2026/07/09
第29回学習物理領域セミナー＋第81回DLAP

機械学習手法を用いた量子多体問題の解析

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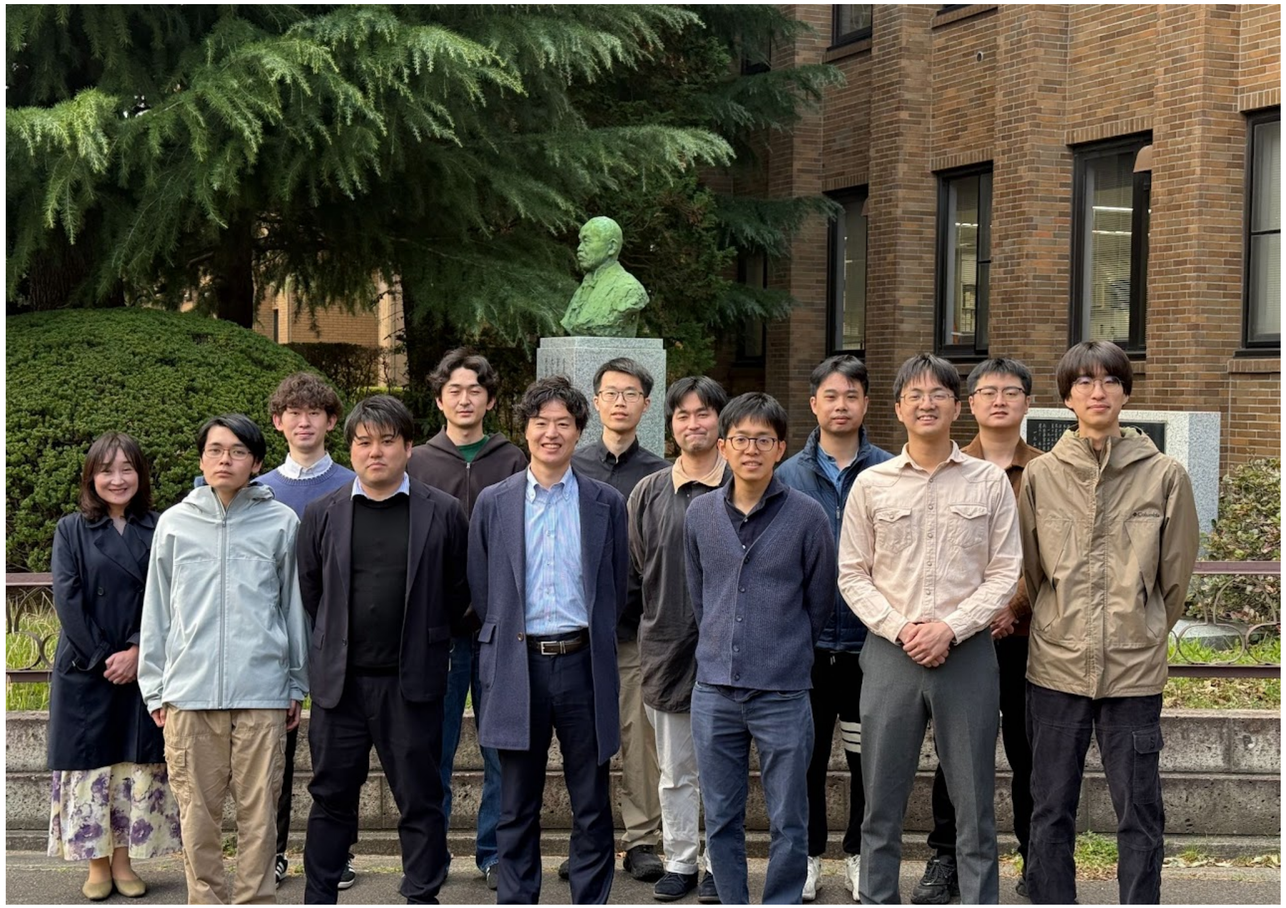
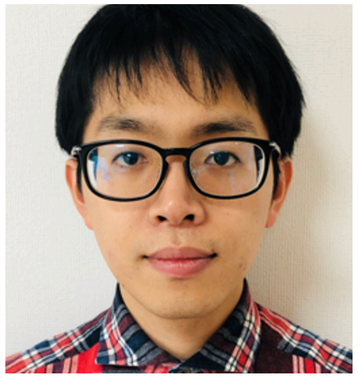


Yusuke Nomura

Strongly correlated materials
Machine learning

Yuta Murakami



Many-body calculations
Nonequilibrium

Hsiao-Yi Chen

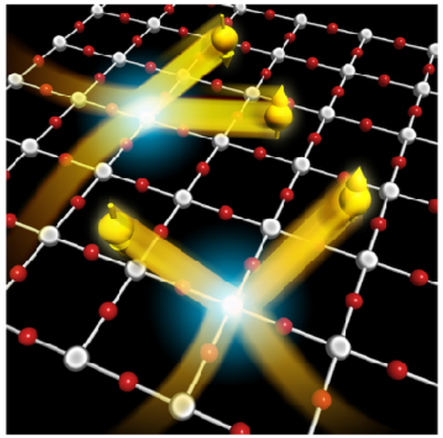
Ab initio calculations
(exciton, magnon, …)

Hitoshi Mori

Ab initio calculations
(phonon)

Quantum many-body problems

Materials = quantum many-body systems



Quantum many-body problems

$$\mathcal{H}\psi = E\psi$$

quantum many-body Hamiltonian

quantum state

Exponential computational cost on classical PC

— quantum and many-body nature → Emergent quantum phenomena

— Various quantum phases compete with each other within small energy scale

Bias from human insight may result in wrong understanding/prediction → machine learning/neural network

Reviews

IOP Publishing
J. Phys.: Condens. Matter **36** (2024) 073001 (14pp)
Journal of Physics: Condensed Matter
https://doi.org/10.1088/1361-648X/ad0916

Topical Review

Boltzmann machines and quantum many-body problems

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Abstract

Analyzing quantum many-body problems and elucidating the entangled structure of quantum states is a significant challenge common to a wide range of fields. Recently, a novel approach using machine learning was introduced to address this challenge. The idea is to 'embed' nontrivial quantum correlations (quantum entanglement) into artificial neural networks. Through intensive developments, artificial neural network methods are becoming new powerful tools for analyzing quantum many-body problems. Among various artificial neural networks, this topical review focuses on Boltzmann machines and provides an overview of recent developments and applications.

Journal of the Physical Society of Japan **94**, 031001 (2025)
https://doi.org/10.7566/JPSJ.94.031001
Special Topics
Machine Learning Physics

Quantum Many-Body Solver Using Artificial Neural Networks and its Applications to Strongly Correlated Electron Systems

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With the evolution of numerical methods, we are now aiming at not only qualitative understanding but also quantitative prediction and design of quantum many-body phenomena. As a novel numerical approach, machine learning techniques have been introduced in 2017 to analyze quantum many-body problems. Since then, proposed various novel approaches have opened a new era, in which challenging and fundamental problems in physics can be solved by machine learning methods. Especially, quantitative and accurate estimates of material-dependent physical properties of strongly correlated matter have now become realized by combining first-principles calculations with highly accurate quantum many-body solvers developed with the help of machine learning methods. Thus developed quantitative description of electron correlations will constitute a key element of materials science in the next generation.

本日のトピック

1. 量子多体問題とそれに対する機械学習を用いた波動関数法：導入

2. 精度を向上させるためには？
   - 物理の知見を利用
   - 大規模化

3. どのように性能を統一的に評価するか？

4. ベンチマークを超えた応用の取り組み

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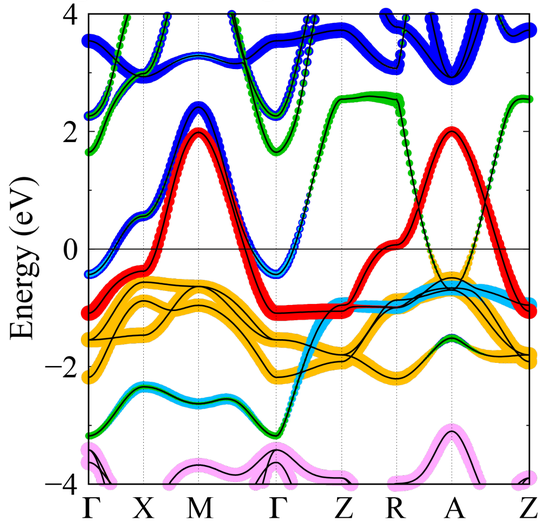
Microscopic picture for understanding physical properties

$$i\hbar\frac{\partial\Psi_{\rm el}(\{\boldsymbol{r}\},t)}{\partial t}=\left[\sum_i\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\boldsymbol{r}_i^2}-\sum_I\frac{Z_Ie^2}{|\boldsymbol{r}_i-\boldsymbol{R}_I|}\right)+\sum_{i<j}\frac{e^2}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}\right]\Psi_{\rm el}(\{\boldsymbol{r}\},t)$$

Kinetic Energy — Attraction from Nuclei (crystal structure) — Electron-electron Interaction

Band structure (wave-like picture)

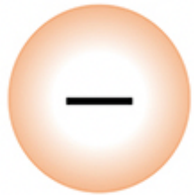
tight-binding Hamiltonian



+

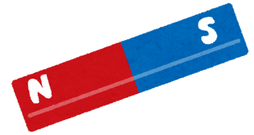
Interaction among charge, spin, orbital (particle-like picture)

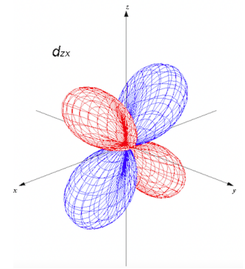
repulsion between charges, spin exchange, …



Charge

Spin





Orbital

Simulations are performed based on the above picture (interactions are difficult to handle)

Difficulty in solving microscopic equations

Quantum many-body problems in condensed matter physics : Many-body Schrödinger equation

Kinetic Energy　Attraction from nuclei (crystal stcutrue)　El-el repulsion

$$\left[\sum_i\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \boldsymbol{r}_i^2}-\sum_I\frac{Z_I e^2}{|\boldsymbol{r}_i-\boldsymbol{R}_I|}\right)+\sum_{i<j}\frac{e^2}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}\right]\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)=E\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)$$

(Material dependent) quantum many-body Hamiltonian

Wave function（representing quantum states）

The wave function can be expressed as a complex vector. The element for (r_1, …, r_N) is $\psi(r_1, \ldots, r_N)$.
Even if the mesh points in real space are only 10 points, at N=15 the dimension is 10^{15} → PB-order memory.

Bra–ket notation

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

Quantum many-body Hamiltonian
(complex matrix with enormous dimensions)

Quantum State
(complex vector with enormous dimension, vector representation=wave function)

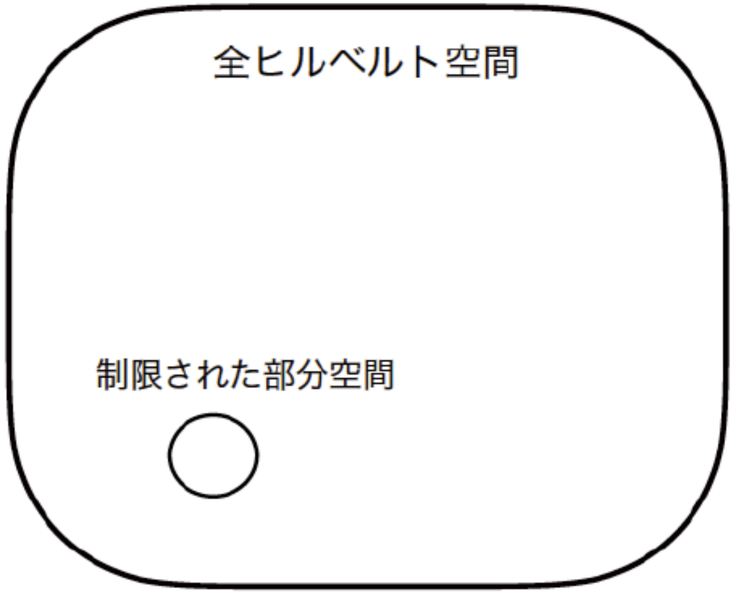
Cannot be solved exactly (takes exponentially long time)

Challenge = Accurate representation of quantum states

Approximation of quantum states: conventional vs ML

従来の変分法

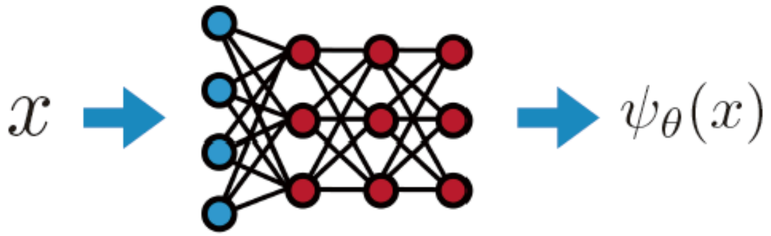
変換のルールは人間が決める（計算科学）



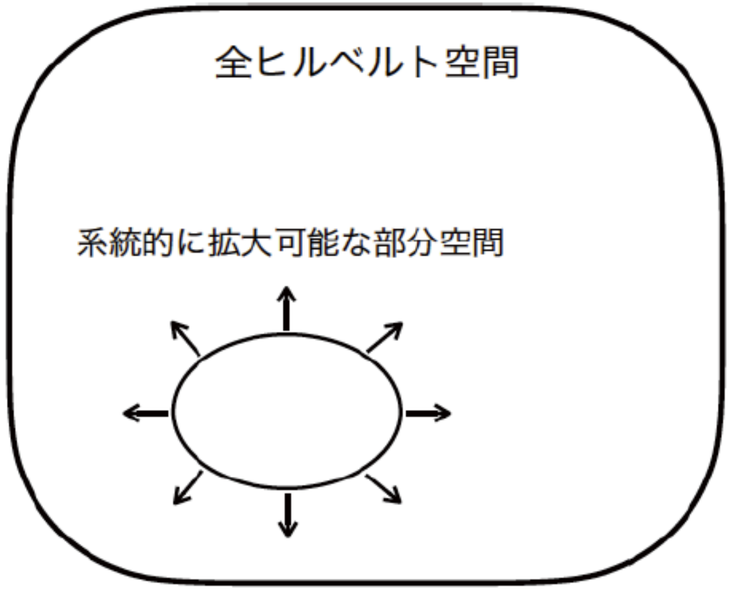
2017~

Carleo and Troyer
Science **355**, 602 (2017)

人工ニューラルネットワークによる変分法



変換のルールはデータが決める（情報科学）



To approximate quantum states by neural networks

Settings required in machine learning tasks (in case of quantum state approximation)

1. Define inputs for neural networks

   → Particle real-space configurations

2. Define outputs of neural networks and their architecture (# of hidden layers, …)

   → Wave function

3. Define cost function

   → Energy expectation value <H> (since ground state is the lowest energy state)

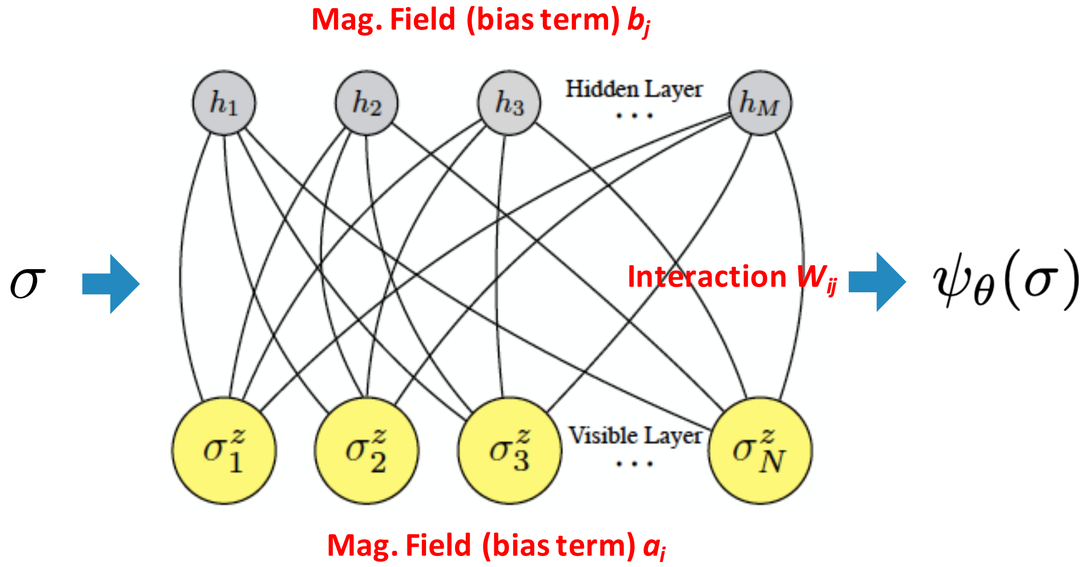
4. Select optimization method

   → Natural gradient method = approximate imaginary-time Hamiltonian evolution

$$\underbrace{\delta\theta}_{\text{network parameter}} = \arg\min_{\delta\theta} \mathcal{F}\left(\underbrace{e^{-2\delta_\tau \mathcal{H}}|\psi_\theta\rangle}_{\text{exact evol.}}, \underbrace{|\psi_{\theta+\delta\theta}\rangle}_{\text{approx. evol.}}\right) = -\delta_\tau \underbrace{S^{-1}}_{\text{metric tensor}} \underbrace{\partial_\theta \langle \mathcal{H} \rangle}_{\text{gradient}}$$

S. Sorella, Phys. Rev. B 64, 024512 (2001); S.-I. Amari, Neural Comput. **10**, 251 (1998)

RBM wave function for quantum spin systems



G. Carleo and M. Troyer Science **355**, 602 (2017)

RBM (restricted Boltzmann machine) wave function

$$\psi_\theta(\sigma) = \sum_h \underbrace{\exp\left(\sum_i a_i \sigma_i^z + \sum_{i,j} \sigma_i^z W_{ij} h_j + \sum_j h_j b_j\right)}_{e^{-E_{\mathrm{RBM}}(\sigma,h)}}$$

(Boltzmann weight)

$\sigma = (\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z)$: real space spin config.

$h_j = \pm 1$: spin of hidden units

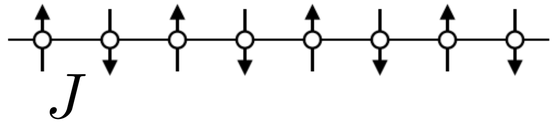
When a=0, RBM wave function can be recast as

$$\psi_\theta(\sigma) = \prod_j \cosh\left(b_j + \sum_i W_{ij}\sigma_i^z\right)$$

A more general wave function based on neural networks is written as

$$\psi_\theta(\sigma) = \mathcal{N}_L \circ \mathcal{L}_L \circ \cdots \circ \mathcal{N}_1 \circ \mathcal{L}_1(\sigma)$$

Example: 1D Heisenberg model (8 site)



$$\mathcal{H} = \sum_i (-\sigma_i^x \sigma_{i+1}^x - \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z)$$

Loss function = Energy $E_\theta = \dfrac{\langle \psi_\theta | \mathcal{H} | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle}$

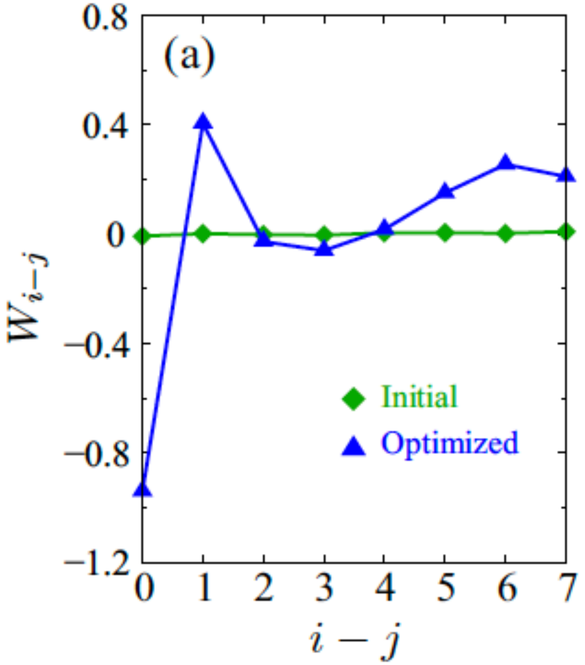
Variational principle: $E_\theta \geq E_0$

※ data for training can be produced by Monte Carlo

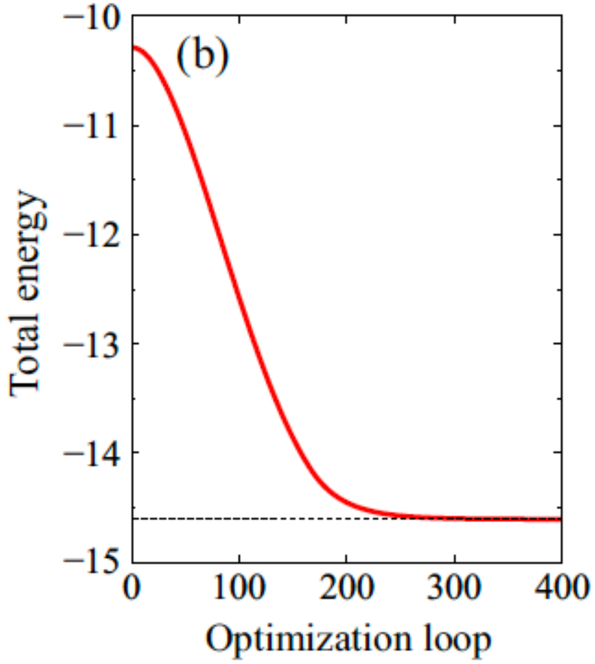
$$E_\theta = \sum_\sigma P_\theta(\sigma) E_\theta^{\mathrm{loc}}(\sigma)$$

$$P_\theta(\sigma) = \frac{|\psi_\theta(\sigma)|^2}{\sum_\sigma |\psi_\theta(\sigma)|^2} \qquad E_\theta^{\mathrm{loc}}(\sigma) = \sum_{\sigma'} \mathcal{H}_{\sigma\sigma'} \frac{\psi_\theta(\sigma')}{\psi_\theta(\sigma)}$$

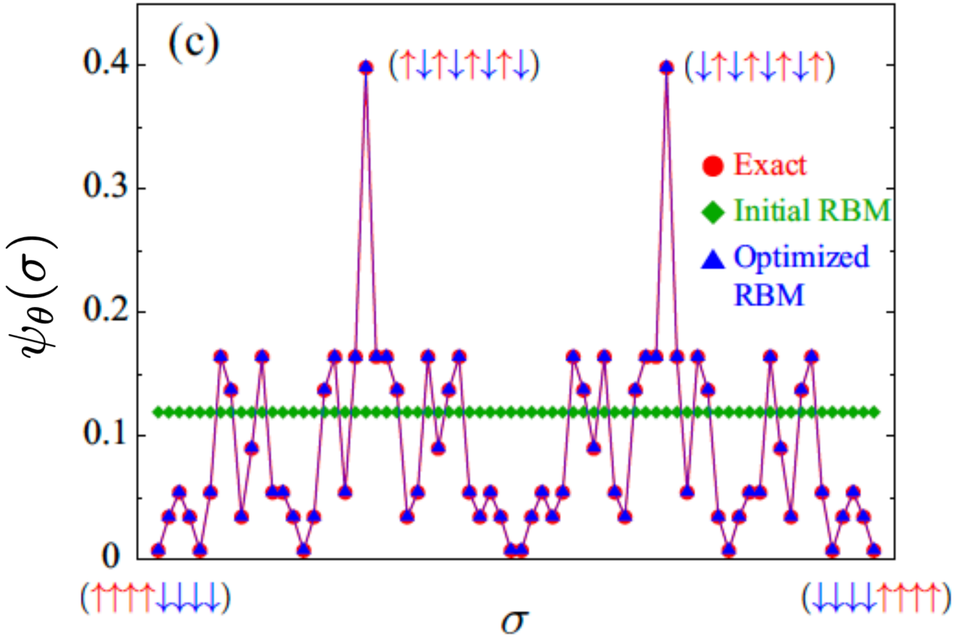
Network parameters



Cost function = Energy



Wave function (output)



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   - 物理の知見を利用
   - 大規模化

cf. 第12回学習物理領域セミナー＋第64回DLAP, 今田先生, 「フェルミマシン」
隠れ層の自由度をフェルミオンに

3. どのように性能を統一的に評価するか？

4. ベンチマークを超えた応用の取り組み

RBM＋PP wave function

YN, A. Darmawan, Y. Yamaji, and M. Imada,
PRB **96**, 205152 (2017)

RBM+PP wave function

$$\Psi(x) = \mathcal{N}(x)\phi_{\mathrm{pair}}(x)$$

Neural network (RBM) Bosonic

Pair-product (PP) state (geminal) Fermionic

cf. many variable VMC wave function

$$\Psi(x) = \mathcal{P}_{\mathrm{G}}(x)\mathcal{P}_{\mathrm{J}}(x)\phi_{\mathrm{pair}}(x)$$

Gutzwiller fac. Jastrow fac.

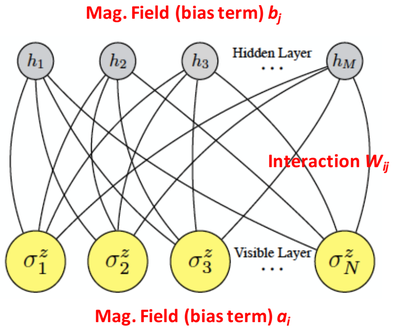
D. Tahara and M. Imada JPSJ **77**, 114701 (2008)

RBM part（incorporating nontrivial correlations）

$$\mathcal{N}(x) = \prod_k 2\cosh\left(b_k + \sum_i W_{ik}\sigma_i\right)$$

(# visible spins)= $2N_{\mathrm{site}}$

$$\sigma_{2i} = 2n_{i\uparrow} - 1 = \pm 1$$
$$\sigma_{2i-1} = 2n_{i\downarrow} - 1 = \pm 1$$



Carleo and Troyer Science **355**, 602 (2017)

PP part（incorporating important correlations in advance）

$$|\phi_{\mathrm{pair}}\rangle = \left(\sum_{i,j=1}^{N_{\mathrm{site}}} \sum_{\sigma,\sigma'=\uparrow,\downarrow} f_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger}\right)^{N_{\mathrm{e}}/2} |0\rangle$$

RBM representation of Gutzwiller and Jastrow factors

Gutzwiller factor

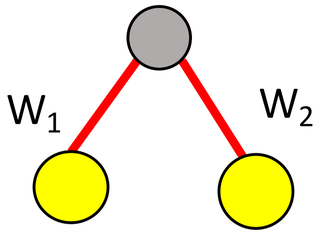
$$\mathcal{P}_{\mathrm{G}} = \exp(-g n_{i\uparrow} n_{i\downarrow}) \longrightarrow \mathcal{P}_{\mathrm{G}} = \exp\left(-\frac{g}{4}\sigma_{2i}\sigma_{2i-1}\right)$$

except for constant factor and one-body potential

$$(\sigma_{2i}, \sigma_{2i-1}) = (2n_{i\uparrow} - 1, 2n_{i\downarrow} - 1)$$

RBM representation of Gutwiller factor (the same transformation can be applied to Jastrow factor)

except for constant factor



$$\mathcal{P}_{\mathrm{G}} = \exp\left(-\frac{g}{4}\sigma_{2i}\sigma_{2i-1}\right)$$

$$\mathcal{P}_{\mathrm{G}} = \sum_{h=\pm 1} \exp(W_1\sigma_{2i}h + W_2\sigma_{2i-1}h)$$

$$= 2\cosh(W_1\sigma_{2i} + W_2\sigma_{2i-1})$$

$$\begin{cases} W_1 = \frac{1}{2}\mathrm{arcosh}(\exp(|g|/2)) \\ W_2 = -\mathrm{sgn}\ g \times W_1 \end{cases}$$

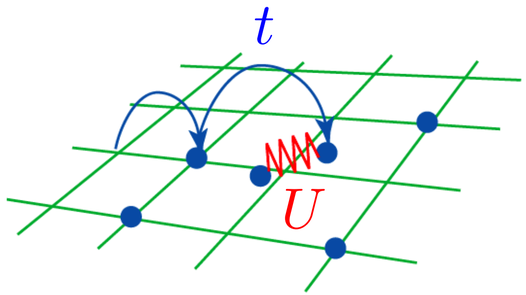
Benchmark using 2D Hubbard model

YN, A. Darmawan, Y. Yamaji, and M. Imada,
PRB **96**, 205152 (2017)

Hubbard model on a square lattice

8x8 square lattice, half-filling (periodic, anti-periodic)

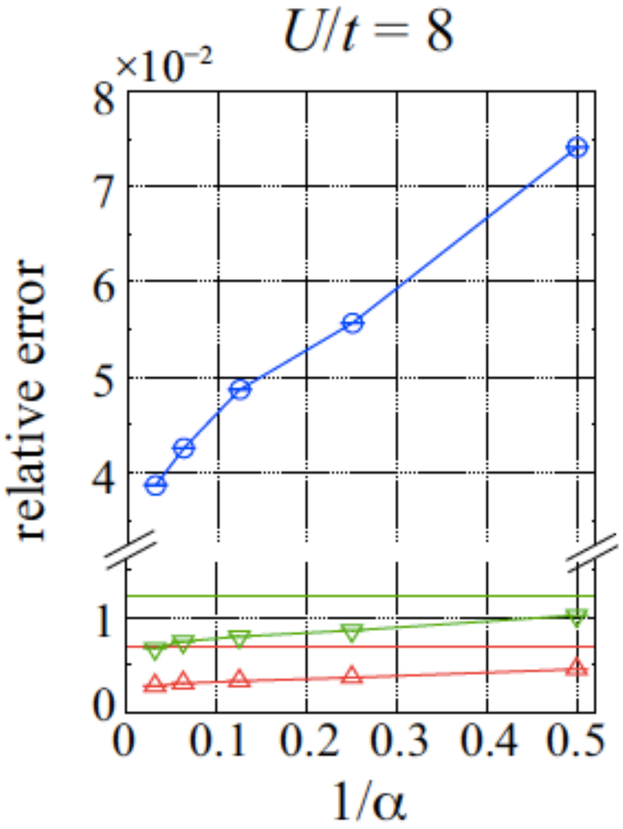
$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Benchmark: Correlation function

	$S(\pi,\pi)/N_{\rm site} \times 10^2$				
	$\alpha = 2$	$\alpha = 8$	$\alpha = 32$	mVMC	AF-QMC
$U/t=4$	3.078(5)	3.057(5)	3.021(5)	3.107(4)	2.92(2)
$U/t=8$	5.233(9)	5.206(9)	5.20(1)	5.30(1)	5.0(1)

Benchmark : Energy



RBM(+Fermi sea)

RBM+PP

RBM+
symmetrized PP

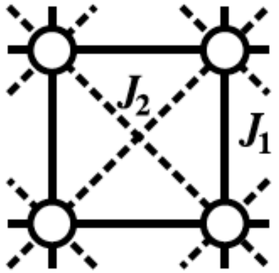
α = (# hidden units)/(# visible units)

PP state helps RBM to learn ground state

Benchmark using 2D J_1-J_2 Heisenberg model ①

Antiferromagnetic J_1-J_2 Heisenberg model on square lattice ($J_1 > 0$, $J_2 > 0$, J_1 and J_2 competes)

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



RBM+PP wave function

$$\Psi(\sigma) = \mathcal{N}(\sigma) \times P_{\mathrm{G}} \phi_{\mathrm{pair}}(\sigma)$$

neural-network (RBM)

Gutzwiller-projected PP state (physics-inspired, RVB type)

$$\sigma_i = 2S_i^z = \pm 1$$ (# visible spins)= N_{site}

YN and M. Imada Phys. Rev. X **11**, 031034 (2021)

momentum and spin-parity projections

spin-parity (+ : S even, − : S odd)

$$\Psi_{\mathbf{K}}^{S_\pm}(\sigma) = \sum_{\mathbf{R}} e^{-i\mathbf{K}\cdot\mathbf{R}} [\Psi(T_{\mathbf{R}}\sigma) \pm \Psi(-T_{\mathbf{R}}\sigma)]$$

total momentum

wave func. w/o symmetry

YN JPCM **33**, 174003 (2021)

Benchmark using 2D J_1-J_2 Heisenberg model ②

YN and M. Imada
Phys. Rev. X **11**, 031034 (2021)

ground-state energy, 10x10 lattice, J_2=0.5

Energy per site	Wave function	Reference
−0.494757(12)	**Neural quantum state**	[72]
−0.49516(1)	**CNN**	[67]
−0.49521(1)	VMC($p=0$)	[23]
−0.495530	DMRG	[25]
−0.49575(3)	**RBM-fermionic wave function**	[70]
−0.497549(2)	VMC($p=2$)	[23]
−0.497629(1)	**RBM + PP**	Present study

→ 13,132 parameters

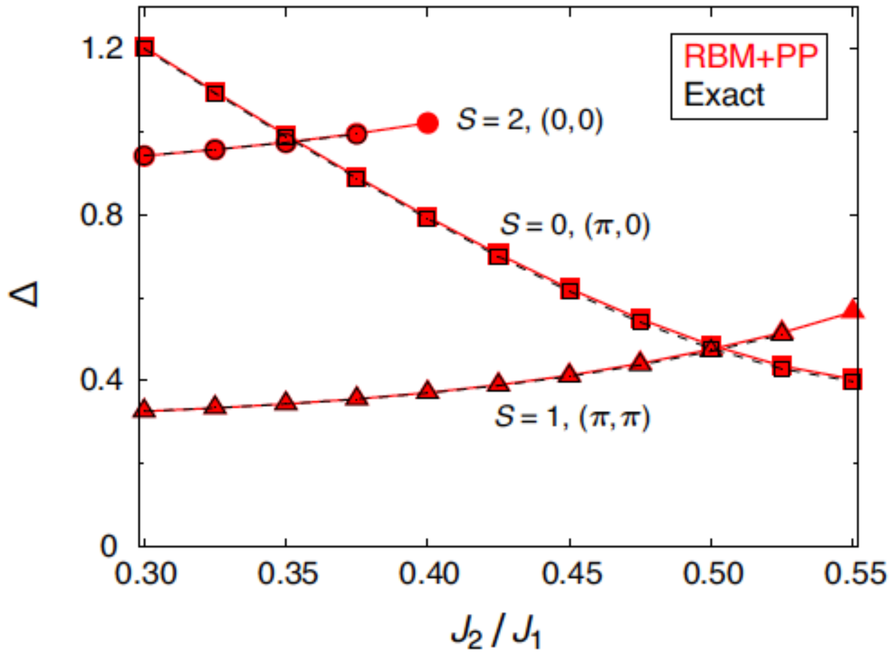
−0.497634(1) **Vision Transformer** R. Rende et al.

→ 267,720 parameters

−0.4976921(4) **Residual neural networks** A. Chen et al.

→ 1,071,488 parameters

excited-state energy, 6x6 lattice



[72] Szabó and Castelnovo PRR 2020 [67] Choo et al., PRB 2019
[23] Hu et al., PRB 2013 [25] Gong et al., PRL 2014 [70] Ferrari et al., PRB 2019

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Minimum-step stochastic reconfiguration (MinSR) method

Chen and Heyl
Nat. Phys. **20**, 1476 (2024)

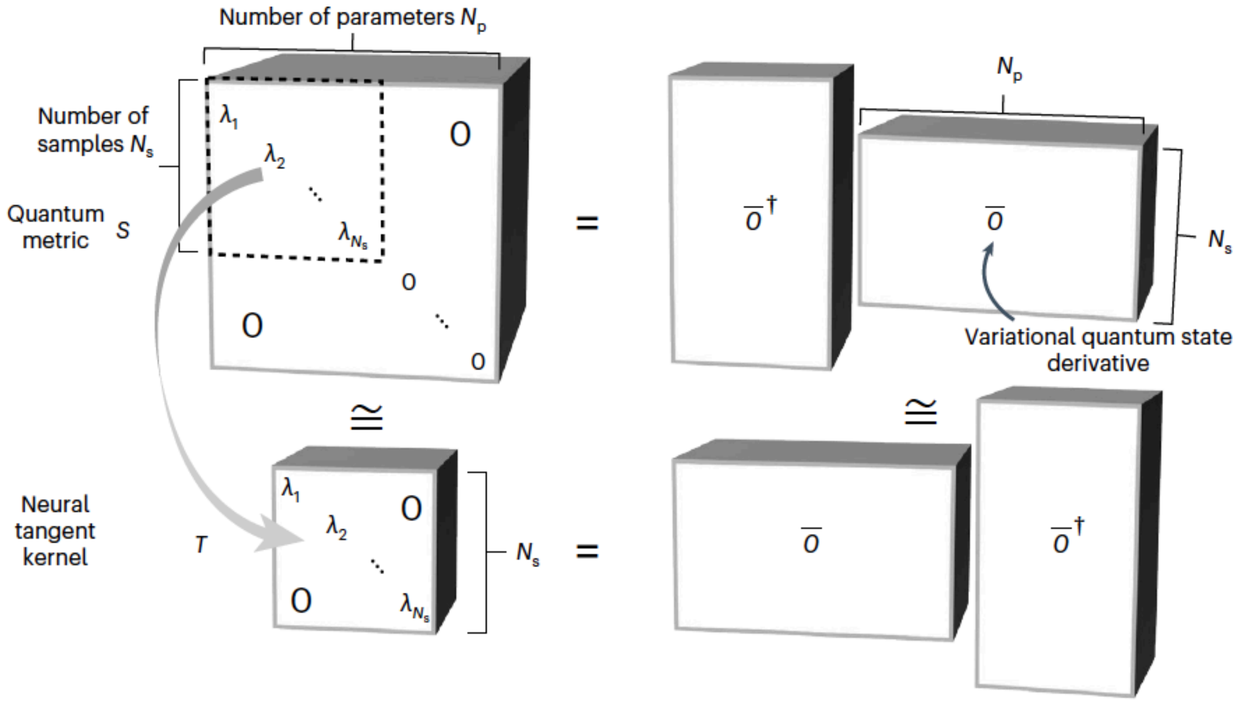
Stochastic Reconfiguration (SR) method (Natural Gradient)

$$\delta\theta = -\delta_\tau S^{-1}\partial_\theta\langle\mathcal{H}\rangle$$

S : Fubini–Study metric tensor
→Np×Np matrix (Np: number of variational param.)

$$|\psi_{\theta+\delta\theta}\rangle = |\psi_\theta\rangle + |d\psi\rangle \qquad d^2 = \delta\theta^\dagger S\delta\theta$$

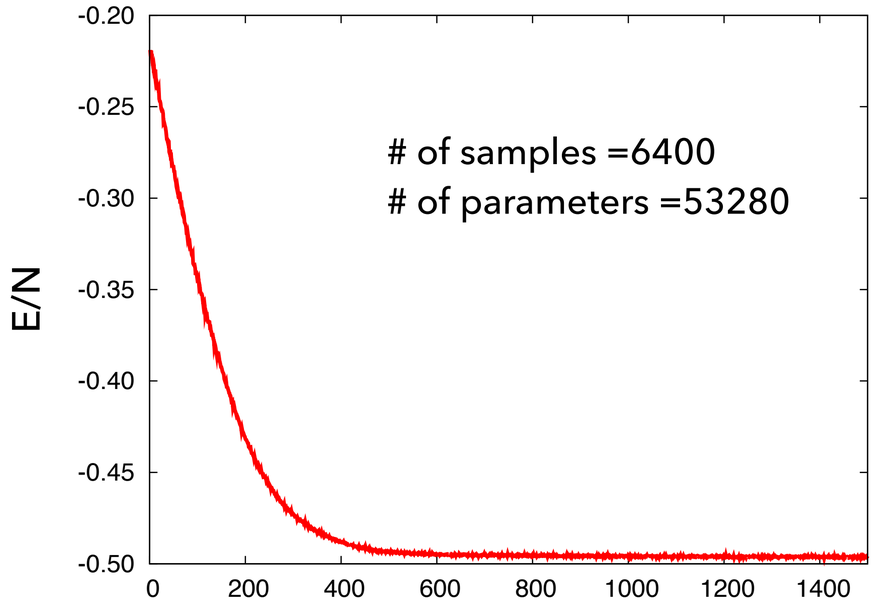
MinSR method



Exploiting metric rank deficiency in the Np > Ns case

Benchmark

J_1-J_2 Heisenberg model on 6x6 square lattice (J_2=0.5)



Benchmark using 2D J_1-J_2 Heisenberg model ②

ground-state energy, 10x10 lattice, J_2=0.5

Energy per site	Wave function	Reference
−0.494757(12)	**Neural quantum state**	[72]
−0.49516(1)	**CNN**	[67]
−0.49521(1)	VMC($p=0$)	[23]
−0.495530	DMRG	[25]
−0.49575(3)	**RBM-fermionic wave function**	[70]
−0.497549(2)	VMC($p=2$)	[23]
−0.497629(1)	**RBM + PP**	Present study

→ 13,132 parameters

Optimized by SR method

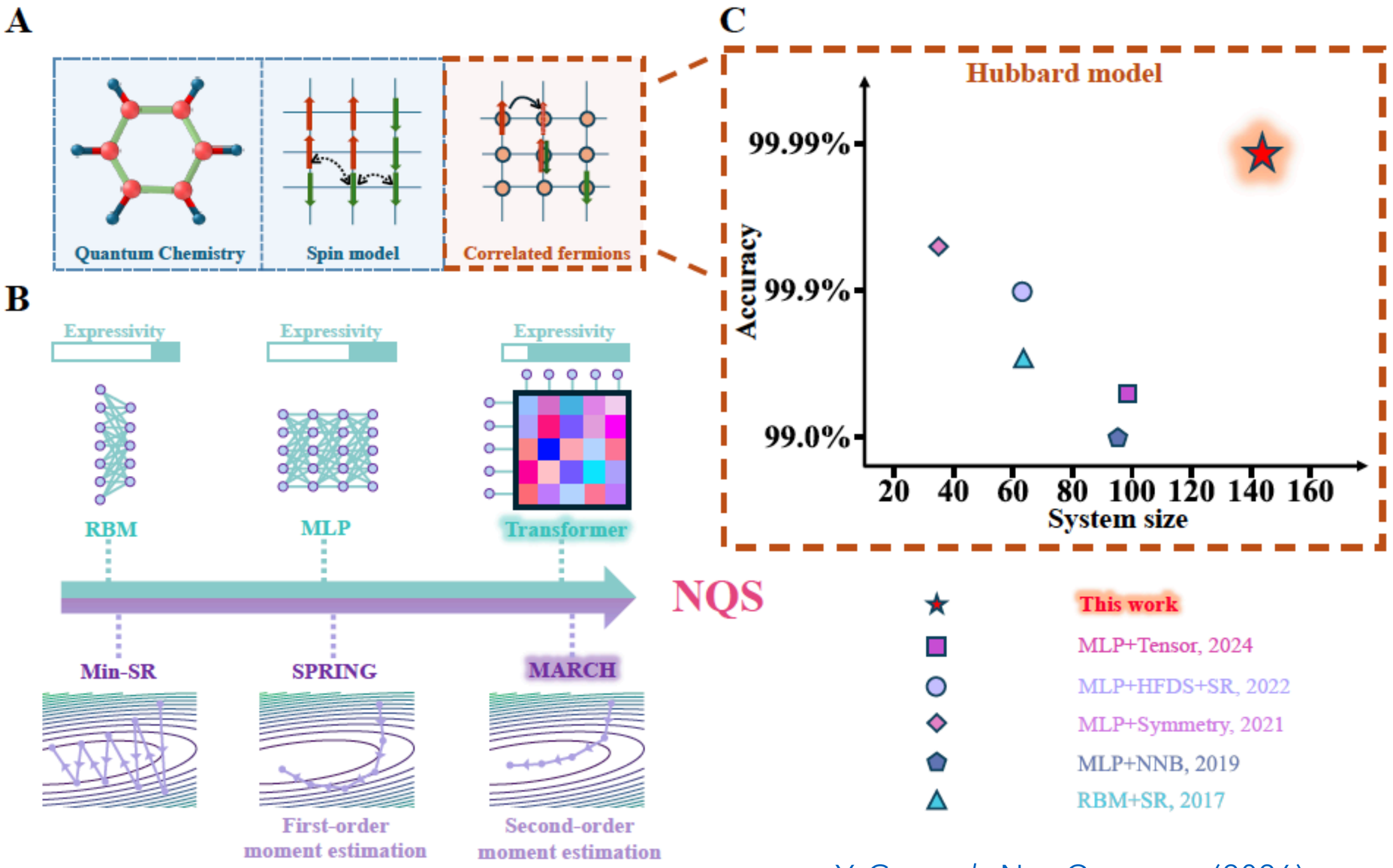
−0.497634(1)	**Vision Transformer**	R. Rende et al.
	→ 267,720 parameters	
−0.4976921(4)	**Residual neural networks**	A. Chen et al.
	→ 1,071,488 parameters	

Optimized by minSR method

cf. talk by Luciano Viteritti @ MLP2026

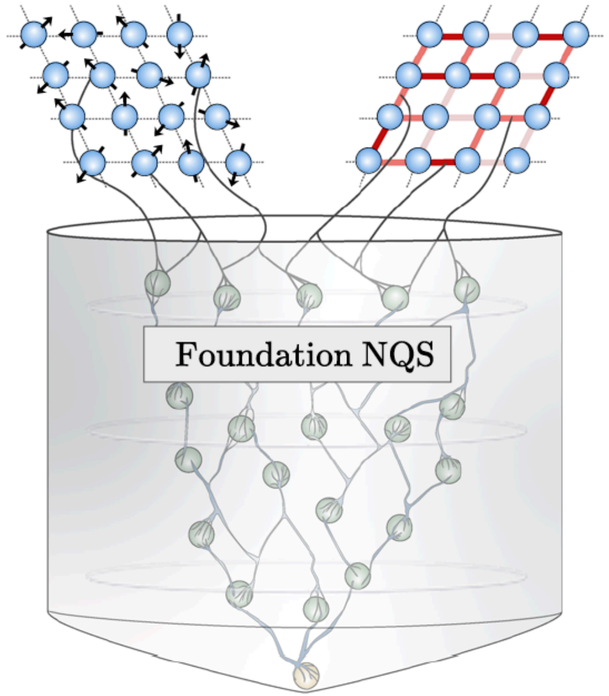
[72] Szabó and Castelnovo PRR 2020 [67] Choo et al., PRB 2019
[23] Hu et al., PRB 2013 [25] Gong et al., PRL 2014 [70] Ferrari et al., PRB 2019

Application of Transformer-based w.f. to Hubbard model



Y. Gu *et al.*, Nat. Commun. (2026)

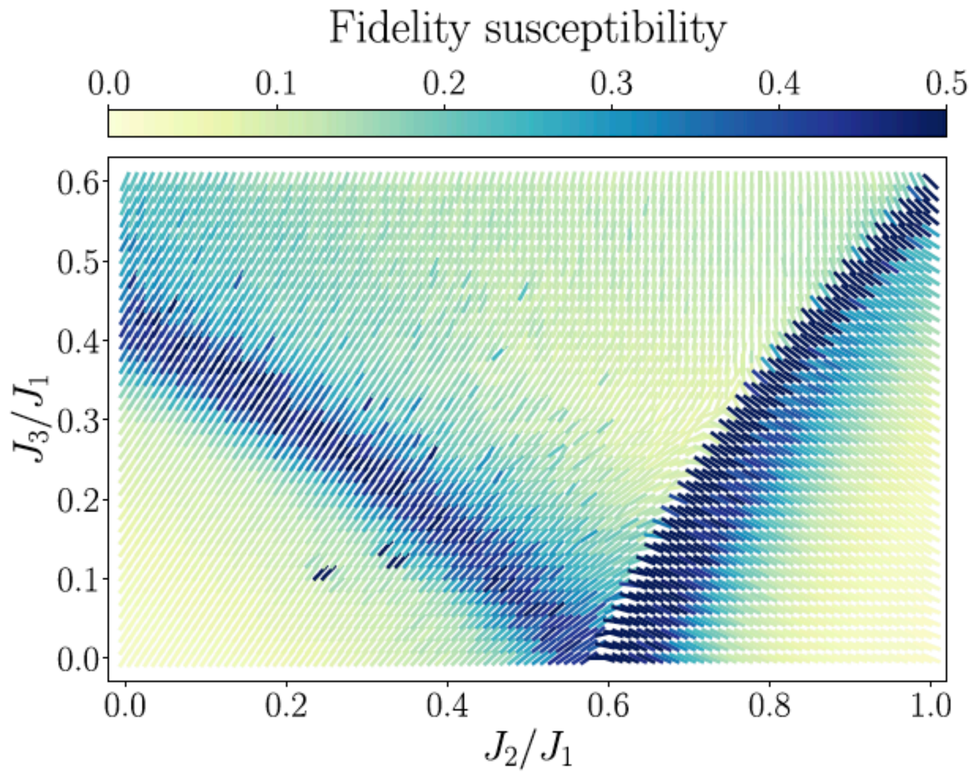
（大規模化とも関係ある最新の面白い動向）Multimodality



$\psi_\theta(\sigma \mid \gamma)$

σ　γ (Hamiltonian param.)

cf. usual definition $\psi_{\theta(\gamma)}(\sigma)$



R. Rende *et al.*, Nat. Commun.**16**, 7213 (2025)

Related works: dynamics simulation: $\psi_{\theta(t)}(\sigma) \rightarrow \psi_\theta(\sigma, t)$

A. Van deWalle *et al.*, Mach. Learn.: Sci. Technol. **6**, 045011 (2025); A. Sinibaldi *et al.*, Phys. Rev. Lett. **136**,120402 (2026)

本日のトピック

1. 量子多体問題とそれに対する機械学習を用いた波動関数法：導入

2. 精度を向上させるためには？
   - 物理の知見を利用
   - 大規模化

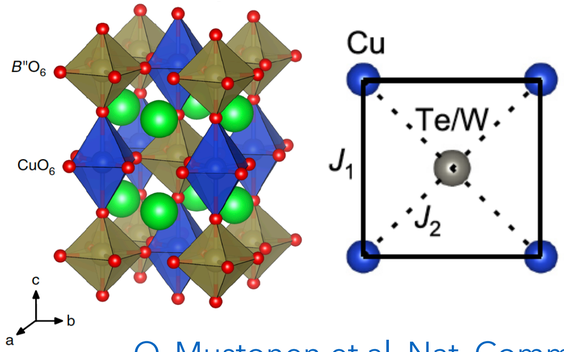
3. どのように性能を統一的に評価するか？

4. ベンチマークを超えた応用の取り組み

High diversity in models and algorithms

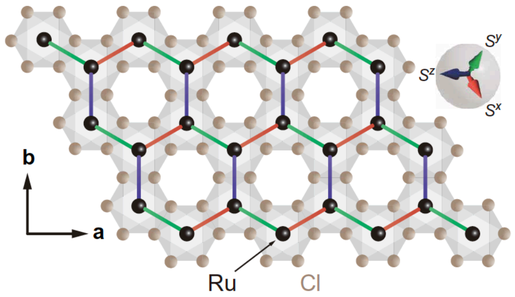
Various models (structure dependence)

Square lattice



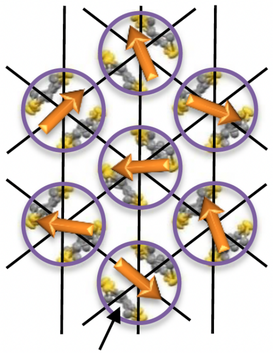
O. Mustonen et al, Nat. Commun. (2018)

Honeycomb lattice



Imamura et al., Sci. Adv. (2024)

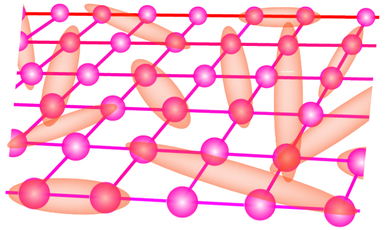
Triangular lattice



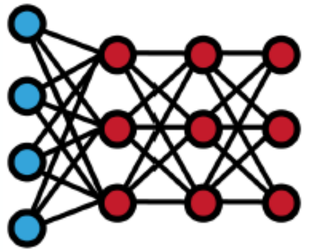
https://www.nims.go.jp/press/2018/04/201804230.html

Various variational methods

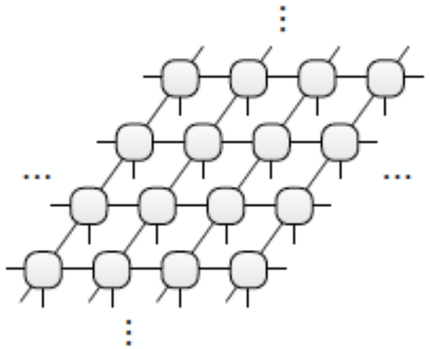
Conventional



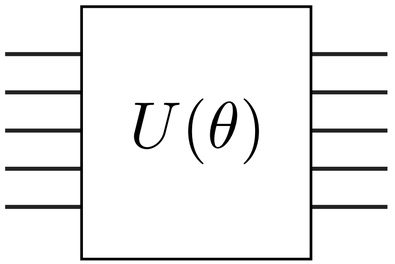
Neural networks



Tensor networks



Quantum Circuits



Unified Accuracy Metric

Performance evaluations are conducted independently across different papers, models, and methods.

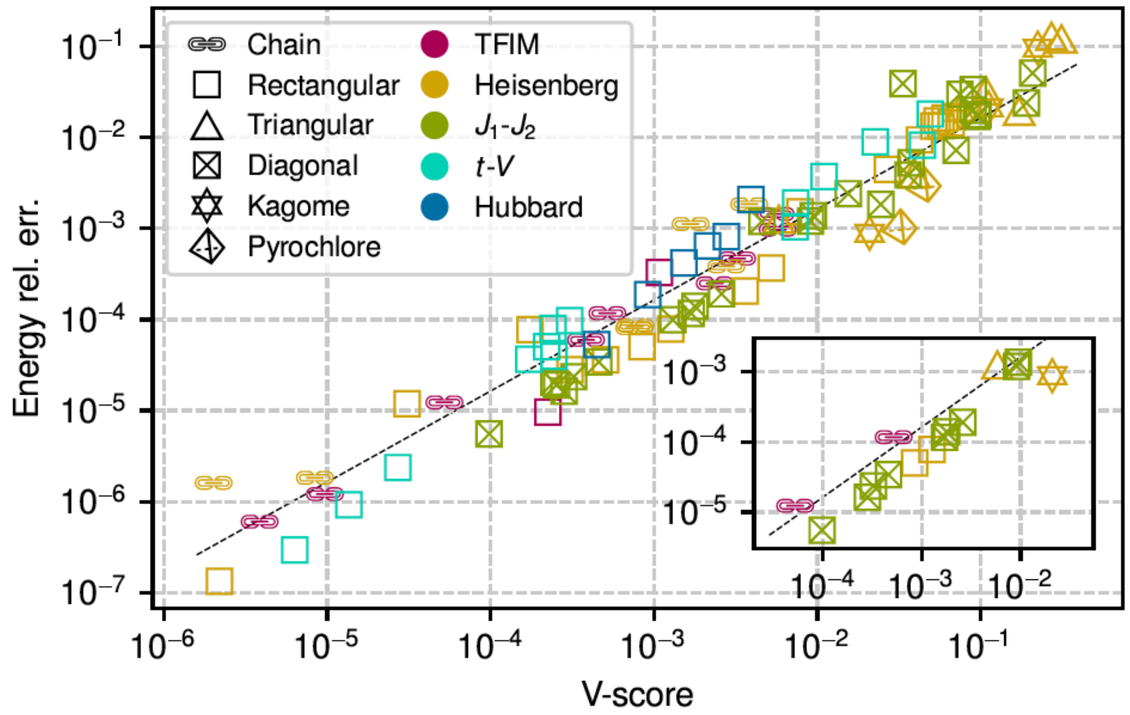
→Introducing the **"V-score"**, a unified numerical metric to consistently compare performance

D. Wu et al., Science **386**, 296 (2024)

Unified Accuracy Metric：V-Score

$$\text{V-score} := \frac{N \operatorname{Var} E}{(E - E_\infty)^2}$$

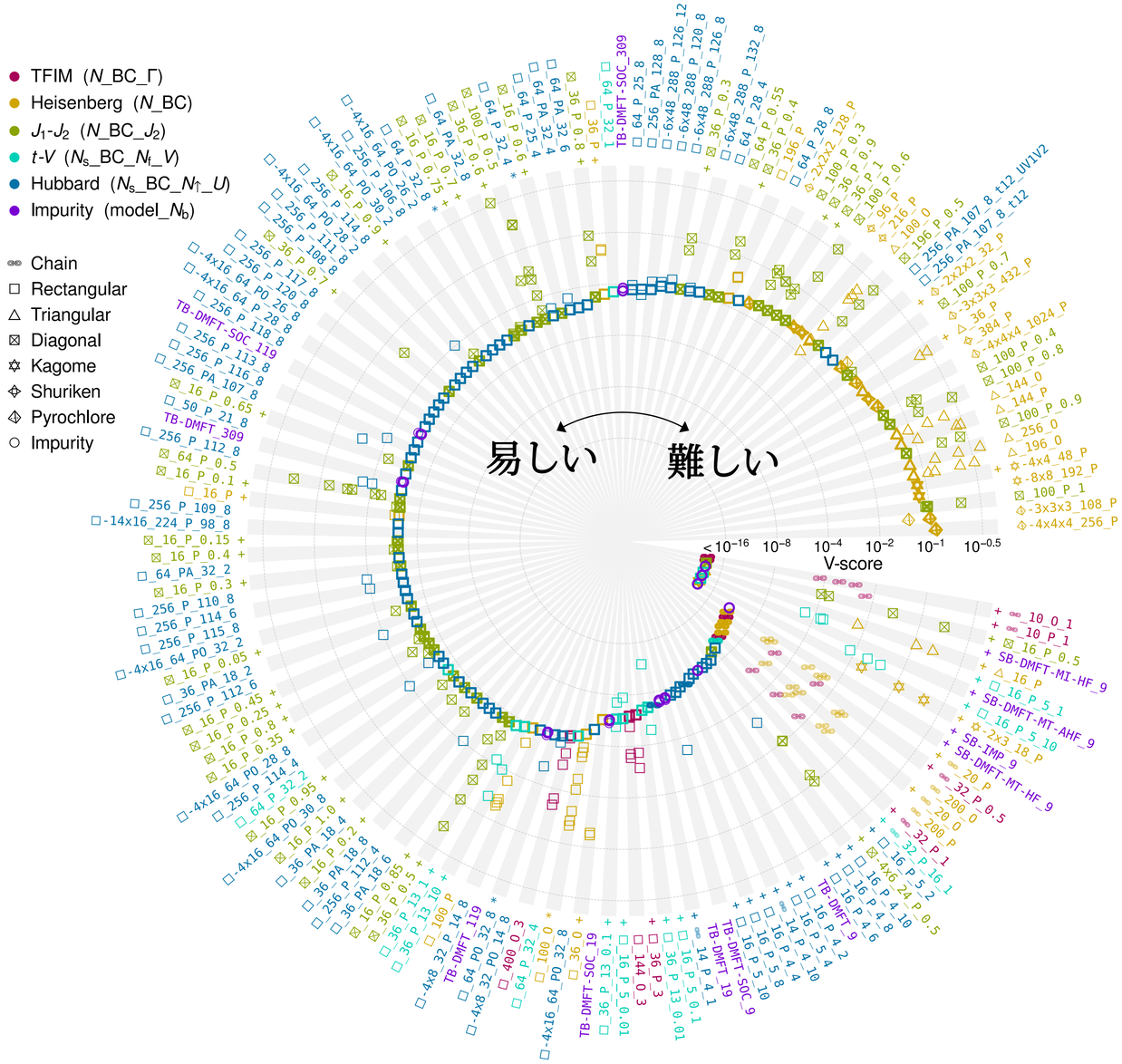
Variational energy　Energy at infinite temperature



cf. variance extrapolation

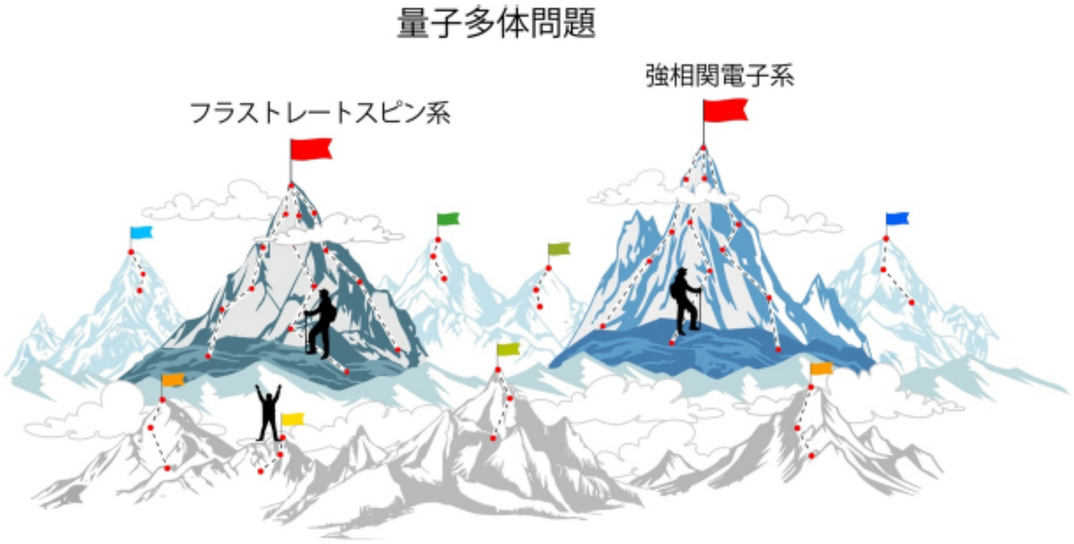
Imada and Kashima, JPSJ **69**, 2723 (2000); Kashima and Imada, JPSJ **70**, 2287 (2001)

Identifying Hard Problems for State-of-the-Art Algorithms



In condensed matter physics,

Strongly correlated electron systems
Frustrated quantum spin systems



D. Wu et al., Science **386**, 296 (2024)

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Downfolding to obtain effective Hamiltonian

RESPACK:
https://sites.google.com/view/kazuma7k6r

RESPACK
First-principles many-body perturbation calculation

Ab initio Hamiltonian

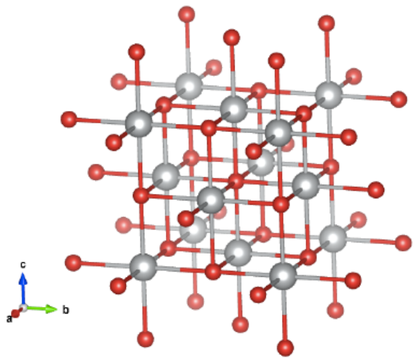
$$\hat{\mathcal{H}} = \sum_i \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}_i^2} - \sum_I \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} \right) + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Effective Hamiltonian

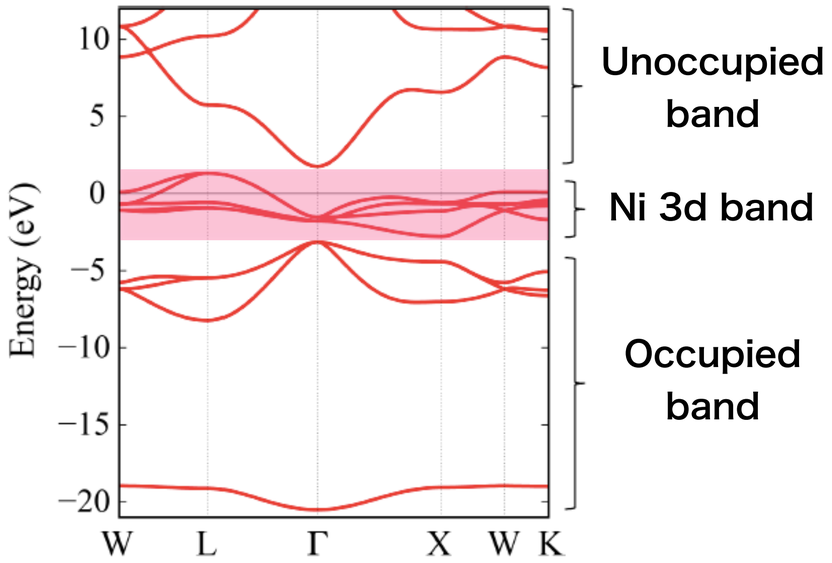
$$\hat{\mathcal{H}} = \sum_{i \neq j} \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{ijkl} \sum_{\sigma\rho} U_{ijkl} c_{i\sigma}^{\dagger} c_{j\rho}^{\dagger} c_{l\rho} c_{k\sigma}$$

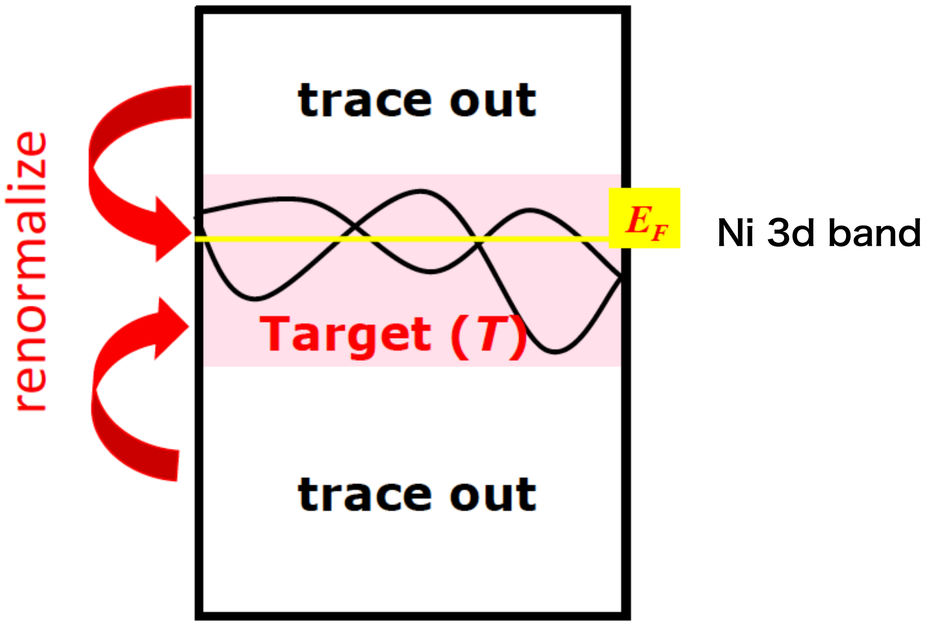
e.g.: NiO

Ni^{2+} → [Ar] $3d^8$
O^{2-} → $1s^2 2s^2 2p^6$
(closed shell)



Band structure from DFT





When the system is a Mott insulator,
we can further map it to a spin model

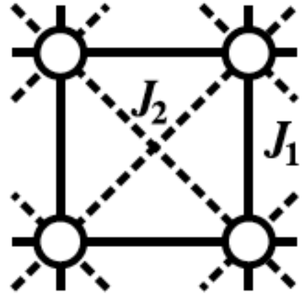
M. Imada and T. Miyake, JPSJ **79**, 112001 (2010)

Application to 2D J_1-J_2 Heisenberg model

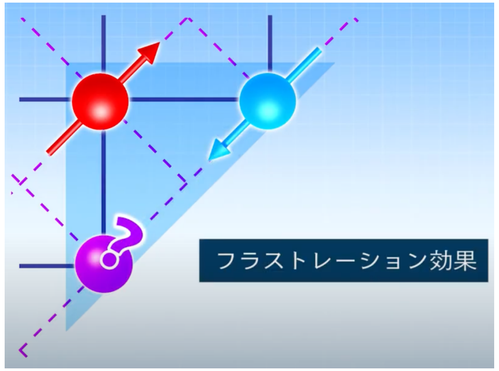
YN and M. Imada
Phys. Rev. X **11**, 031034 (2021)

Antiferromagnetic J_1-J_2 Heisenberg model on square lattice $(J_1 > 0, J_2 > 0)$

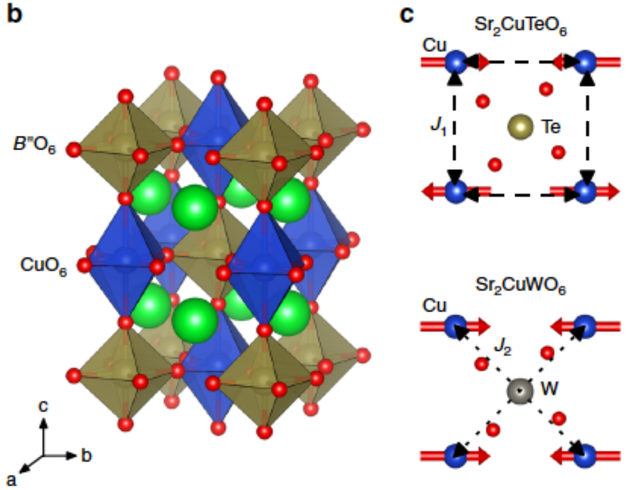
$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



J_1 and J_2 competes



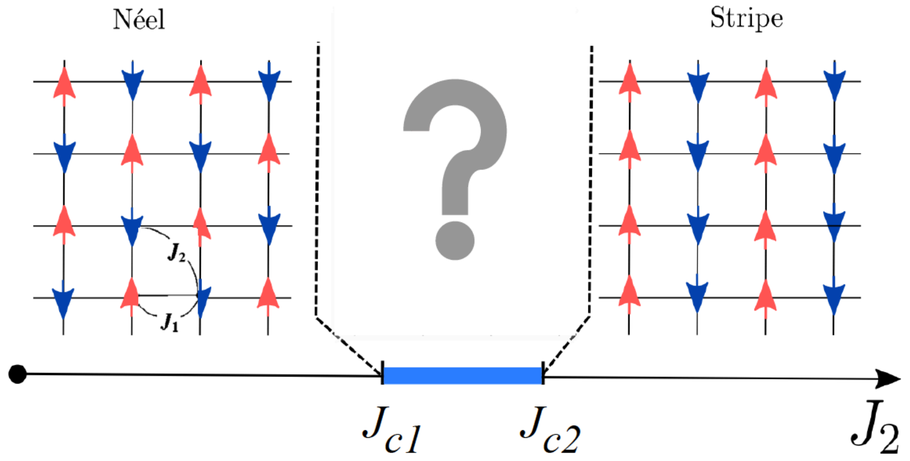
Candidate Materials



O. Mustonen et al, Nat. Commun. **9**, 1085 (2018)

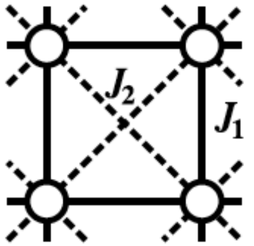
Realization of quantum spin liquid?

Long-standing mystery for decades

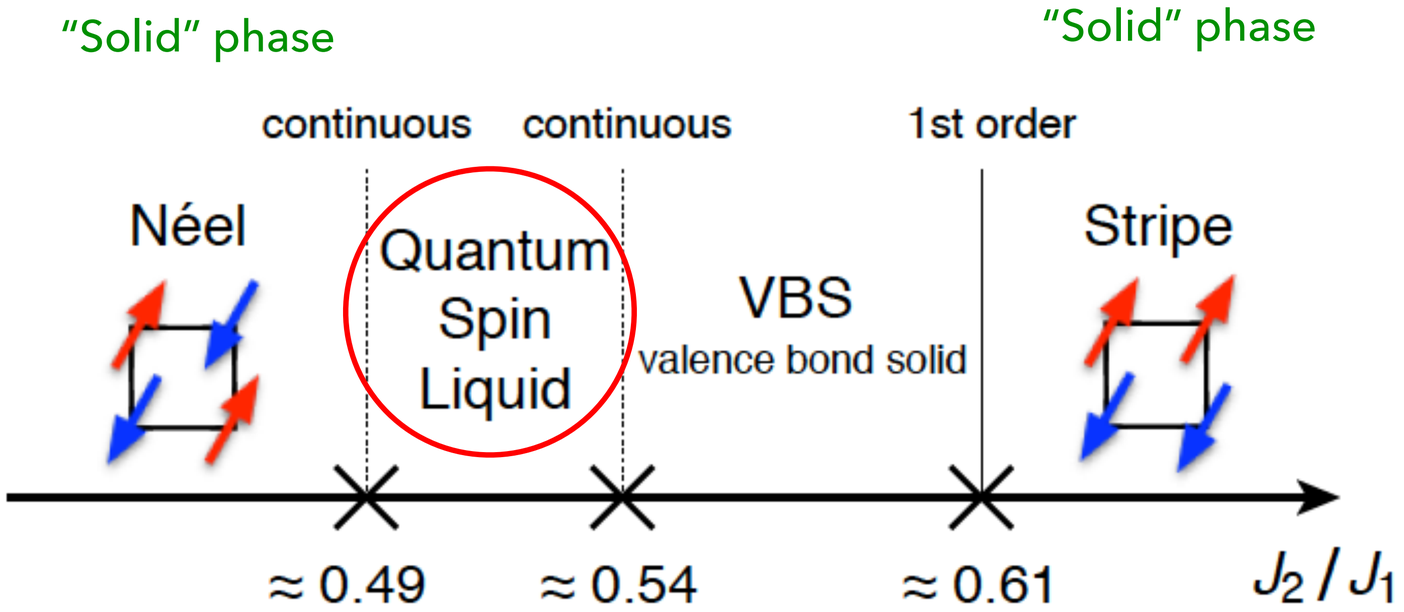


Usually, the orientation of interacting spins is fixed at absolute zero
(a "solid" state with long-range order is realized)

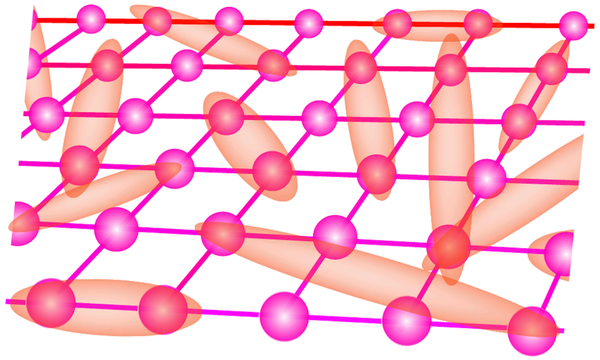
Quantum spin liquid phase where spin order is “melted”



Phase diagram at 0 K obtained from neural-network method



Fluctuating spins even at 0 K



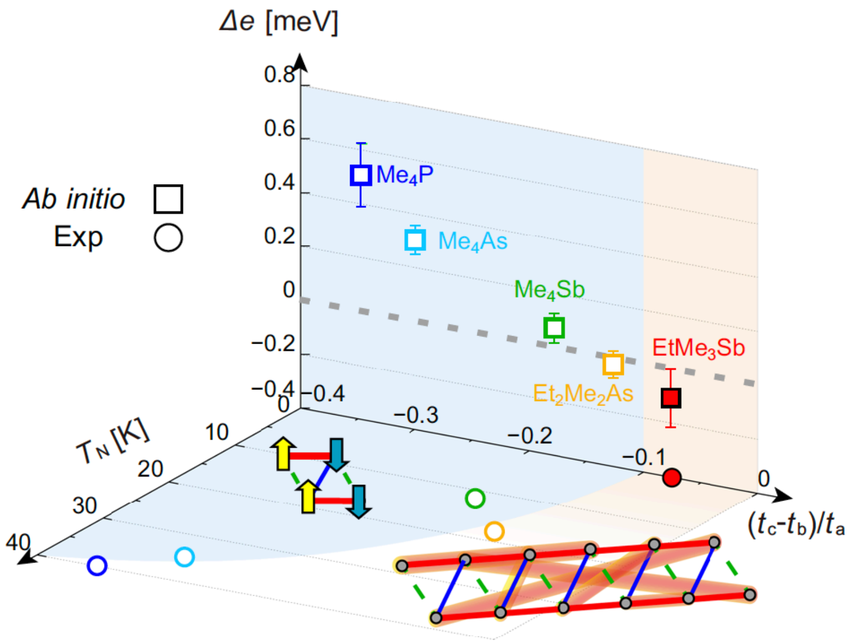
YN and M. Imada Phys. Rev. X **11**, 031034 (2021)

Highly accurate calculations reveal unusual “liquid” phase of quantum spins even at zero temperature

- Quantum spin liquid (QSL) + doping (metallization) → high-temperature superconductivity?
- QSL entanglement and topology may offer pathways to quantum computing.

Applications (beyond benchmark) to material-specific Hamiltonians

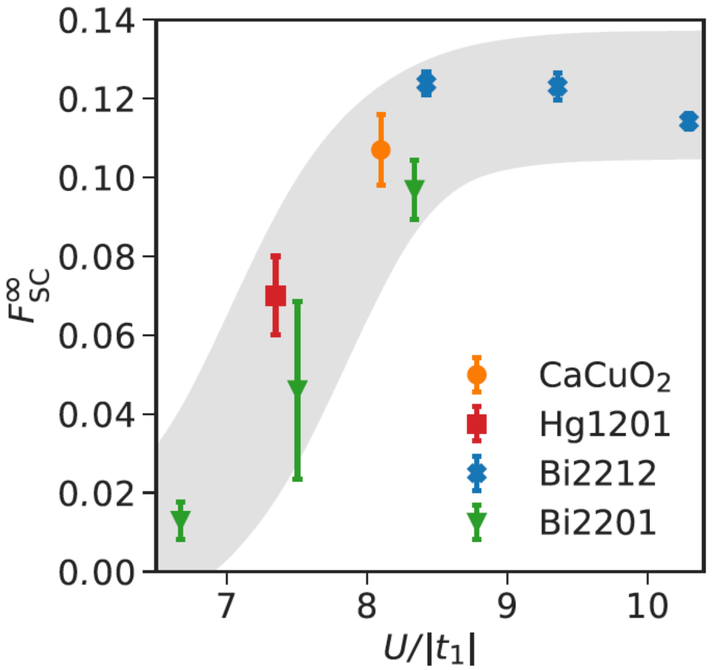
Pd(dmit)$_2$ salts (organic solids)



Quantum spin liquid in real materials

K. Ido et al., npj Quantum Mater. **7**, 48 (2022)

High-T_c cuprates



Identifying key factors for controlling pairing strength

M.-T. Schmid *et al.*, Phys. Rev. X **13**, 041036 (2023)

→ Entering a phase of research where we can utilize neural networks for challenging problems in physics

Summary and open questions

Summary

Machine learning (ML) + proper setting → state-of-the-art performance

ML can play an essential role in resolving a problem beyond human intuition

Open questions

Best architecture ? (For the moment, performance is optimized through trial and error)

How to reduce computational cost without loosing accuracy?
We need to achieve calculations with $O(10^3)$ site/orbital/spin degrees of freedom

What quantities determine the representational power of neural networks?

cf. entanglement entropy for tensor networks