

# Information Compression #7

## #7 Information compression & low-rank nature in materials science

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0. (Revisited) Random vector
1. Physically motivated coarse-graining
  - Hierarchy
  - Renormalization
2. Mathematical measure of low-rank nature of many-body systems
  - Compression of basis set
3. Naïve assumption of low-rank nature

.

# (Revisited) Some Remarks on Random Vector and Distribution of Eigenstates

# Distribution of Eigenvalues of Hermitian Matrices

An important relationship between distribution or density of states and statistical mechanics

$$P(E) = \frac{\rho(E)e^{-\beta E}}{\int dE' \rho(E')e^{-\beta E'}} \sim \frac{\exp[-(E - \langle E \rangle)^2/2CT^2]}{\sqrt{2\pi CT^2}}$$

$$k_B = 1$$

$$C = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{T^2}$$

$$\langle \hat{H}^m \rangle \sim \int E^m P(E) dE$$

# Nature of Random Vector

M. Imada and M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).  
A. Hams and H. De Raedt, Phys. Rev. E 62, 4365 (2000).

## Random wave function

$$|\phi_0\rangle = \sum_x c_x |x\rangle \quad \sum_x |c_x|^2 = 1$$
$$|x\rangle = |\sigma_0 \sigma_1 \cdots \sigma_{N-1}\rangle$$

## Infinite-temperature result

$$\mathbb{E}[\langle \phi_0 | \hat{O} | \phi_0 \rangle] = N_H^{-1} \sum_n \langle n | \hat{O} | n \rangle = \langle \hat{O} \rangle_{\beta=0}^{\text{ens}}$$

$$\mathbb{E}[|c_x|^2] = N_H^{-1}$$
$$|n\rangle = \sum_x U_{xn} |x\rangle$$

Complexity  
Memory

$$\mathcal{O}(N_H)$$

N. Ullah, Nucl. Phys. 58, 65 (1964).  
-Uniform distribution on  
unit sphere in  $\mathbb{R}^{2N_H}$

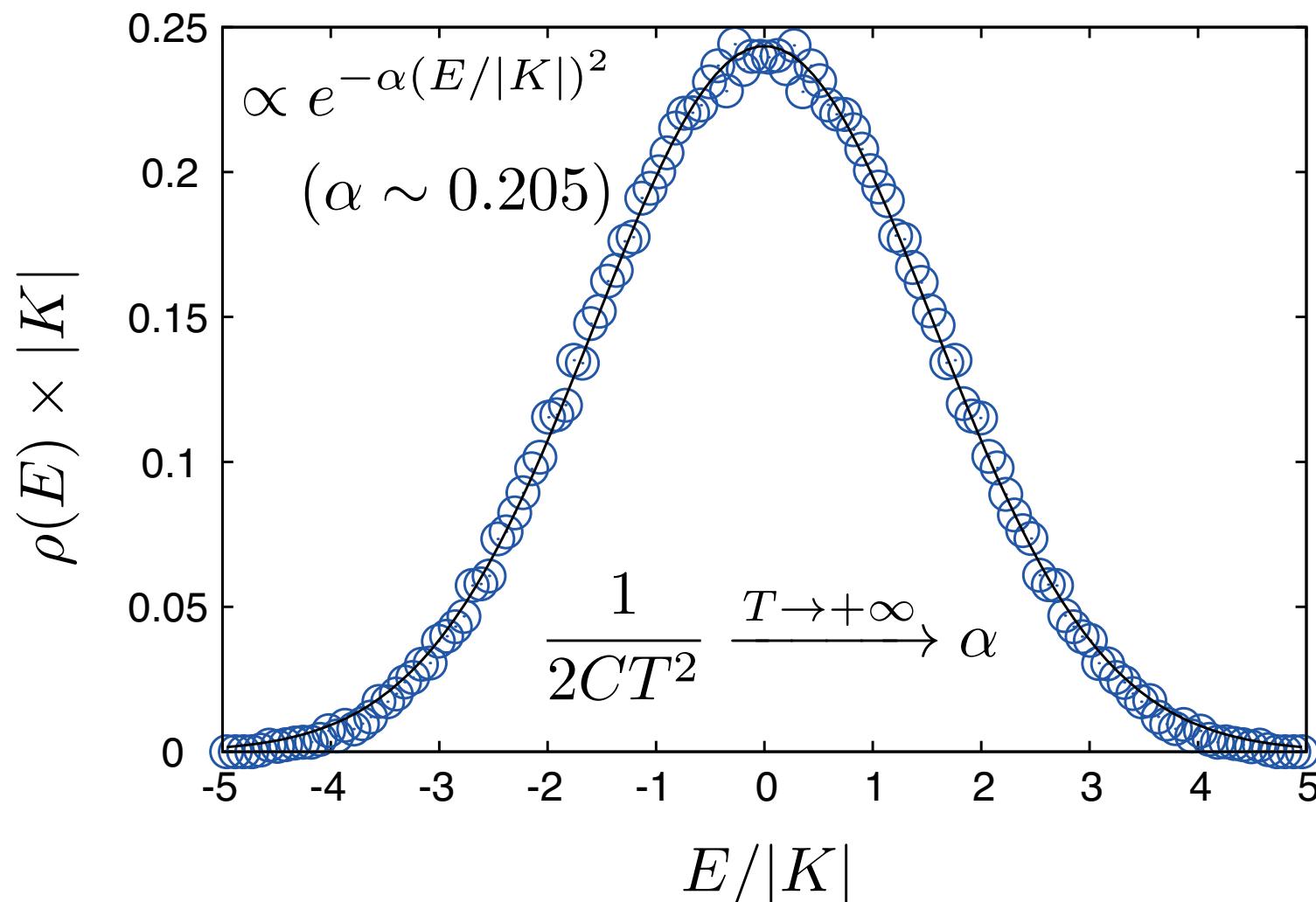
$$\mathbb{E}[|c_x|^{2n}] = \frac{\Gamma(N_H)\Gamma(n+1)}{\Gamma(N_H+n)}$$

# An Example of Density of State

24 site cluster of Kitaev model  
(frustrated  $S=1/2$  spins)

A. Kitaev, Annals Phys. 321, 2 (2006).

$$2^{24} = 16,777,216$$



# Example of Dense Matrix: Random Symmetric Matrices

Eugene P. Wigner, Annals of Mathematics, 2nd Series, 67, 325 (1958)

Wigner's random matrix  $(A)_{ij} = a_{ij}$

$$\underline{a_{ij} = a_{ji}}$$

(Not necessarily sparse)

$$\int p_{ij}(a)da = 1$$

$$p_{ij}(+a) = p_{ij}(-a)$$

$$\langle a_{ij}^n \rangle = \int p_{ij}(a)a^n da \leq B_n$$

$$\langle a_{ij}^2 \rangle = \int p_{ij}(a)a^2 da = 1$$

# Example of Dense Matrix: Random Symmetric Matrices

Eugene P. Wigner, Annals of Mathematics, 2nd Series, 67, 325 (1958)

Density of states of  $L \times L$  symmetric random matrix

$$A\vec{v} = E\vec{v}$$

$$\sigma(E) = \begin{cases} \frac{\sqrt{4L - E^2}}{2\pi L} & (E^2 < 4L) \\ 0 & (E^2 > 4L) \end{cases}$$

Comment:

Sparse matrices in quantum many-body problems show smaller density of states than random matrices around the both ends of the distribution

- Sparse around maximum/minimum eigenvalues
- Lanczos method may work well

# Approximate SVD by Krylov Subspace Method

## Low-rank approximation by *block* Krylov subspace

C. Musco & C. Musco,  
NIPS'15 Proceedings of 28th International Conference on  
Neural Information Processing Systems 1, 1396 (2015)

$$\|A - ZZ^T A\|_2 \leq (1 + \epsilon) \|A - A_k\|_2 \quad \begin{matrix} \text{Operator norm defined by 2-norm} \\ \text{(Spectral norm)} \end{matrix}$$

$$A \in \mathbb{R}^{L \times M} \quad Z \in \mathbb{R}^{L \times k} \quad \text{rank } k \leq L, M$$

$$q = \mathcal{O}(\ln d / \sqrt{\epsilon})$$

random matrix  $\Pi \in \mathbb{R}^{M \times k}$

$$\mathcal{K}_{q+1} = \text{span}\{A\Pi, (AA^T)A\Pi, \dots, (AA^T)^q A\Pi\}$$

$Q \in \mathbb{R}^{N \times qk}$  Orthogonalized basis set of the block Krylov subspace

$$M = Q^T AA^T Q \in \mathbb{R}^{qk \times qk}$$

$U_k$  : the top  $k$ singular vectors of  $M$

$$Z = QU_k$$

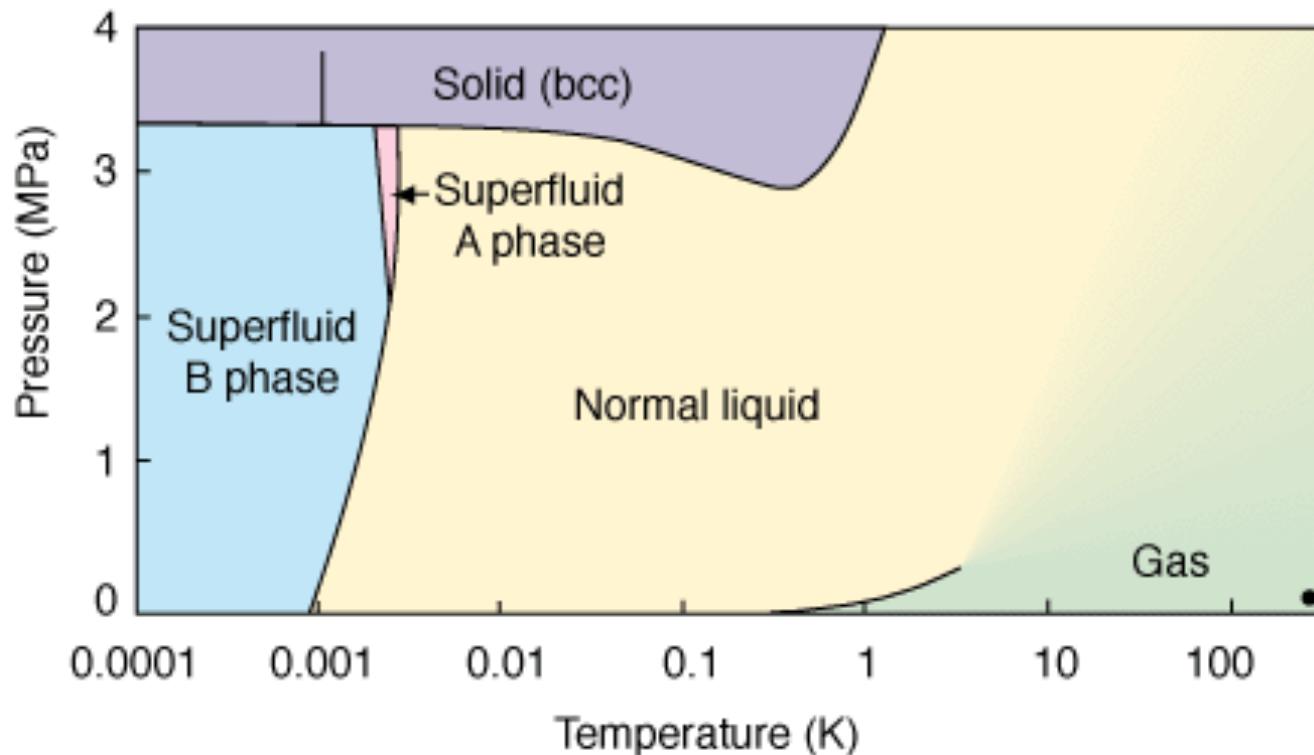
$(\Pi)_{ij}$  : Random number generated by  $e^{-x^2/2} / \sqrt{\pi}$

# Target: Many-Body Systems in Condensed Matter Physics

- Electrons and ions    Qubits, plasma
- Atoms                      Cold atoms
- Molecules
- Gases, liquids, solids

# Low-Temperature Phases

Phase diagram of  ${}^3\text{He}$



D. D. Osheroff, R. C. Richardson, and D. M. Lee,  
Phys. Rev. Lett. 28, 885 (1972).

From atoms to full systems (multiscale)

Hierarchy  
(階層構造)

Renormalization  
(繰り込み)

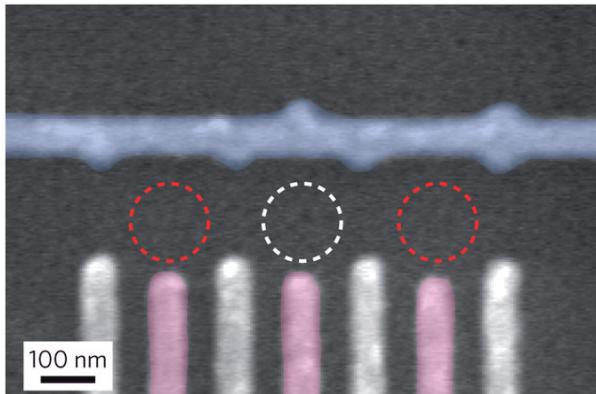
Reduction of number of bases (基底数)

Entanglement  
(もつれ)

# Quantum Many-Body Problems

## Quantum dots

F. R. Braakman, et al., Nat. Nano. 8, 432 (2013)

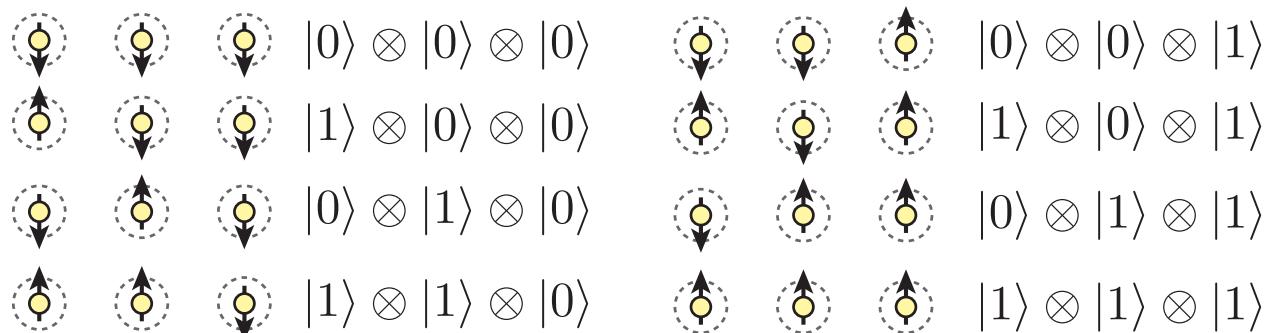


Quantum dot:

- A quantum box can confine a single electron
- Utilized for single electron transistor, quantum computers

Three-body problem:

→ Number of states =  $2^3$  (factor 2 from spin)



States represented by superposition

$$\mathcal{F} = \left\{ \sum_{n_0=0,1} \sum_{n_1=0,1} \sum_{n_2=0,1} C_{n_0 n_1 n_2} |n_0\rangle \otimes |n_1\rangle \otimes |n_2\rangle : C_{n_0 n_1 n_2} \in \mathbb{C} \right\}$$

# How Large Fock Space Dimension Is

Example: Water ( $\text{H}_2\text{O}$ ) molecule

(5  $\uparrow$ -spin electrons & 5  $\downarrow$ -spin electrons)

Accuracy of quantum chemistry calculation is controlled by  
1) choice of basis set (基底関数系) and 2) solver (数值解法)

G. K.-L. Chan & M. Head-Gordon, J. Chem. Phys. 118, 8551 (2003).

A choice: 41 orbitals per spin (4s3p2d on O and 3s2p on H)

Fock space dimension:

$$\left( \frac{41!}{5! \times 36!} \right)^2 \sim 5.6 \times 10^{11}$$

A single wave function  $\sim$  4TB  
(double precision real number)

# Physically Motivated Information Compression: Coarse-graining

# To What Extent We Can Compress Information of Many-Body Systems

Macroscopic phenomena  
(巨視的)

Coarse-graining  
(疎視化)

Microscopic Hamiltonian  
(微視的)

Thermodynamics

Small number of variables:  
 $P, V, T$

Quantum mechanics



# To What Extent We Can Compress Information of Many-Body Systems

Coarse-graining from physics  
(疎視化)

Hierarchy  
(階層構造)

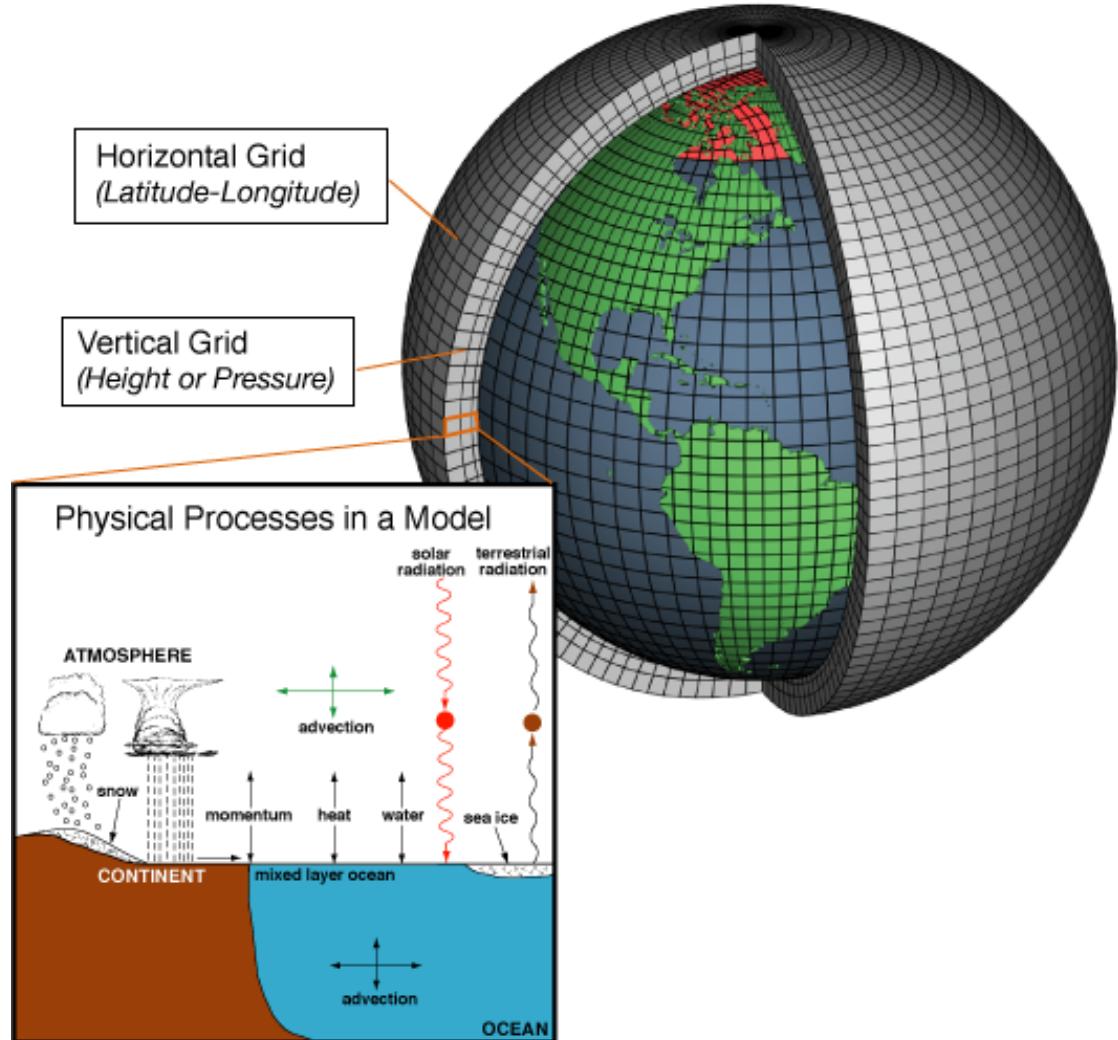
cf.) Global climate model

Renormalization  
(繰り込み)

Starting point:  
Ginzburg-Landau theory

# Example of Hierarchy: Multiscale Modeling

## Global climate model



[https://celebrating200years.noaa.gov/breakthroughs/climate\\_model/modeling\\_schematic.html](https://celebrating200years.noaa.gov/breakthroughs/climate_model/modeling_schematic.html)

# Example of Renormalization: Ginzburg-Landau Theory

Ginzburg-Landau-Wilson (GLW) free energy functional  
(pseudo free energy)

$$F[\phi] = \frac{1}{2} \int \phi(\vec{r})(r + c\nabla^2)\phi(\vec{r})d^d r + \mathcal{O}(\phi^4)$$

$\phi$ : Order parameter field (秩序変数場)

Real/complex scalar, real/complex vector

Real scalar: Ising

Minimum as a functional →  
Free energy in thermodynamics

Microscopic details in the origin of  $\phi$  do not affect GLW

# Example of Order Parameter Field

$$\phi(\vec{r}) = \phi_0$$

crystal

$$\phi(\vec{r}) = -\phi_0$$

liquid

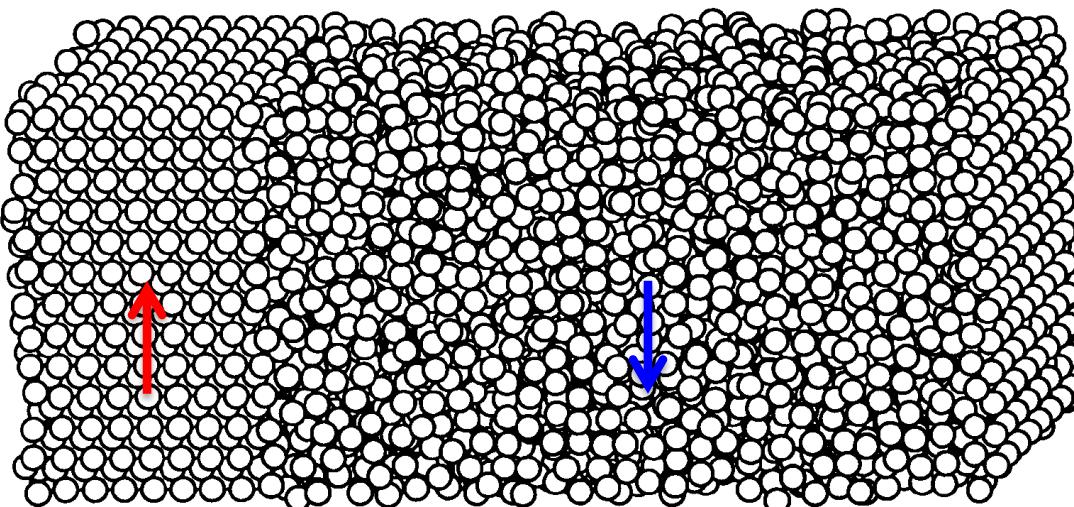
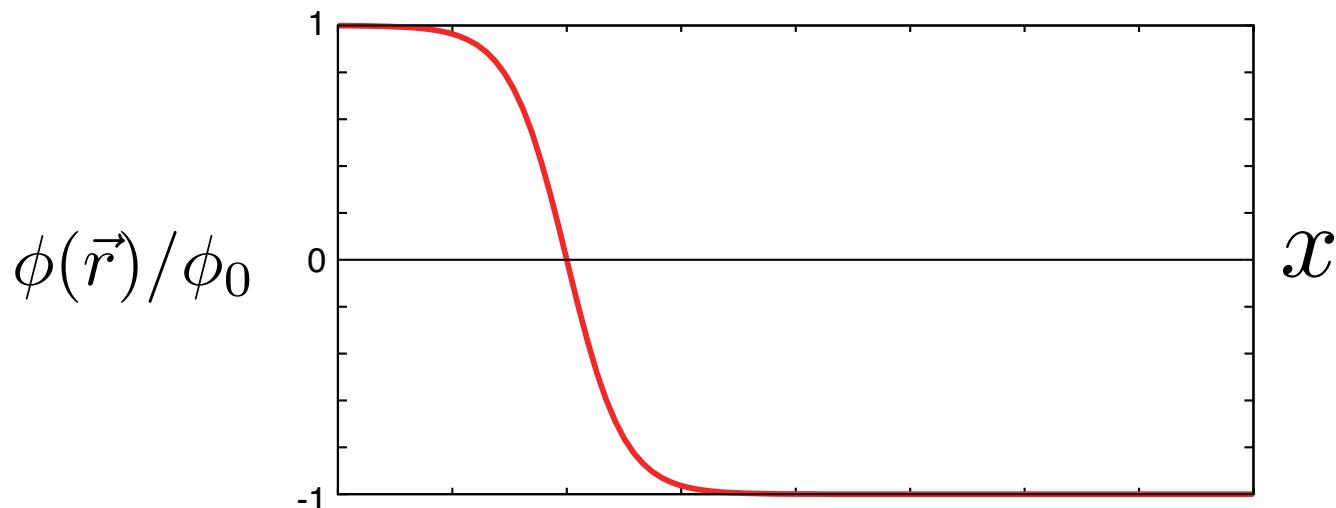
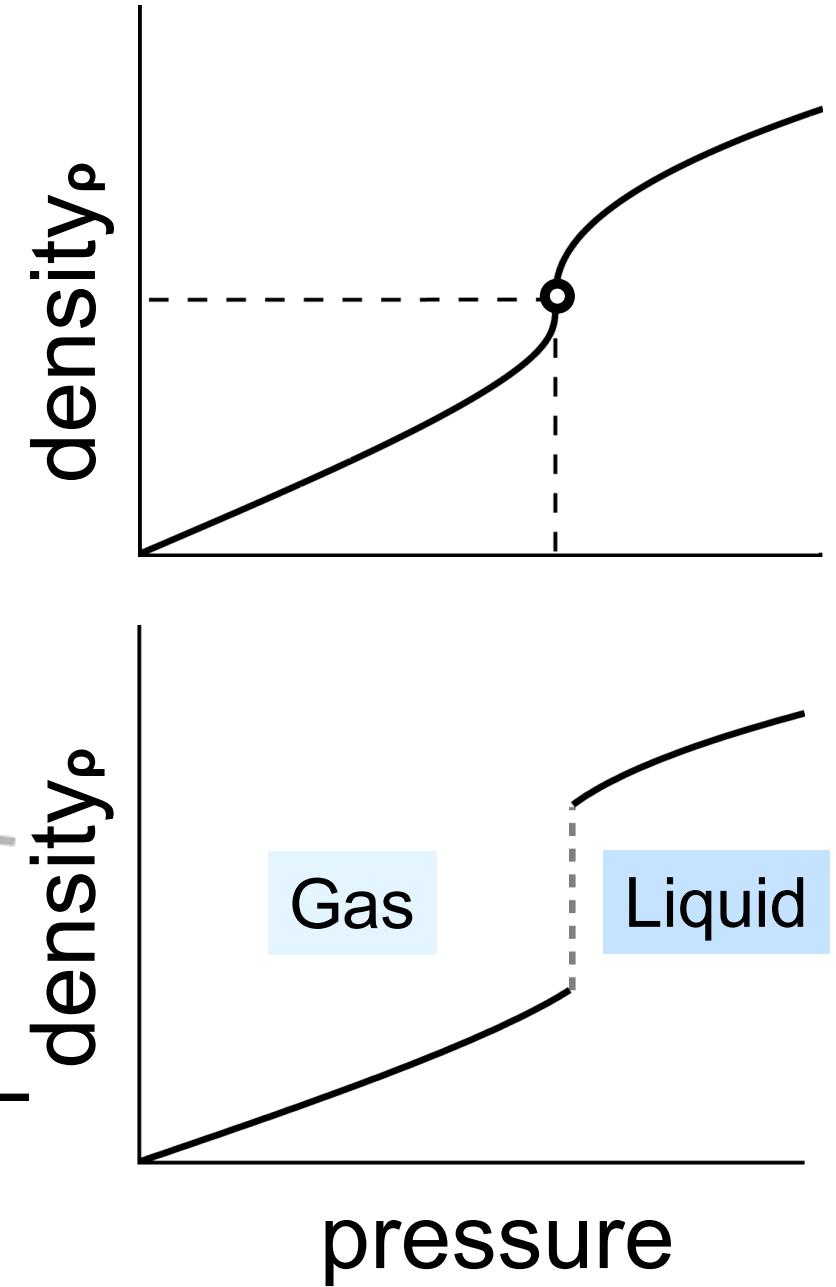
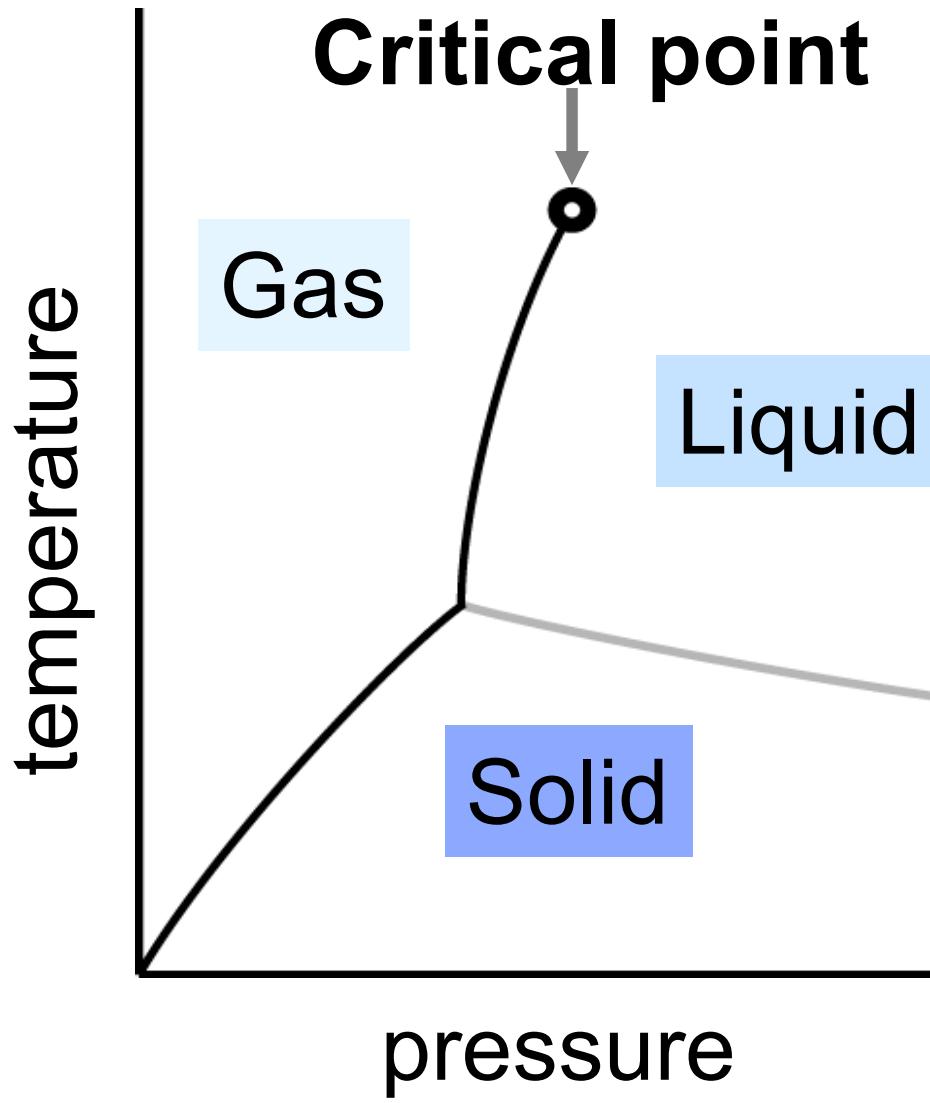


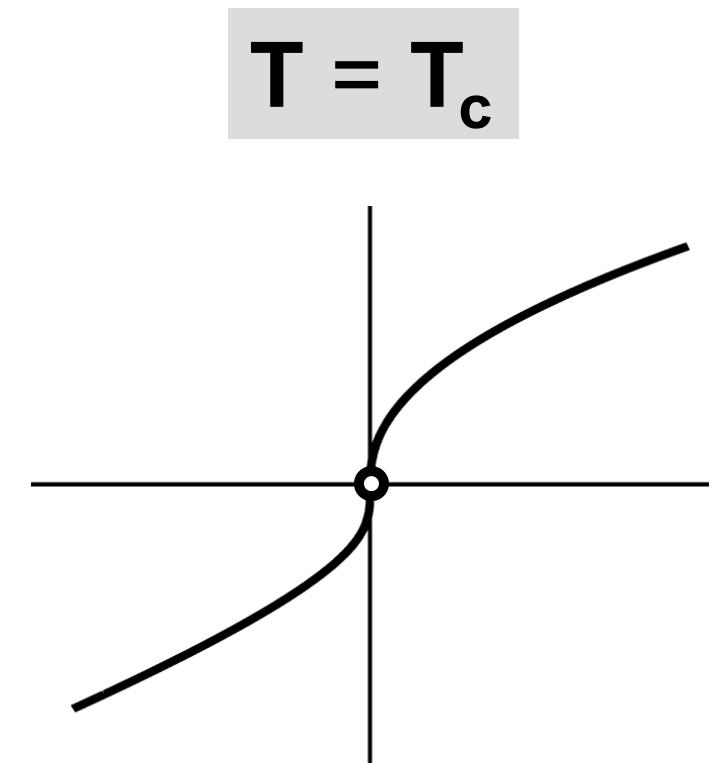
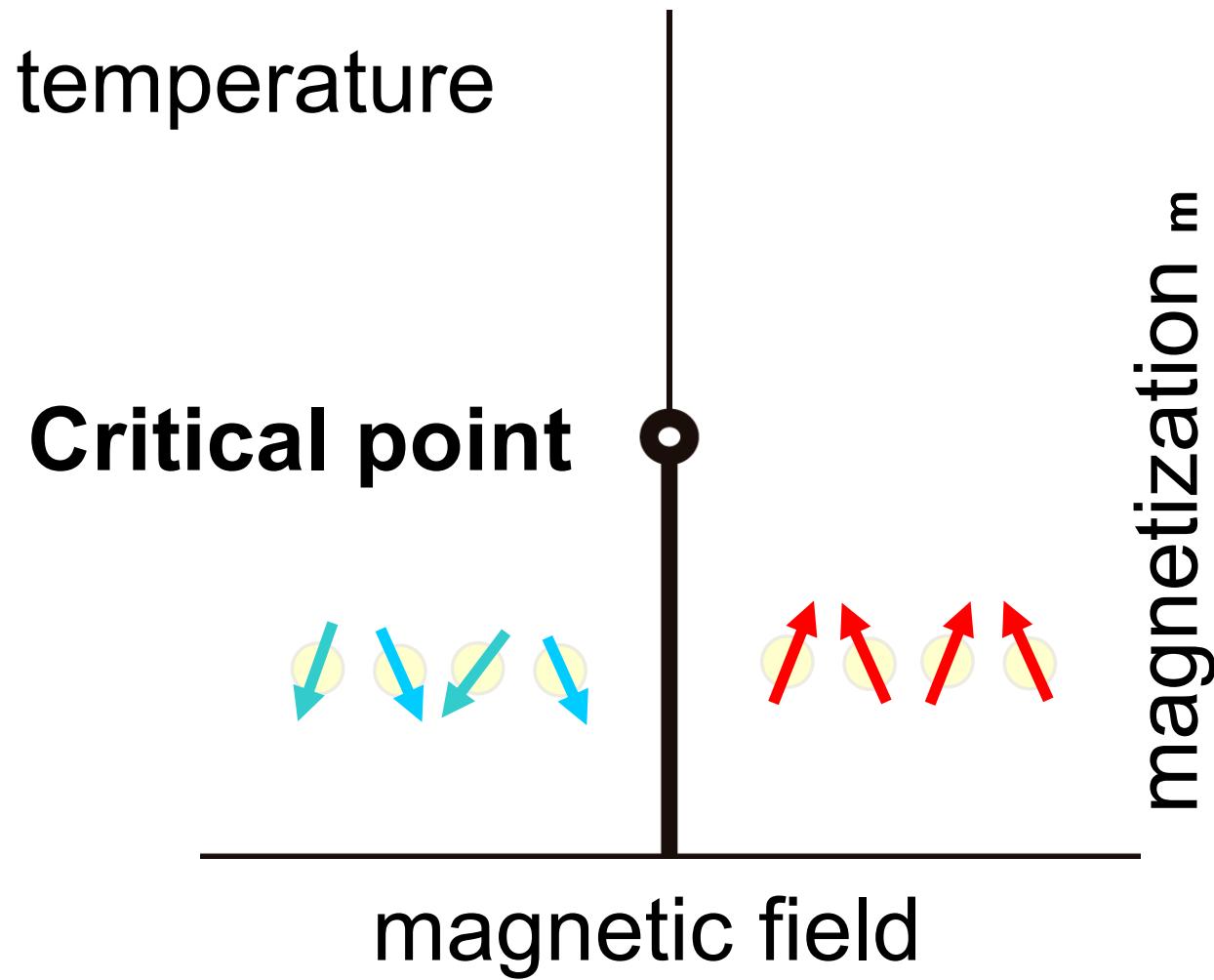
Fig. 1. The initial configuration of atoms used in the simulation of solid–liquid interface motion. The example shown is for 100 Ni at 1500 K.



# Critical Phenomena: Gas-Liquid



# Critical Phenomena: Ising FM



# GLW Free Energy in Momentum Space

Ginzburg-Landau-Wilson free energy functional  
(pseudo free energy)

$$\begin{aligned} F[\phi] = & \frac{1}{2} \int \tilde{\phi}(\vec{q})(r + c|\vec{q}|^2)\tilde{\phi}(\vec{q}) \frac{d^d q}{(2\pi)^d} \\ & + \frac{u}{4} \int \tilde{\phi}(\vec{q}_1)\tilde{\phi}(\vec{q}_2)\tilde{\phi}(\vec{q}_3)\tilde{\phi}(-\vec{q}_1 - \vec{q}_2 - \vec{q}_3) \frac{d^d q_1}{(2\pi)^d} \frac{d^d q_2}{(2\pi)^d} \frac{d^d q_3}{(2\pi)^d} \end{aligned}$$

# Revisit Ginzburg-Landau Theory

$$f = F/V = \frac{1}{2}r\phi^2 + \frac{u}{4}\phi^4 - h\phi$$

$$\frac{\partial f}{\partial \phi} = r\phi + u\phi^3 - h = 0 \quad \Rightarrow \quad \frac{d\phi}{dh} = \frac{1}{r + 3u\phi}$$

$$\phi|_{h \rightarrow +0} = \begin{cases} 0 & (r > 0) \\ \sqrt{-r/u} & (r < 0) \end{cases} \quad \text{Susceptibility (感受率)}$$

$$f|_{h \rightarrow 0} = \begin{cases} 0 & (r > 0) \\ -\frac{r^2}{4u} & (r < 0) \end{cases}$$

Phase transition (相転移) occurs at  $r = 0$

Ordered phase (秩序相)  $r < 0$

# Revisit Ginzburg-Landau Theory

GL theory for real space fluctuation

$$f_{\vec{q}} = \frac{1}{2}(r + c|\vec{q}|^2)\phi_{\vec{q}}^2 + \frac{u}{4}\phi_{\vec{q}}^4 - h_{\vec{q}}\phi_{\vec{q}}$$

$$\frac{\partial f_{\vec{q}}}{\partial \phi_{\vec{q}}} = 0$$

$$\Rightarrow \chi_{\vec{q}} = \frac{d\phi_{\vec{q}}}{dh_{\vec{q}}} = \frac{1}{r + c|\vec{q}|^2 + 3u\phi_{\vec{q}}} \quad \text{Susceptibility (Ornstein-Zernike form)}$$

$$\chi_{\vec{q}} = \frac{1}{c|\vec{q}|^2} \quad (h_{\vec{q}} = 0, r = 0) \quad \text{Power-law behavior  
No length scale}$$

Gaussian fluctuation

# Renormalization

Kenneth G. Wilson

$$F[\phi] = \frac{1}{2} \int \tilde{\phi}(\vec{q})(r + c|\vec{q}|^2)\tilde{\phi}(\vec{q}) \frac{d^d q}{(2\pi)^d}$$

Separation of slow ( $q < \Lambda/s$ ) and fast ( $q > \Lambda/s$ ) mode

$$F[\phi] = F[\phi_<] + F[\phi_>]$$

$$F[\phi_<] = \frac{1}{2} \int_0^{\Lambda/s} \tilde{\phi}(\vec{q})(r + c|\vec{q}|^2)\tilde{\phi}(\vec{q}) \frac{d^d q}{(2\pi)^d}$$

$$F[\phi_>] = \frac{1}{2} \int_{\Lambda/s}^{\Lambda} \tilde{\phi}(\vec{q})(r + c|\vec{q}|^2)\tilde{\phi}(\vec{q}) \frac{d^d q}{(2\pi)^d}$$

\*If you have  $\phi^4$  term, you will have *mode couplings*

# Renormalization at *Tree Level*

$$\vec{q}' = s\vec{q} \quad \text{Scale transformation } (s > 1)$$

Keep the GLW functional invariant at the critical point  
 $r = 0$

$$F[\phi_<] = s^{-2-d} \frac{1}{2} \int_0^\Lambda \tilde{\phi}(\vec{q}'/s) (s^2 r + c|\vec{q}'|^2) \tilde{\phi}(\vec{q}'/s) \frac{d^d q'}{(2\pi)^d}$$

$$\tilde{\phi}(\vec{q}'/s) = \zeta \tilde{\phi}'(\vec{q}')$$

$$F[\phi_<] = s^{-2-d} \zeta^2 \frac{1}{2} \int_0^\Lambda \tilde{\phi}'(\vec{q}') (s^2 r + c|\vec{q}'|^2) \tilde{\phi}'(\vec{q}') \frac{d^d q'}{(2\pi)^d}$$

$$\zeta = s^{(d+2)/2}$$

$$r' = s^2 r$$

$$F[\phi_<] = \frac{1}{2} \int_0^\Lambda \tilde{\phi}'(\vec{q}') (r' + c|\vec{q}'|^2) \tilde{\phi}'(\vec{q}') \frac{d^d q'}{(2\pi)^d}$$

# Renormalization at *Tree Level* (0th order approximation)

$$F[\phi_<] = \frac{1}{2} \int_0^{\Lambda/s} \tilde{\phi}(\vec{q})(r + c|\vec{q}|^2 + c_4|\vec{q}|^4)\tilde{\phi}(\vec{q}) \frac{d^d q}{(2\pi)^d}$$

$$\vec{q}' = s\vec{q}$$

$$\tilde{\phi}(\vec{q}'/s) = s^{(d+2)/2}\tilde{\phi}'(\vec{q}')$$

$$F[\phi_<] = \frac{1}{2} \int_0^{\Lambda} \tilde{\phi}'(\vec{q}') (r' + c'|\vec{q}'|^2 + c'_4|\vec{q}'|^4)\tilde{\phi}'(\vec{q}') \frac{d^d q'}{(2\pi)^d}$$

$$r' = s^2 r \quad \text{Relevant}$$

$$c' = c \quad \text{Marginal (Gaussian fixed point)}$$

$$c'_4 = s^{-2}c_4 \quad \text{Irrelevant (becoming smaller after ST)}$$

Long-wave-length limit (**not exact!!**) is captured by

$$F[\phi] = \frac{1}{2} \int \tilde{\phi}(\vec{q})(r + c|\vec{q}|^2)\tilde{\phi}(\vec{q}) \frac{d^d q}{(2\pi)^d}$$

# Coarse-Graining in Material Science

Multiscale modeling of solidification of metals

## 1. Molecular dynamics

$10^{-10}\text{m/fs}$  scale

J. J. Hoyt, B. Sadigh, M. Asta, & S. M. Foiles,  
Acta Mater. 47, 3181 (1999)

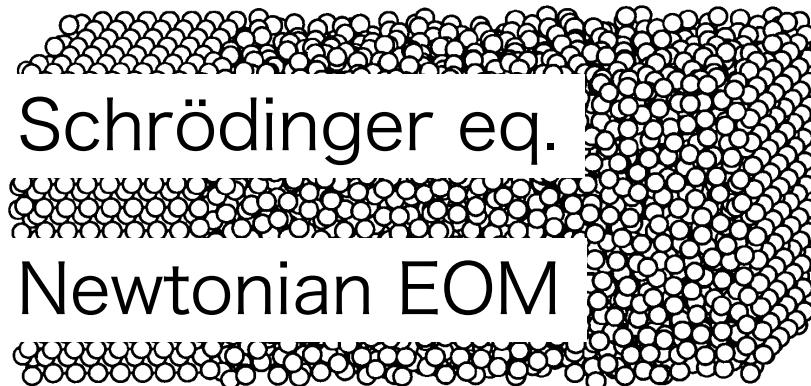


Fig. 1. The initial configuration of atoms used in the simulation of solid–liquid interface motion. The example shown is for 100 Ni at 1500 K.

*Ab Initio* MD: Classical atoms and quantum electrons  
MD with force field: Classical atoms

## 2. Phase field (order parameter field)

$10^{-6}\text{m}/10^{-6}\text{sec}$  scale

J. Bragard, A. Karma, Y. H. Lee, & M. Plapp,  
Interface Science 10, 121 (2002)



# Measure of Low-Rank Nature in Many-Body Systems

# Measuring Entanglement

Density matrix of pure state

$$\rho = |\psi\rangle\langle\psi|$$

von Neumann entropy

$$S = -\text{tr}[\rho \log_2 \rho]$$

System + Environment

cf.) Density matrix of canonical ensemble

$$\rho_{ce} = \sum_n e^{-\frac{E_n}{k_B T}} |n\rangle\langle n|$$

Invariant under changes in basis set

Reduced density matrix by partial trace of Environment

$$\rho_S = \text{tr}_E[\rho]$$

Entanglement entropy between System and Environment

$$S_S = -\text{tr}[\rho_S \log_2 \rho_S]$$

# Schmidt Decomposition

$$\begin{aligned} |\psi\rangle &= \sum_{i=1}^{n_S} \sum_{j=1}^{n_E} \beta_{ij} |\psi_S\rangle_i |\psi_E\rangle_j \\ &= \sum_{j=1}^m \alpha_j |\psi'_S\rangle_j |\psi'_E\rangle_j \quad (m \leq \min\{n_S, n_E\}) \end{aligned}$$
$$\begin{aligned} {}_{j_1} \langle \psi'_S | \psi'_S \rangle_{j_2} &= \delta_{j_1, j_2} \\ {}_{i_1} \langle \psi'_E | \psi'_E \rangle_{i_2} &= \delta_{i_1, i_2} \end{aligned}$$

$$\alpha_j : \text{singular value of } M \quad (M)_{ij} = \beta_{ij}$$

Reduced density matrix by partial trace of Environment

$$\rho_S = \sum_{j=1}^m |\alpha_j|^2 |\psi'_S\rangle_j \langle \psi'_S|$$

Entanglement entropy between System and Environment

$$S_S = - \sum_{j=1}^m |\alpha_j|^2 \log_2 |\alpha_j|^2$$

# Entanglement

Example: Two qubits (0th bit: System, 1st bit: Environment)

$$|n_0\rangle \otimes |n_1\rangle$$

1) Product state/classical state

$$|\psi\rangle = |0\rangle \otimes |0\rangle$$

$$\rho_S = |0\rangle\langle 0|$$

$$S_S = -\text{tr}[|0\rangle\langle 0| \log_2 |0\rangle\langle 0|] = 0$$

2) Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle \otimes |0\rangle - |0\rangle \otimes |1\rangle)$$

$$\rho_S = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$$

$$S_S = \log_2 2$$

Entanglement entropy:

Measuring how many bases we need to represent the pure state  
(Larger entanglement entropy  $\rightarrow$  larger basis set)

# Compression of Basis Set Based on Entanglement

Numerical *Renormalization* Group (NRG)

Kenneth G. Wilson (1975)

Density Matrix *Renormalization* Group (DMRG)

Steven White (1992)

- In the light of matrix product state (MPS), they are closely related each other
- Be careful of the terminology “renormalization;” Essentially both methods (can) keep the almost all information of the ground state wave function

# Dimension of Fock Space

Fock space dimension can be stored in memory

- Hubbard-like hamiltonian  
 $N (< 30\text{-}40)$  orbital systems
- Heisenberg-like hamiltonian  
 $N (< 50)$  *spin* systems

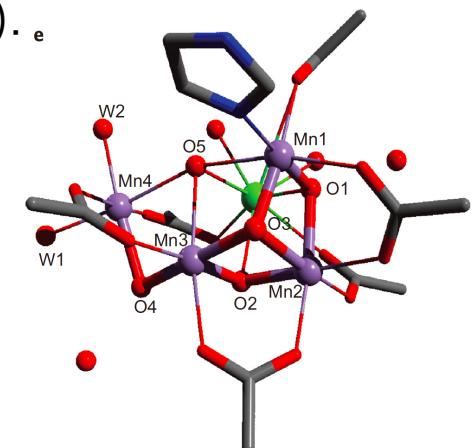
## Examples of finite size systems from chemistry

-A H<sub>2</sub>O molecule: 5  $\uparrow$  & 5  $\downarrow$  electrons in 41 orbitals  
 $\rightarrow 5.6 \times 10^{11}$  dimensional ( $\sim 2^{39}$ )

G. K.-L. Chan & M. Head-Gordon, J. Chem. Phys. 118, 8551 (2003).

-Manganese cluster in photosystem II:  
44 electrons in 35 orbitals  
 $\rightarrow 2 \times 10^{18}$  dimensional ( $\sim 2^{61}$ )

Y. Kurashige, G. K.-L. Ghan, & T. Yanai, Nat. Chem. 5, 660 (2013).



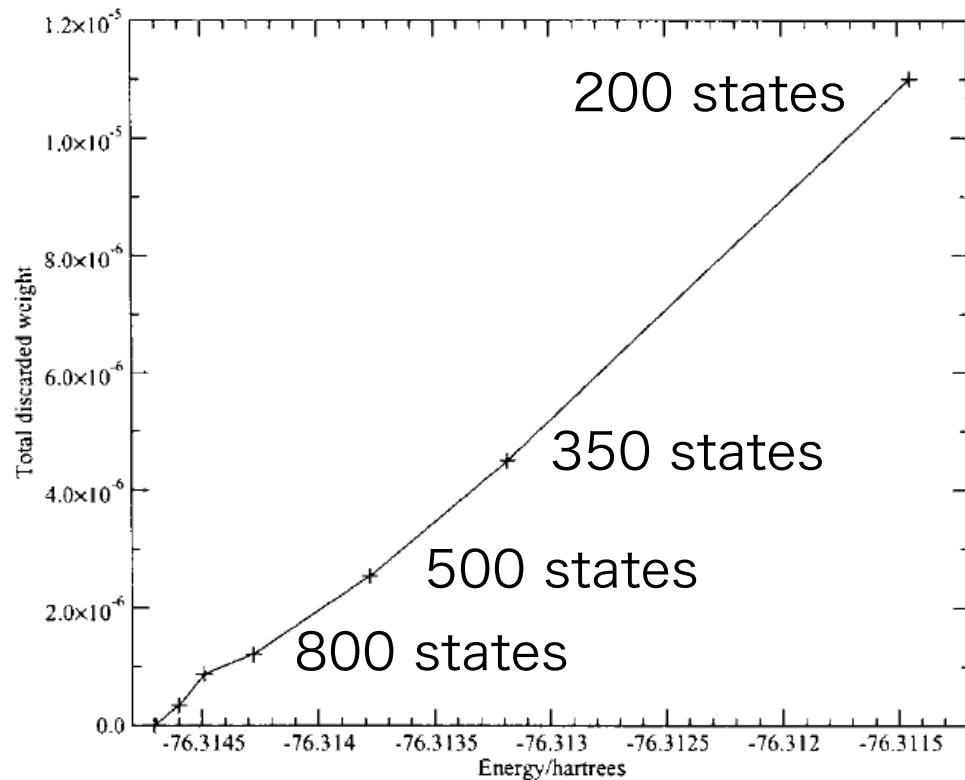
# How Much DMRG Reduces Number of States

Water ( $\text{H}_2\text{O}$ ) molecule

(5  $\uparrow$ -spin electrons & 5  $\downarrow$ -spin electrons)

Fock space dimension of  $\text{H}_2\text{O}$  (by 41 orbitals):

$$\left( \frac{41!}{5! \times 36!} \right)^2 \sim 5.6 \times 10^{11}$$

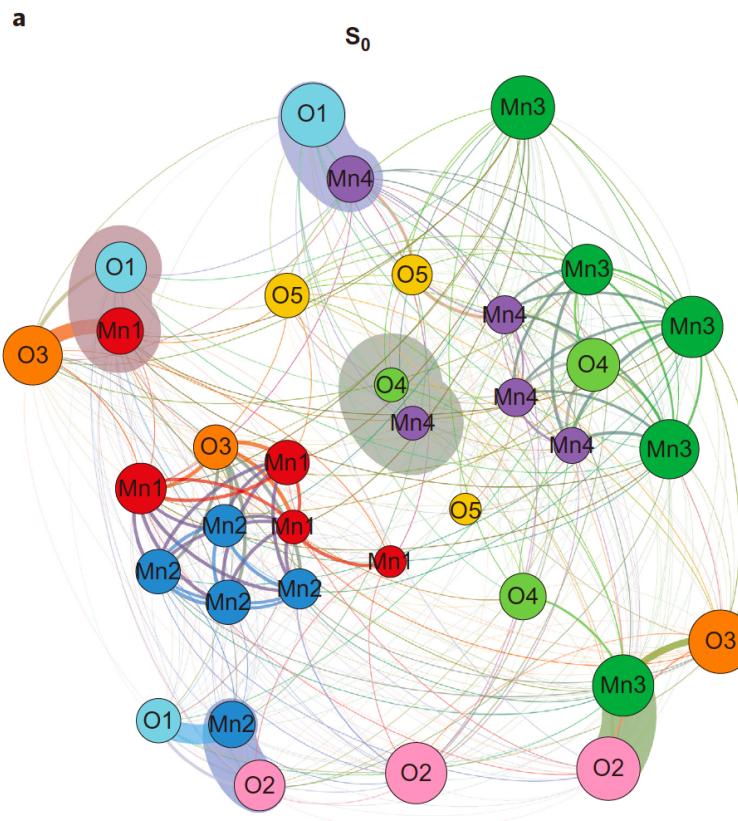
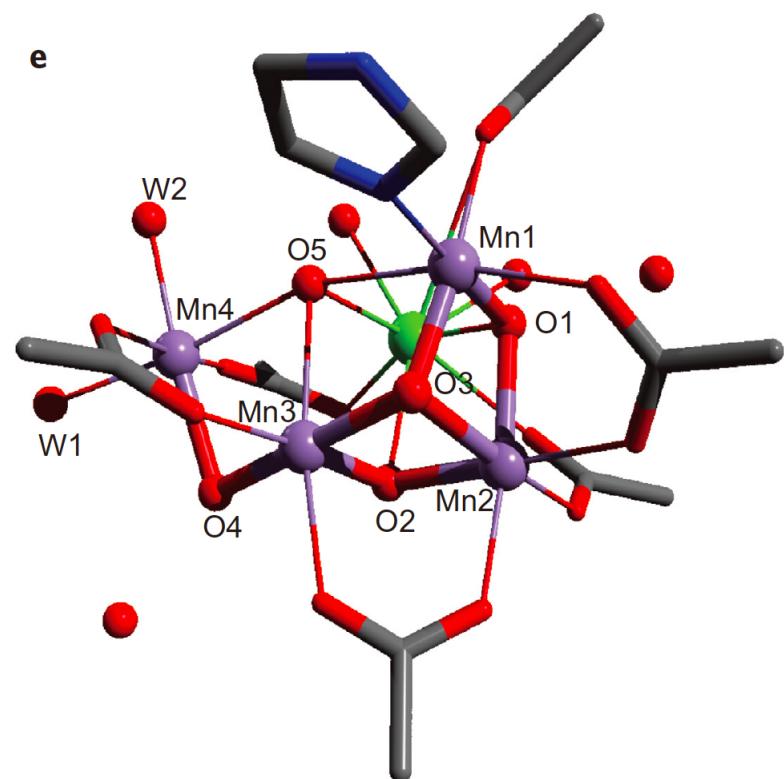


# How Much DMRG Reduces Number of States

## Manganese cluster in photosystem II

Y. Kurashige, G. K.-L. Ghan, & T. Yanai, Nat. Chem. 5, 660 (2013)

44 electrons in 35 orbitals  $\rightarrow 2 \times 10^{18}$  dimensional



# Nearsightedness

Fock space dimension can be stored in memory

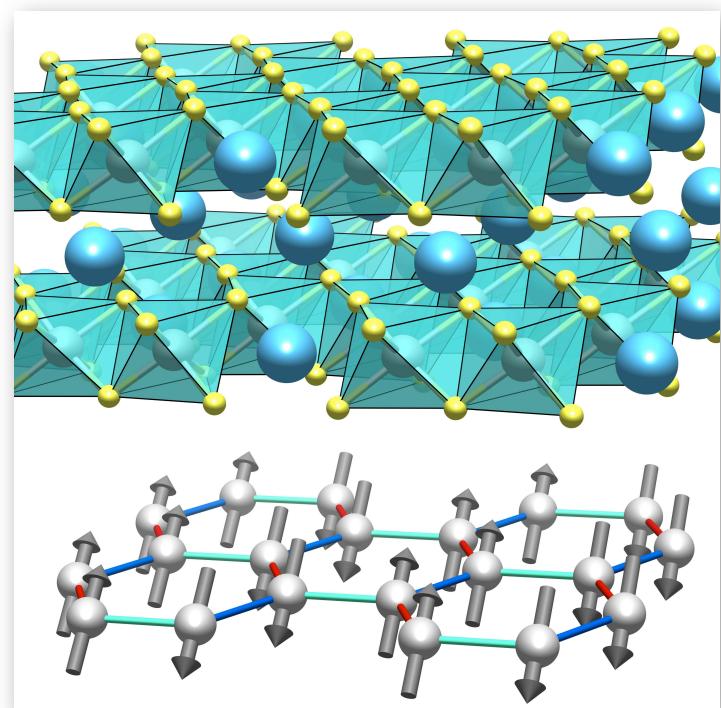
- Hubbard-like hamiltonian  
 $N (< 30\text{-}40)$  orbital systems
- Heisenberg-like hamiltonian  
 $N (< 50)$  *spin* systems

How about crystalline lattice ?  
(with periodic boundary)

- Finite  $N$  calculations are useful?

## Nearsightedness

W. Kohn, Phys. Rev. Lett. 76, 3168 (1996).



# Naïve Assumption on Low-Rank Nature & Interpolation Based on Low-Rank Nature

# Recommendation System by Collaborative Filtering

As a review,

Chih-Chao Ma, *A Guide to Singular Value Decomposition for Collaborative Filtering*.

Problem:

Recommend *objects* to *users* based on the rating matrix

Example of rating matrix

	Madmax: Fury Road	Pacific Rim	Les Miserables	Skyfall	Creed	Logan
Alice	5			3		
Bob		2			3	
Charlie	3		4			4
Damon	5	5		3		
Eddie			2		5	3

-Number of non-zero entries is small

-Sparseness is not clear *a priori* (演繹的に), at least, for me

Should be validated *a posteriori* (帰納的に)

## Data sets for the rating matrix

From Chih-Chao Ma, *A Guide to Singular Value Decomposition for Collaborative Filtering.*

Dataset	# user	# object	# training score	# test score	density
<i>Movielens</i>	6,040	3,706	982,089	18,120	4.61%
<i>Netflix</i>	480,189	17,770	99,072,112	1,408,395	1.18%
<i>small1</i>	2,917	167	9,734	138	2.00%
<i>small2</i>	4,802	178	702,956	138	82.24%
<i>small3</i>	56	178	9,809	138	98.40%

-Number of non-zero entries is really small!

# Singular Value Decomposition of Partially Unknown Matrix

As a review,

Chih-Chao Ma, *A Guide to Singular Value Decomposition for Collaborative Filtering.*

## Mathematical formulation: Input

Rating matrix

$$V = \begin{bmatrix} 5 & 0 & 0 & 3 & 0 & 0 \\ 0 & 2 & 0 & 0 & 3 & 0 \\ 3 & 0 & 4 & 0 & 0 & 4 \\ 5 & 5 & 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 & 5 & 3 \end{bmatrix} \quad V \in \mathbb{R}^{n \times m}$$

Indicator

$$I = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix} \quad I \in \{0, 1\}^{n \times m}$$

# Singular Value Decomposition of Partially Unknown Matrix

As a review,

Chih-Chao Ma, *A Guide to Singular Value Decomposition for Collaborative Filtering.*

## Mathematical formulation

Rating matrix

$$V = \begin{bmatrix} 5 & 0 & 0 & 3 & 0 & 0 \\ 0 & 2 & 0 & 0 & 3 & 0 \\ 3 & 0 & 4 & 0 & 0 & 4 \\ 5 & 5 & 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 & 5 & 3 \end{bmatrix} \quad V \in \mathbb{R}^{n \times m}$$

Infer the SVD of the *complete* rating matrix from  $V$

$$\tilde{V} \simeq U^T M$$

$$U \in \mathbb{R}^{f \times n}$$

$$M \in \mathbb{R}^{f \times m}$$

-Rank  $f$  approximation

# Singular Value Decomposition of Partially Unknown Matrix

As a review,

Chih-Chao Ma, *A Guide to Singular Value Decomposition for Collaborative Filtering*.

## Mathematical formulation

Minimize the cost function

$$E = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^m I_{ij} [V_{ij} - p(U_i, M_j)]^2$$

$$+ \frac{k_u}{2} \sum_{i=1}^n \|U_i\|_2^2 + \frac{k_m}{2} \sum_{j=1}^m \|M_j\|_2^2$$

Feature vectors

$$U_i = (U_{1i}, U_{2i}, \dots, U_{fi})^T$$

$$M_j = (M_{1j}, M_{2j}, \dots, M_{fj})^T$$

- $L_2$  regularization

A prediction function for the rating (You need to choose)

$$p(U_i, M_j) = \begin{cases} 1 & \text{if } U_i^T M_j < 0 \\ 1 + U_i^T M_j & \text{if } 0 < U_i^T M_j < 4 \\ 5 & \text{if } 4 < U_i^T M_j \end{cases}$$

# Singular Value Decomposition of Partially Unknown Matrix

$$\text{RMSE}(p, V) = \sqrt{\frac{\sum_{i,j} I_{ij} [V_{ij} - p(U_i, M_j)]^2}{\sum_{i,j} I_{ij}}}$$

Optimization:  
Steepest descent

$$U_i \leftarrow U_i - \mu \nabla_U E$$

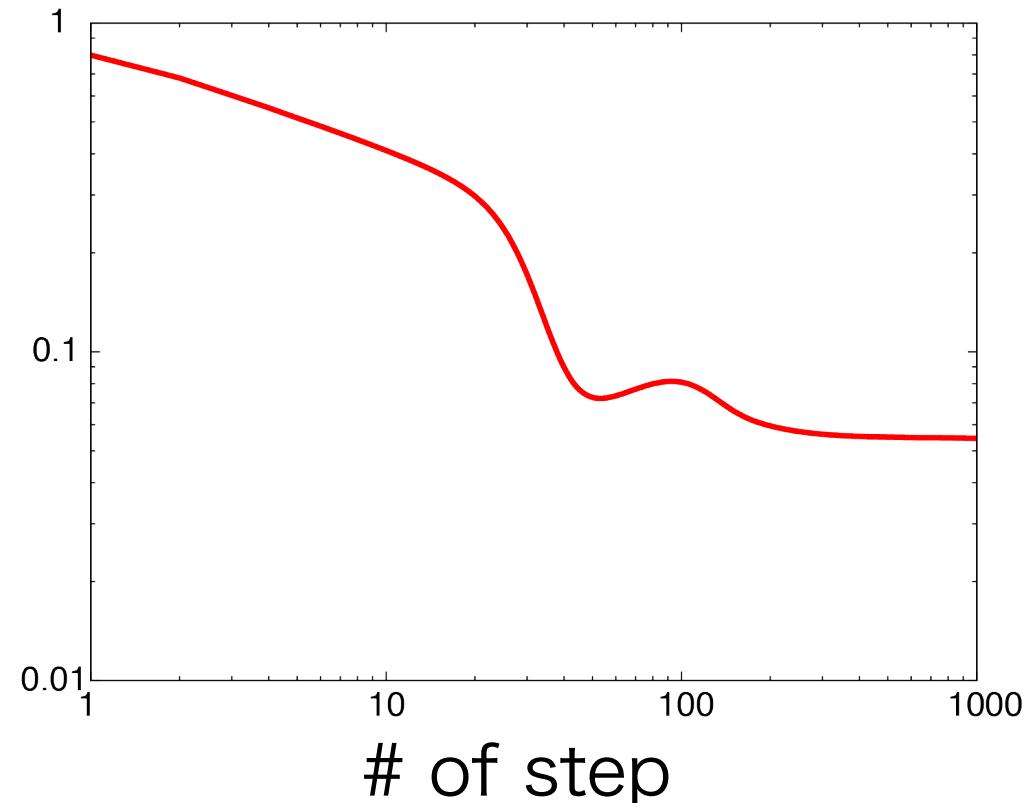
$$M_j \leftarrow M_j - \mu \nabla_M E$$

Parameters

$$f = 3$$

$$\mu = 0.1$$

$$k_u = k_m = 0.1$$



# Singular Value Decomposition of Partially Unknown Matrix

Original rating matrix

$$V = \begin{bmatrix} 5 & 0 & 0 & 3 & 0 & 0 \\ 0 & 2 & 0 & 0 & 3 & 0 \\ 3 & 0 & 4 & 0 & 0 & 4 \\ 5 & 5 & 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 & 5 & 3 \end{bmatrix}$$

A predicted rating matrix

$$p(U_i, M_j) = \begin{bmatrix} \textcolor{blue}{4.92} & 4.39 & 2.29 & \textcolor{blue}{2.96} & 4.93 & 3.23 \\ 2.57 & \textcolor{blue}{2.02} & 1.07 & 1.78 & \textcolor{blue}{2.94} & 1.60 \\ \textcolor{blue}{3.01} & 3.82 & \textcolor{blue}{3.92} & 2.05 & 2.55 & \textcolor{blue}{3.94} \\ \textcolor{blue}{4.98} & \textcolor{blue}{4.91} & 3.11 & \textcolor{blue}{3.00} & 4.64 & 3.85 \\ 4.55 & 3.85 & 2.01 & 2.78 & 4.92 & \textcolor{blue}{2.98} \end{bmatrix}$$

- $f > 2$  is enough (for Netflix,  $f \sim 100-1000$ )

-Should be validated (but the data set is too small)

# Application of Recommendation System to Materials Science

A goal of materials science:  
Synthesize a compound with desired functions

Difficulty:  
Process of synthesis is complicated  
and costs much time and resources

→ *Virtual screening* is desirable

Virtual screening by recommendation system  
A recommendation system tells us whether  
a given chemical composition (化学組成)  
is synthesizable or not

A. Seko, H. Hayashi, H. Kashima, & I. Tanaka, Phys. Rev. Materials 2, 013805 (2018).

-Crystal structure is another important problem

# Application of Recommendation System to Material Science

A. Seko, H. Hayashi, H. Kashima, & I. Tanaka, Phys. Rev. Materials 2, 013805 (2018).

Example: Ternary compounds (3元化合物)  $A_aB_bX_x$

-Generating possible chemical compositions

-Synthesis is reported  
→ non-zero entry 1

TABLE I. Elements included in the datasets of known CRCs. Rare-earth elements shown in parentheses are excluded in the candidate quaternary and quinary compositions.

Cations	Li,Na,K,Rb,Cs,Be,Mg,Ca,Sr,Ba,Zn,Cd,Hg, B,Al,Sc,Y,La,Ga,In,Tl,Si,Ge,Sn,Pb,P,As,Sb,Bi Ti,Zr,Hf,V,Nb,Ta,Cr,Mo,W,Mn,Tc,Re, Fe,Ru,Os,Co,Rh,Ir,Ni,Pd,Pt,Cu,Ag,Au, (Ce,Pr,Nd,Pm,Sm,Eu,Gd,Tb,Dy,Ho,Er,Tm,Yb,Lu)
Anions	C,N,O,S,Se,Te,F,Cl,Br,I

	Ternary	Quaternary	Quinary
ICSD	9,313	7,742	1,321
ICDD	2,369 (9,278)	2,647 (7,864)	639 (1,326)
SpMat	2,708 (10,461)	3,066 (8,141)	1,169 (1,893)
ICDD+SpMat	4,134 (12,573)	4,961 (11,307)	1,616 (2,562)
Candidates	7,405,200	1,188,038,460	23,104,706,560

# Application of Recommendation System to Material Science

A. Seko, H. Hayashi, H. Kashima, & I. Tanaka, Phys. Rev. Materials 2, 013805 (2018).

Example: Ternary compounds (3 元化合物)  $A_a B_b X_x$

-Schematic rating matrix

Li <sub>2</sub> O (1,1,1)	Li <sub>2</sub> O (1,1,2)	Li <sub>2</sub> O (1,2,2)	Li <sub>2</sub> O (1,3,3)	Li <sub>2</sub> O (1,4,3)	...	In <sub>2</sub> O (1,1,2)	In <sub>2</sub> O (1,1,3)	In <sub>2</sub> O (1,2,4)	In <sub>2</sub> O (2,2,5)	In <sub>2</sub> O (3,3,8)	
0	0	0	0	0	...	1	0	0	0	0	Na
0	0	0	0	0	...	0	0	1	0	0	Mg
0	1	0	0	0	...	0	0	0	0	0	Al
:	:	:	:	:	..	:	:	:	:	:	
1	1	1	1	0	...	1	0	1	1	1	Cu
0	0	0	0	1	...	0	0	1	0	0	Zn
0	1	0	0	0	...	0	1	0	0	0	Ga

# References

Renormalization and GLW:

P. M. Chaikin, & T. C. Lubensky,

*Principles of condensed matter physics*,

Cambridge University Press 1995

Reasonable low-rank nature in materials science:

M. Shiga, *et al.*, Ultramicroscopy 170, 43 (2016);

M. Shiga, *et al.*, Trans. Mat. Res. Soc. Japan 41, 333 (2016).

# Announcement on ITC-LMS

## Additional lectures related to quantum algorithms

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Pilot lectures organized by

**Quantum Software Endowed Chair**  
(量子ソフトウェア寄付講座)

<https://qsw.phys.s.u-tokyo.ac.jp>

- On Dec. 14, 21, Jan. 11, 25, we will organize lectures related to quantum algorithms.
  - The lectures will start from 17:00, and they are 90 min each.
  - The lectures will be given by Prof. Todo and Okubo.
  - They will be given in Japanese, although we will prepare lecture materials in English.

### Topics

- (12/14) Tensor network renormalizaiton
- (12/21) Quantum computers and simulations
- (1/11) Quantum error corrections and tensor network
- (1/25) Quantum-classical hybrid algorithms and tensor network

# Announcement on ITC-LMS

Workshop on tensor network and quantum computation

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## 第1回量子ソフトウェアワークショップ： テンソルネットワークと量子計算の展望

<https://qsw.phys.s.u-tokyo.ac.jp/workshop202112>

「テンソルネットワーク」と「量子計算」をキーワードとして、大学・  
産業界から登壇者を招き、最先端の情報交換と緊密な議論を行うこと  
で、量子ソフトウェア分野の今後の発展と展望を探ります。

### 開催概要

- ・日時: 2021年12月7日(火) 13:00-17:10
- ・場所: オンライン (Webex Meetings)
- ・定員: 200名 (事前の参加申し込みが必要です)
- ・参加費用: 無料
- ・参加申し込み締切: 2021年12月6日(月) 13:00

ワークショップの詳細および参加申し込みについては上のページをご参照ください

# Next Next Week (No lecture on Nov. 25)

1st: Huge data in modern physics

2nd: Information compression in modern physics

3rd: Review of linear algebra

4th: Singular value decomposition and low rank approximation

5th: Basics of sparse modeling

6th: Basics of Krylov subspace methods

7th: Information compression in materials science

**8th: Accelerating data analysis:**

## **Application of sparse modeling**

9th: Data compression: Application of Krylov subspace method

10th: Entanglement of information and matrix product states

11th: Application of MPS to eigenvalue problems

12th: Tensor network representation

13th: Information compression by tensor network renormalization