New algorithm of the high-temperature expansion

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1. Introduction

- **Analytic parameter expansion**

  e.g. – High-temperature expansion

  – Low-temperature expansion

  – Strong coupling expansion

  – Hopping parameter expansion

  $\Rightarrow$ not only qualitative but also quantitative results, if we have long enough series.

- **High-temperature expansion of Spin models**

  - **In two dimensions**

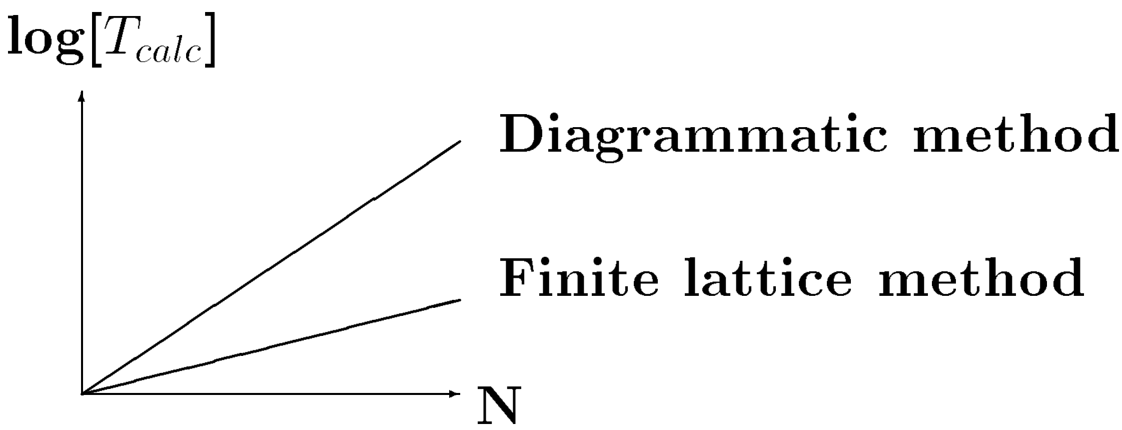
    – Diagrammatic method :

    T_{calc} **: Total amount of the calculation**

    $$\sim \exp(aN)$$

    – $\boxed{\textbf{Finite lattice method}}$ **:**

    $$T_{calc} \sim \exp(bN)$$

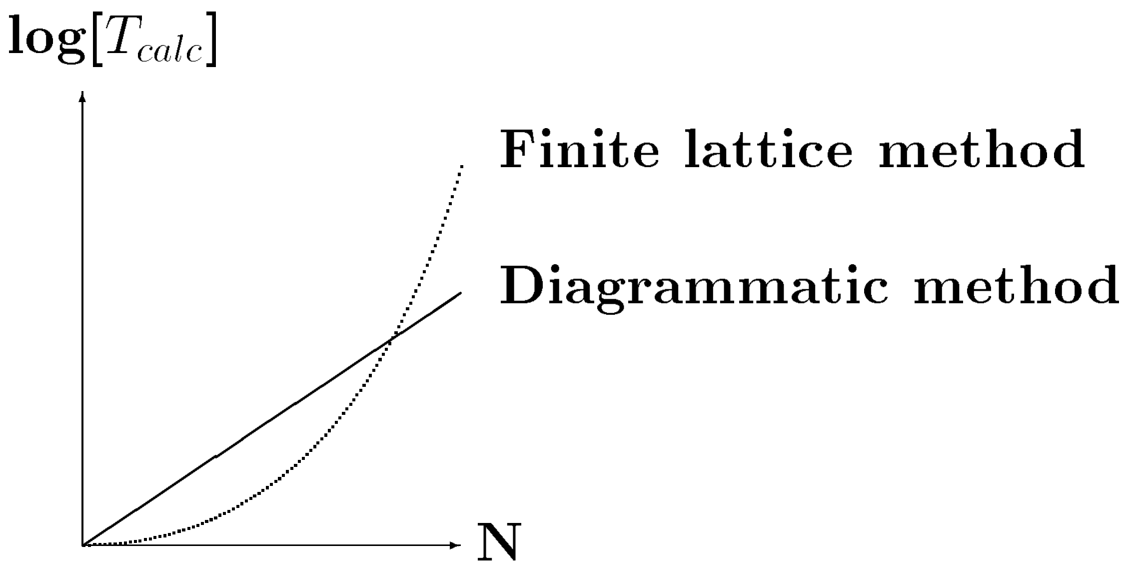


- **In three dimensions**
  - **Diagrammatic method :**

    $$T_{calc} \sim \exp(aN)$$

  - **Finite lattice method :**

    $$T_{calc} \sim \exp(bN^2)$$



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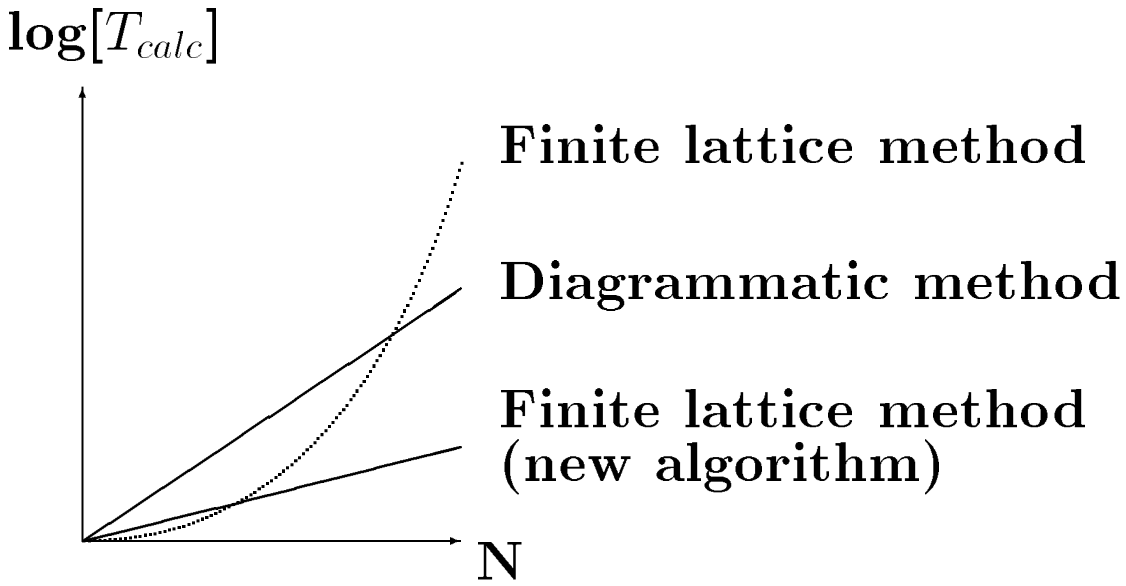
◇ **$\boxed{\text{New algorithm}}$ of the finite lattice method for the Ising model**

$$T_{calc} \sim \exp(cN \log N)$$


$\log[T_{calc}]$
Finite lattice method
Diagrammatic method
Finite lattice method
(new algorithm)
N

Orders of the high-temperature expansion for the Ising model in three dimensions

	Diagrammatic method	Finite lattice method: old algorithm	Finite lattice method: new algorithm
free energy	$N = 18$	$N = 26$	$N = 46$
susceptibility	$N = 25$	$N = 13$	$N = 32$

- **free energy**

  $N = 26$: **Guttmann and Enting (1994)** $\cdots$ **Finite lattice method**

- **magnetic susceptibility**

  $N = 25$: **Butera and Comi (2002)** $\cdots$ **Diagrammatic method**

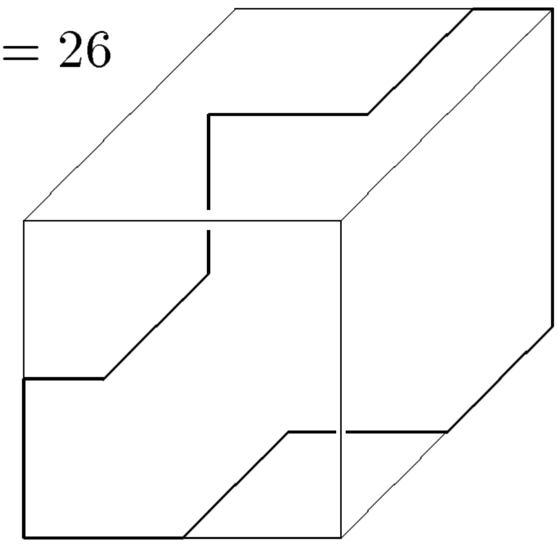
◇ **In the finite lattice method (with the old algorithm)**

- **maximum size of the lattice whose partition function is calculable:**

$$l_x \times l_y \times l_z = 4 \times 4 \times 5$$

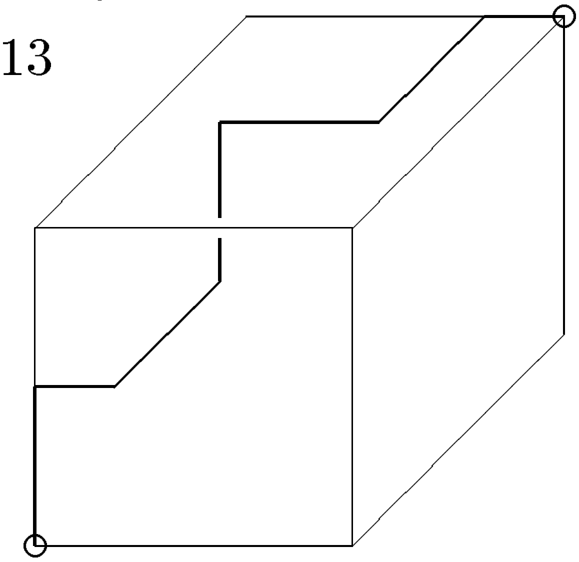
- **free enenrgy**

$$N = 2(l_x + l_y + l_z) = 26$$



- **magnetic susceptibility**

$$N = l_x + l_y + l_z = 13$$



2. Finite lattice method

- **Low- and high-temperature expansion in spin systems**
  - **Enting (1978)**
  - **Creutz (1991)**
- **Strong coupling expansion in lattice gauge theory**
  - **Fujiwara and H.A. (1984)**

$$\downarrow$$

< Ising model in two dimensions >

Partition function

$$Z(\beta) = \sum_{\{s_i\}} \exp\left(\beta \sum_{i,j} s_i s_j\right)$$

Boltzmann factor

$$\exp\left(\beta\ s_i s_j\right) = \cosh\left(\beta\right)\ \left(1\ +\ t\ s_i s_j\right)$$

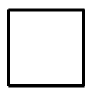
$$t = \tanh\left(\beta\right)$$

$$\left(\beta \equiv \frac{J}{k_B T}\right)$$

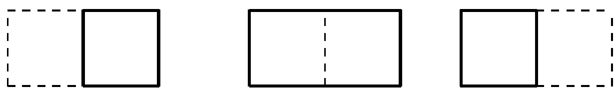
♢ Finite lattice method
(= non-diagramatic method)

- **Calculate the partition function** $Z(l_x \times l_y)$ **for the finite size lattices with** $2(l_x + l_y) \le N$ **to order** t^N

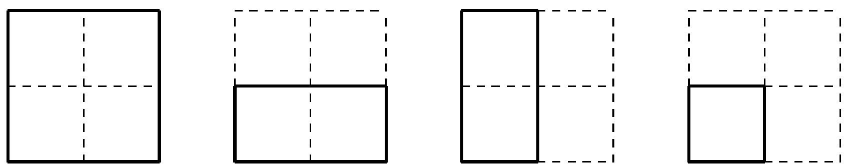
- **Calculate** $\phi(l_x \times l_y)$ **recursively as**



$$\phi(1 \times 1) = \log Z(1 \times 1)$$



$$\phi(2 \times 1) = \log Z(2 \times 1) - 2\phi(1 \times 1)$$



$$\begin{aligned} \phi(2 \times 2) \;=\; & \log Z(2 \times 2) \\ & -2\phi(2 \times 1) - 2\phi(1 \times 2) - 4\phi(1 \times 1) \end{aligned}$$

For general $l_x \times l_y$ lattice,

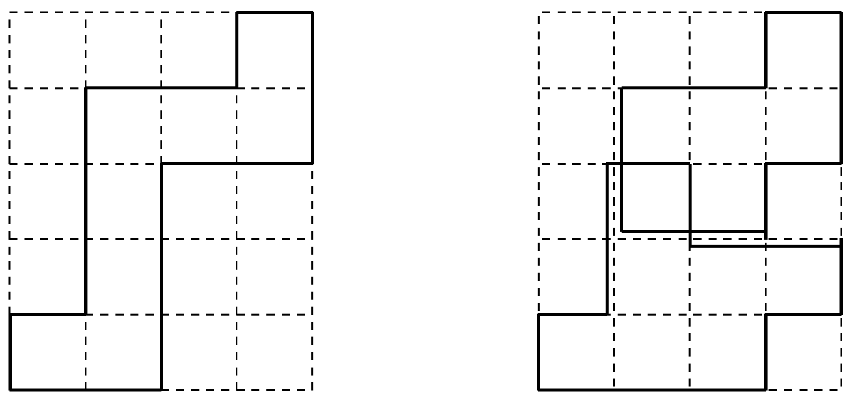
$$\begin{aligned}\phi(l_x \times l_y) &= \log Z(l_x \times l_y) \\ &\quad - \sum_{\substack{l'_x \le l_x, l'_y \le l_y \\ (l'_x, l'_y) \neq (l_x, l_y)}} (l_x - l'_x + 1)(l_y - l'_y + 1)\phi(l'_x \times l'_y)\end{aligned}$$

Then, the free energy density in the infinite volume limit:

$$f = \sum_{2(l_x + l_y) \le N} \phi(l_x, l_y)$$

$$\Uparrow$$

The Taylor expansion of $\phi(l_x \times l_y)$ w.r.t. t gives automatically the contribution to the free energy density in the infinite volume limit from all the connected diagrams (clusters of polymers) that just fit the $l_x \times l_y$ lattice.



- **Partition function** $Z(l_x \times l_y)$ **is calculated by the transfer matrix formalism (in bond-by-bond construction)**

$$Z = V_{0i} V_{ij} V_{ik} \cdots V_{l0} \,.$$

All of the configurations with the order $n \leq N$ **are taken into account in the finite lattice method.**

- **Maximum size of the lattice to be considered:**

$$l_x \sim l_y \sim \frac{N}{4} \quad \textbf{in two dimensions}$$
$$l_x \sim l_y \sim l_z \sim \frac{N}{6} \quad \textbf{in three dimensions}$$

- **Total amount of the calculation**

$$\propto \textbf{ the number of states } \{i\}$$
$$\begin{cases} \propto 2^{l_x} \sim \exp{(cN)} & \textbf{in two dimensions} \\ \propto 2^{l_x \times l_y} \sim \exp{(c' N^2)} & \textbf{in three dimensions} \end{cases}$$

3. New algorithm of the finite lattice method

- **In order to obtain the series to a given order, however, it is enough to consider only a restricted number of bond configurations for $Z(l_x \times l_y)$.**

  i.e. Most of the bond configurations do not contribute to $\phi(l_x \times l_y)$ and can be neglected systematically.

- **Consider the anisotropic model $(t_x \neq t_y)$ in two dimensions**

  To obtain the series to order

  $$N = N_x + N_y = 20,$$

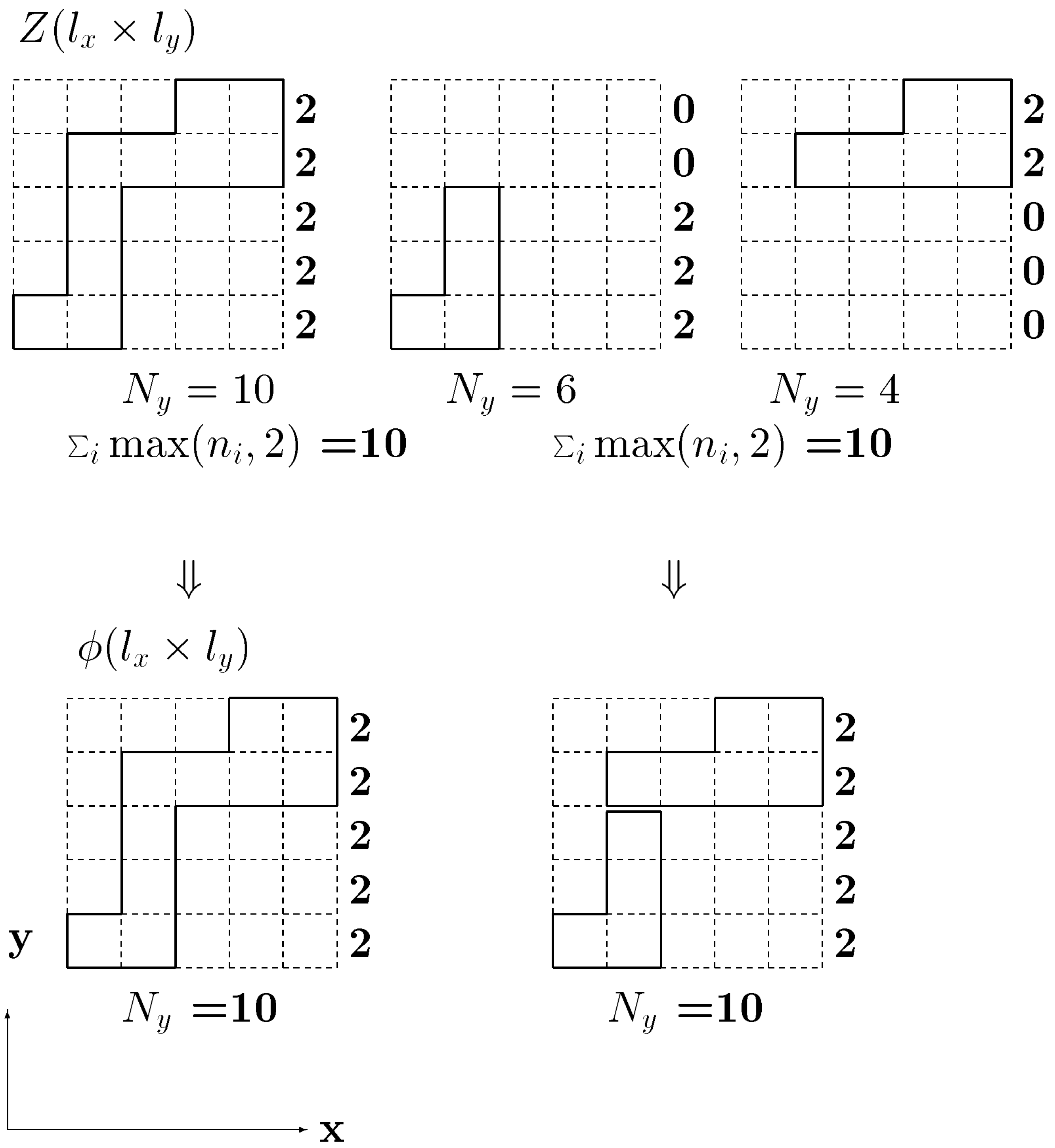
  the largest size of the lattice is

  $$l_x \times l_y = 5 \times 5$$

  and

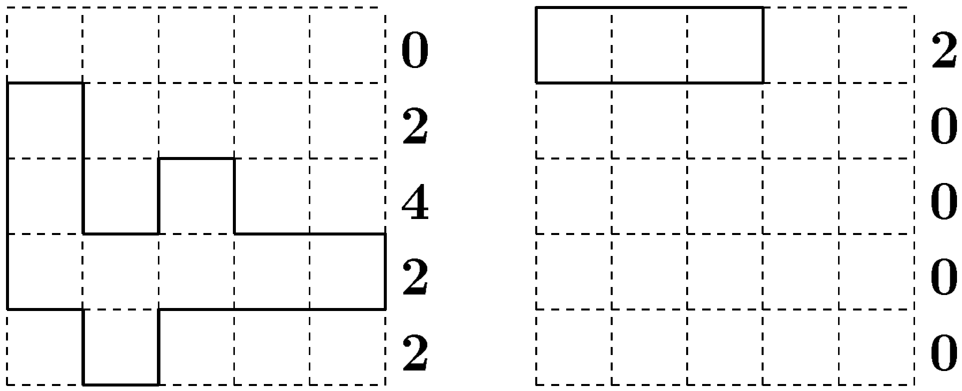
  $$N_x = 2l_x = 10,$$
  $$N_y = 2l_y = 10.$$

- **Configurations for $Z(l_x\times l_y)$ that contribute to the lowest order term of $\phi(5\times 5)$ in ${t_y}^{N_y}$ $(N_y = 2l_y = 10)$**



- **Configurations for $Z(l_x \times l_y)$ that do <u>not</u> contribute to the lowest order term of $\phi(l_x \times l_y)$ in t_y ($N_y = 2l_y = 10$)**

$Z(l_x \times l_y)$



$N_y = 10$

$\Sigma_i \max(n_i, 2)$ **=12**

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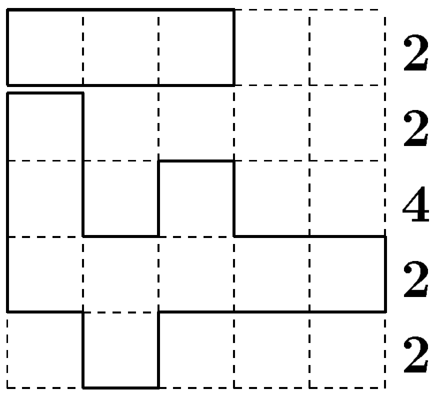
$\phi(l_x \times l_y)$



$N_y = 12$

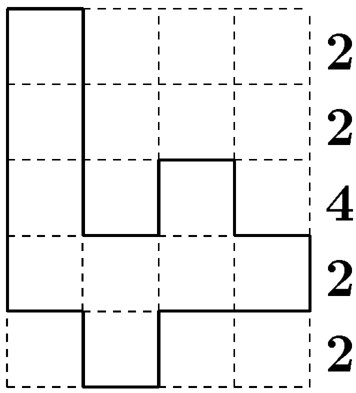
- **The second largest lattice size is**

$$l_x \times l_y = 4 \times 5$$

and

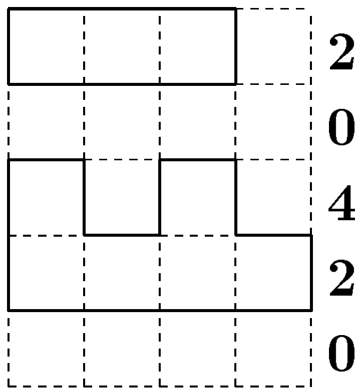
$$N_x = 2l_x = 8,$$
$$N_y = 2l_y + 2 = 12.$$

$Z(l_x \times l_y)$



N_y **=12**

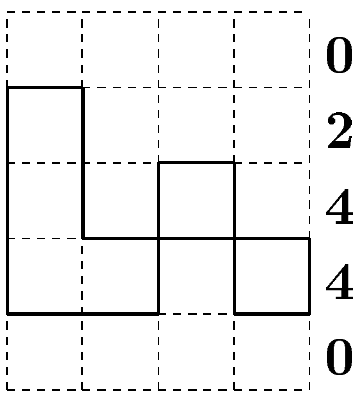
$\Sigma_i \max(n_i, 2)$ **=12**



N_y **= 8**

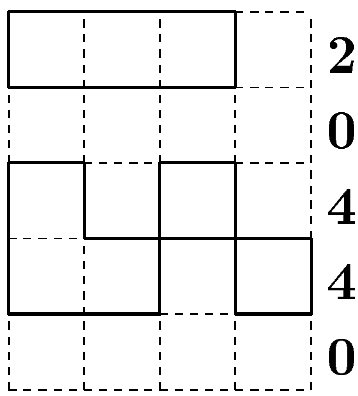
$\Sigma_i \max(n_i, 2)$ **=12**

should be included



N_y **=10**

$\Sigma_i \max(n_i, 2)$ **=14**



N_y **=10**

$\Sigma_i \max(n_i, 2)$ **=14**

can be neglected

To obtain $\phi(l_x \times l_y)$ in the order of N_y in t_y, only the configurations for $Z(l_x \times l_y)$ that have the order n_i of the i-th layer that satisfy

$$\sum_{i=1}^{l_y} \max(n_i, 2) \le N_y$$

should be taken into account.

♢ In three dimensions

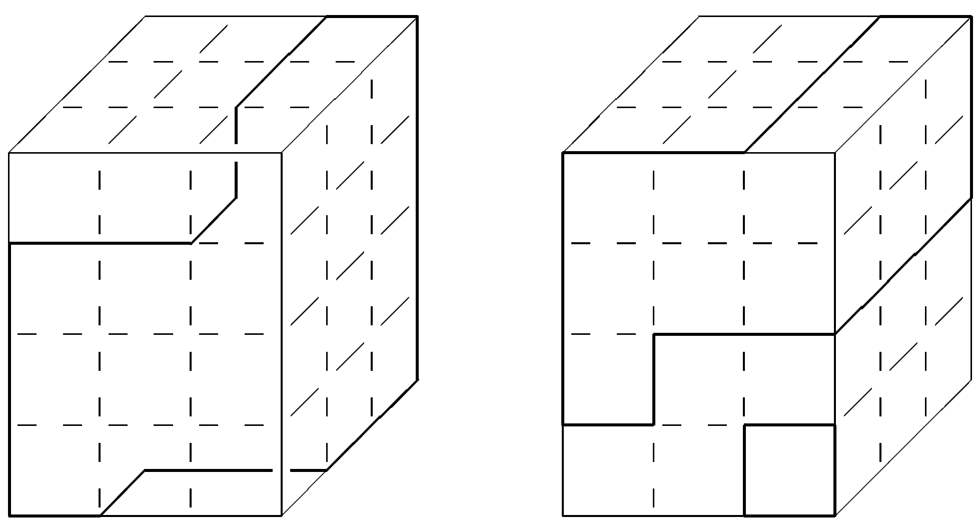
- **Largest size of the lattice to be considered:**

$$l_x \sim l_y \sim l_z \sim N/6$$

$$\text{with } 2(l_x + l_y + l_z) = N$$

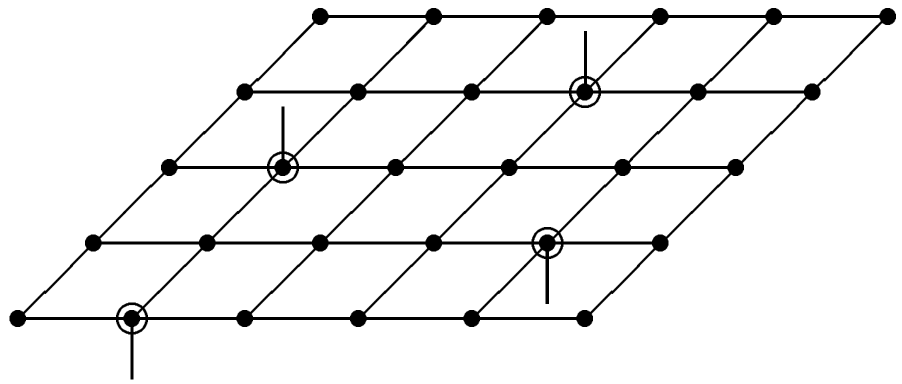
- **Partition function is calculated by the transfer matrix formalism taking into account only the bond configurations with**

$$n_{zi} \le 2$$



$$Z = V_{0,2}\ \ V_{2,2}\ \ \cdots\ \ V_{2,2}\ \ V_{2,0}$$

– **Transfer matrix $V_{2,2}$ is like**



This transfer matrix itself is the 'partition function' in two dimensions and can be calculated by another transfer matrix formalism.

- **Amount of the calculation for the transfer matrices**

$$\propto C(l_x\ l_y,\ 4)\ 2^{\,l_x} \propto N^4 2^{N/6} \sim \exp\left(cN + c' \log N\right)$$

4. Results

• free energy

$$f = 3\cosh(\beta) + \sum_n a_n t^n$$

$$t = \tanh(\beta)$$

n	a_n
2	0
4	3
6	22
8	375/2
10	1980
12	24044
14	319170
16	18059031/4
18	201010408/3
20	5162283633/5
22	16397040750
24	266958797382
26	4437596650548
28	525549581866326/7
30	6448284363491202/5
32	179577198475709847/8
34	395251648062268272
36	21093662188820520521/3
38	126225408651399082182
40	4569217533196761997785/2
42	291591287110968623857940/7
44	8410722262379235048686604/11
46	14120314204713719766888210

• Critical exponent α of the specific heat

$$\begin{aligned} C &= \beta^2 \frac{d^2 f}{d\beta^2} \\ &\sim (\beta_c - \beta)^{-\alpha} \left[1 + \mu(\beta_c - \beta)^{\Delta} + \cdots \ \right] \end{aligned}$$

$$\beta_c = \begin{cases} 0.2216546(\ 1) \\ 0.2216595(15) \end{cases}$$

$$\Delta \sim 0.5$$

(correction-to-scaling exponent)

$$\begin{aligned} \alpha_n &\equiv [\beta_c^2 \frac{a_{2n}}{a_{2n-2}} - 1]n + 1 \\ &\sim \alpha + \frac{b}{n^{\Delta}} + \frac{c}{n} + \cdots \end{aligned}$$

		α
H-T expansion	$\beta_c = 0.2216546(\ 1)$	0.1035 ± 0.0010
	$\beta_c = 0.2216595(15)$	0.1082 ± 0.0010
Monte Carlo		0.125 ± 0.025
ϵ-expansion		0.1088 ± 0.0039
hyper scaling relation		0.1096 ± 0.0005

$\alpha = 2 - d\nu$ with $d = 3$ and

ν: critical exponent for the correlation length

Magnetic susceptibility

n	a_n
0	1
1	6
2	30
3	150
4	726
5	3510
6	16710
7	79494
8	375174
9	1769686
10	8306862
11	38975286
12	182265822
13	852063558
14	3973784886
15	18527532310
16	86228667894
17	401225368086
18	1864308847838
19	8660961643254
20	40190947325670
21	186475398518726
22	864404776466406
23	4006394107568934
24	18554916271112254
25	85923704942057238
26	397637244058624494
27	1839992653230056950
28	8509528288325589438
29	39350934581190850230
30	181885145332015353030
31	840628109226856546326
32	3883554493872938687622

◇ **Analysis of the series (ratio method)**

$$\chi \sim (\beta_c - \beta)^{-\gamma}\left[1 + \mu(\beta_c - \beta)^{\Delta} + \cdots \ \right]$$

$$\Delta \sim 0.5$$

(correction-to-scaling exponent)

- **Critical point** β_c

$$(\beta_c)_n \equiv \left(\frac{a_{n-2}a_{n-3}}{a_n a_{n-1}}\right)\exp\left[\frac{(s_n + s_{n-2})}{2s_n(s_n - s_{n-2})}\right]$$
$$\sim \beta_c + \frac{b}{n^{1+\Delta}} + \cdots$$

$$s_n = \left(\ln\left(\frac{a_{n-2}^2}{a_n a_{n-4}}\right)^{-1} + \ln\left(\frac{a_{n-3}^2}{a_{n-1}a_{n-5}}\right)^{-1}\right)/2$$

H-T expansion	$N = 32$	0.2216550(5)
Monte Carlo		0.2216546(1)
		0.2216595(15)

• Critical exponent γ

$$\begin{aligned}\gamma_n &\equiv 1+\frac{2(s_n+s_{n-2})}{(s_n-s_{n-2})^2}\\ &\sim \gamma+\frac{b}{n^{\Delta}}+\cdots\end{aligned}$$

<table>
<tr><td rowspan="2">H-T expansion</td><td>$N = 25$</td><td>1.2378(10)</td></tr>
<tr><td>$N = 32$</td><td>1.2370(2)</td></tr>
<tr><td colspan="2">perturbative RG</td><td>1.2396(13)</td></tr>
<tr><td colspan="2">ϵ-expansion</td><td>1.2380(50)</td></tr>
<tr><td colspan="2">Monte Carlo(FSS)</td><td>1.2353(25)</td></tr>
<tr><td colspan="2">H-T expansion
(generalized Ising model):20th</td><td>1.2371(4)</td></tr>
</table>

5. Summary and Discussions

- A new algorithm of the finite lattice method has been presented to generate long series of the high-temperature expansions for the Ising model in three dimensions.

- It has been applied to:
  - free energy $N = 26 \to N = 46$
    ($\to N = 50$ calculating on CP-PACS)
  - magnetic susceptibility $N = 25 \to N = 32$
    ($\to N = 40$)

- It can also be applied to other quantities: i.e.
  - second moment correlation length
  - true correlation length

- It can also be applied to the models with a continuous symmetry: i.e.
  - X-Y model
    (Space Shuttle ^{4}He experiment
    $\alpha = -0.01056(38)$)

- It can also be applied to other parameter expansions: i.e.
  - low-temperature expansion