2020/08/06

ボルツマンマシンを用いた量子多体波動関数表現：

深層ボルツマンマシンによる厳密な表現と制限ボルツマンマシンによる数値的近似表現

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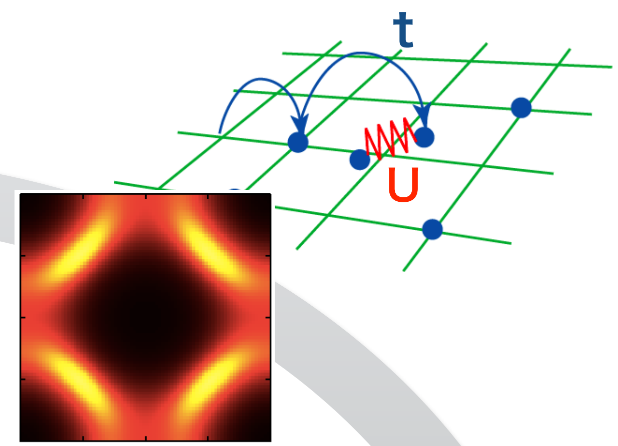
理研 CEMS

関連する発表：7/9 吉岡さん、9/3 斎藤先生

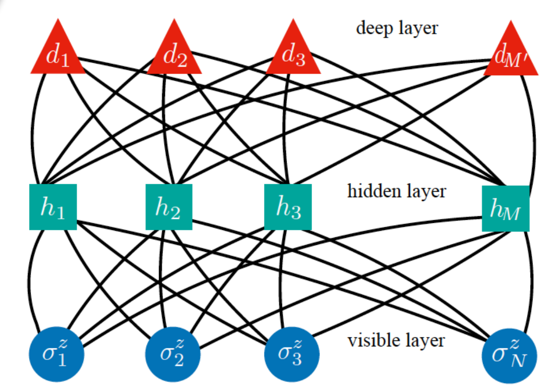
研究内容

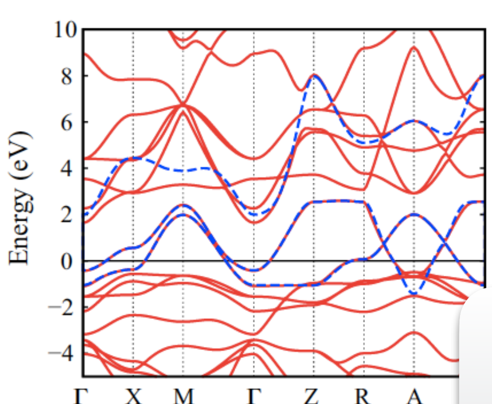
量子多体論
DMFT, FLEX, …

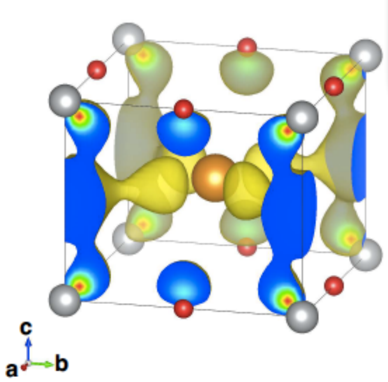


新たな計算物質科学のフレームワーク

機械学習
RBM, neural network, …







第一原理計算
DFT, DFPT, …

機能物性予測・設計へ

Machine Learning

Modeling unknown relationship between data

$$y(\mathbf{x}) = \mathcal{F}[\phi(\mathbf{x}), \mathbf{x}]$$

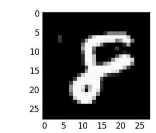
$\mathbf{x},\ y(\mathbf{x})$: data

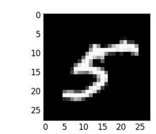
$\mathcal{F}$: functional (nonlinear)

Example: Handwritten digit recognition

$\mathbf{x}$: pixel data of images $\qquad$ $y(\mathbf{x})$: 0-9 digits

$\mathbf{x}$ $\qquad$ $y(\mathbf{x})$

 $\rightarrow$ 8

 $\rightarrow$ 5

https://note.mu/sadaaki/n/n362a3f0fa5a9

$\rightarrow$ useful in extracting essential pattern from data

Application to quantum many-body systems

$\mathbf{x}$: Basis of the Hamiltonian

$y(\mathbf{x})$: Amplitude of quantum many-body wave function

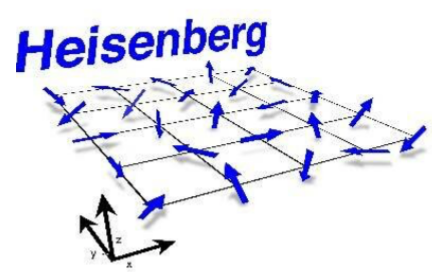
Extract essential pattern of wave functions (data compression) and obtain accurate representations with a finite number of parameters

Quantum many body problems

$$\underbrace{\mathcal{H}}_{\text{Hamiltonian}}|\Psi\rangle = E\underbrace{|\Psi\rangle}_{\text{Eigenstate}}$$

Example of many-body Hamiltonian : Heisenberg model (interacting S=1/2 quantum spins, effective model for Mott insulator)

$$\mathcal{H} = J\sum_{(i,j)} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$



Ground state :

Lowest-energy eigenstate (vector with exponentially large dimension) of Hamiltonian (matrix with exponentially large dimension)

→ Most stable quantum states at zero temperature

$$\mathcal{H}|\Psi_{\mathrm{GS}}\rangle = E_0|\Psi_{\mathrm{GS}}\rangle$$

Accurate ground-state calculations : Grand challenges in physics as well as in quantum chemistry

$$|\Psi\rangle = \underbrace{\sum_x}_{\text{sum over } 2^N \text{ configurations (Heisenberg)}} \Psi(x)|x\rangle \xrightarrow{\text{model relation between x and } \Psi(x) \text{ (machine learning)}} \Psi(x) \approx \psi_{\boldsymbol{\gamma}}(x)$$

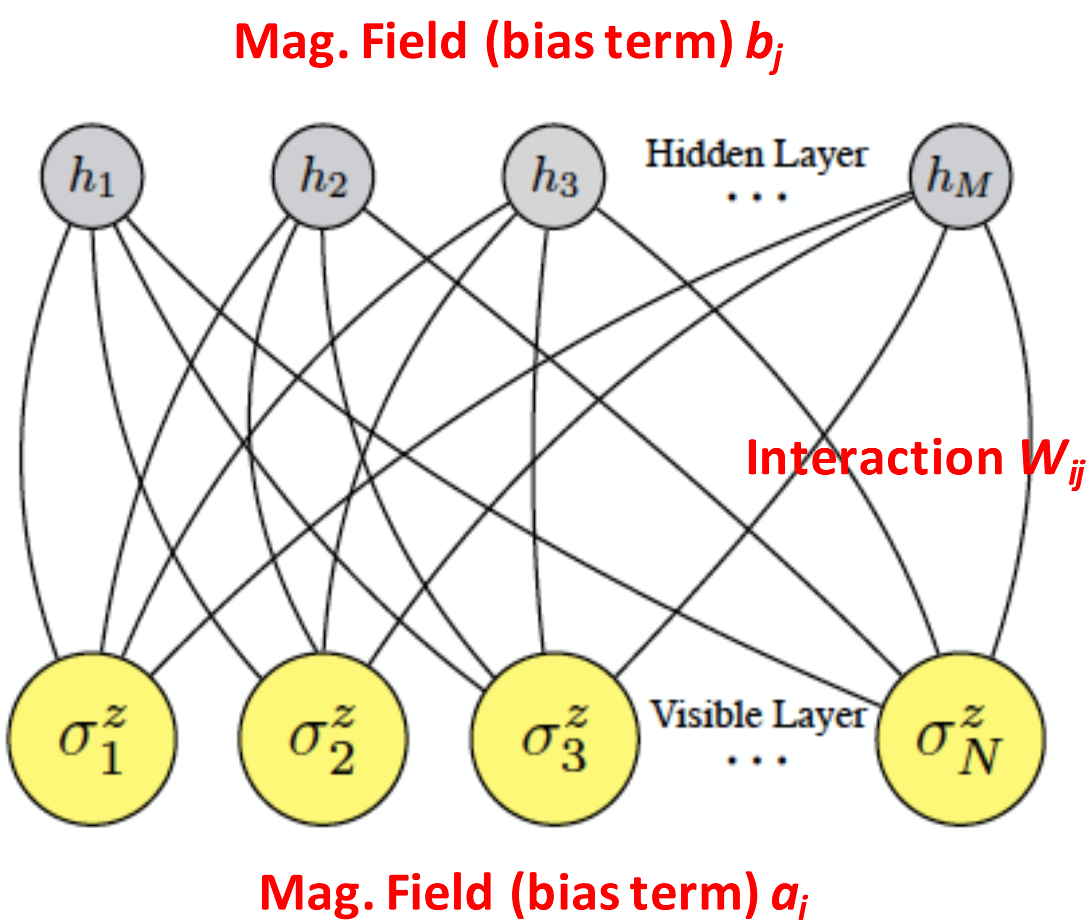
sum over 2^N configurations (Heisenberg)

$|x\rangle = |\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z\rangle$

γ : parameter set (finite number)

Restricted Boltzmann machine (RBM)

Paul Smolensky (1986)
G. E. Hinton, R. R. Salakhutdinov, Science. 313, 504 (2006)



- Energy function

$$E(\boldsymbol{\sigma}, \boldsymbol{h}) = -\sum_{i=1}^{N} a_i \sigma_i - \sum_{i=1}^{N} \sum_{k=1}^{M} W_{ik} \sigma_i h_k - \sum_{k=1}^{M} b_k h_k$$

$$\boldsymbol{\sigma} \in \{0,1\}^N \qquad \boldsymbol{h} \in \{0,1\}^M$$

- Boltzmann distribution

$$p(\boldsymbol{\sigma}, \boldsymbol{h}) = \frac{e^{-E(\boldsymbol{\sigma}, \boldsymbol{h})}}{Z} \qquad Z = \sum_{\boldsymbol{\sigma}, \boldsymbol{h}} e^{-E(\boldsymbol{\sigma}, \boldsymbol{h})}$$

- Marginal distribution

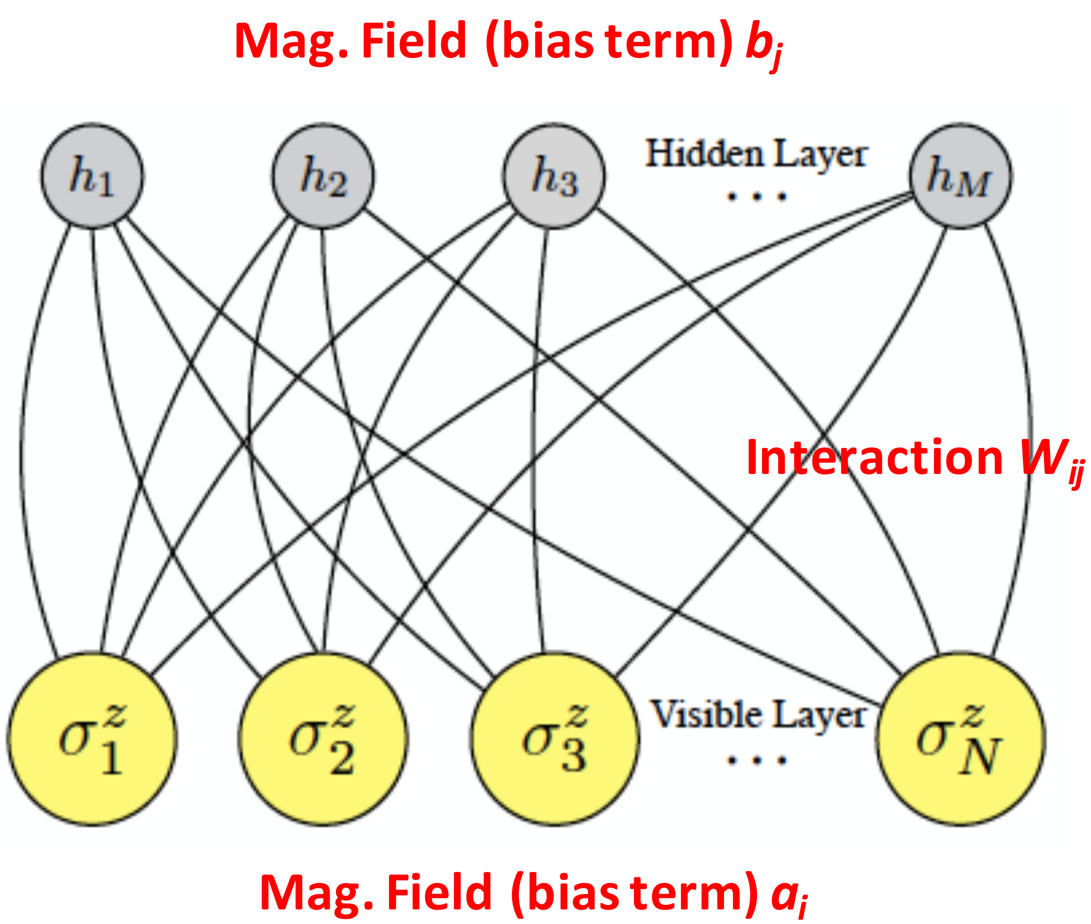
$$\tilde{p}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{h}} p(\boldsymbol{\sigma}, \boldsymbol{h})$$

- Single hidden layer + interlayer coupling only → restricted Boltzmann machine (RBM)
- Marginal distribution $\tilde{p}(\boldsymbol{\sigma})$ can represent any distribution over $\{0,1\}^N$ with infinite M

K. Hornik, Neural Networks 4, 251 (1991); G. Cybenko, Mathematics of Control, Signals and Systems 2, 303 (1989); N. L. Roux and Y. Bengio, Neural Computation 20, 1631(2008).

Using artificial neural network to solve quantum many-body problems

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



RBM

Spin config. σ^z $\longleftrightarrow$ wave function $\Psi(\sigma^z)$

RBM wave function

$$\Psi(\sigma^z) = \sum_{\{h_j\}} \exp\Big(\sum_i a_i \sigma_i^z + \sum_{i,j} \sigma_i^z W_{ij} h_j + \sum_j b_j h_j\Big)$$

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

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

- Learning quantum states: Optimization of RBM parameters using nonlinear loss function (Energy)
- Quantum correlations among physical spins via artificial neural network
- Can represent any wave function with infinite number of hidden units (universal approximation)

$$\Psi(\sigma^z) = e^{\sum_i a_i \sigma_i^z} \times \prod_j 2\cosh\Big(b_j + \sum_i W_{ij} \sigma_i^z\Big)$$

Example: 1D Antiferromagnetic Heisenberg model (8site)

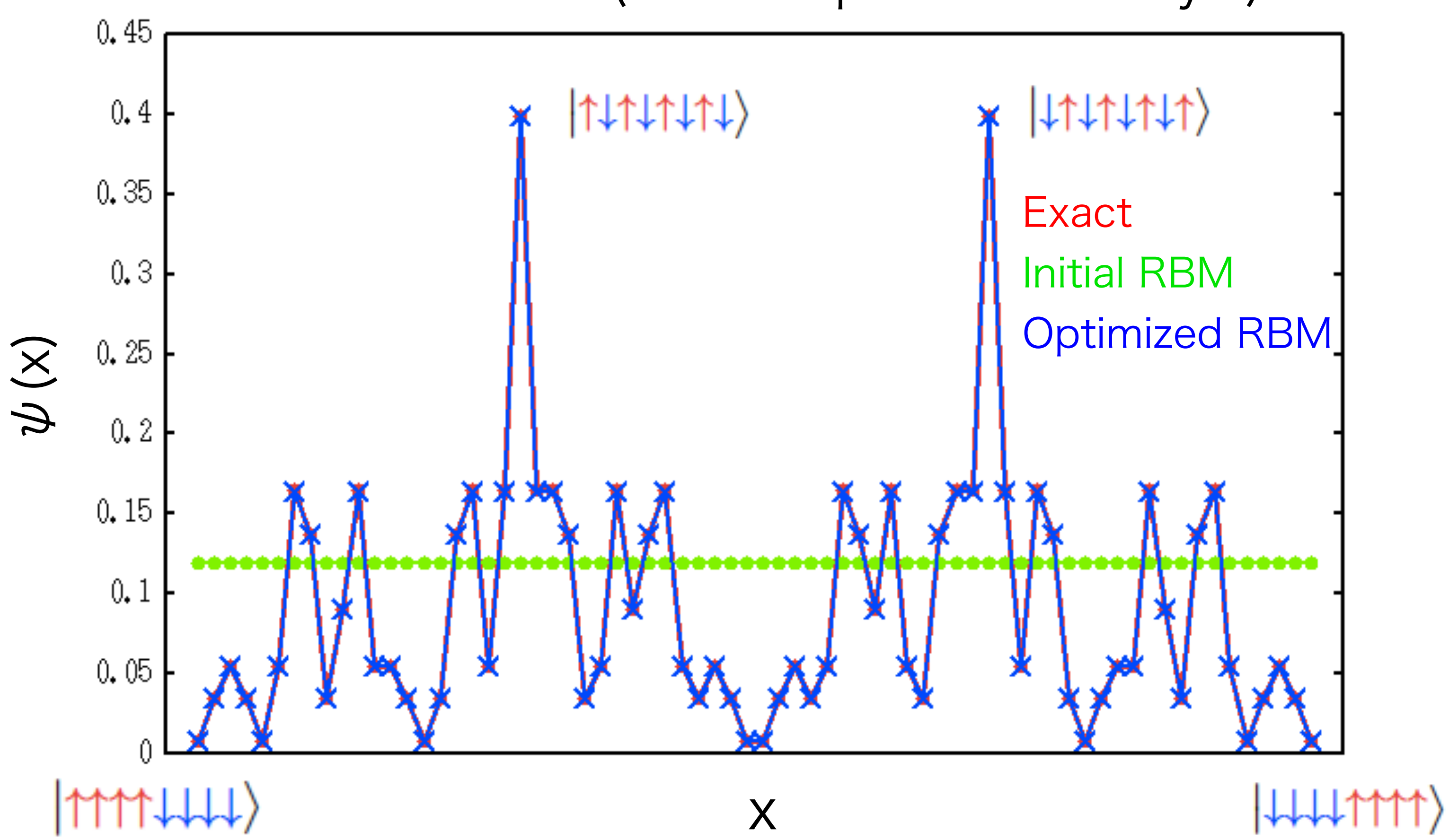
gauge transformation
$\sigma^{x,y} \rightarrow -\sigma^{x,y}$ for one of sublattice

$$\mathcal{H}_{\mathrm{Heisenberg}} = J \sum_{(i,j)} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j = J \sum_{(i,j)} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z) \quad (J > 0) \quad \Rightarrow \quad \mathcal{H}_{\mathrm{Heisenberg}} = J \sum_{(i,j)} (-\sigma_i^x \sigma_j^x - \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z)$$

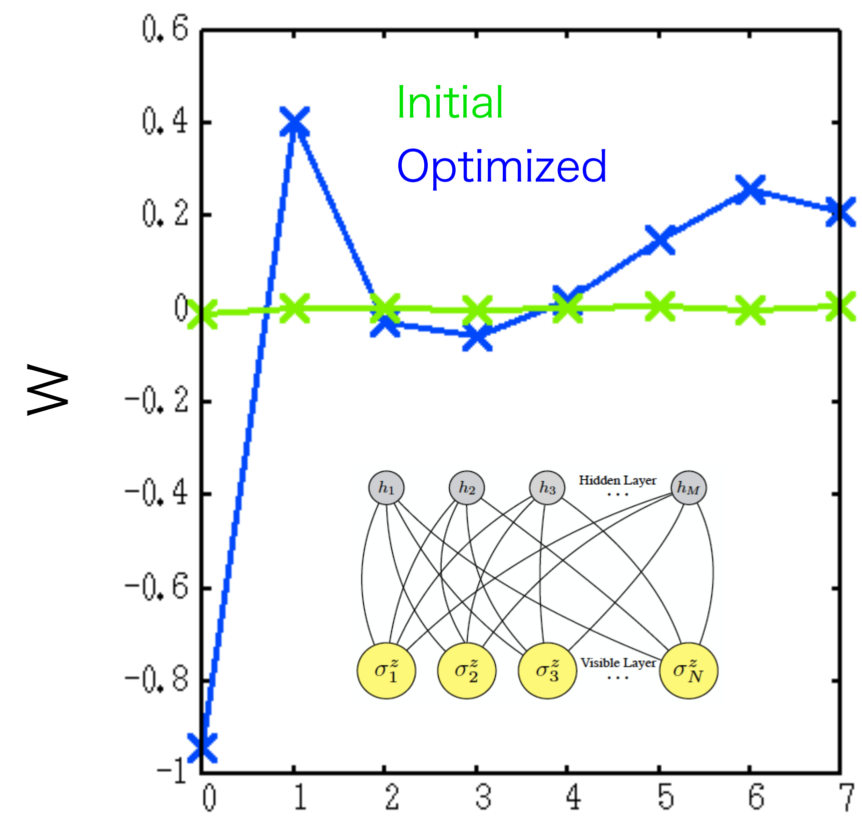
Optimization following variational principle : $\langle \mathcal{H} \rangle = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0$ $\quad$ E_0: ground state energy

optimization of nonlinear function using nonlinear cost function
→ equivalent to machine learning task

wave function (real and positive for any x)



RBM interaction parameter



Extensions to various systems

②

Boson system

- Spin system (localized Mott insulator)
  - without frustration (Heisenberg model)
    Carleo and Troyer (2017), …
  - **with frustration**
    (J_1-J_2 Heisenberg model)
    YN and Imada arXiv, …
- Bose-Hubbard model (itinerant)
  Saito (2017), …

Fermion system

- **Itinerant electrons in solids**
  (Hubbard model)
  YN et al., (2017), …
- Molecules (H_2, LiH, …)
  Han et al., Choo and Carleo, …

Boson and fermion system

- **Electron-phonon coupling**
  (Holstein model)
  YN JPSJ (2020)
  Editor's Choice

From benchmark to "true" applications to challenges in physics

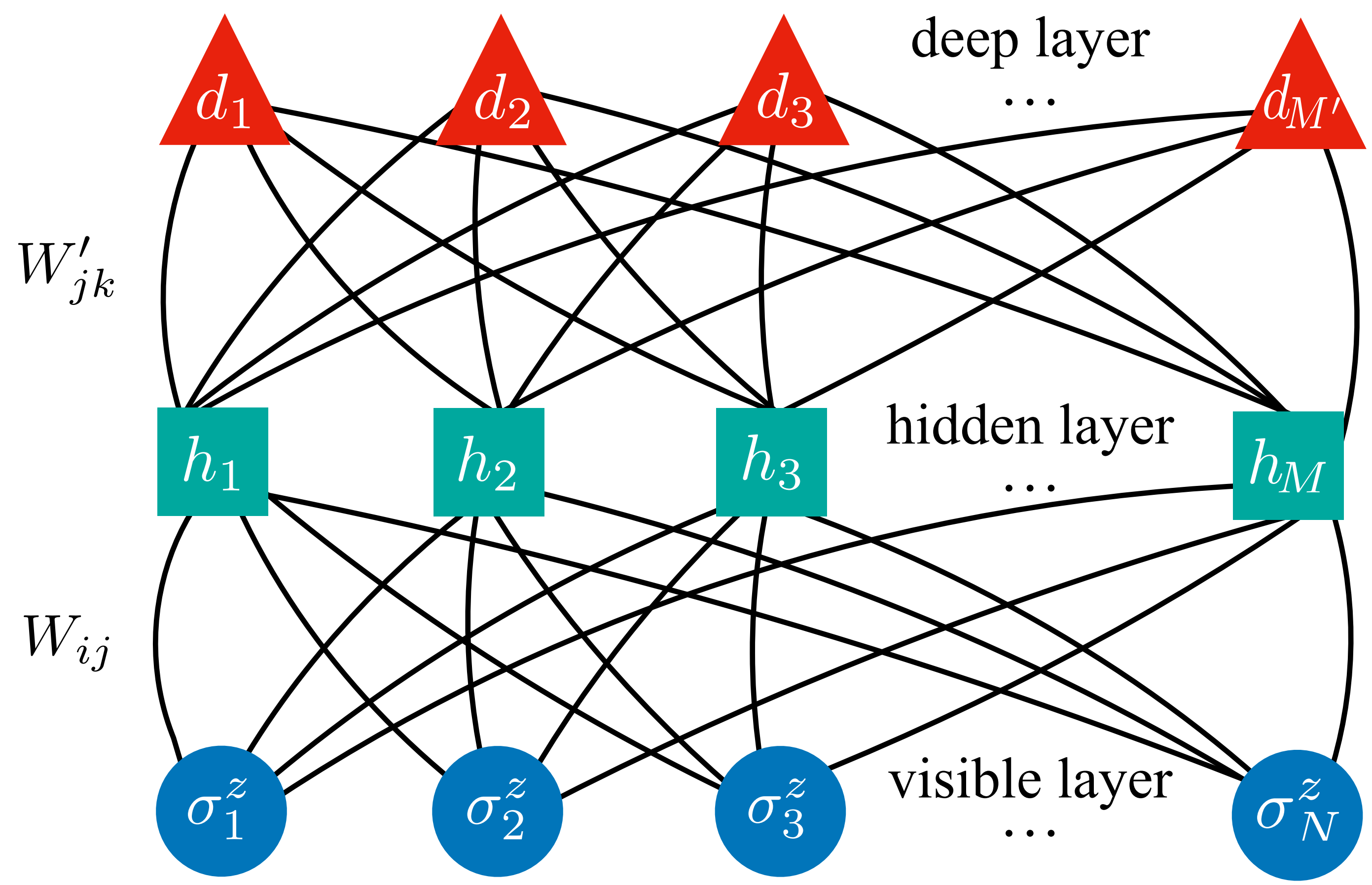
①

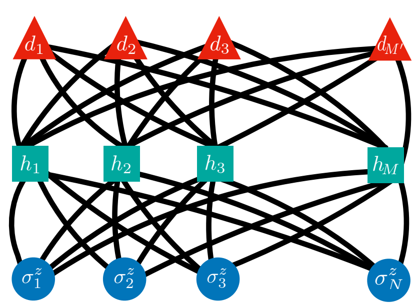
※ Why is the machine learning powerful？

→ Exact quantum-classical mapping using deep Boltzmann machine (c.f. numerical mapping using RBM)

G. Carleo, YN, and M. Imada, Nat. Commun, **9**. 5322 (2018)

DBM (deep Boltzmann machine) wave function



$$\Psi(\sigma) = \sum_{h,d}$$  $$= \sum_{h,d} e^{\sum_i a_i \sigma_i^z + \sum_{i,j} \sigma_i^z W_{ij} h_j + \sum_j b_j h_j + \sum_{j,k} h_j W'_{jk} d_k + \sum_k b'_k d_k}$$

DBM representation of ground states

DBM compared with RBM

- Pros

  much more flexible representability

  X. Gao and L.-M. Duan, Nat. Commun. **8**, 662 (2017).

- Cons

  cannot trace out both h and d analytically

  (need to sample hidden spins to obtain wave function)

Key idea

- reproduce imaginary-time evolution by dynamically modifying DBM network

  (no need to perform stochastic optimization of parameters! everything deterministic !)

$$|\Psi(\tau)\rangle = e^{-\mathcal{H}_1 \frac{\delta_\tau}{2}} e^{-\mathcal{H}_2 \delta_\tau} \ldots e^{-\mathcal{H}_2 \delta_\tau} e^{-\mathcal{H}_1 \frac{\delta_\tau}{2}} |\Psi_0\rangle$$

- Physical quantities are measured by MC sampling of classical visible and hidden spins

Novel class of quantum-to-classical mapping

G. Carleo, Y. Nomura, and M. Imada, Nat. Commun. **9**, 5322 (2018) (see also N. Freitas et al., arXiv:1803.02118)

Example: Transverse-Field Ising model

G. Carleo, YN, and M. Imada, Nat. Commun, **9**. 5322 (2018)

Hamiltonian: $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$

Interaction (classical): $\mathcal{H}_1 = \sum_{l<m} V_{lm} \sigma_l^z \sigma_m^z$

Transverse-field: $\mathcal{H}_2 = -\sum_l \Gamma_l \sigma_l^x$

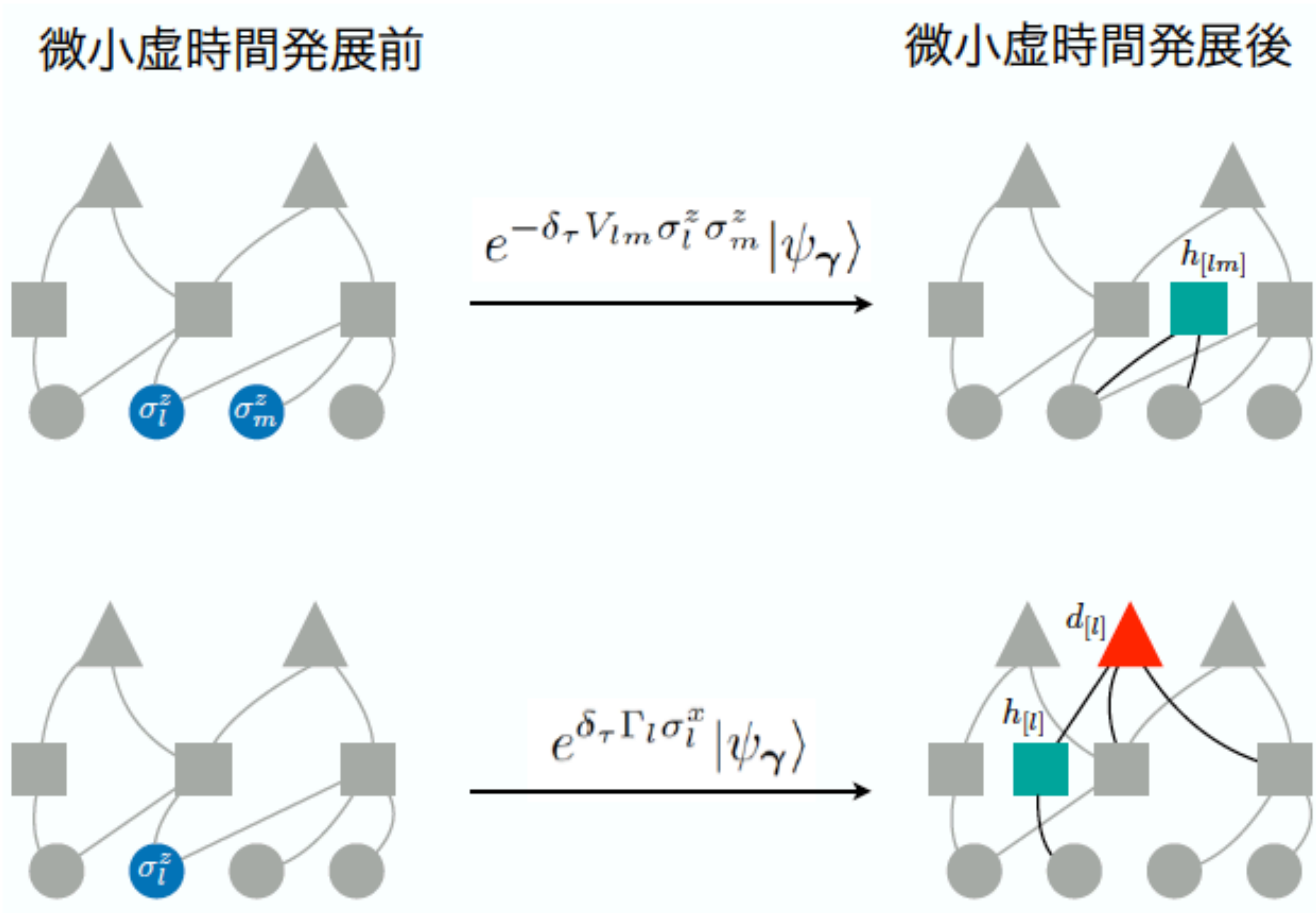
How to express short time propagators by DBM ?

Interaction propagator: $e^{-\delta_\tau V_{lm} \sigma_l^z \sigma_m^z} |\mathrm{DBM}\rangle$

Transverse-field propagator: $e^{\delta_\tau \Gamma_l \sigma_l^x} |\mathrm{DBM}\rangle$

Example: Transverse-Field Ising model

G. Carleo, YN, and M. Imada, Nat. Commun, **9**. 5322 (2018)



$$W_{l[lm]} = \frac{1}{2}\mathrm{arcosh}\left(e^{2|V_{lm}|\delta_\tau}\right)$$
$$W_{m[lm]} = -\mathrm{sgn}(V_{lm}) \times W_{l[lm]}$$

$$W'_{j[l]} = -W_{lj}$$

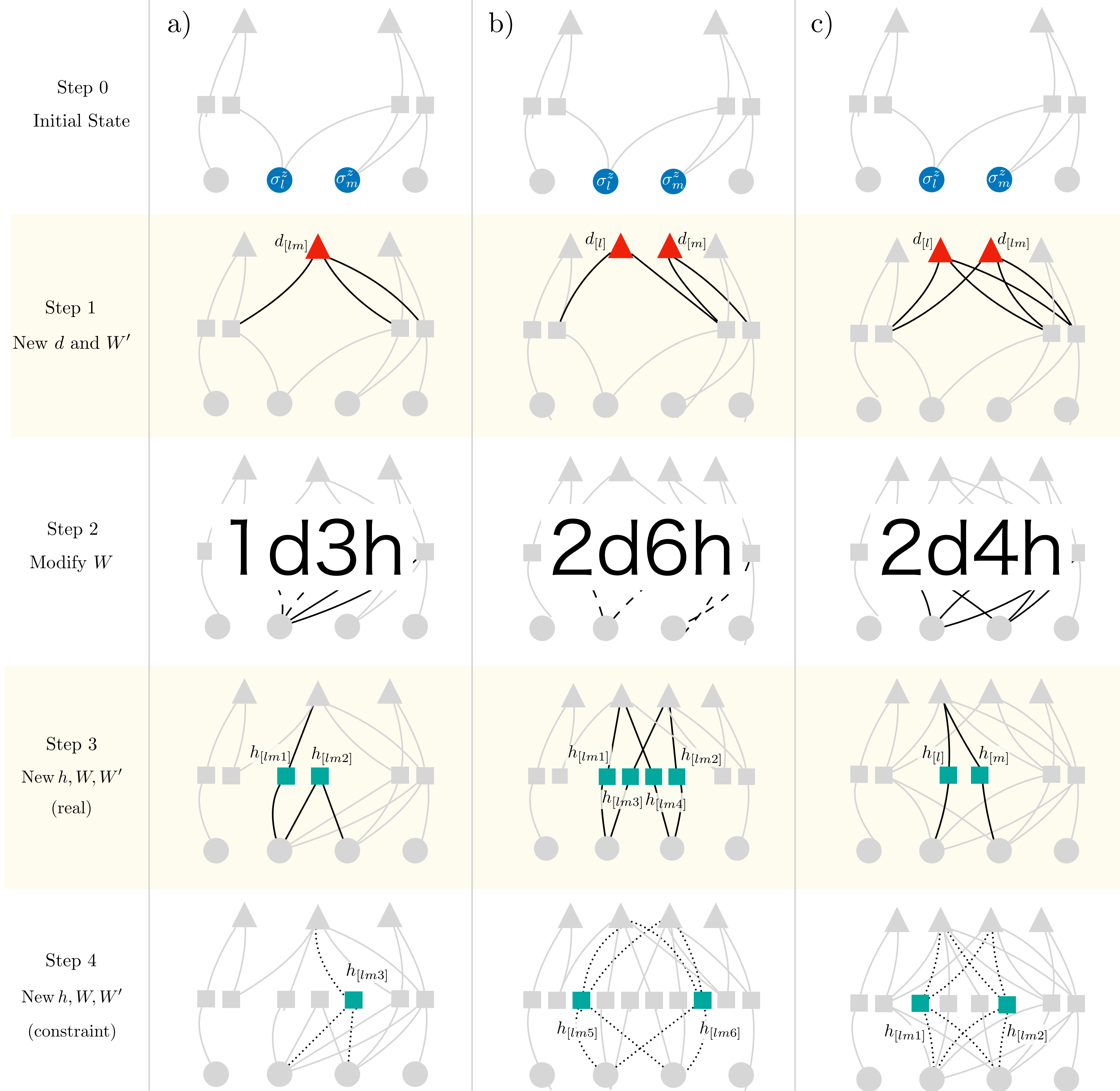
$$\bar{W}_{lj} = W_{lj} + \Delta W_{lj} = 0$$

$$W_{l[l]} = \frac{1}{2}\mathrm{arcosh}\left(\frac{1}{\tanh(\Gamma_l\delta_\tau)}\right)$$
$$W'_{[l][l]} = -W_{l[l]}.$$

DBM construction for Heisenberg model

G. Carleo, YN, and M. Imada, Nat. Commun, **9**. 5322 (2018)

Initial network



network after time evolution

$e^{-\delta_\tau J \vec{\sigma}_l \vec{\sigma}_m}|\mathrm{DBM}\rangle$

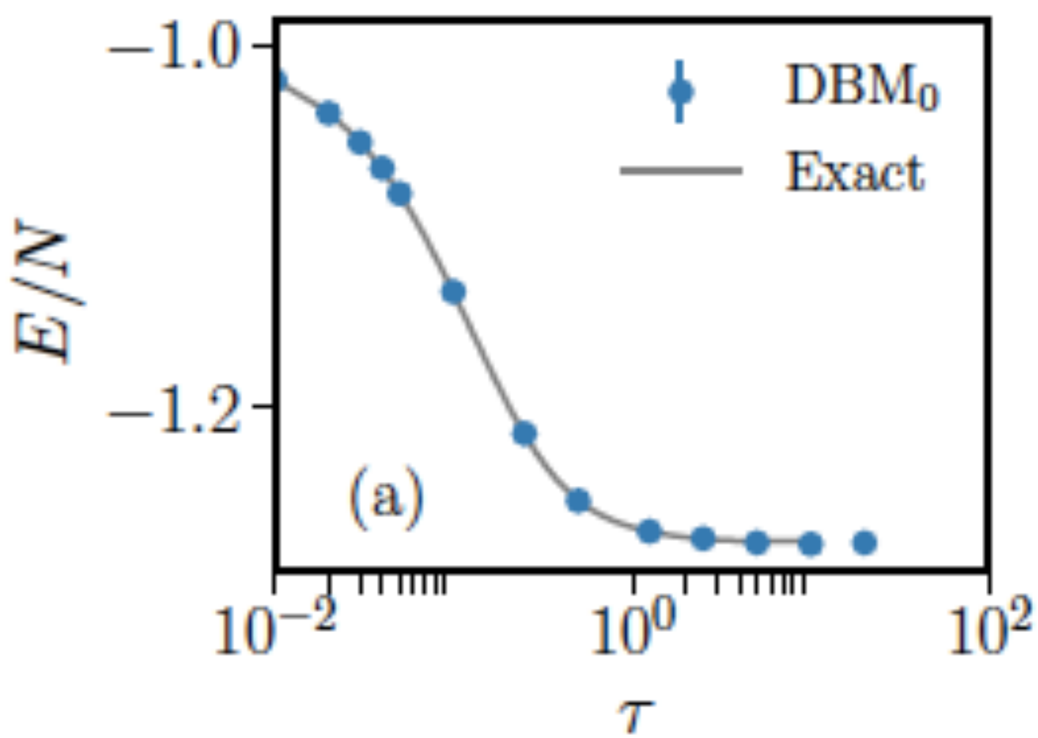
Numerical result

G. Carleo, YN, and M. Imada, Nat. Commun, **9**. 5322 (2018)

(# hidden units) ∝ (system size) x (imaginary time)

1D Transverse-Field Ising

N = 20, Jδτ = 0.01



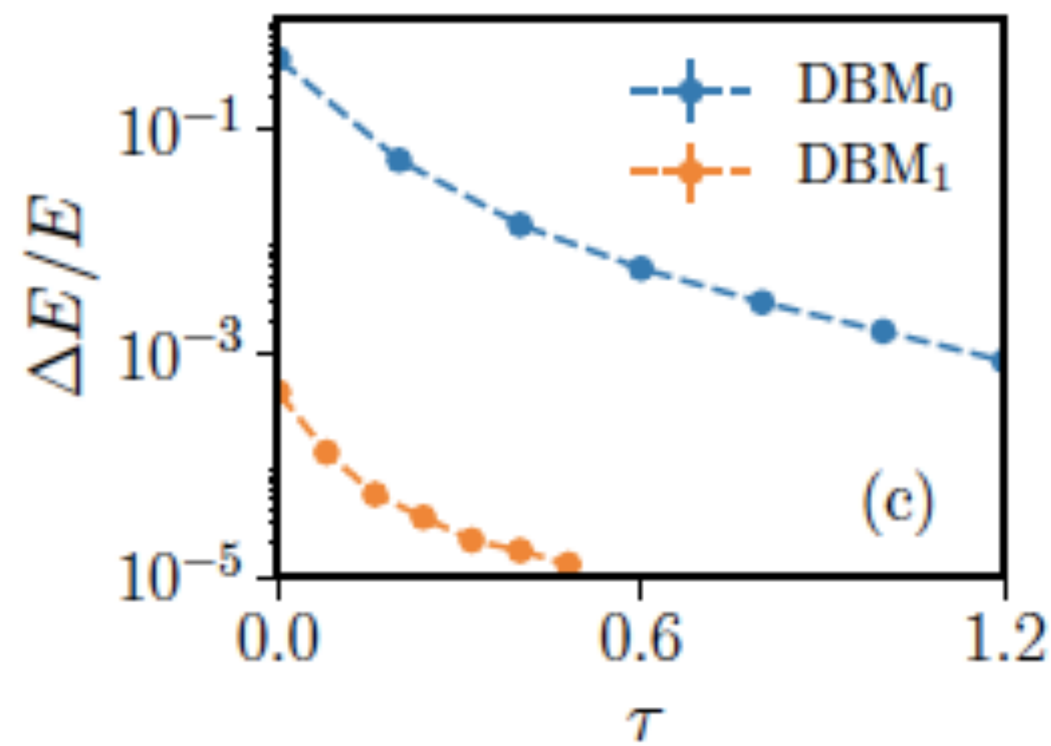
DBM reproduces exact time-evolution

1D Antiferromagnetic Heisenberg

N = 80, Jδτ = 0.01

from empty network

from pre-optimized RBM



better initial state => faster convergence

Short Summary

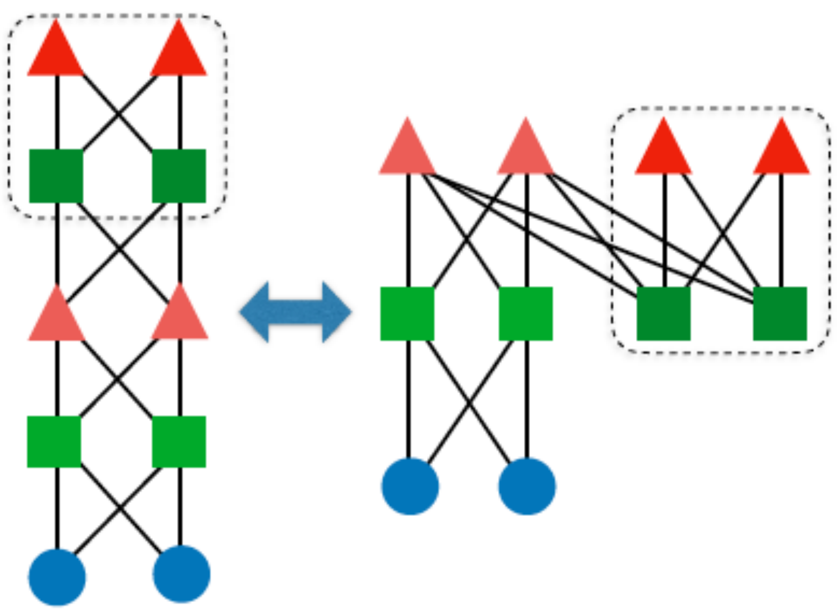
- Show deterministic construction of DBM to represent ground states

  The number of hidden units grows linearly with system size and imaginary time, respectively

- Additional hidden (deep) layer : “additional dimension” in statistical mechanics

- DBM representation => New quantum-to-classical mapping

- Unfortunately, there exist negative sign problem for e.g. frustrated spin systems



G. Carleo, Y. Nomura, and M. Imada, Nat. Commun. **9**, 5322 (2018) (see also N. Freitas et al., arXiv:1803.02118)

Extensions to various systems

②

Boson system

- Spin system (localized Mott insulator)

  without frustration

  (Heisenberg model)

  Carleo and Troyer (2017), …

  with frustration

  (J_1-J_2 Heisenberg model)

  YN and Imada arXiv, …

- Bose-Hubbard model (itinerant)

  Saito (2017), …

Fermion system

- **Itinerant electrons in solids**

  (Hubbard model)

  YN et al., (2017), …

- Molecules (H_2, LiH, …)

  Han et al., Choo and Carleo, …

Boson and Fermion system

- **Electron-phonon coupling**

  (Holstein model)

  YN JPSJ (2020)

  Editor's Choice

From benchmark to "true" applications to challenges in physics

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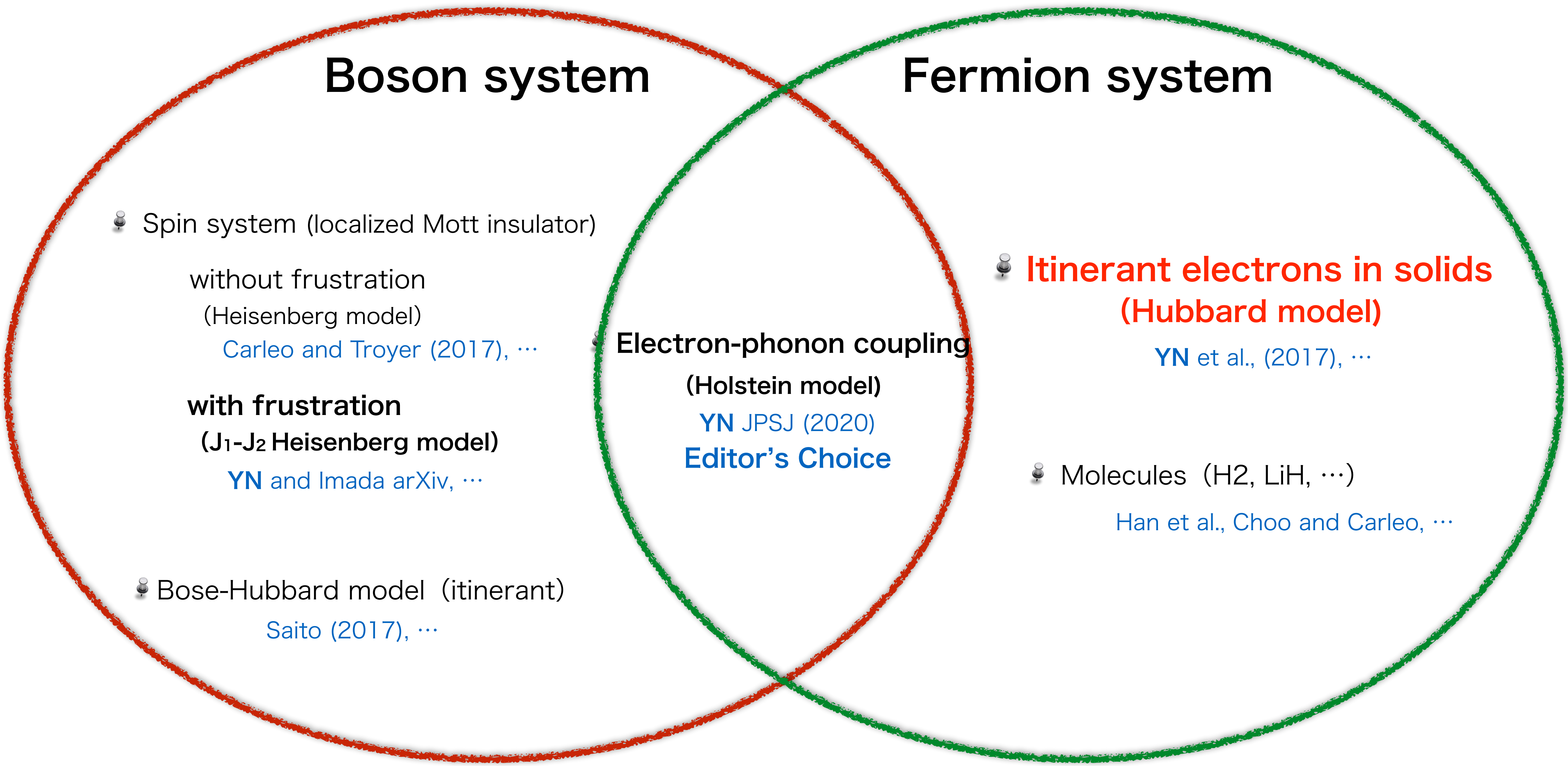
G. Carleo, YN, and M. Imada, Nat. Commun, **9**. 5322 (2018)

Extensions to various systems



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

See also Luo and Clark PRL (2019), …

Bosonic wave function vs Fermionic wave function

Boson

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = +\Psi(\mathbf{x}_2, \mathbf{x}_1)$$

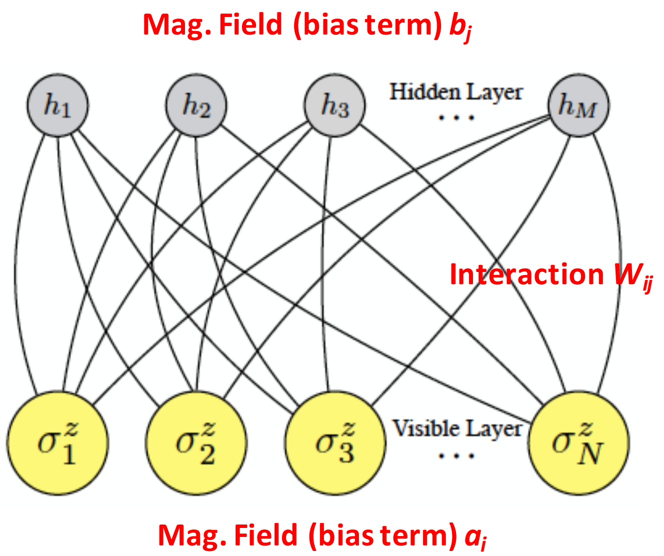
Fermion

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = -\Psi(\mathbf{x}_2, \mathbf{x}_1)$$

RBM wave function

$$\Psi(\sigma^z) = \sum_{\{h_j\}} \exp\left(\sum_i a_i \sigma_i^z + \sum_{i,j} \sigma_i^z W_{ij} h_j + \sum_j b_j h_j\right)$$

$\rightarrow$ Bosonic wave function



Application to Fermion systems

Mapping to interacting spin systems using Jordan-Wigner transformation

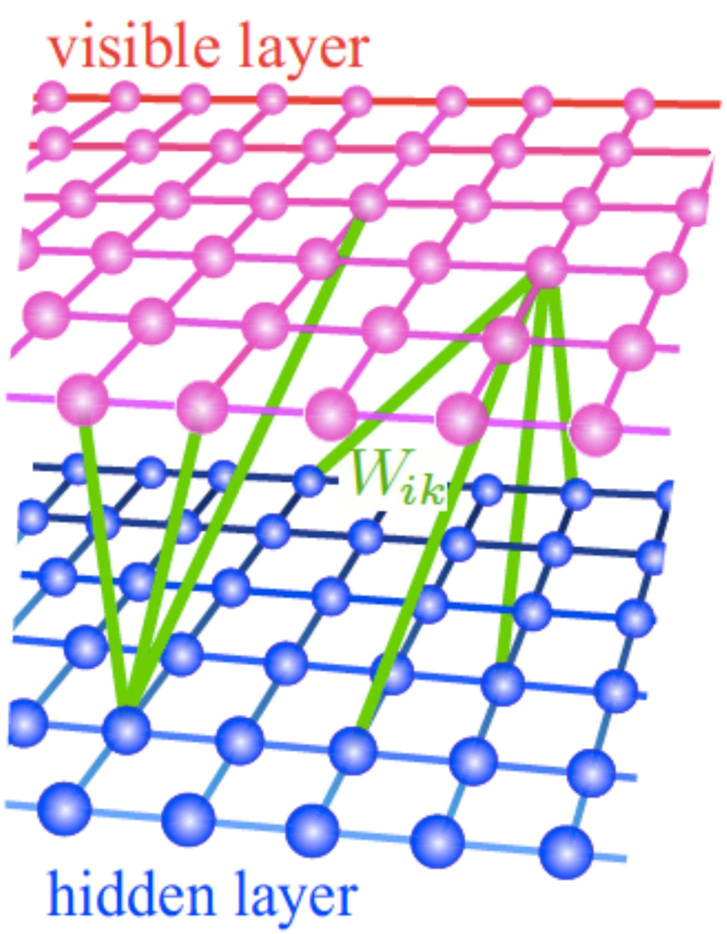
K. Choo et al, Nat. Commun. (2020)
Yoshioka et al.,

RBM+PP wave function

restricted Boltzmann machine + pair-product

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

RBM



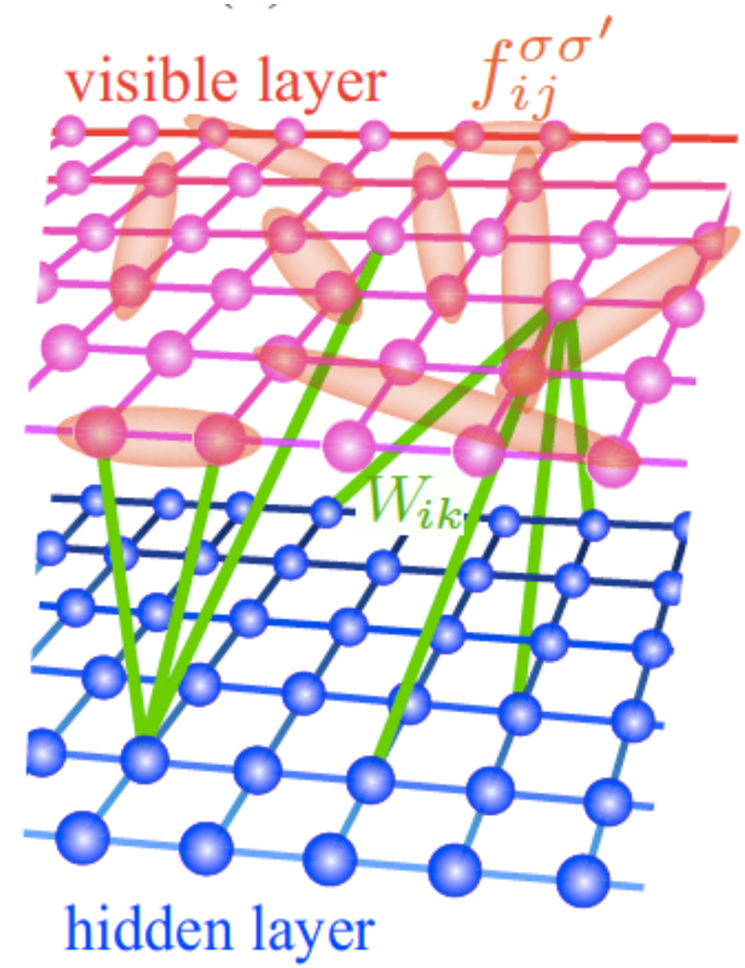
combine concepts from machine learning (RBM) and physics (pair-product(PP) state)

$$|\Psi\rangle = \sum_x |x\rangle\, \mathcal{N}(x)\, \phi_{\mathrm{product}}(x)$$

Boson wave function

no entanglement if hidden layer is absent

RBM+PP



$$|\Psi\rangle = \sum_x |x\rangle\, \mathcal{N}(x)\, \phi_{\mathrm{pair}}(x)$$

Pair-Product state (geminal wave function):

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

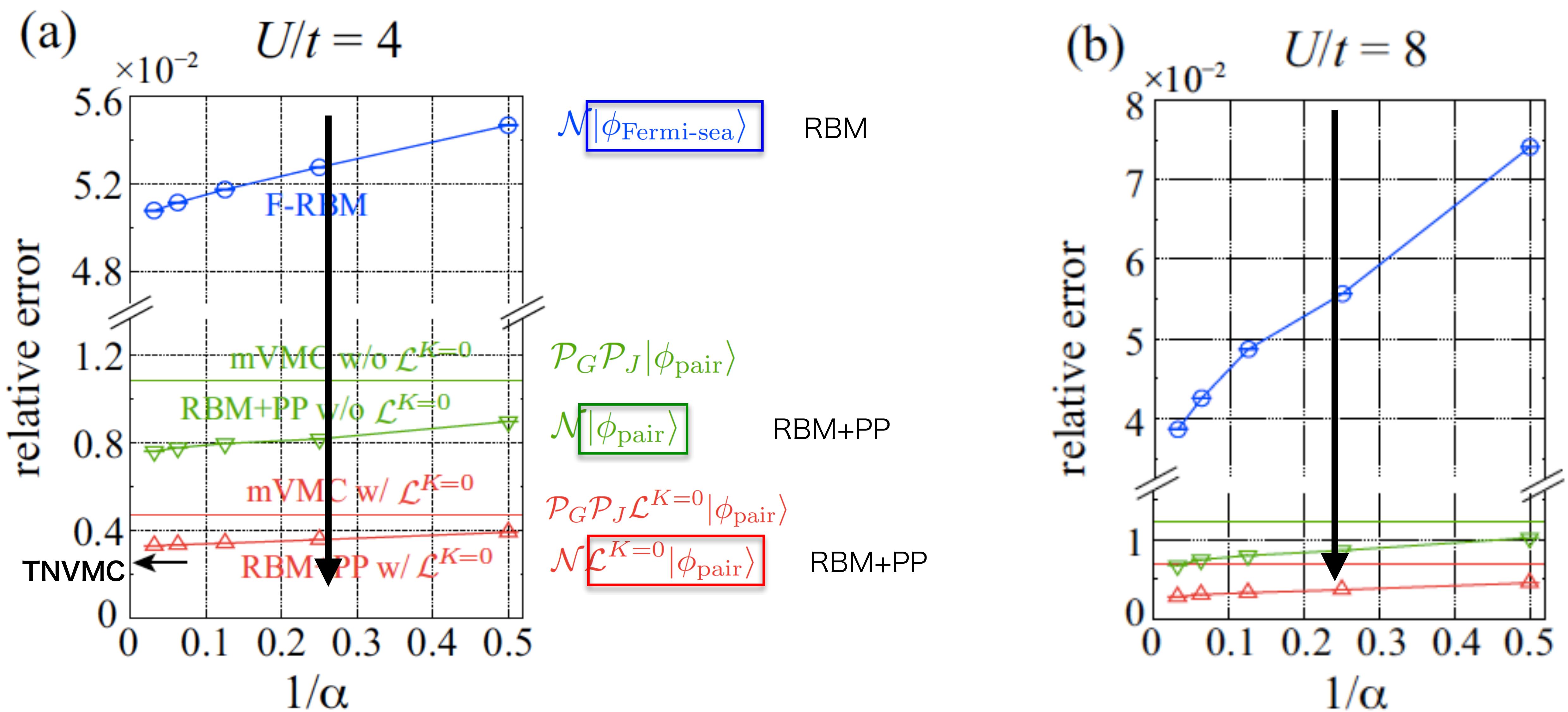
Fermion wave function

PP helps RBM to learn ground state

Application to 2D Hubbard model

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

YN, A. Darmawan, Y. Yamaji, and M. Imada, PRB **96**, 205152 (2017)
TNVMC data: H.-H. Zhao et al., PRB **96**, 085103 (2017).



α = (# hidden units)/(# physical spins)

- RBM+PP substantially improves accuracy compared to RBM
- Using combination saves # of parameters (important when simulate large system size)

Extensions to various systems

Boson system

- Spin system (localized Mott insulator)

  without frustration
  (Heisenberg model)
  Carleo and Troyer (2017), …

  with frustration
  (J_1-J_2 Heisenberg model)
  YN and Imada arXiv, …

- Bose-Hubbard model (itinerant)
  Saito (2017), …

Boson system ∩ Fermion system

- **Electron-phonon coupling**
  (Holstein model)
  YN JPSJ (2020)
  Editor's Choice

Fermion system

- **Itinerant electrons in solids**
  (Hubbard model)
  YN et al., (2017), …

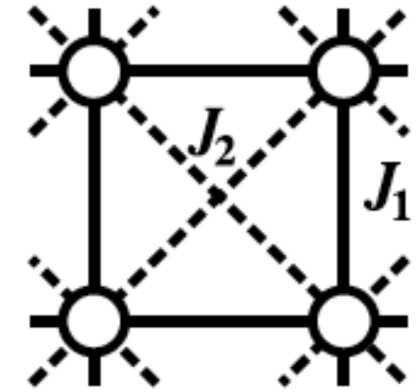
- Molecules (H2, LiH, …)
  Han et al., Choo and Carleo, …

YN and M. Imada, arXiv:2005.14142

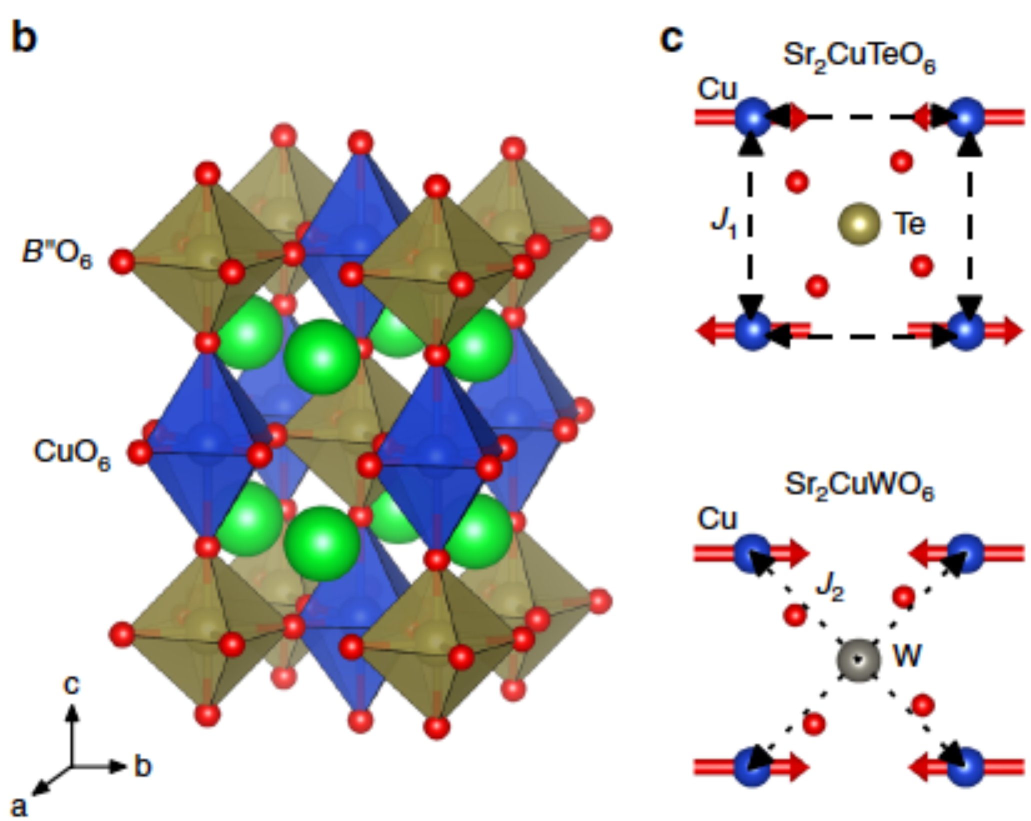
See also Liang et al., PRB (2018), Choo et al., PRB (2019), Ferrari et al., PRB (2019), Westerhout et al, Nat. Commun. (2020), Szabó and Castelnovo, arXiv.2002.04613, …

2D square-lattice J_1-J_2 Heisenberg model

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

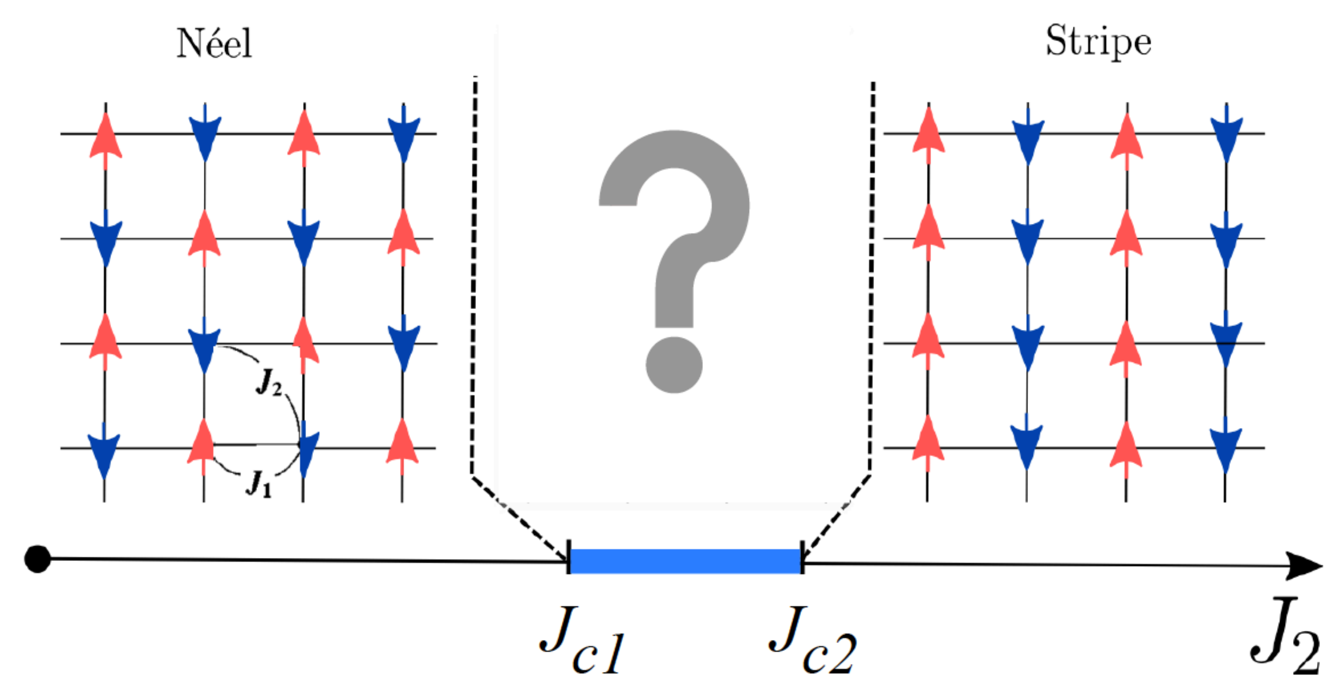


Materials



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

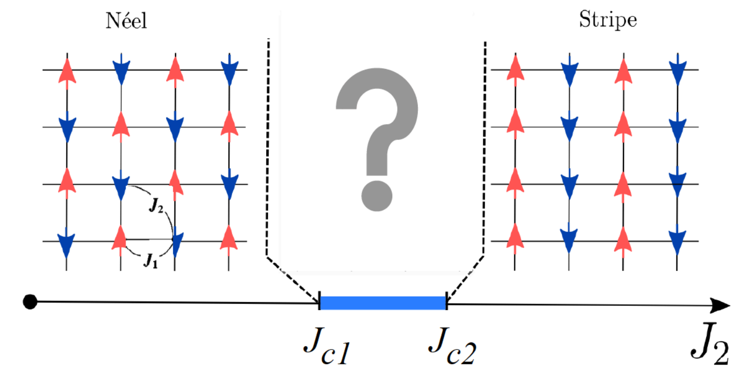
Unsettled phase diagram (J_1=1)



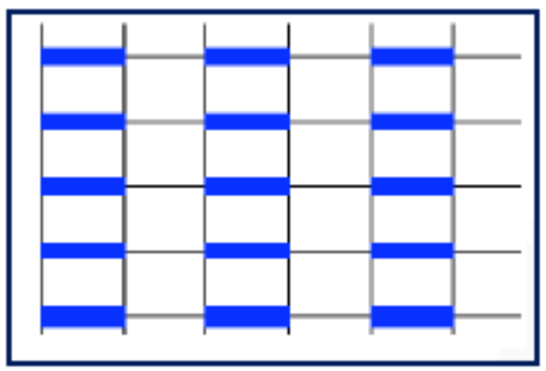
Quantum spin liquid (QSL) around J_2 = 0.5 ?

Relation between QSL and superconductivity ?

Candidates for intermediate phase(s)

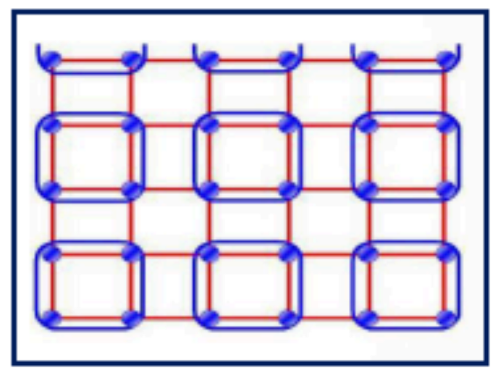


Columnar Dimer State



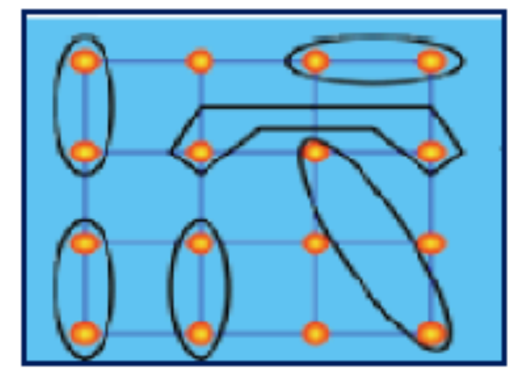
Gelfand, Singh, Huse, PRB 1989
Sachdev & Bhatt, PRB 1990
Valeri, *et al.*, PRB 1999
Murg, Verstraete, Cirac, PRB 2009
Haghshenas & Sheng, PRB 2018
Wang, Gu, Verstraete, Wen, PRB 2016
……

Plaquette Bond Crystal



Read & Sachdev, PRL 1989
Zhitomirsky & Ueda, PRB 1996
Doretto, PRB 2014
Mambrini et. al., PRB 2006
Gong, Sheng, *et. al.*, PRL 2014
……

Quantum Spin Liquid

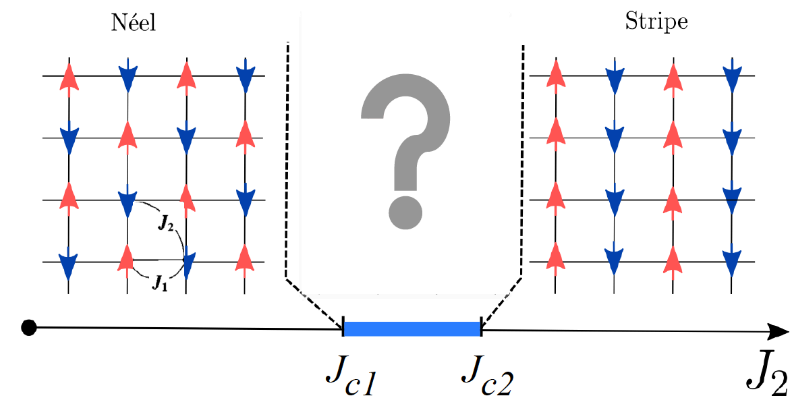


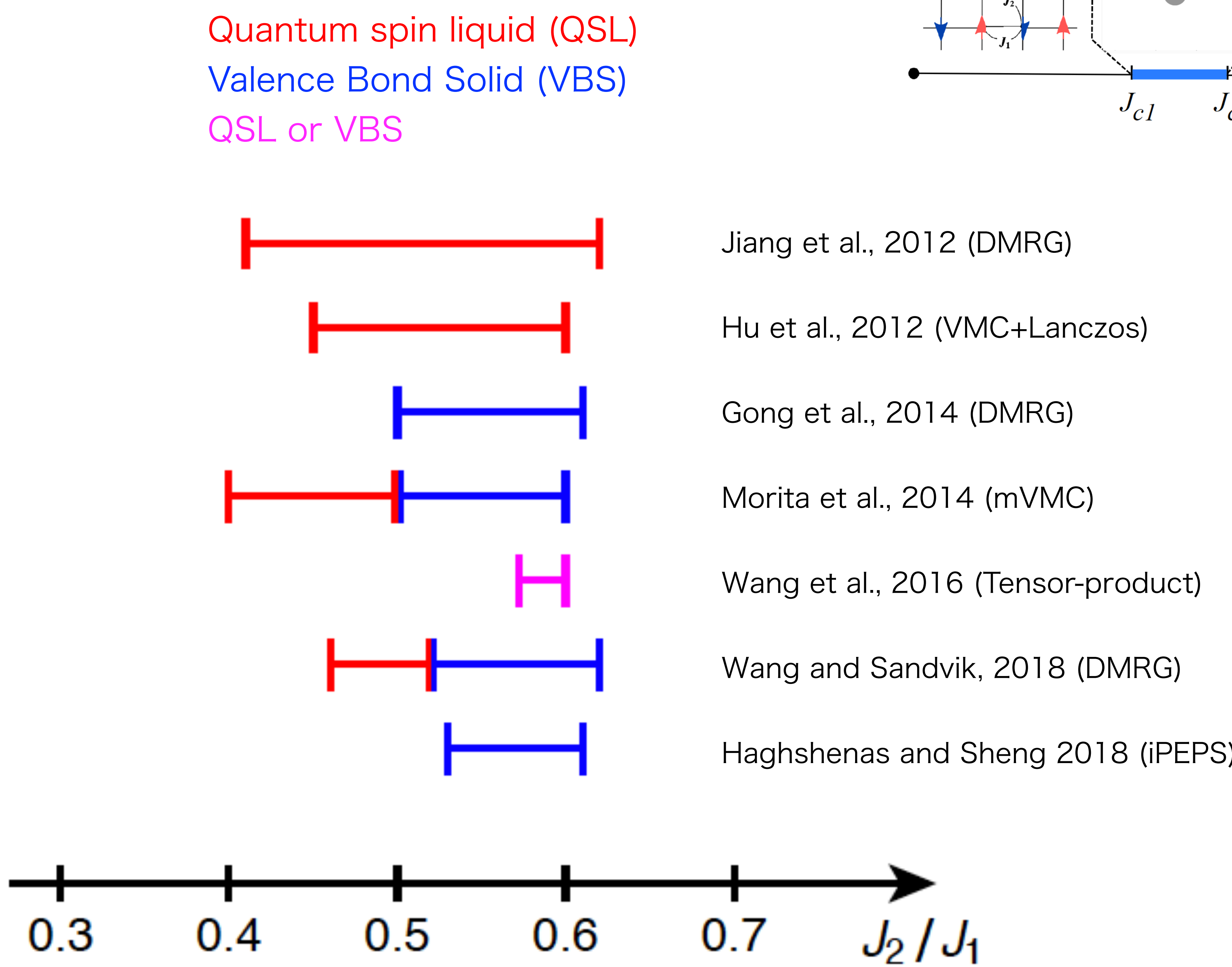
Chandra & Doucot, PRB 1988
Gochev, PRB 1993
Figueirido, Kivelson, et al., PRB 1989
Richter & Schulenburg, PRB 2010
Li, Becca, Hu, Sorella, PRB 2012
Jiang, Yao, Balents, PRB 2012
Wang & Sandvik, PRL 2018
……

$\underbrace{\hspace{10em}}$
Valence Bond Solid (VBS)

From Tao Xiang's lecture at ISSP

Controversy



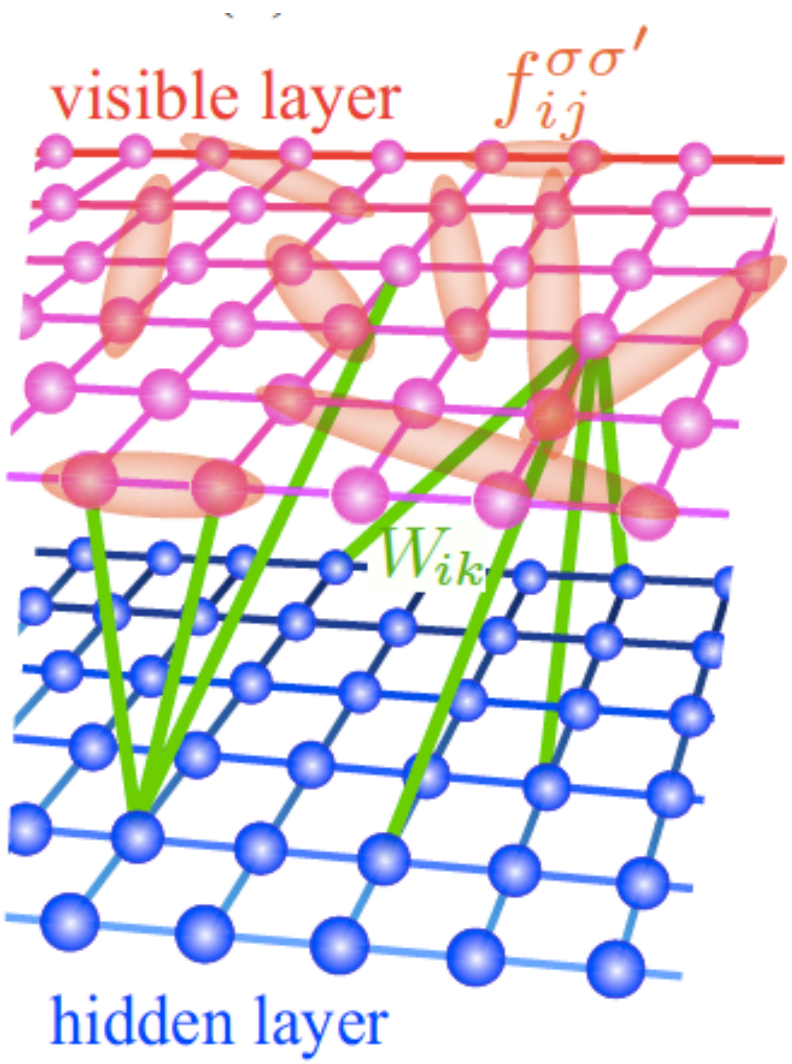


→ Let’s apply machine learning method !

RBM+PP wave function

restricted Boltzmann machine + pair-product

YN and M. Imada, arXiv:2005.14142



RBM+PP wave function

$$\Psi(\sigma) = \underbrace{\mathcal{N}(\sigma)}_{\text{neural-network (RBM)}} \times \underbrace{P_{\mathrm{G}}\phi_{\mathrm{pair}}(\sigma)}_{\text{Gutzwiller-projected PP state}}$$

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

Imposing quantum numbers (symmetry)

Choo et al., PRL (2018), Ferarri et al., PRB (2019), YN JPSJ (2020), ···

spin-parity (+ : S even, – : S odd)

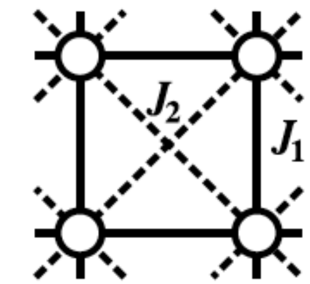
$$\Psi_{\mathbf{K}}^{S\pm}(\sigma) = \sum_{\mathbf{R}} e^{-i\mathbf{K}\cdot\mathbf{R}} [\underbrace{\Psi}_{\text{wave func. w/o symmetry}}(T_{\mathbf{R}}\sigma) \pm \Psi(-T_{\mathbf{R}}\sigma)]$$

total momentum

Ground state : S=0(even), **K=0**

Excited states : other quantum numbers

Benchmarks



Number hidden units = 16 Nsite

Ground-state energy (J_2=0.5, 10x10 lattice)

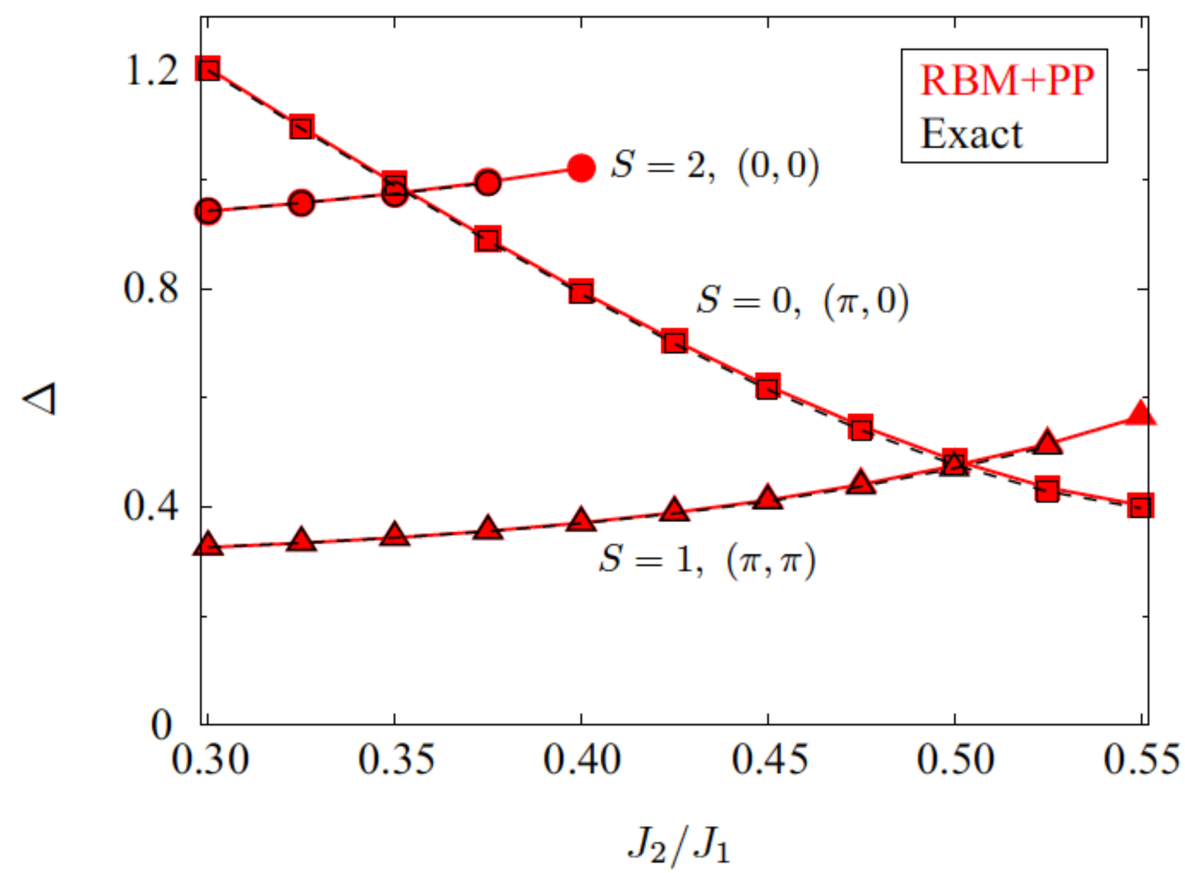
Green: using neural network

−0.49476(1)	Neural quantum states [1]
−0.49516(1)	CNN [2]
−0.49521(1)	VMC [3]
−0.495530	DMRG [4]
−0.49575(3)	RBM+fermion wave func. [5]
−0.49718(2)	**RBM+PP (present study)**
−0.497549(2)	VMC+2nd order Lanczos [3]

accurate

[1] Szabó and Castelnovo, arXiv [2] Choo et al., PRB 2019
[3] Hu, et al., PRB 2013 [4] Gong et al., PRL 2014 [5] Ferrari et al., PRB 2019

Excitation energy (6x6 lattice)

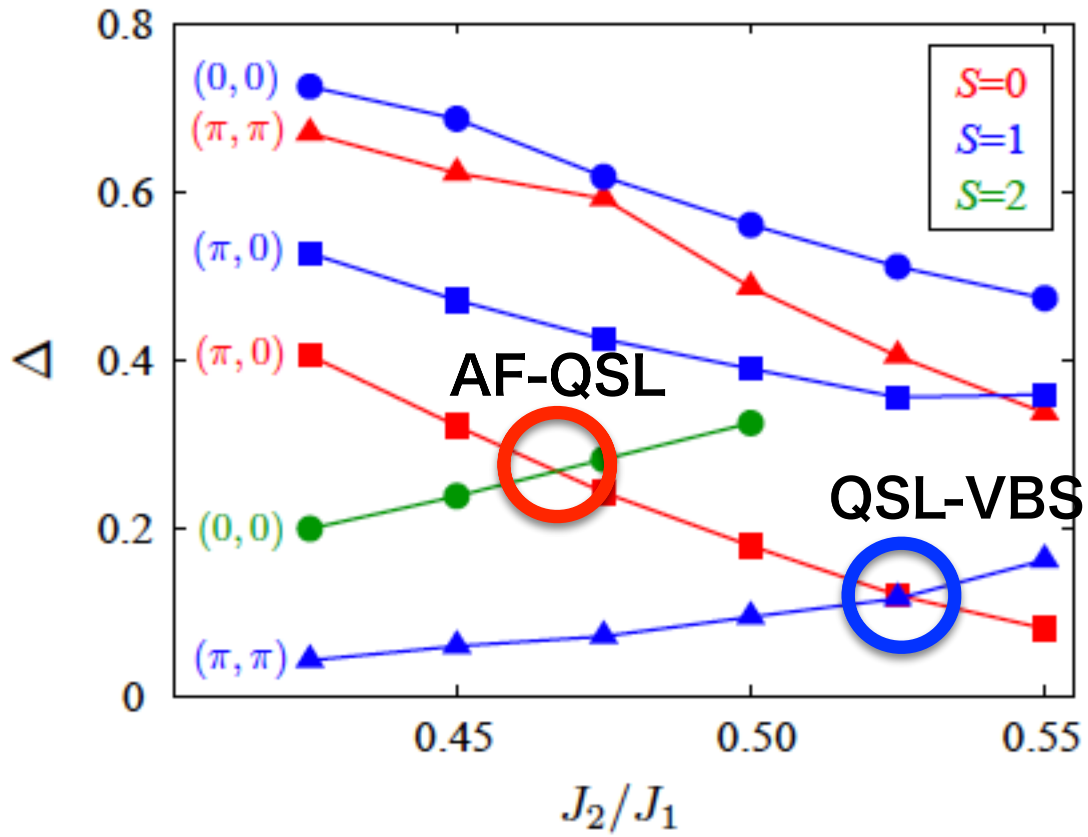


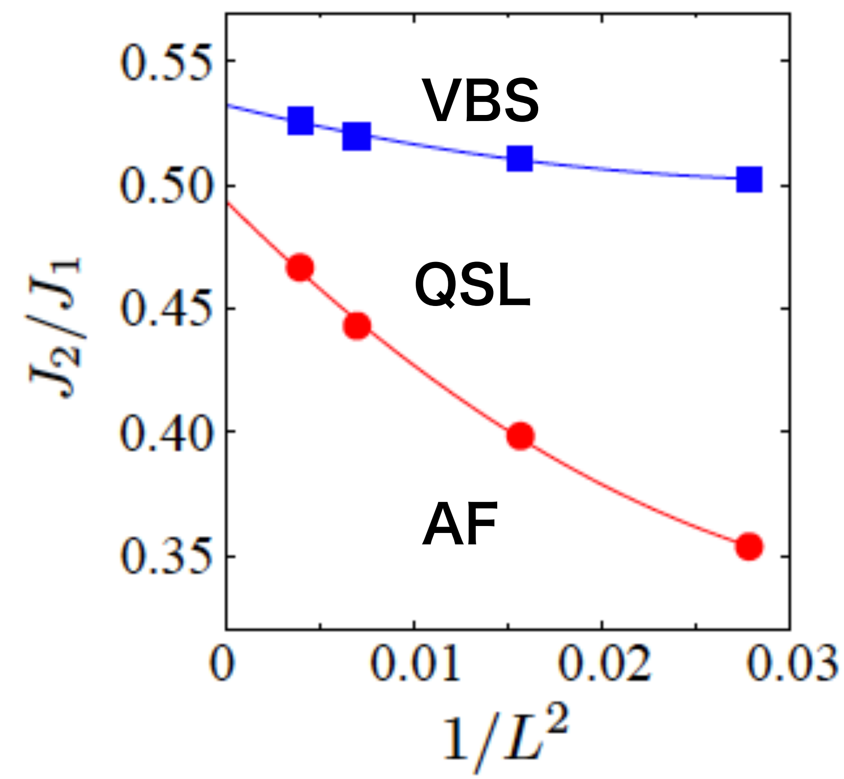
- RBM+PP can accurately represent not only the ground state but also excited states
  → enables excited-state level spectroscopy

Excited-state level spectroscopy

Suwa et al PRB (2016); Wang and Sandvik PRL (2018)

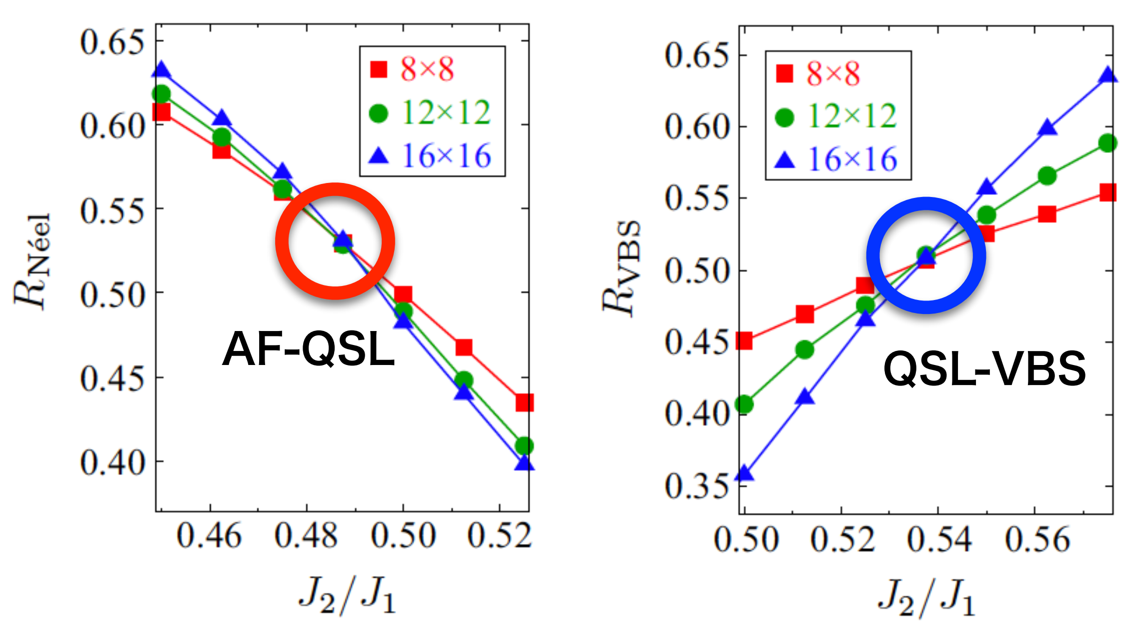
Excitation energy at 16x16 lattice





cf. Analysis of correlation ratio $1 - S(\mathbf{q}_{\text{peak}} + \delta\mathbf{q})/S(\mathbf{q}_{\text{peak}})$

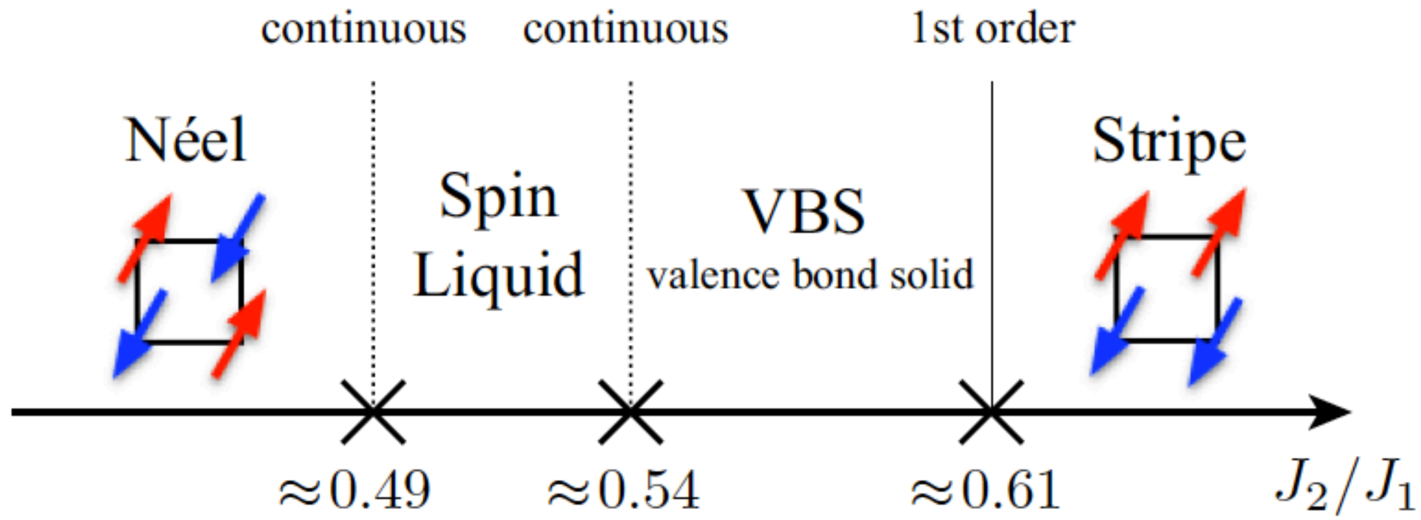
(ground state property)

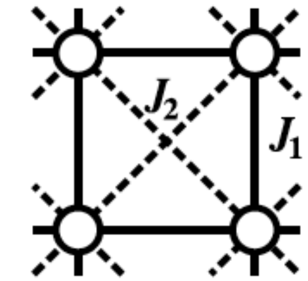


- **Two independent analyses agree**

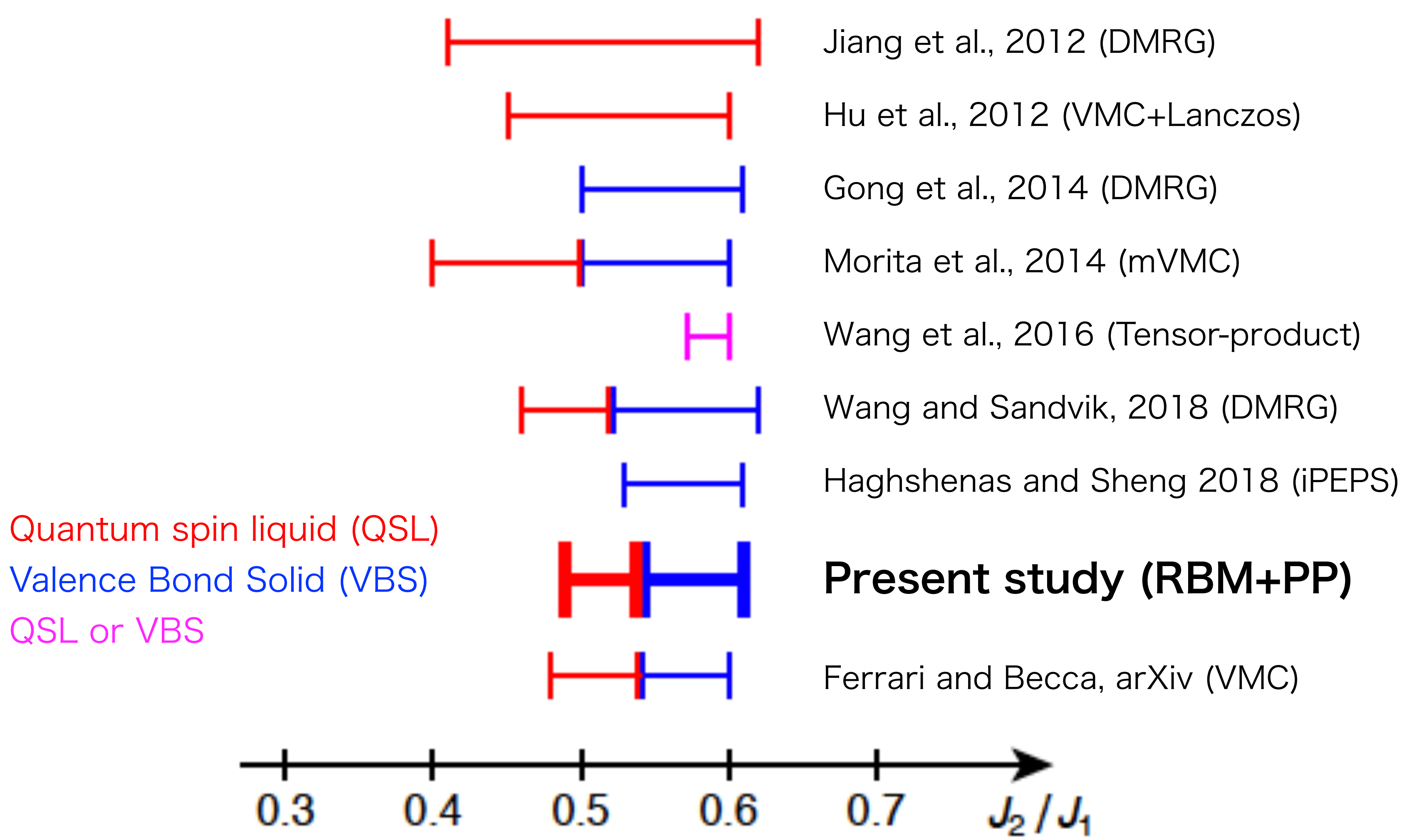
(one-to-one correspondence between ground-state phase and excitation structure)

Ground-state phase diagram

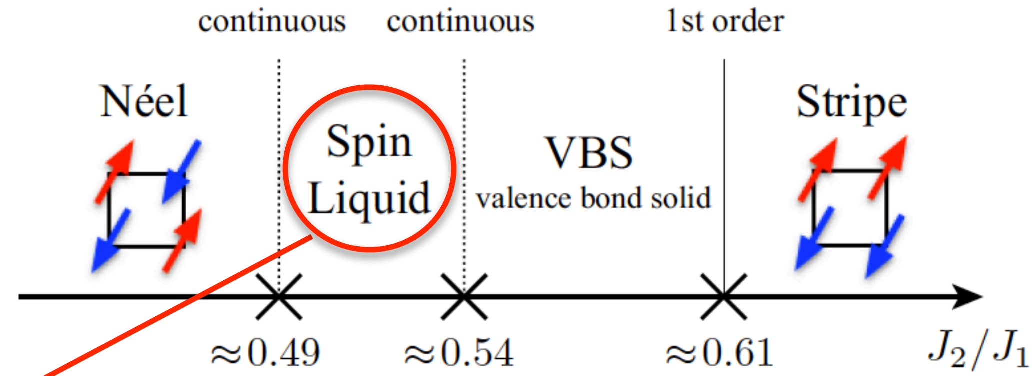




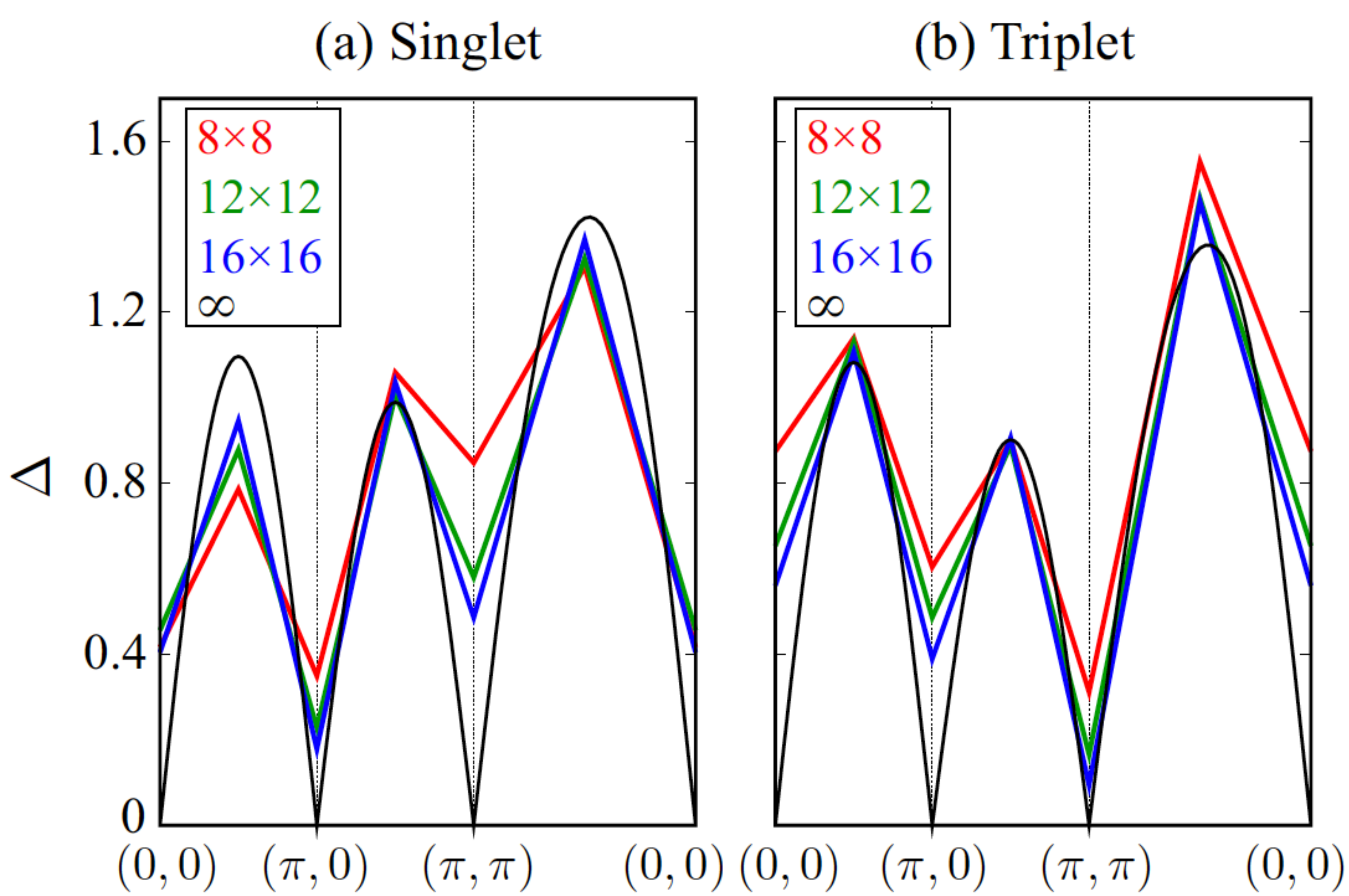
Comparison to previous results



Nodal quantum spin liquid

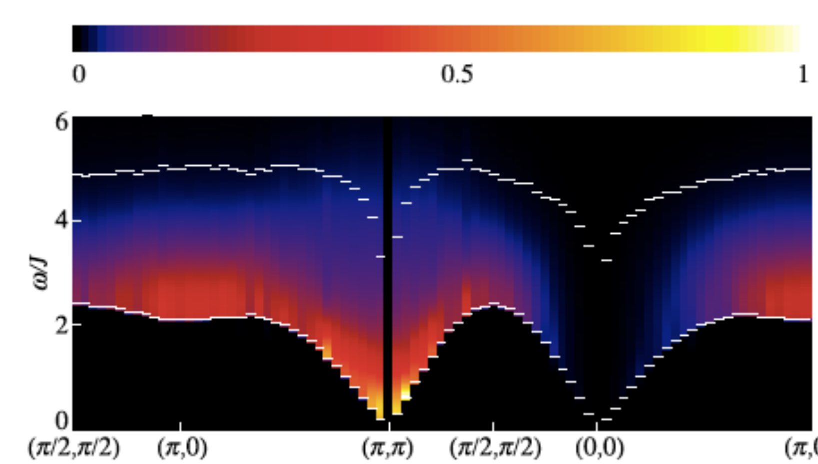


Excitation spectra (J2=0.5)



Qualitatively consistent with Ferrari and Becca, PRB **98**, 100405 (2018)

c.f. S(q,ω) in Heisenberg model



H. Shao et al., PRX **7**, 041072 (2017)

- **Accurate excited-states calculations clarify the nature of QSL**

Summary

Boson system

- Spin system (localized Mott insulator)

  without frustration
  (Heisenberg model)
  Carleo and Troyer (2017), …

  with frustration
  (J_1-J_2 Heisenberg model)
  YN and Imada arXiv, …

- Bose-Hubbard model (itinerant)
  Saito (2017), …

Fermion system

- **Itinerant electrons in solids**
  (Hubbard model)
  YN et al., (2017), …

- Molecules (H2, LiH, …)
  Han et al., Choo and Carleo, …

Boson and fermion system

- **Electron-phonon coupling**
  (Holstein model)
  YN JPSJ (2020)
  Editor's Choice

Machine-learning method shows its power in grand challenges in physics !

YN and M. Imada, arXiv:2005.14142