### **Tensor Networks for Statistical Mechanics**

Tomotoshi. Nishino (Kobe Universty)

#### Part I. 17:00 PM (Kobe), 22 Feb. 2021

Tensor network structure in statistical systems — [Ising Model]

Elementary algorithms for the calculation of partition functions (from Baxter)

to higher dimension PEPS/TePS and TRG

Application examples (if there is some time)

#### Part II. 17:00 PM (Kobe), 24 Feb. 2021

Exotic systems:

Random-bond Ising model

ANNNI models (effect of frustration)

Fractal lattices / Hyperbolic lattices

... HaPPY ...



### why do I have to (?) speak about statistical mechanics?

to confirm that Quantum Mechanics is only a part of physics

... but it is difficult of earn billions with the title "statistical ..."

"Strong correlation" also exists in statistical mechanics and other fields.

Tensor Network Structure is naturally contained in statistical systems. (Path Integral representation of quantum systems)

Variational Formulation for a QM system "produces" a Statistical system.

(Most of the descriptions on TN are actually statistical.)



just I love statistical physics from the time I had rich hair.



### a century? of the Ising Model

W. Lenz, Phys. Z. 21, 613 (1920):

W. Lenz (Rostock), Beitrag zum Verständnis der magnetischen Erscheinungen in festen Körpern.

E. Ising, Z. 31, 253 (1925): Beitrag zur Theorie des Ferromagnetismus<sup>1</sup>).

Von Ernst Ising in Hamburg.

### See Rev. Mod. Phys. 39, 883 (1967):

REVIEWS OF MODERN PHYSICS

VOLUME 39, NUMBER 4

OCTOBER 1967

### History of the Lenz-Ising Model

STEPHEN G. BRUSH

Department of Physics and Department of History of Science, Harvard University, Cambridge, Massachusetts

Many physico-chemical systems can be represented more or less accurately by a lattice arrangement of molecules with nearest-neighbor interactions. The simplest and most popular version of this theory is the so-called "Ising model," discussed by Ernst Ising in 1925 but suggested earlier (1920) by Wilhelm Lenz.

Major events in the subsequent history of the Lenz-Ising model are reviewed, including early approximate methods of solution, Onsager's exact result for the two-dimensional model, the use of the mathematically equivalent "lattice gas" model to study gas-liquid and liquid-solid phase transitions, and recent progress in determining the singularities of thermodynamic and magnetic properties at the critical point. Not only is there a wide range of possible physical applications of the model, there is also an urgent need for the application of advanced mathematical techniques in order to establish its exact properties, especially in the neighborhood of phase transitions where approximate methods are unreliable. **Ising Spin:** up (1) and down (-1)

**Hamiltonian** 
$$H = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \dots + \sigma_{N-1}\sigma_N) = -J\sum_{i=1}^{N-1} \sigma_i\sigma_{i+1}$$

**\*\* Partition Function** of 1D Ising Model is obtained as the trace of the products among transfer matrices *T*.

$$Z'' = \sum_{\sigma_1 \cdots \sigma_N} T(\sigma_1 | \sigma_2) T(\sigma_2 | \sigma_3) \cdots T(\sigma_{N-1} | \sigma_N) T(\sigma_N | \sigma_1)$$

corresponding diagram (under periodic boundary condition)



this is an example of tensor network, which is formed by the contraction among two-leg tensors, the transfer matrices *T*.

### **2D Ising model on Diagonal Lattice**

Putting Ising spins on the diagonal lattice, and putting local Boltzmann weights for **shaded** squares.



shaded square: interaction among 4 spins



### corresponding Boltzmann weight

$$W_{i}^{(j)} = \exp\left[\frac{J}{kT} \left(\sigma_{i}^{(j-1)} s_{i-1}^{(j)} + s_{i-1}^{(j)} \mathbf{f}_{i}^{(j)} + \sigma_{i}^{(j)} s_{i}^{(j)} + s_{i}^{(j)} \sigma_{i}^{(j-1)}\right)\right]$$

$$\mathbf{j}$$

$$\mathbf{i-1} - \mathbf{i}$$

#### **Partition Function: 2D Tensor Network**

j-1





Tensor Network structure naturally emerges from the lattice statistical models.

(transfer matrix)



**2^N-dimensional** real (symmetric)



example: ice model Lieb, Phys. Rev. **162**, 162 (1967) To obtain the largest eigenvalue of the transfer matrix (precisely), when the system width N is large enough, is a main purpose of numerical calculation. Variational estimation is often considered.

### vertex - face transformation

## \* Depending on Physics behind, either face or vertex representation is more natural than the other.

\*\* unnatural representation might introduce "troublesome" constraints.

\* It is possible to map a face model to a vertex model. (vertex-IRF transformation, duality transformation, etc.)



Owczarek and Baxter, J. Stat. Phys. 49, 1093 (1987)

A Class of Interaction-Round-a-Face models and Its Equivalence with an Ice-Type Model

\* In the case of Ising model, a way of performing the transformation is to considering the model on the Lieb (Fisher?) lattice.
(Taking configuration sum for either black or white spins in the figure.)

PHYSICAL REVIEW

VOLUME 113, NUMBER 4

FEBRUARY 15, 1959

#### **Transformations of Ising Models**

MICHAEL E. FISHER Wheatstone Physics Laboratory, King's College, London, England (Received August 29, 1958)

The "star-triangle" and "decoration" transformations are generalized so as to apply to arbitrary mechanical systems coupled to the spins of a standard Ising net. This leads to exact solutions for further plane Ising nets and also for lattices in which the spins on alternate sites have a magnitude greater than  $S = \frac{1}{2}$ . A general class of antiferromagnetic Ising models is constructed; exact closed expressions can be derived for all the thermodynamic and magnetic properties of these models in an arbitrary magnetic field.

The magnetizations and susceptibilities of Ising nets in which different spins have different magnetic moments are investigated and a valuable relation between the susceptibilities of the honeycomb and triangular lattices is derived. It is shown how correlation functions involving a given spin can be expressed in terms of correlations involving the nearest-neighbor spins instead.

### Face model (IRF model)





#### **Transfer Matrix**



No contraction is performed

### **Partition Function**



### Local Boltzmann Weight is specified by 4 spins that surrounds a face

Interaction-round-a-face (IRF) Hamiltonian  

$$H_{\rm IRF} = -\frac{J}{2}(\sigma\sigma' + \sigma'\sigma'' + \sigma''\sigma''' + \sigma'''\sigma)$$
1/2: Prevent Double Counting

IRF weight : Boltzmann weight for a "face"  $W_{\sigma \sigma' \sigma'' \sigma'''} = \exp\left[-\frac{E_{\sigma \sigma' \sigma'' \sigma'''}}{kT}\right]$ 

Configuration Sum is taken over all the spins after multiplying all the faces.

It is possible to perform variational analysis without mapping the system to a vertex model.

Kramers-Wannier, PR60, 252 (1941)

### **Eigenvector as natural MPS**



\* The eigenvector of the TM can be constructed as the (partial) contractions among half **column** transfer matrices.

### Face contracted state

Baxter, J. Stat. Phys. 19, 461 (1978)

(black spins are summed up)



\* By means of duality transformation or SVD, one can map a face contracted state to a vertex contracted state.

### **Vertex contracted state**



#### **Variational Construction**

 $T \, V_0 \, = \lambda \, V_0 \,$  eigenvalue problem for a Transfer Matrix

### **Kramers-Wannier Approximation** Phys. Rev. **60**, 263 (1941) "Statistics of the Two-Dimensional Ferromagnet. Part II"

\* Variational state is represented as the simplest case of the **face contracted state** (without auxiliary variable). Note that the state is **finitely correlated**.

$$V(\cdots \sigma \, \sigma' \sigma'' \sigma''' \cdots) = \cdots M^{\sigma \, \sigma'} M^{\sigma' \, \sigma''} M^{\sigma'' \, \sigma'''} \cdots$$

**Baxter introduced auxiliary degree of freedom** 

$$\begin{aligned} & \operatorname{Face}_{(1976-)} V(\cdots \sigma \, \sigma' \sigma'' \sigma''' \cdots) = \sum_{\operatorname{Greek}} \cdots M^{\sigma \, \sigma'}_{\alpha \beta} M^{\sigma' \, \sigma''}_{\beta \, \gamma} M^{\sigma'' \, \sigma'''}_{\gamma \, \delta} \cdots \\ & \operatorname{vertex}_{(1968-)} V(\cdots \sigma \, \sigma' \sigma'' \sigma''' \cdots) = \sum_{\operatorname{Greek}} \cdots M^{\sigma}_{\alpha \beta} M^{\sigma'}_{\beta \, \gamma} M^{\sigma''}_{\gamma \, \delta} M^{\sigma'''}_{\delta \, \epsilon} \cdots \\ & \operatorname{This is MPS!} \end{aligned}$$

One might feel that the **Face** representation is more complicated than **Vertex** one. Please do not hear your voice from the heart. The **Face-type** variational state works as well as the **Vertex** one, as long as d=2 classical lattice models are concerned.

### Kramers-Wannier Approximation Phys. Rev. 60, 263 (1941)

(\*part I: K-W duality)

### Statistics of the Two-Dimensional Ferromagnet. Part II

H. A. KRAMERS, University of Leiden, Leiden, Holland

AND

G. H. WANNIER, University of Texas, Austin, Texas (Received June 12, 1941)

The study of the two-dimensional Ising model is continued. Its specific heat at the Curie point is investigated. The quantity in question is computed for six successive finite matrix problems and the conclusion is drawn that the specific heat is infinite at the Curie point. A new closed form approximation of the partition function  $\lambda$  is then developed by using the matrix method in its variational form. The two power series for  $\lambda$  at extreme temperatures are used as a test for this and various other approximations, and it is found that the new result is a considerable improvement over the existing solutions. Finally it is pointed out that these closed form solutions support our conclusion as to the place and nature of the Curie point transition.

### What is "the Matrix Method in its Variational Form"??

### **Kramers-Wannier Approx**<sup>1</sup> to the 2D Ising Model



in R.J.Baxter: J. Stat. Phys. **19**, 461 (1978), it is stated that the **Face** contracted state without auxiliary variable coincides with Kramers-Wannier approximation.

Another interesting example is the case  $J_0 = J'' = H_3 = J_4 = 0$ . The model then becomes the usual nearest-neighbor Ising model and it turns out that the n = 0 solution of (30) is precisely the Kramers-Wannier approximation.<sup>(7)</sup>

### a basic tool in TNS: Corner Transfer Matrix

### applied to Vertex model

R.J.Baxter: "Dimers on a Rectangular Lattice" J. Math. Phys. 9, 650 (**1968**) applied to **Face** (and vertex) model

R.J.Baxter: J. Stat. Phys. 15, 485 (**1976**) (the term CTM appears!) applied to **Face** model

R.J.Baxter: J. Stat. Phys. 19, 461 (1978)

\* The following figure in this article tells everything. Half-infinite system is represented as the product of two CTMs, and their extension scheme is also shown.



Fig. 4. Graphical representation of Eqs. (30a) and (30c).

### Corner Transfer Matrix Formulation

### R.J.Baxter: "Dimers on a Rectangular Lattice" J. Math. Phys. 9, 650 (1968)

A set of matrix equations is derived which yields the statistical mechanical properties of a system of monomers and dimers on a rectangular lattice in the thermodynamic limit. As the matrices are strictly of infinite dimensionality, the equations cannot be solved directly, but if they are restricted to be of finite and quite small dimensionality, very good approximations to the thermodynamic properties are obtained.

# The problem is to analyze the thermal equilibrium of dimers distributed on the square lattice.

Energy: E = 0 when empty.

E = -2 kT ln t when occupied vertically.

E = -2 kT ln s when occupied horizontally.

Corresponding Boltzmann Weight W = exp(-E/kT)

W = 1 when empty.

W = t \* t when occupied vertically.

w = s \* s when occupied horizontally.

### [[ We skip the detail! ]]



### [[ The model naturally contains the Tensor Network Structure. ]]

It is convenient to attribute a **4-leg Tensor** (Boltzmann Weight) for each Vertex.

We denote horizontal bond variable (= 0 or 1) by 'a' and vertical one by 'b'.



system can be written as

$$Z = \sum_{\{\alpha\},\{\beta\}} \prod_{i,j} K(\alpha_{ij}, \alpha_{i,j+1} | \beta_{ij}, \beta_{i+1,j}), \quad (2.1)$$

... we use images from Baxter's paper to remind his originality .... (and to reduce typing task)

Row-to-Row Transfer Matrix: a horizontal product of Boltzmann weights (Periodic BC)

$$V_{\tau\tau'} = V_{\beta_1 \cdots \beta_n | \beta_1' \cdots \beta_n'}$$
  
=  $\sum_{\alpha_1 \cdots \alpha_n} \prod_{j=1}^n K(\alpha_j, \alpha_{j+1} | \beta_j, \beta'_j),$   
b'1 b'2 b'3 b'4 b'5 b'6 b'7 b'8  
-  $\bigvee_{j=1}^{n} V_{j}(\alpha_j, \alpha_{j+1} | \beta_j, \beta'_j),$   
b'1 b'2 b'3 b'4 b'5 b'6 b'7 b'8  
-  $\bigvee_{j=1}^{n} V_{j}(\alpha_j, \alpha_{j+1} | \beta_j, \beta'_j),$   
b'1 b'2 b'3 b'4 b'5 b'6 b'7 b'8  
-  $\bigvee_{j=1}^{n} V_{j}(\alpha_j, \alpha_{j+1} | \beta_j, \beta'_j),$ 

Partition function obtained from the transfer matrix V

$$Z = \sum_{\tau_1, \dots, \tau_m} V_{\tau_1 \tau_2} V_{\tau_2 \tau_3} \cdots V_{\tau_m \tau_1} = \operatorname{Tr} \mathbf{V}^m \sim \Gamma^m$$
  
where  $\Gamma$  is the greatest eigenvalue of  $\mathbf{V}$ .

Variational evaluation of the largest eigenvalue

As the matrix V is symmetric, it is possible to obtain its greatest eigenvalue from the variational principle

$$\Gamma = \mathbf{x}' \mathbf{V} \mathbf{x} / \mathbf{x}' \cdot \mathbf{x}, \qquad (3.1) \quad [[ Rayleigh Ratio ]]$$

where the  $2^n$ -dimensional vector x is chosen so as to maximize the right-hand side of the equation. If x

How to obtain the variational state x?

(This is the Time Evolution Scheme that we know.)

$$\mathbf{x} \propto \mathbf{V}^k \mathbf{y}, \qquad (3.2)$$

where y is some vector which cannot be orthogonal to x but is otherwise arbitrary.

### **The Matrix Product Ansatz**

$$x(\beta_1, \cdots, \beta_n) \propto \operatorname{Tr} \{G_{\beta_1}G_{\beta_2}\cdots G_{\beta_n}\}$$
 Eq. (3.3)

Half-Column Transfer Matrix = "Local Tensor" in Tensor Network State

$$G^{\beta}_{\alpha_1\cdots\alpha_k|\alpha_1'\cdots\alpha_{k'}} = \sum_{\beta_1\cdots\beta_k} \prod_{i=1}^k K(\alpha_i, \alpha'_i \mid \beta_i, \beta_{i+1})$$

Variational Freedom, Exactness, and Expected Efficiency

real, symmetric, infinite-dimensional matrices. It follows that if these symmetric matrices are regarded as arbitrary, then (3.3) should provide a good trial function for the variational principle (3.1). In fact, if they are allowed to have infinitely great dimensionality, then the results obtained should be formally exact. Further, and more significantly, if the matrices are restricted to be of finite and quite small dimensionality, then it should still be possible to obtain good approximations to  $\Gamma$  and the thermodynamic properties. That this is the case will be shown in



Column-to-Column Transfer Matrix  $R_{\lambda\mu|\lambda'\mu'} = \sum_{\beta} G^{\beta}_{\lambda\lambda'} G^{\beta}_{\mu\mu'}$ Extended C-T-C Transfer Matrix  $S_{\alpha\lambda\mu|\alpha'\lambda'\mu'} = \sum_{\beta,\beta'} K(\alpha, \alpha' \mid \beta, \beta') G^{\beta}_{\lambda\lambda'} G^{\beta'}_{\mu\mu'}$ 

Variational Ratio  $\Gamma = \mathbf{x}' \mathbf{v} \mathbf{x} / \mathbf{x}' \cdot \mathbf{x} = \operatorname{Tr} \mathbf{S}^n / \operatorname{Tr} \mathbf{R}^n$ 



.... this is an origin of MPS in statistical mechanics .... (another one is by Derrida.)

It follows that in the limit of *n* large,

$$\Gamma \sim \kappa^n,$$
 (3.8)

Eigenvalue of the C-T-C Transfer Matrix

where

$$\kappa = \eta/\xi \tag{3.9}$$

and  $\xi$  and  $\eta$  are the greatest eigenvalues of **R** and **S**,

Eigenvectors; X for R and P for S

$$\sum_{\alpha'\beta\beta'} K(\alpha, \alpha' \mid \beta, \beta') \mathbf{G}_{\beta} \mathbf{P}_{\alpha'} \mathbf{G}_{\beta'} = \eta \mathbf{P}_{\alpha}$$

(\*\*) these equations are written in the matrix form. Please look and guess!

$$\sum_{\beta} \mathbf{G}_{\beta} \mathbf{X} \mathbf{G}_{\beta} = \xi \mathbf{X}$$



Variational Estimate of the Partition Function per Vertex



The rest of the task is to find out the **variational minimum**, adjusting G and obtaining the eigenvectors of CTC matrices. Direct optimization is straightforward; Baxter went further!

### Introduction of the CORNER TRANSFER MATRIX

The CTM corresponds to a Quadrant of the system.

One rather unsatisfactory feature of the transfer matrix technique is that it treats the rows of the lattice on a different basis from the columns, and so destroys the symmetry that exists between them. It is therefore very gratifying to find that this symmetry is restored in the above equations. To show this, introduce two further matrices  $G_0^*$  and  $G_1^*$  by defining

$$\mathbf{P}_{\alpha} = \mathbf{X}^{\frac{1}{2}} \mathbf{G}_{\alpha}^{*} \mathbf{X}^{\frac{1}{2}}. \tag{3.15}$$

"Gauge" degree of freedom,

"Gauge" fixing by the diagonalization of CTM, which is equivalent to the diagonalization of the Density Matrix.

> Inspection of Eqs. (3.19)-(3.21) reveals that they are unaffected by applying the same orthogonal transformation to each of the r by r matrices **A**, **G**, and **H**. It follows that it is possible to choose **A** to be diagonal, and this representation clearly reduces the amount of numerical work involved in evaluating the various matrix products.





Evolution (or extension) Scheme for CTM itself

$$L = GAG + s(GAH + HAG), \qquad (4.1)$$

$$\mathbf{M} = s\mathbf{G}\mathbf{A}\mathbf{G} \qquad \mathbf{C} = \begin{pmatrix} \mathbf{L} & \mathbf{M} \\ \mathbf{M} & \mathbf{O} \end{pmatrix}, \qquad (4.2)$$

... GKG induces an evolution for CTM. Every after this extension, the matrix dimension is doubled.

Diagonalization of the extended CTM matrix of the form

CQ = QD,

$$\mathbf{D} = \eta \begin{pmatrix} \mathbf{A} & \mathbf{O} \\ \mathbf{O} & \cdots \end{pmatrix}. \tag{4.6}$$

G

**D** is a 2r by 2r diagonal

Α

G

тппп

А

Cut off the irrelevant parts: **Renormalization!!** 

Using (4.6) and the condition that  $A_{11}$  be unity, calculate  $\eta$  and **A** from the first *r* diagonal elements of **D**.

From the eigenvectors in Q, obtain the "improved" G. (This is a bit different from CTMRG.)



Baxter's numerical result on the dimer problem

r	$\kappa/s$			
	s = 1.0	s = 4.0	s = 10.0	$s = \infty$
1	1.937416664	1.444670083	1.356095932	1.299038106
2	1.940215341	1.460590906	1.381143005	1.335033348
3	1.940215344	1.460623453	1.381458447	1.337338271
4	1.940215351	1.460629381	1.381506501	1.337984697
5	1.940215351	1.460629397	1.381508315	1.338250017
6	1.940215351	1.460629398	1.381508512	1.338380390
Extrap-				
olated	1.940215351	1.460629398	1.381508536	1.338506344

One finds a careful statement on his numerical result.

It is clearly not possible to deduce rigorously from the above working whether or not the dimer system undergoes a phase transition, but the fact that the successive approximations vary smoothly with s and tend towards the known results at both the highand low-density limits suggests very strongly that no transition occurs in this system.

... can anyone here can be as careful as Baxter? Apparently, I cannot ...

#### DMRG applied to 2D Ising Model

Nishino, J. Phys. Soc. Jpn. 64, 3598 (1995)

**Face** representation is used for **Transfer Matrix**.

**Vertex** representation is used for variational MPS.

\* m = 60 states are kept.



\* as long as one uses DMRG, variational state is always MPS regardless of TM.

\* Infinite System Algorithm is employed.



- \* Eigenvector of the renormalized TM can be obtained by the power method, which is the vertical stack of TM.
- \* One finds that **Face**-type variational state is naturally formed for the colum-to-colum transfer matrix.
- \* Similarity with Baxter's CTM formulation in **Face** representation is apparent.
- \* This is our (historical?) route to CTMRG.

### **Diagrams in vertex representation**

#### **Transfer Matrix**

**Variational MPS** 





#### **Variational Partition Function per raw**

#### **Renormalized Transfer Matrix**





### CTMRG: Face and Vertex

(First trial)

**Face** representation is used for **Corner Transfer Matrix**.

Nishino Okunishi,

J. Phys. Soc. Jpn. 65, 891 (1996)

\* m = 98 states are kept.



- \* Fixed point of CTMRG is the same as Baxter's original CTM method. This is natural because the variational construction is the same.
- \* Convergence speed in CTMRG is a bit faster.



(Second Trial)

### **Vertex** representation is used for **Corner Transfer Matrix**.

Nishino Okunishi, J. Phys. Soc. Jpn. 66, 3040 (1997)

\* m = 200 states are kept.

### **Environment for a central vertex**

#### Toward 3D: Vertex Scheme

Nishino et al, Prog. Theor. Phys. **105**, 409 (2001)

- \* Local Boltzmann Weights and TM are written by **Vertex** scheme, via Fisher model.
- \* Variational State is chi=2 **Infinite Tensor Product State**.

\* Inner Product: a 2-layer statistical system.

Variational Partition Function: a 3-layer statistical system. \*







#### Toward 3D: Vertex Scheme

(D=2) Nishino et al, Prog. Theor. Phys. **105**, 409 (2001) (D=3) Gendiar, Maeshima, Nishino, Prog. Theor. Phys. **110**, 691 (2003)





\* **Variational tensor** is improved gradually according to the Generalized Eigenvalue Problem shown above.

$$\sum_{s \{\eta_{c}\}} B_{\bar{s}s}\{\bar{\eta}_{c}|\eta_{c}\}v^{s}\{\eta_{c}\} = \lambda[\Psi] \sum_{s \{\eta_{c}\}} A_{\bar{s}s}\{\bar{\eta}_{c}|\eta_{c}\}v^{s}\{\eta_{c}\}$$

\* **Obtained variational state is fully optimized within the parameter space**. (full variational update)

\* Note that the calculated spontaneous magnetization sharply drops to zero. This is the right (mean-field) behavior with the fully optimized variational TPS.



(additional Note)

\* Current World Record: Vanhecke et al, arXiv:2102.03143 (4 digits in Tc up to D=4)

https://arxiv.org/abs/2102.03143

### TRG / TERG / HOTRG / etc.

Levin, Nave (2006)

Xie et al (2012)

Modern developments in Real-space renormalization.





(diagrams are schematic: in actual calculation the RG transformation is performed independently for vertical and horizontal directions.)

isometries are created by (higher-order) Singular Value Decomposition (SVD).



Tree tensor network is hidden in the renormalized tensor.





### **Further Developments**

Environ should be considered for the right construction of isometries.

isometries are optimized in a self-consistent manner.

Evenbly, Vidal (2014) Tensor Network RG



Xie et al, Second RG (2006)



Morita et al: Higher-order moments TRG (arxiv:1806.10275)

lino et al: Boundary TRG (arxiv:1905.02351)

Adachi et al: Bond weighted TRG (arxiv:2011.01679)

Lyu et al: Linearized RG transformation (arxiv:2102.08136)

... ... ...

### a discussion:

\* How can we find out an appropriate isometry which correctly produce the right local tensor that is fully updated?



