ($\tilde{L}^* = 1$).

IV. Numerical Results and Conclusion.

Our numerical calculation is performed directly on the average magnetization in the cell ω_{α} , and ω_{ξ}^A of the either side of the scaling relation while the external fields acting to a point k assumed the form

$$\sum_{\beta=1}^N \sum_{j \in \omega_{\beta}} 2k^{i_{\alpha} j_{\beta}} (1 - S_{j_{\beta}}^0) S_{j_{\beta}}^0 .$$

It is very easy to verify for the Ising Model that

$$\frac{1}{\omega_{\alpha}} \sum_{i \in \omega_{\alpha}} |\langle S_{i_{\alpha}} \rangle| = \frac{1}{\omega_{\xi}} \sum_{i \in \omega_{\xi}} |S_{i_{\alpha}}^0 \langle S_{i_{\alpha}} \rangle| \quad (1)$$

since $S_{i_{\alpha}}^0 = 1$. If we calculate $\langle S_{i_{\alpha}} \rangle$ under the field mentioned above, and expanded up to first order, we recover the equation (II.10), provided $S_{i_{\alpha}}^0 \langle S_{i_{\alpha}} \rangle$ is non-negative. Nevertheless, the correct order parameter and equation of state invariance is the one that have been discussed in I, and II that lead to the equation (II.10). However for the very special case we concern in III, both would be expected to give the same results. Accordingly, the future work would be the numerical calculation base directly on the equation (II.10) for various classical spin system, i.e. infinitely-weak-long-range interaction Ising model, planar model, or extention to higher dimensionality.

By using the computer CDC 170/720, we calculate to find the solution of

$$\frac{1}{\omega_{\alpha}} \sum_{i \in \omega_{\alpha}} |\langle S_{i_{\alpha}} \rangle| = \frac{1}{\omega_{\xi}^A} \sum_{i \in \omega_{\xi}^A} |\langle S_{i_{\xi}}^A \rangle| \quad (2)$$

for various square cell up to 3×3 , with and without periodic condition in vertical direction. The solution is K_1^* , K_2^* , L^* which define a critical surfaces

We present the numerical results only for the isotropic interaction, $K_1 = K_2 = K$, case. Various square cell, $2 \times 2 \rightarrow 1 \times 1$, $3 \times 3 \rightarrow 1 \times 1$, $3 \times 3 \rightarrow 2 \times 2$, scaling transformation is used, and the results is shown in Figure I for the normal square cell, and Figure II for the square cell with periodic condition in vertical direction. The full critical surfaces is just a strianigh forward of our calculation(the 3-dimension graphical drawing).

For the normal square cells, it gives a good results at high temperature region: comparing to the exact results at $L = 0$, or at $K = 0$ which is ~ 0.44 , we are at the error of $\sim 20\%$. At low temperature, it gives a correct estimate of assymtotic approach to the line $L = -\frac{1}{2}K$ for the ferro-magnetic ground state while it is not for the layered I ground state. More than that, the case of $3 \times 3 \rightarrow 2 \times 2$ scaling, at high $K > 1$, it go across the assymtotic solution, which is wrong.

For the square cell with periodic condition in vertical direction, it shows a correcect assymtotic solution: approach the line $L = -\frac{1}{2}K$ very fast, and all assymtotic solution go together within an error of 0.005 for $K > 1.5$.

These numerical results confem our analysis in chapter III that the theory is good in the high temperature region for all ground states, but only anti-ferro- and ferro-magnetic ground states that have a correct, qualitative, results at low temperature. However, becource of the freedom of the choice of the shape of the cells, we are able to reproduce a correct assymtotic behavior at low temperature. The optimized answer to all region must be the large square cell with a periodic condition in vertical direction. For example, $4 \times 4 \rightarrow 2 \times 2$ scaling cells with the periodic condition. Unfortunately, now, we are not able to reduce the computing time to a reasonable scale.

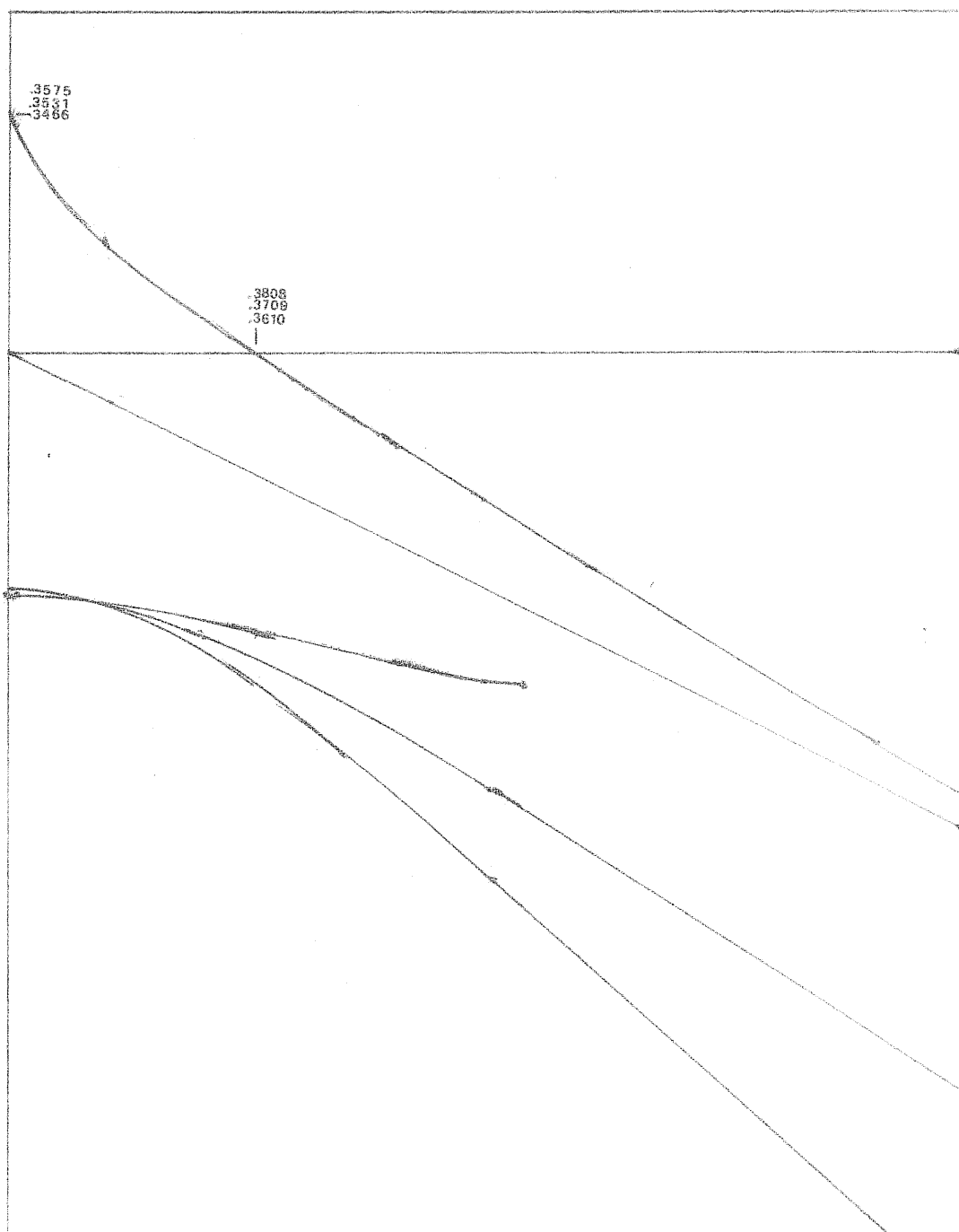


Figure I

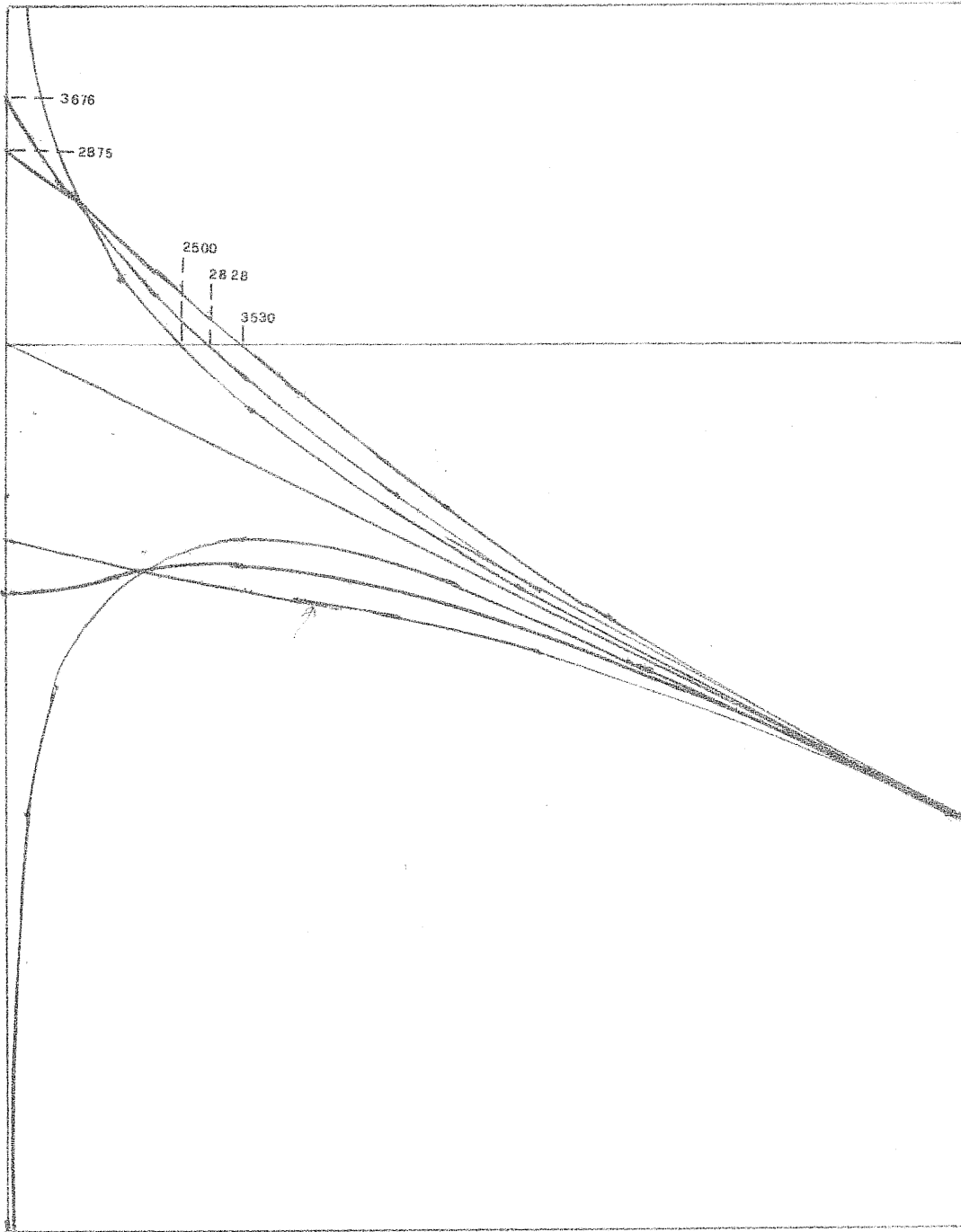


Figure II

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A Derivation of (III.2) from (II.10).

Here we are going to evaluate any side of (II.10) for a cell $\omega_a = \omega_{n,n'}$:

$$I_{n,n'} = \frac{1}{\omega_a} \sum_{B=1}^N \sum_{\substack{x,y \in \omega_a \\ z \in \omega_B}} S_x^0 G_{xy} K^{yz} (1 - \delta^{aB}) S_z^0 \quad (1)$$

for the case mentioned in III.

Because of the translational invariance of K^{yz} , we have

$$I_{n,n'} = \sum_{r \in \Omega} K^{Or} \sum_{y \in \omega_a} \sigma(y) \frac{\theta_{\omega_a}^-(y+r) S_{y+r}^0}{S_y^0} \quad (2)$$

$$\sigma(y) := \frac{1}{\omega_a} \sum_{x \in \omega_a} S_x^0 G_{xy} S_y^0 \quad (3.a)$$

$$\theta_{\Gamma}^-(z) := \begin{cases} 1 & ; \quad z \in \Gamma \\ 0 & ; \quad z \notin \Gamma \end{cases} \quad (3.b)$$

Note that (2) is general since the only assumption taken into account is the translational invariance of K^{yz} which almost all statistical problems do have this property

For the chosen ground states, we have S_{y+r}^0 / S_y^0 is independent of y , and equal to S_r^0 , thus (2) becomes

$$I_{n,n'} = \sum_{r \in \Omega} K^{Or} S_r^0 \sum_{y \in \omega_a} \sigma(y) \theta_{\omega_a}^-(y+r) \quad (4)$$

Let us write down explicitly the characteristic function $\theta_{\omega_a}^-(y+r)$ for the case:

$$\begin{aligned} \sigma_{\omega}^{(y+r)} &= \left\{ \delta_{y_1+r_1, n_1-1} + \delta_{y_1+r_1, n_1'+1} + \delta_{y_2+r_2, n_2-1} + \delta_{y_2+r_2, n_2'+1} \right\} \\ &\quad - \left(\delta_{y_1+r_1, n_1-1} + \delta_{y_1+r_1, n_1'+1} \right) \left(\delta_{y_2+r_2, n_2-1} + \delta_{y_2+r_2, n_2'+1} \right), \quad (5) \end{aligned}$$

where the negative term is the reduction from the double counting of the points at the corners of $\omega_{n-1, n'+1}$ in the bracket $\{\dots\}$.

Using (5), the equation (4) becomes

$$\begin{aligned} I_{n, n'} &= \sum_{\substack{r_1 \leq r_2 \\ r_1 + r_2 = 2}} K^{0r} \mu_1^{r_1} \mu_2^{r_2} \left\{ \sum_{y_2=n_2}^{n_2'} \left[\sigma(n_1-1-r_1, y_2) + \sigma(n_1'+1-r_1, y_2) \right] \right. \\ &\quad + \sum_{y_1=n_1}^{n_1'} \left[\sigma(y_1, n_2-1-r_2) + \sigma(y_1, n_2'+1-r_2) \right] - \left[\sigma(n_1-1-r_1, n_2-1-r_2) \right. \\ &\quad \left. \left. + \sigma(n_1-1-r_1, n_2'+1-r_2) + \sigma(n_1'+1-r_1, n_2-1-r_2) + \sigma(n_1'+1-r_1, n_2'+1-r_2) \right] \right\} \quad (6) \end{aligned}$$

From the knowledge that $\sigma(y)$ is zero if $y \notin \omega_{n, n'}$, the summing up over r gives us the equation (III.2)

B. Evaluation of (III.2) Analytically for the cells 1x1, and 2x2.

For the 1x1 cell, we know that $G_{(1,1)}(1,1) = 1$, thus $\sigma(1,1) = 1$, then $\Sigma^0/2 = \Sigma^1 = \Sigma^2 = 2$, and the equation (III.2) reads

$$I_{1x1} = 2K_1 \mu_1 + 2K_2 \mu_2 + 4L \mu_1 \mu_2 \quad (1)$$

For the 2x2 cell, by summing up (III.3.b) and (III.3.c), comparing to (III.3.a), we found $\Sigma^0 = \Sigma^1 = \Sigma^2$. Factorizing out Σ^0 in (III.2):

$$I_{2 \times 2} = (K_1^{\mu_1} + K_2^{\mu_2} + 3L^{\mu_1 \mu_2}) \Sigma^0 \quad (2)$$

Now the problem is to evaluate Σ^0 . Luckily, Σ^0 can be written as

$$\Sigma^0 = 1 + G^1_{\mu_1} + G^2_{\mu_2} + G^3_{\mu_1 \mu_2} \quad (3)$$

where

$$G^1 = \frac{K_1 + 2K_2L + K_1(K_2^2 + L^2) + 2K_1^2 K_2 L + K_1 K_2 L^2}{1 + 4K_1 K_2 L + K_1^2 K_2^2 + K_1^2 L^2} \quad (4.a)$$

and the G^2, G^3 are the permutation of K_1, K_2, L in G^1 respectively.

C. The Ground State Evaluation of $\Sigma - \Sigma_\Lambda$, to Obtain (III.6).

Since there is no thermal fluctuation, $G_{xy} = S_x^0 S_y^0$, then $\sigma(y) = 1$, we have

$$\Sigma^0 = 4 \quad ; \quad \Sigma^1 = 2(n_2' - n_2 + 1) \quad ; \quad \text{and} \quad \Sigma^2 = 2(n_1' - n_1 + 1) \quad .$$

Similarly, we have from the cell $n/\Lambda, n/\Lambda$. The different of the two side:

$$\Sigma^{0*} - \Sigma_\Lambda^{0*} = 0 \quad ; \quad \Sigma^{1*} - \Sigma_\Lambda^{1*} = 2(n_2' - n_2 + 1)(1 - 1/\Lambda) \quad ; \quad \Sigma^{2*} - \Sigma_\Lambda^{2*} = 2(n_1' - n_1 + 1)(1 - 1/\Lambda) \quad .$$

Consequently, putting this result in to (III.5), and dividing by $\Sigma^{2*} - \Sigma_\Lambda^{2*}$ which is known to be non-zero, we obtain (III.6).