Encoding many-body quantum physics into neural networks

Nobuyuki Yoshioka

University of Tokyo

2021.05.27

東京大学
THE UNIVERSITY OF TOKYO

About me

Nobuyuki Yoshioka

2020.03	Ph.D. in Physics at UTokyo, Katsura group
2020.04-12	Postdoc at RIKEN, Theoretical Quantum Physics Laboratory (Nori group)
2021.01-	Research Associate at UTokyo (Sagawa group)

Interest：Algorithms for the Quantum

- Classifying physical states by neural networks

  NY, Akagi, Katsura, Phys. Rev. B 97, 205110 (2018).

- Efficient representation of many-body states by neural nets

  NY, Akagi, Katsura, Phys. Rev. E 99, 032113 (2019).

  NY, Hamazaki, Phys. Rev. B 99, 214306 (2019).

  NY, Mizukami, Nori, Commun. Phys. 4 106 (2021).

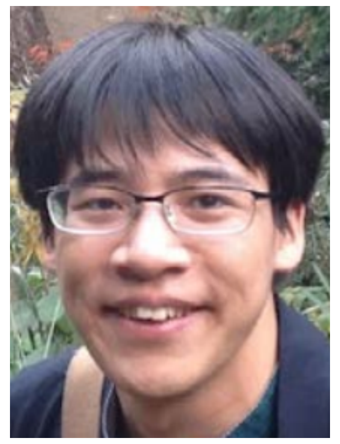
  Nomura*, **NY***, Nori arXiv:2103.04791

- Building quantum algorithms

  NY, Y.O. Nakagawa, K. Mitarai, K. Fujii, PRR 2, 043289 (2020).

  NY, H. Hakoshima, Y.Suzuki, S.Endo in prep.

Collaborators



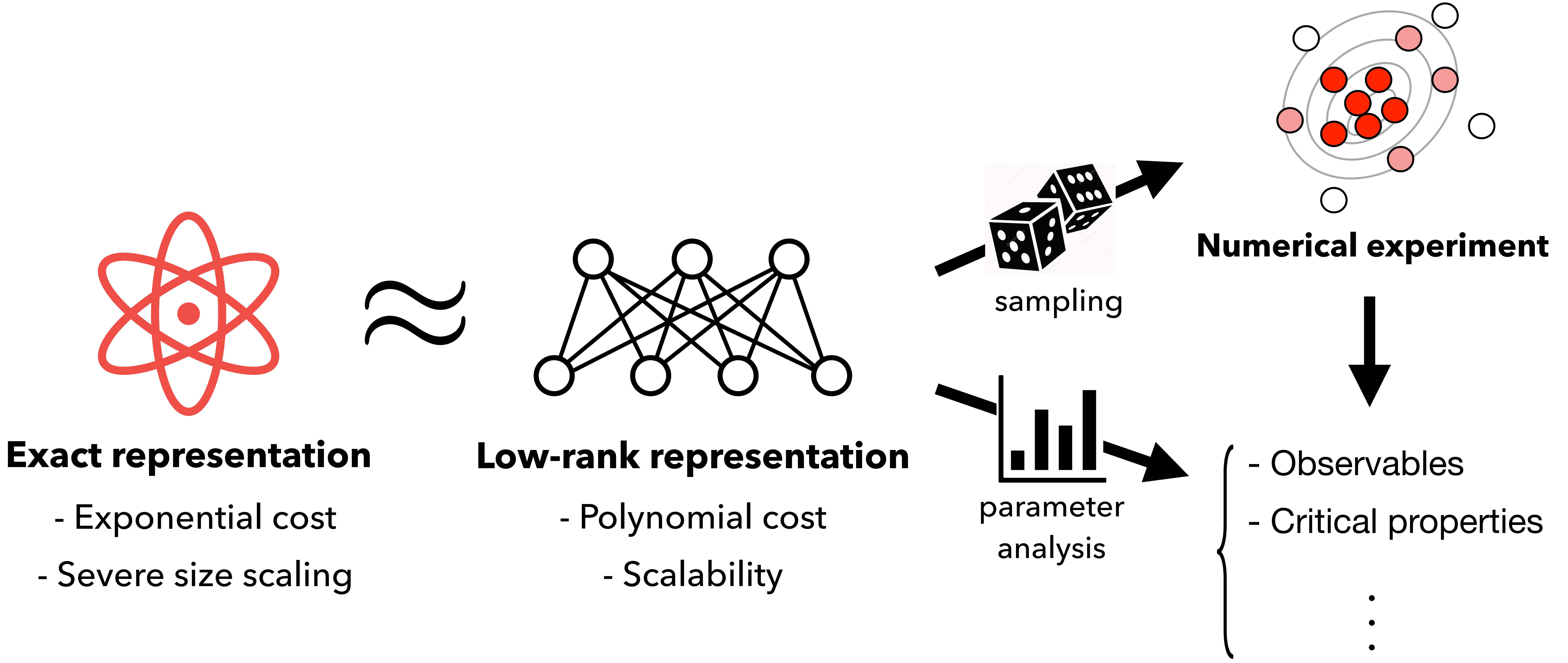
R. Hamazaki

F. Nori

Y. Nomura

W. Mizukami

Compressing quantum many-body states



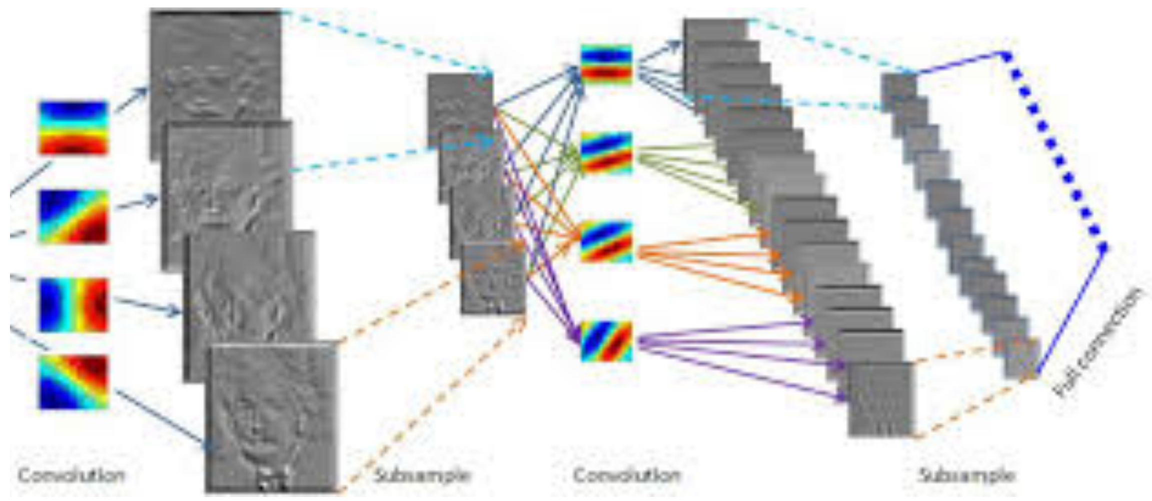
Compressing quantum many-body states

Data-driven

Feature extraction via experiment/synthetic data

e.g. Phase classification

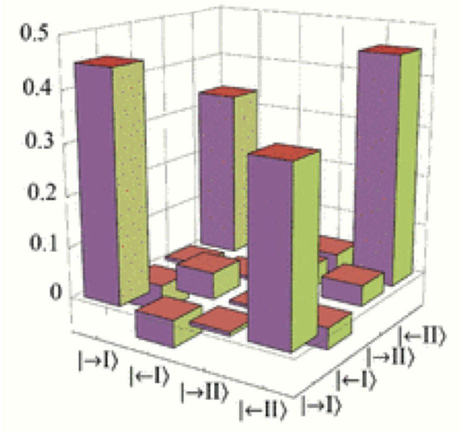
$|\psi\rangle$

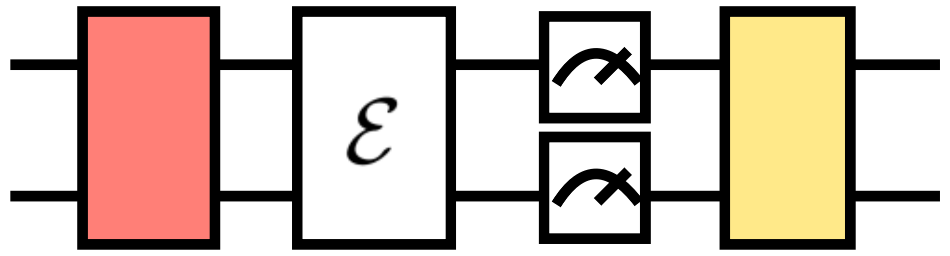


- Constructing "surrogate" order parameters
- One-shot classification from noisy data

Schindler et al., PRB ('17) Rem et al., Nat Phys. 15 ('19)

e.g. Quantum tomography





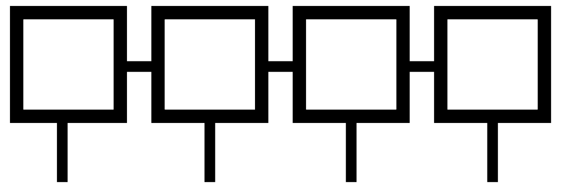
- Exponential cost in naive way
- Polynomial cost by fitting variational forms

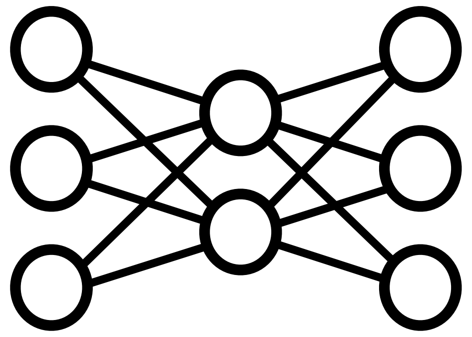
Cramer et al., Nat.Comm ('10) Torlai et al., Nat. Phys. ('18)

Model-driven

Boosting analysis on well-defined models

e.g. Variational calculation





- "Effective equation" in parameter space
- Key: variational principle and approximant

Variational simulation

What is variational simulation?

To solve some equation *within parameter space,* such that solution in Hilbert space is approximated

e.g. Ground state problem in quantum many-body systems

$$H|\Psi_{\mathrm{GS}}\rangle = E_{\mathrm{GS}}|\Psi_{\mathrm{GS}}\rangle$$

Diagonalization

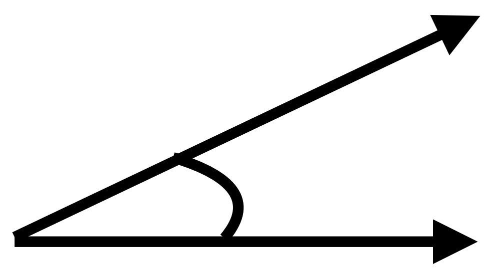
$$|\Psi_{\mathrm{GS}}\rangle = \lim_{\beta\to\infty} \frac{e^{-\beta H}|\Psi_0\rangle}{\||e^{-\beta H}|\Psi_0\rangle\||}$$

Imaginary-time evolution (ITE)

Exponential cost for exact solution

Approximate ITE by variational function $|\Psi_\theta\rangle$ based on Trotterization:

$$e^{-\delta H}|\Psi_\theta\rangle$$

$|\Psi_\theta\rangle$  $|\Psi_{\theta+\delta\theta}\rangle$

Choose $\delta\theta$ that minimize distance
(Polynomial cost)

$$|\Psi_0\rangle \to e^{-\delta H}|\Psi_0\rangle \to \cdots$$

$$\wr\wr \qquad \wr\wr \quad \arg\min_{\delta\theta}\left(\mathcal{F}\left(e^{-\delta_\tau \mathcal{H}}|\Psi_\theta\rangle, |\Psi_{\theta+\delta\theta}\rangle\right)\right)$$

$$|\Psi_{\theta_0}\rangle \to |\Psi_{\theta_0+\delta\theta^{(1)}}\rangle \to \cdots$$

Variational simulation

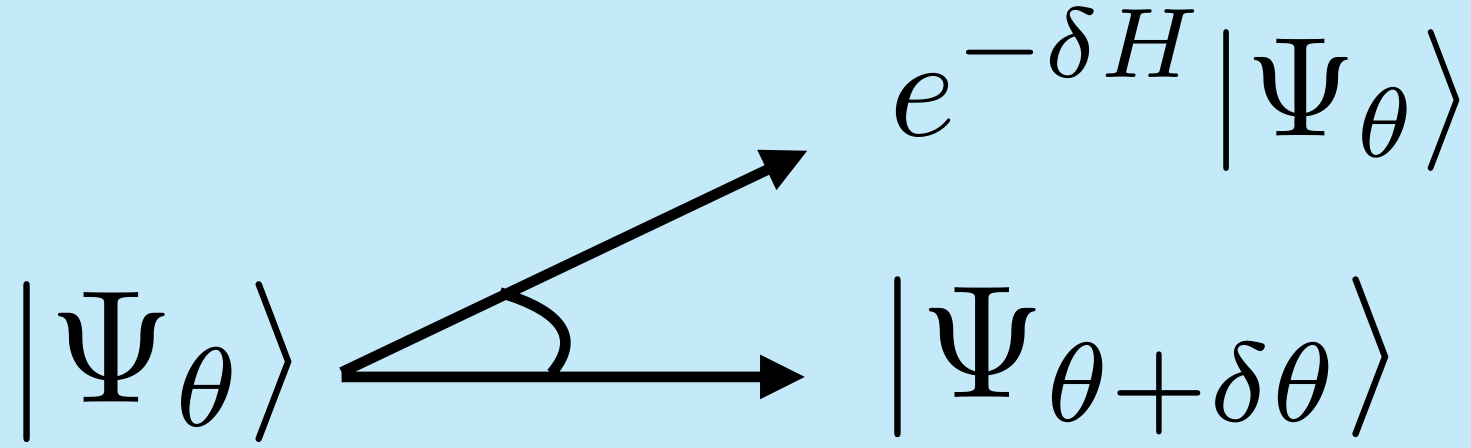
What is variational simulation?

To solve some equation *within parameter space,* such that solution in Hilbert space is approximated

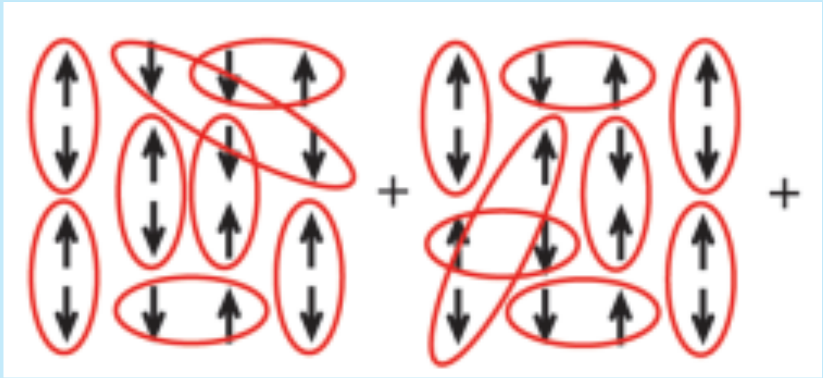
Key steps

1. Choose variational principle

e.g. Choose metric $\mathcal{F}$ for



2. Choose GS approximant $|\Psi_\theta\rangle$



RVB state
(for spin liquid)

Laughlin state
(for fractional QHE)

Conventional ones are *physics-motivated*

→ "biased" search, requires deep physical knowledge

How to construct *physics-agnostic* variational function?

I. Neural-network quantum states

Properties of neural-network quantum states

Ground state problems

II. Beyond GS problems

Finite-temperature simulations by DBM purification

First-principles calculation in solid systems

Requirements for unbiased variational ansatz

Three conditions, in my personal opinion:

[1] Nearly exact for weakly correlated systems

→ Large-scale benchmarks (GS problems without negative sign)

Carleo&Troyer Science 355('17) Sharir et al. PRL ('20) Yang et al. NeurIPS ('20)

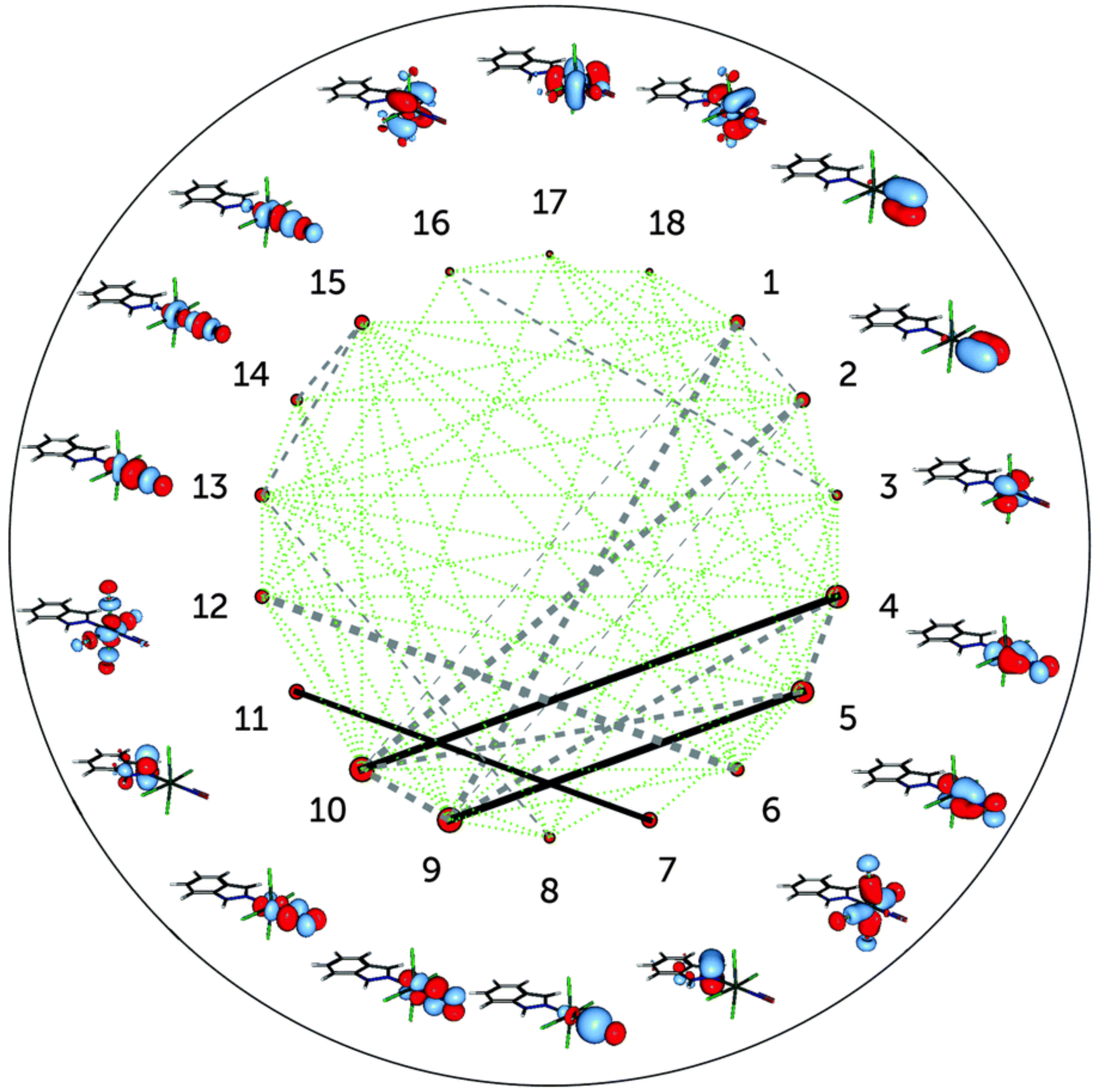
[2] Unbiased in terms of lattice/interaction geometry

→ Ability to express large quantum entanglement

Deng etal. PRX ('17) Levine etal. PRL ('19)

[3] Ability to reflect physical constraints, i.e. symmetry

Torlai&Melko PRL ('18) Viejra etal., PRL ('20)



Freitag etal. PCCP ('15)

Neural networks expected to satisfy all of them

Requirements for unbiased variational ansatz

Three conditions, in my personal opinion:

[1] Nearly exact for weakly correlated systems

→ Large-scale benchmarks (GS problems without negative sign)

Carleo&Troyer Science 355('17) Sharir et al. PRL ('20) Yang et al. NeurIPS ('20)

[2] Unbiased in terms of lattice/interaction geometry

→ Ability to express large quantum entanglement

Deng etal. PRX ('17) Levine etal. PRL ('19)

[3] Ability to reflect physical constraints, i.e. symmetry

Torlai&Melko PRL ('18) Viejra etal., PRL ('20)

Neural networks expected to satisfy all of them

Neural networks as variational ansatz

e.g. Restricted Boltzmann machine (RBM)

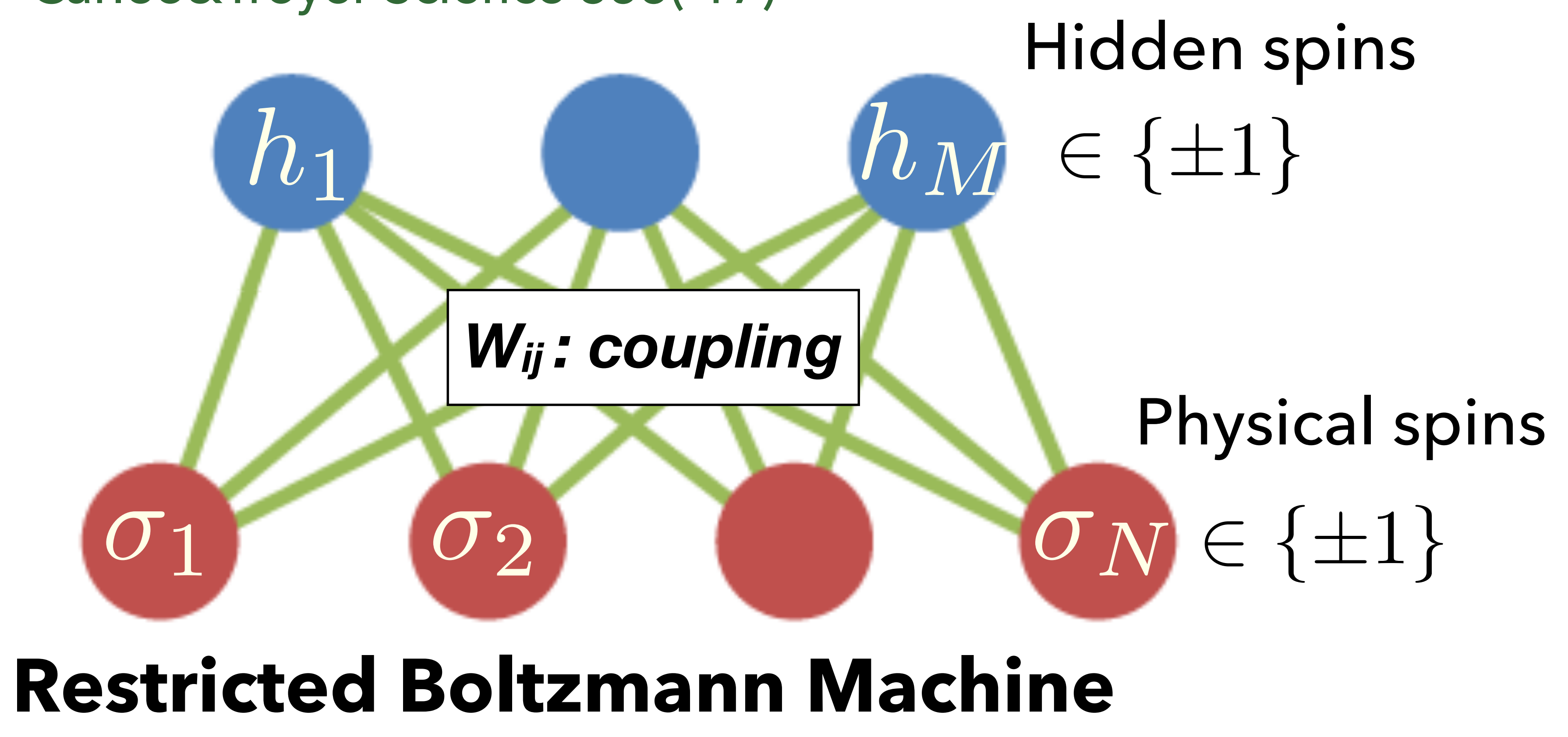
- One of the simplest/shallowest networks used from 80's Smolensky ('86)

- The complex amplitude for spins config $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ Carleo&Troyer Science 355('17)

$$\langle \sigma | \Psi \rangle = \frac{1}{Z} \sum_{h_j} e^{-E(\sigma,h)}$$ "Boltzmann factor"

interaction, magnetic field

$$E(\sigma, h) = \sum_{ij} W_{ij}\sigma_i h_j + a_i\sigma_i + b_j h_j$$



- Universal approximation theorem (complex func. version) Roux&Bengio ('08), Montufar&Ay ('11)

  If we have $O(2^N)$ hidden spins (N: #physical spins),
  arbitrary wave function $\Psi(\sigma)$ can be approximated with arbitrary accuracy.

Solving ground state by variational Monte Carlo

VMC for low-dimensional quantum spin models Carleo&Troyer Science 355('17)

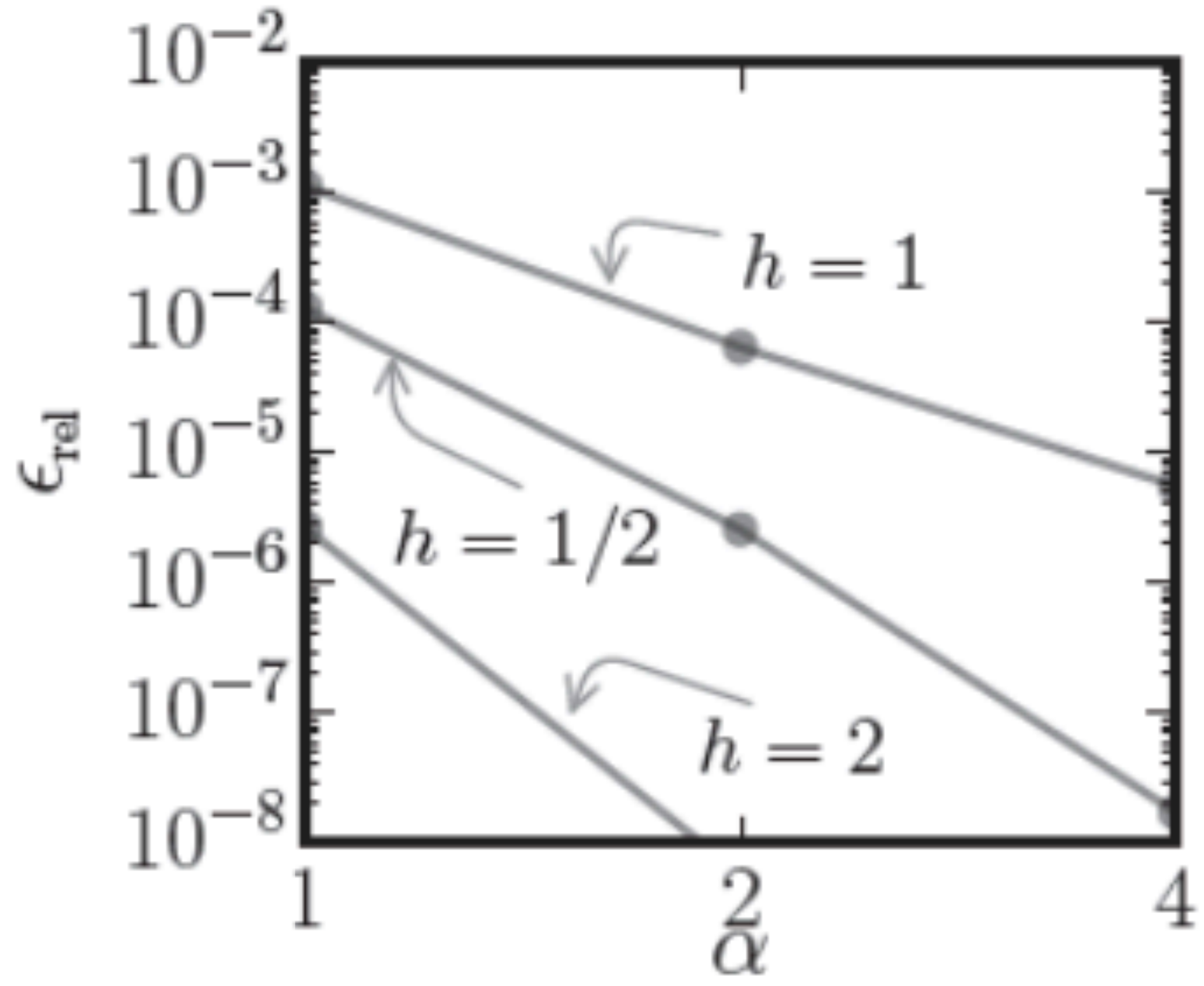
State-of-the-art accuracy compared with tensor network methods (MPS, PEPS)

(Relative error: $\epsilon_{\rm rel} = |E_{\rm RBM} - E_{\rm QMC}|/E_{QMC}$)

1d transverse-field Ising model

80 spins, periodic boundary,

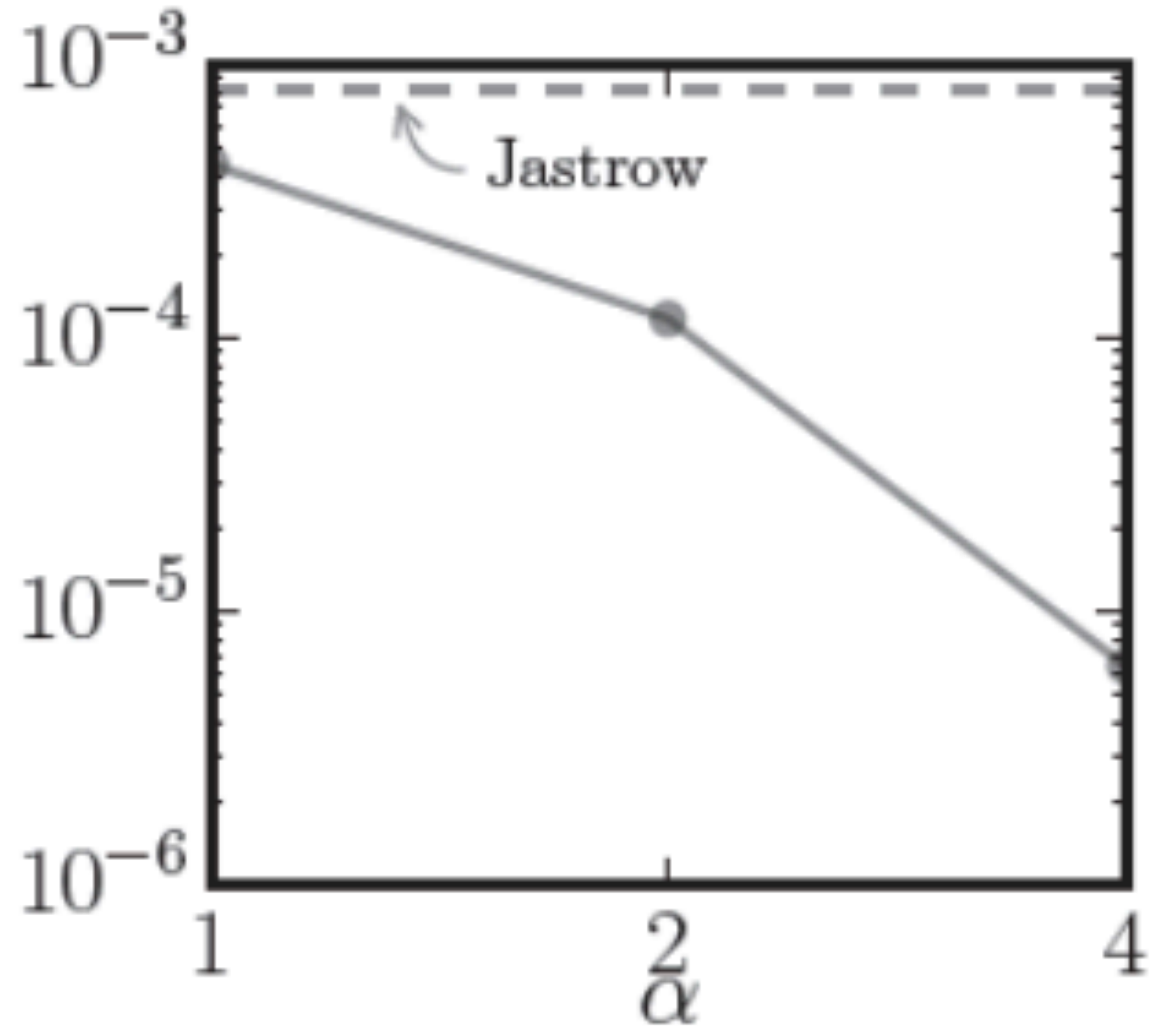
h : field, alpha: (# of hidden neuron)



α :(#hidden)/(#visible)

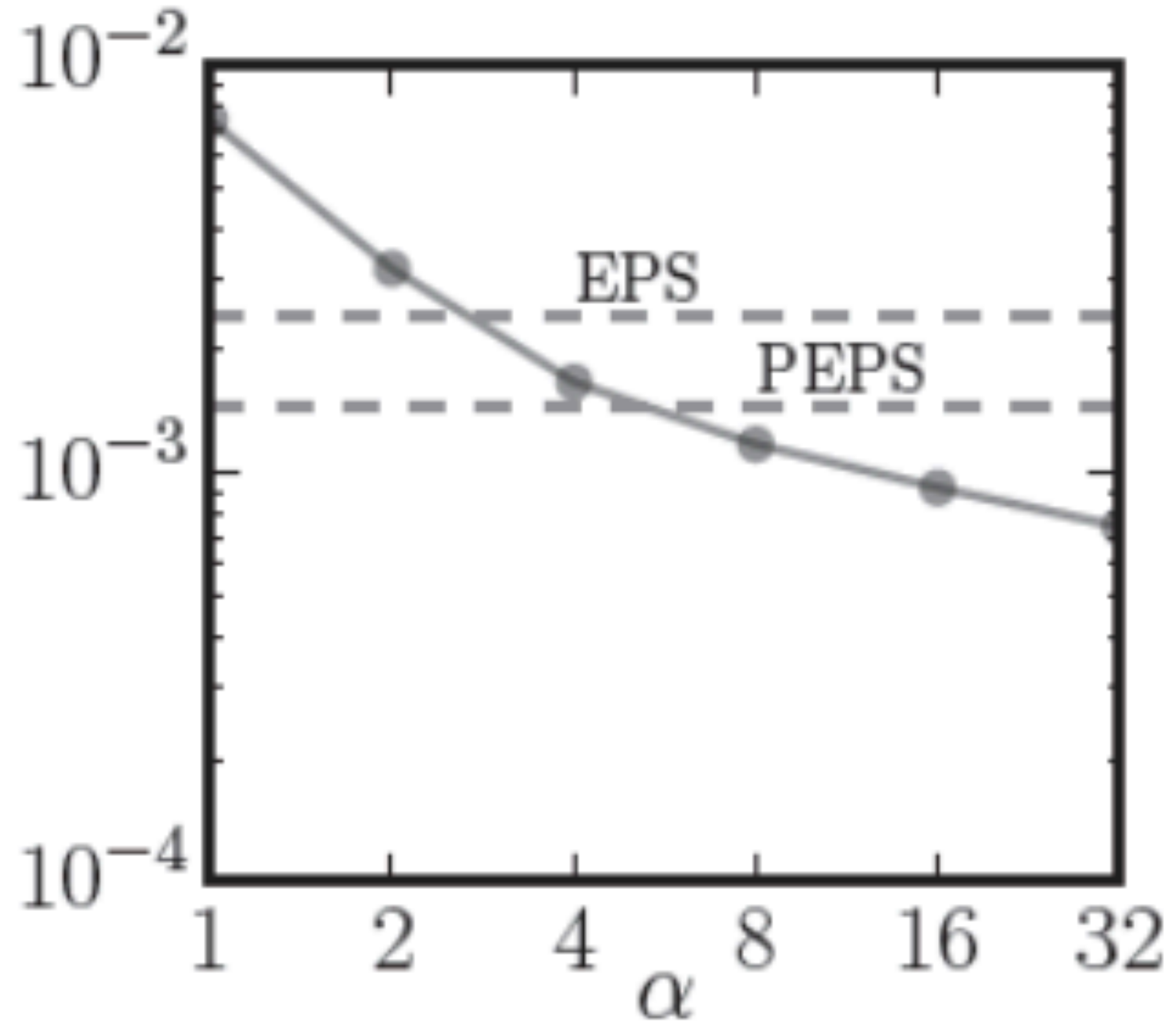
1d antiferro Heisenberg model

80 spins, periodic boundary



2d antiferro Heisenberg model

10x10 spins, periodic boundary



Requirements for unbiased variational ansatz

Three conditions, in my personal opinion:

[1] Nearly exact for weakly correlated systems

→ Large-scale benchmarks (GS problems without negative sign)

Carleo&Troyer Science 355('17)   Sharir et al. PRL ('20)   Yang et al. NeurIPS ('20)

[2] Unbiased in terms of lattice/interaction geometry

→ Ability to express large quantum entanglement

Deng etal. PRX ('17)   Levine etal. PRL ('19)

[3] Ability to reflect physical constraints, i.e. symmetry

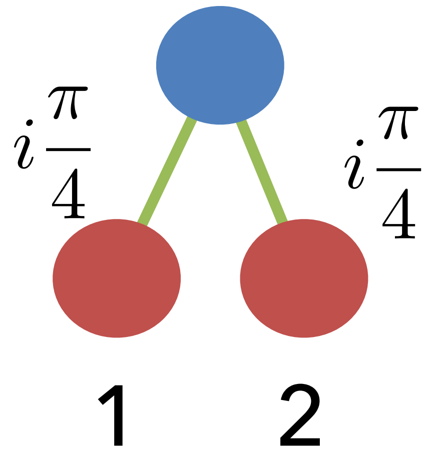
Torlai&Melko PRL ('18)   Viejra etal., PRL ('20)

Neural networks expected to satisfy all of them

Properties of RBM quantum states

Efficient representation of entanglement

e.g. Bell state

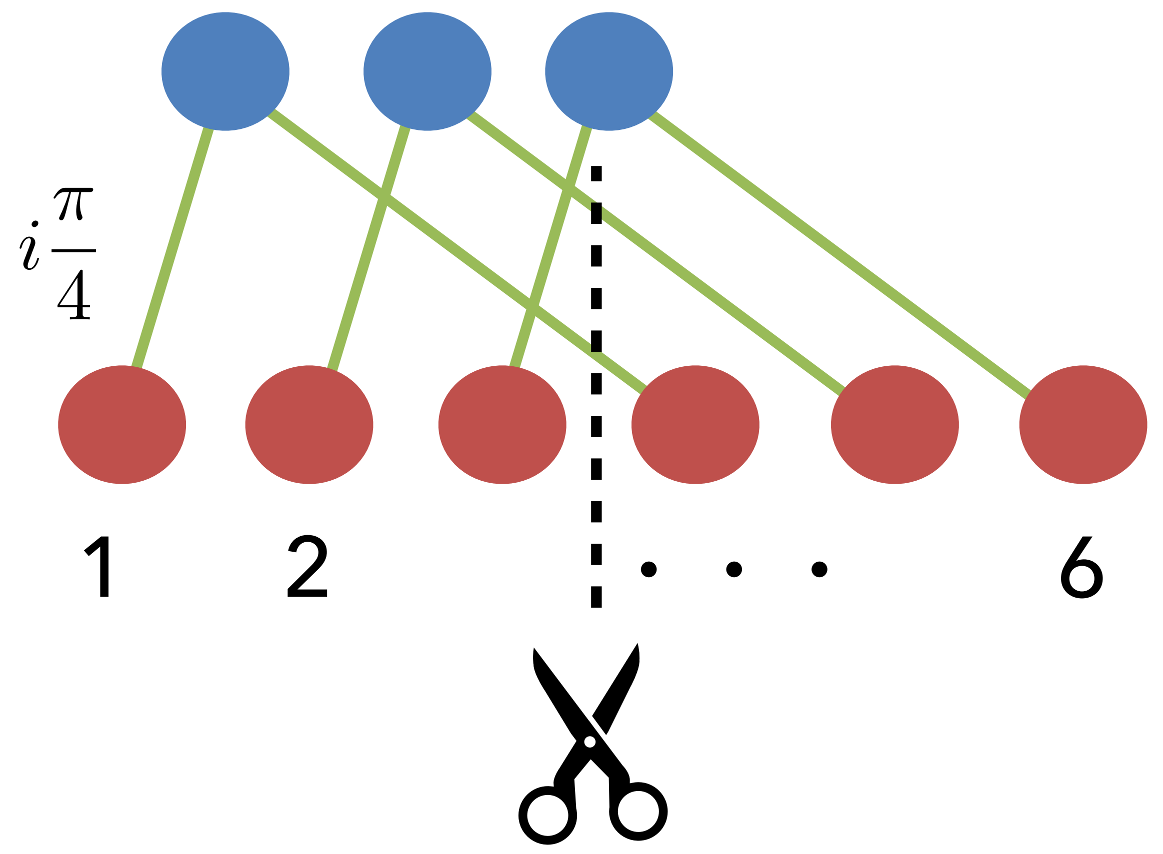


$$= \sum_\sigma \cosh(W_1\sigma_1 + W_2\sigma_2)|\sigma_1, \sigma_2\rangle$$

$$= \sum_\sigma \cosh(i\frac{\pi}{4}\sigma_1 + i\frac{\pi}{4}\sigma_2)|\sigma_1, \sigma_2\rangle$$

$$= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$ (Also capable of GHZ, W states)

e.g. Maximally entangled state for arbitrary bipartition Deng etal. PRX ('17)



$$= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)_{14} \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)_{25} \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)_{36}$$

Reduced density mat. is maximally mixed, and therefore

$$S_\alpha^A := \frac{1}{1-\alpha}\log[\mathrm{Tr}(\rho_A^\alpha)]$$: Renyi entropy

$$= \frac{N}{2}\log 2$$ **Maximal value!**

Properties of RBM quantum states

Random RBM state Deng etal. PRX ('17)

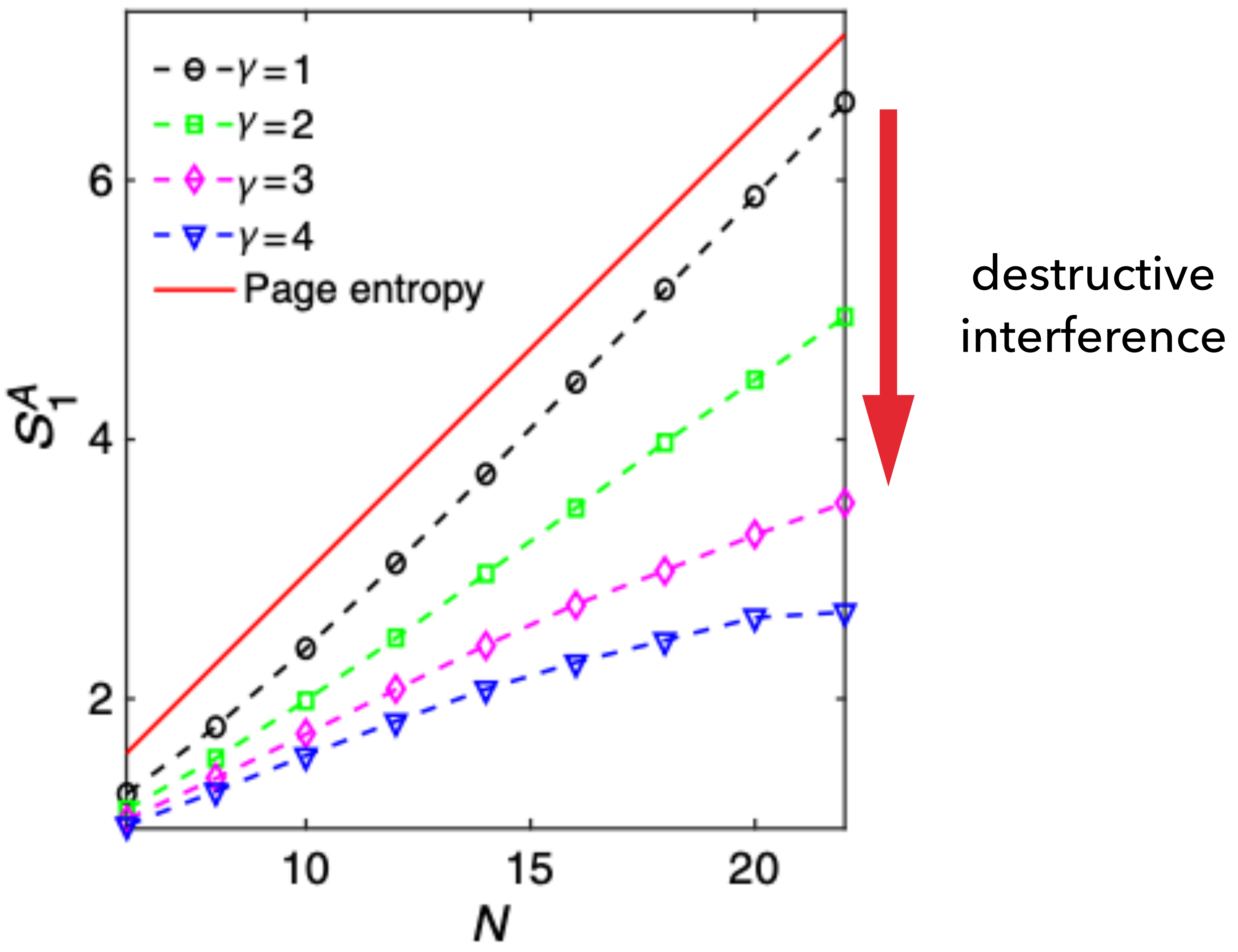
- Satisfies volume-law scaling in general
    - destructive interference by adding hidden spins

- EE(RBM) < Page value (average EE of Haar random)

➡ Haar random states cannot be simulated efficiently
Requires exponentially many parameters

- No "figure of merit" known so far
  (cf. entanglement entropy for tensor networks)

von Neumann Entanglement scaling

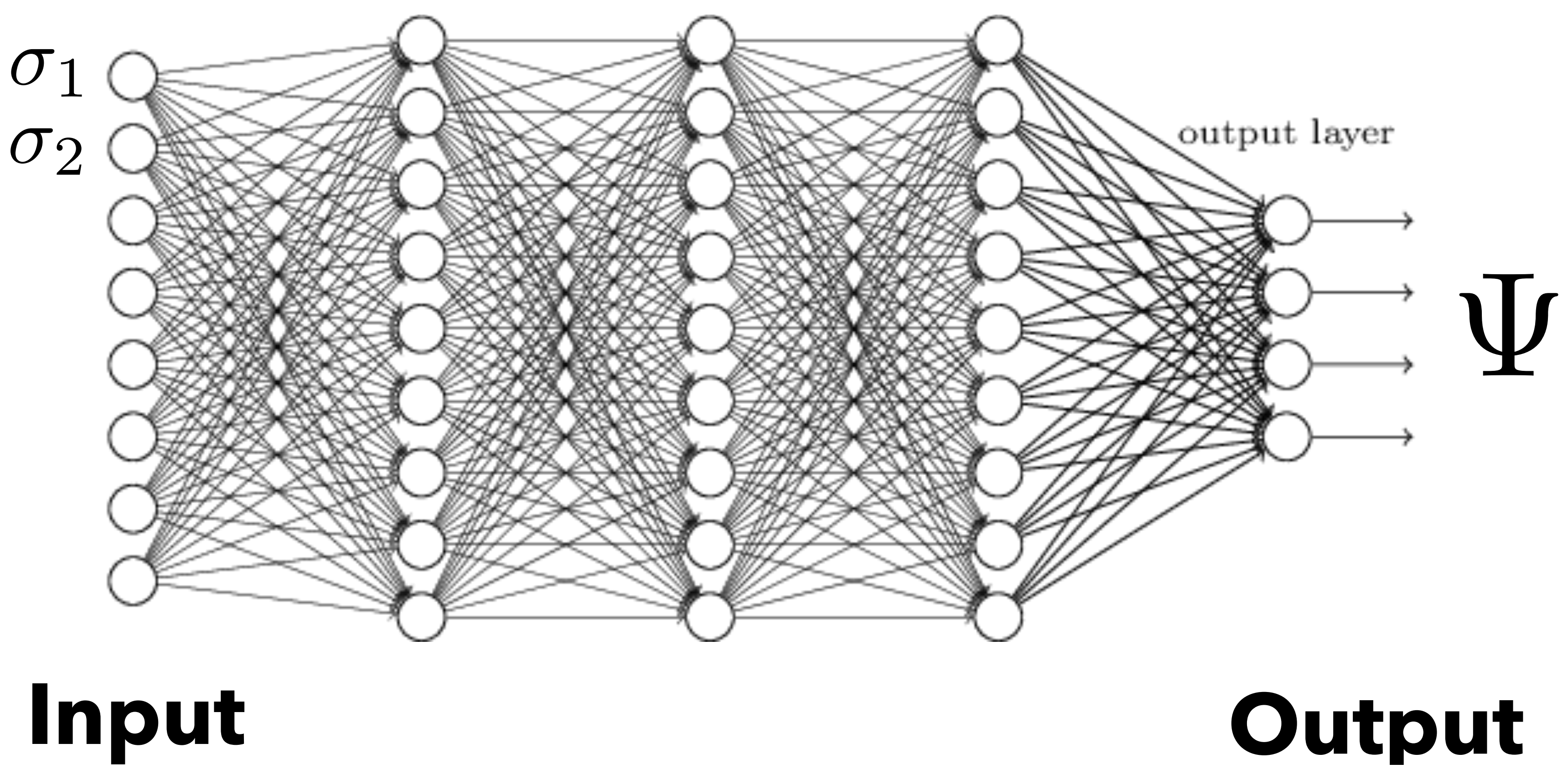


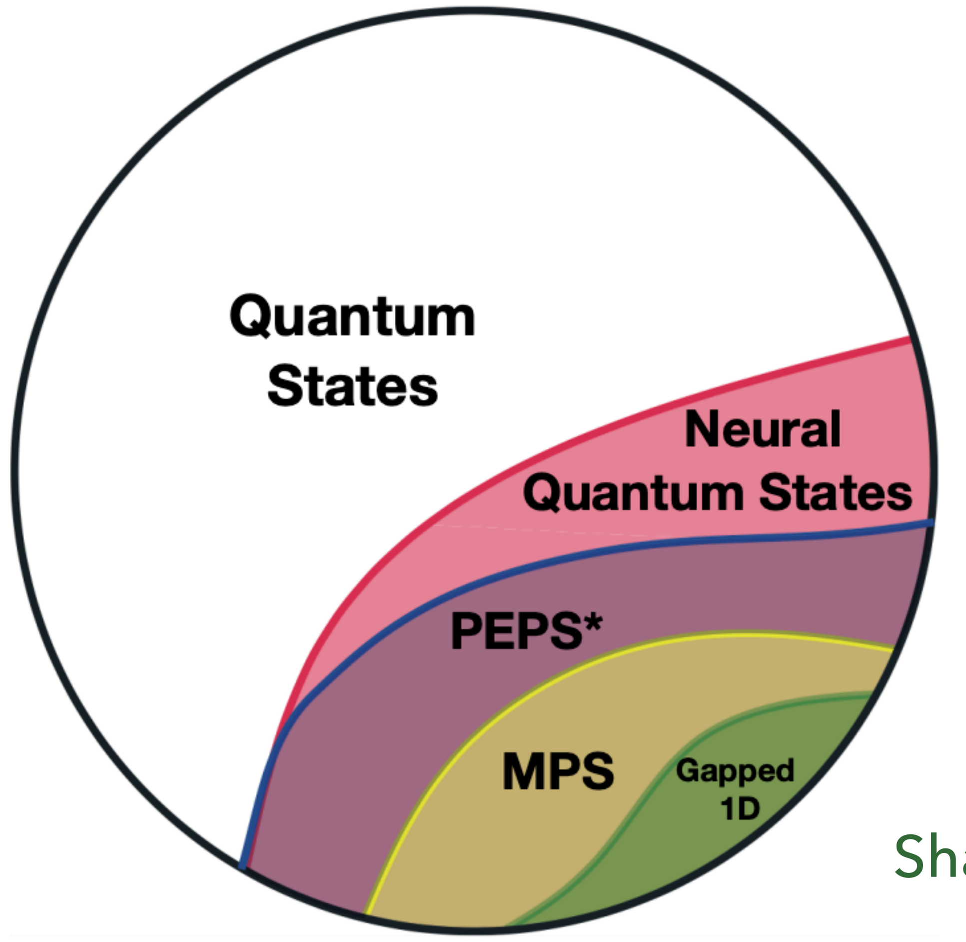
Deep neural-network quantum states

Q. Are deep networks even more powerful?

→ A. Yes! X.Gao&L.-M.Duan, Nat. Commun. ('17) Sharir, Sashua, Carleo ('21)

e.g. Fully-connected neural-network





Sharir, Sashua, Carleo ('21)

Tensor nets contractable with polynomial cost can be efficiently approximated by deep NN

Deep neural-network quantum states

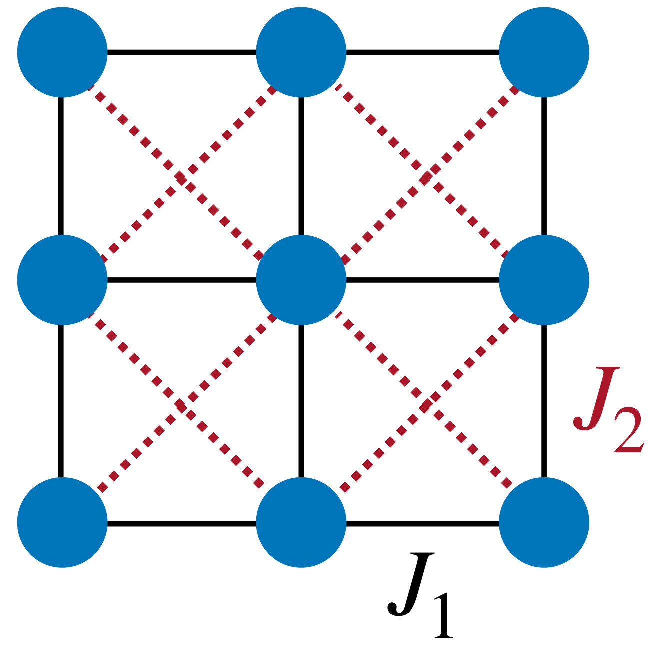
Q. Is deeper always the better?

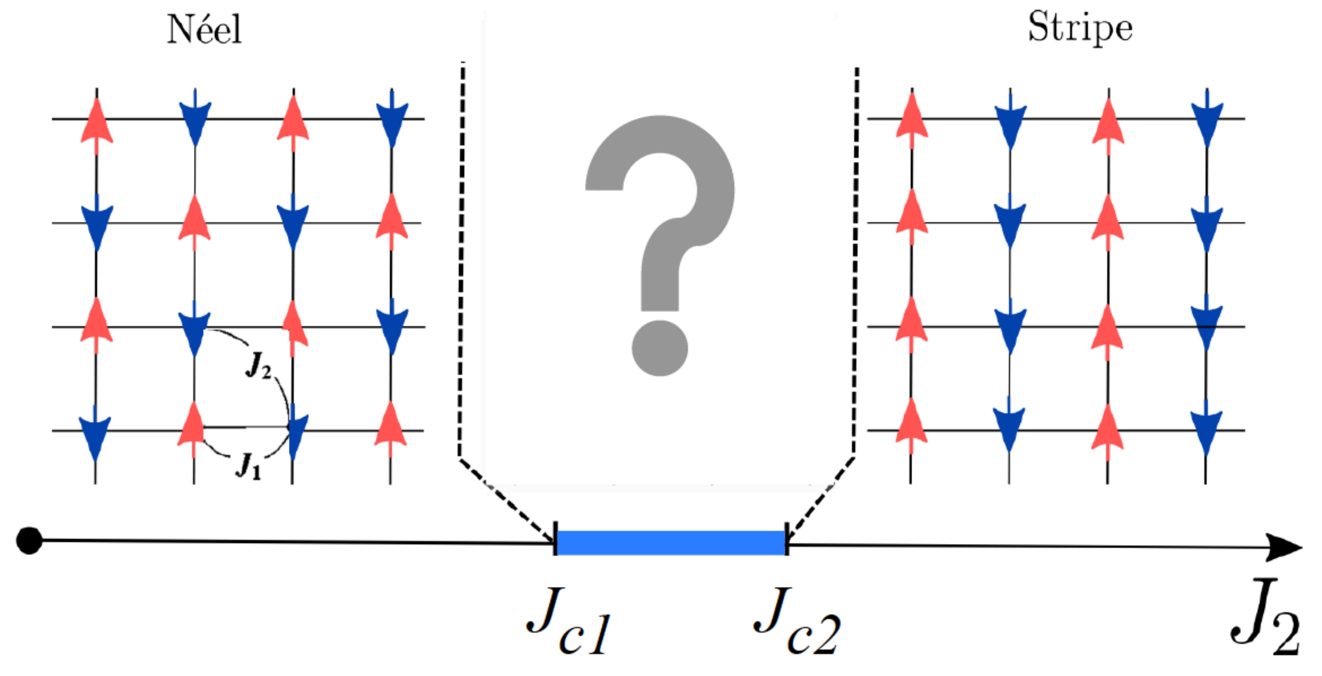
➡ Not necessarily in practical case.
Optimization seems to become more difficult

Ground state in 2d J1J2 Heisenberg model
(J2/J1 = 0.5, 10x10)

Energy per site	Wave function	Reference
−0.494757(12)	**Neural quantum state**	65
−0.49516(1)	**CNN**	60
−0.49521(1)	VMC(p=0)	18
−0.495530	DMRG	22
−0.49575(3)	**RBM-fermionic w.f.**	63
−0.497549(2)	VMC(p=2)	18
−0.497629(1)	**RBM+PP**	present study

Nomura&Imada ('20)



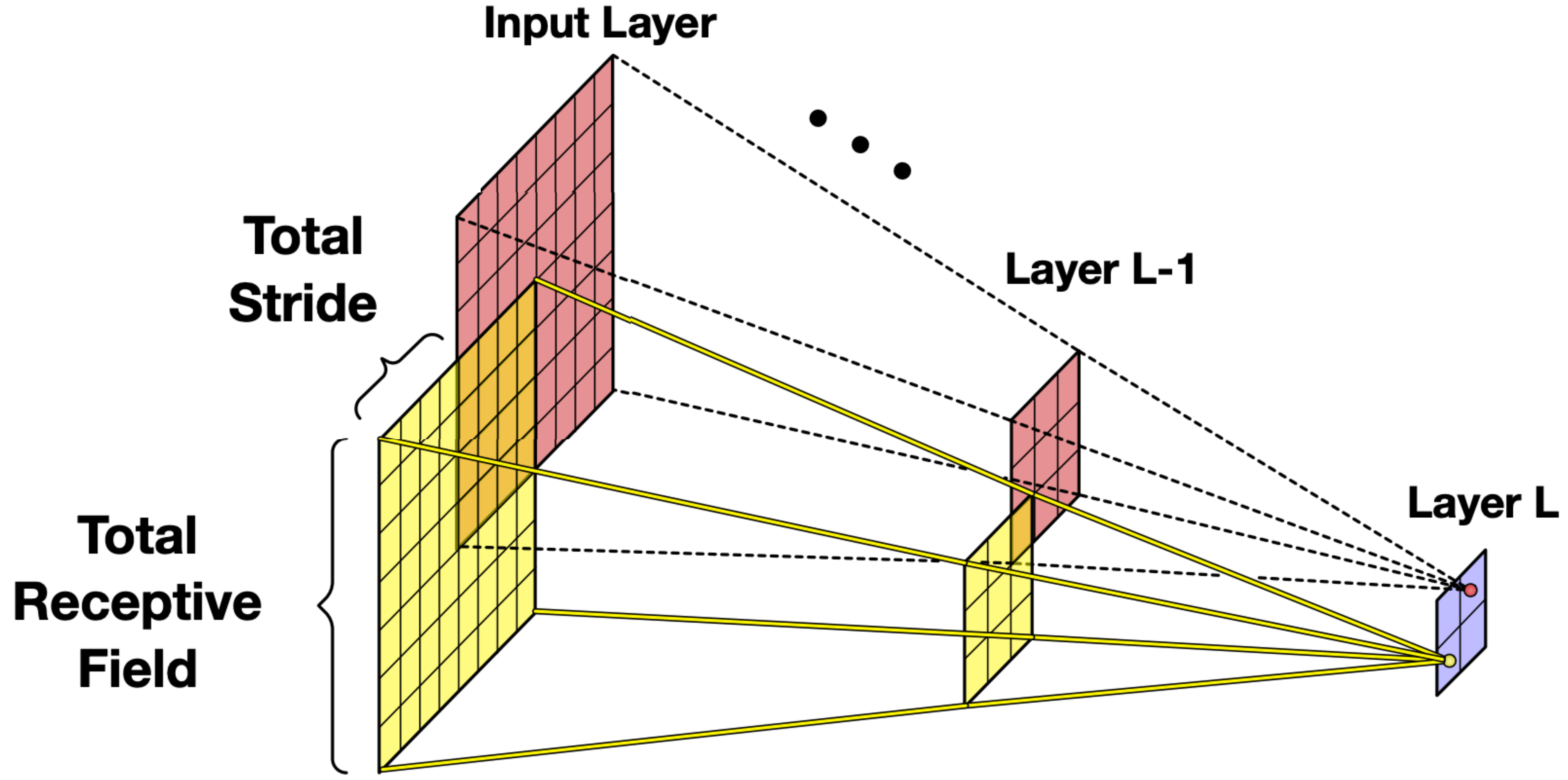


What's next?

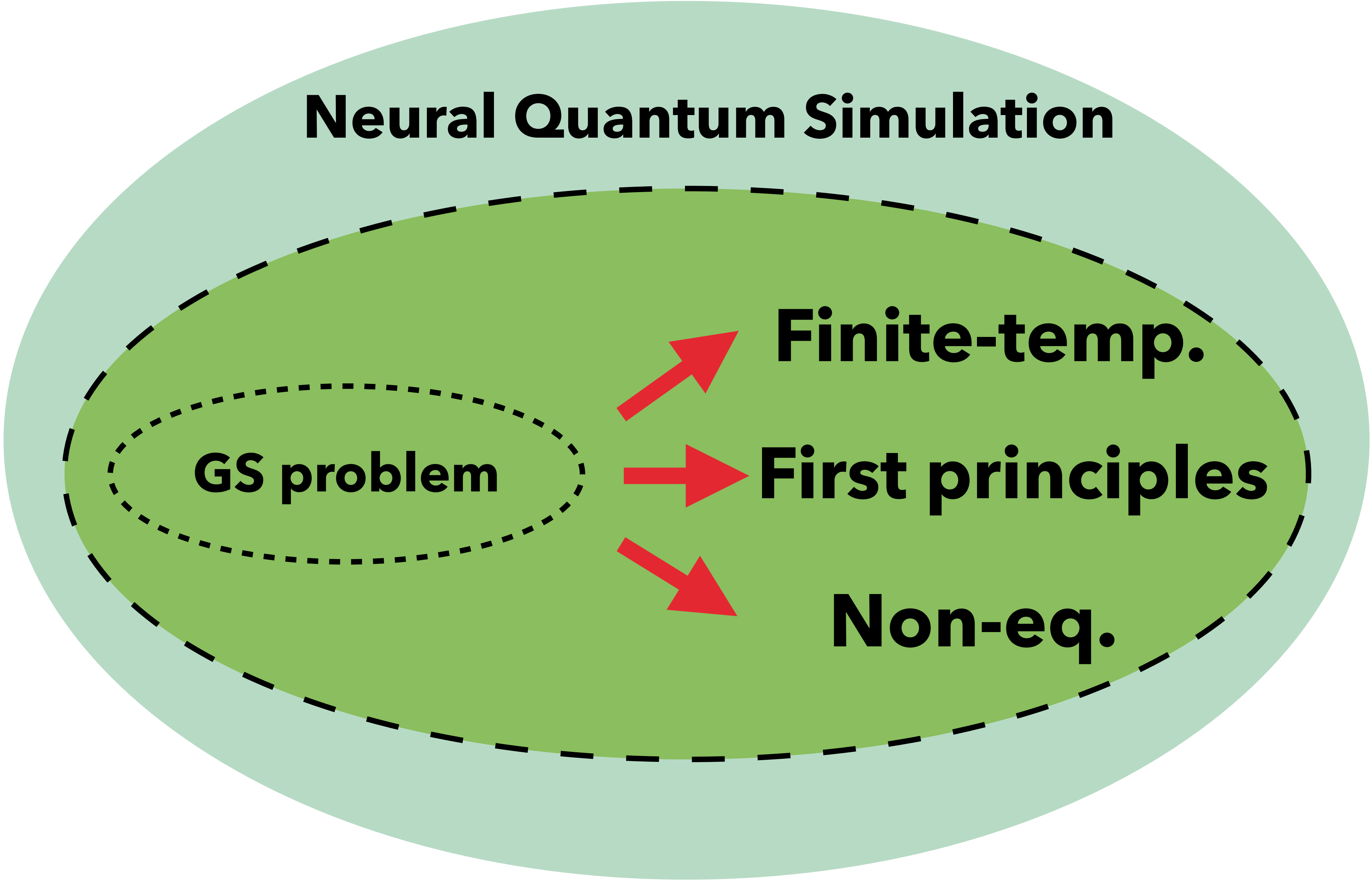
1. Develop qualitative understanding on ansatz

- What is the "figure of merit" that characterize NN representation?

- Is deeper really not better? Representability/trainability trade-off



2. Explore/demonstrate practical simulations



→ Gibbs states as purified Deep BM
Nomura*, **NY***, and Nori, arXiv:2103.04791

→ First-principles calculation for solids
NY, Mizukami, and Nori, Commun. Phys. 4, 106 (2021).

→ Steady-states in open quantum system
NY&Hamazaki, Phys. Rev. B 99, 214306 (2019).

I. Neural-network quantum states

Properties of neural-network quantum states

Ground state problems

II. Beyond GS problems

Finite-temperature simulations by DBM purification

First-principles calculation in solid systems

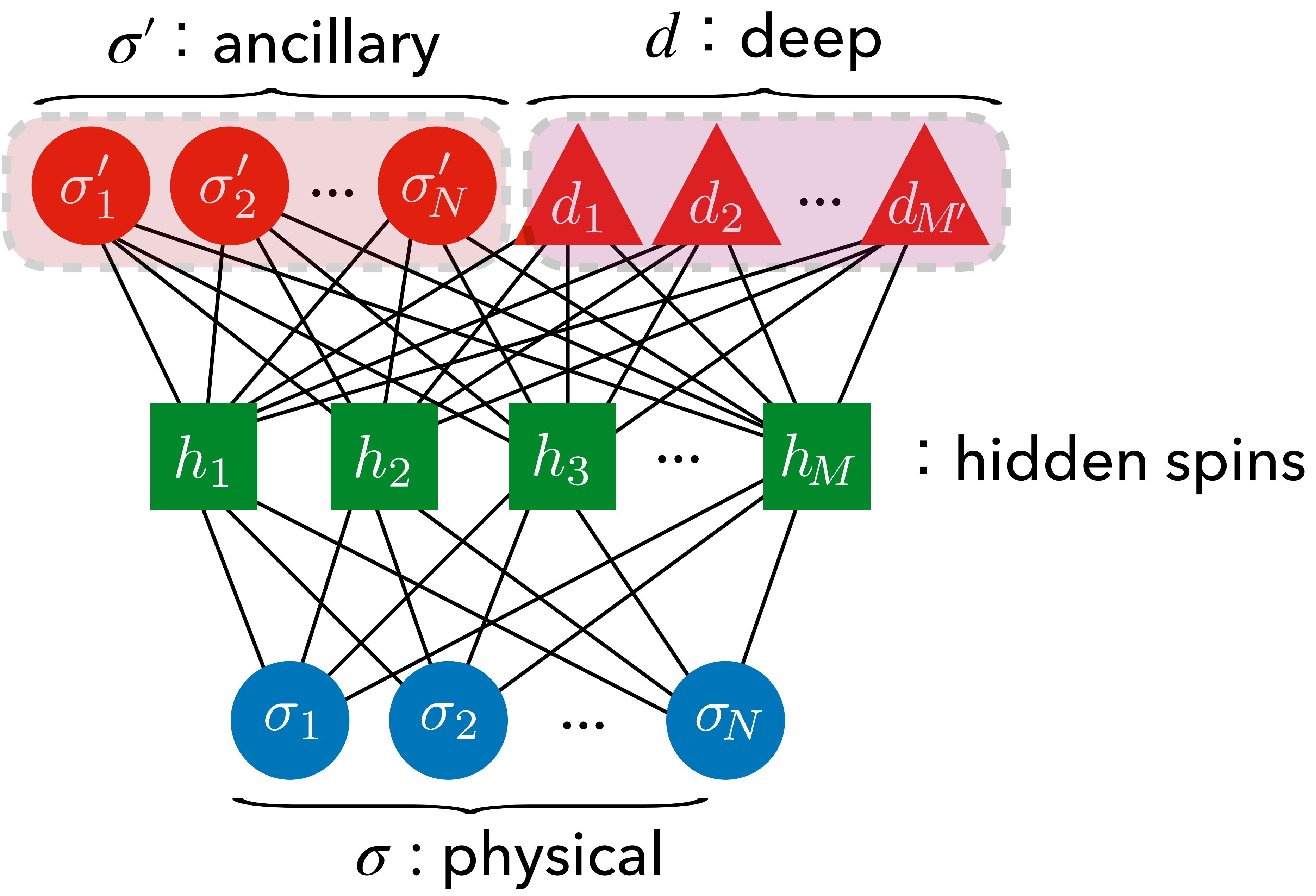
Finite-temperature problems

Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

Why finite-temperature?

- How to conquer the unsolved problems in strongly-correlated 2d systems (e.g. spin liquid, Fermi Hubbard)?
  - tensor-networks → Mainly limited to 1d (MPS)
  - DMFT → Exact in infinite-dim, not quantitative in 2d
  - Neural nets → state-of-the-art for 2d GS problems

Purifying Gibbs states by DBM



$$\rho = \mathrm{Tr}_{\sigma'}\left[|\Psi_{\mathrm{DBM}}\rangle\langle\Psi_{\mathrm{DBM}}|\right]$$

$$|\Psi_{\mathrm{DBM}}\rangle = \sum_{\sigma,\sigma'} \Psi_{\mathrm{DBM}}(\sigma,\sigma')|\sigma,\sigma'\rangle$$

High-level protocol

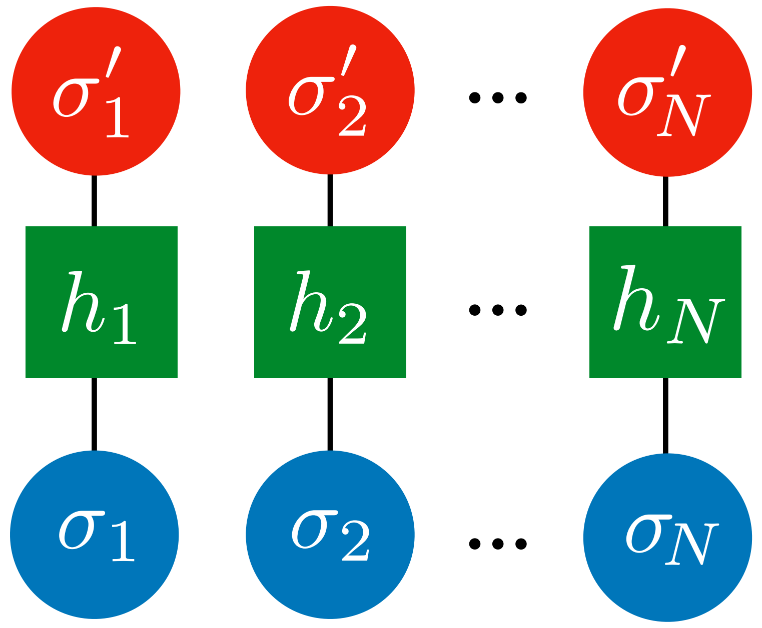
Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

Step (I) : Purify infinite-temperature state

$$|\Psi_{T=\infty}\rangle = \bigotimes_i \frac{(|\uparrow\downarrow'\rangle + |\downarrow\uparrow'\rangle)_i}{\sqrt{2}}$$

Purified state — Product of Bell pairs

Infinite-temperature DBM



$$\Psi(\sigma,\sigma') = \prod_i 2\cosh\left[\mathrm{i}\frac{\pi}{4}(\sigma_i + \sigma'_i)\right]$$

Step (II) : Perform imaginary-time evolution

$$|\Psi_T\rangle = \left(e^{-\mathcal{H}/2T} \otimes \mathbb{I}'\right)|\Psi_{T=\infty}\rangle = \left(\left[e^{-\delta_\tau \mathcal{H}}\right]^{N_\tau} \otimes \mathbb{I}'\right)|\Psi_{T=\infty}\rangle,$$

- Method (I) : Exact representation of Trotter steps as DBM layer growth
- Method (II) : Approximation by fixed-structure DBM

Method (I): Exact Gibbs DBM

Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

DBM representation of Suzuki-Trotter decomposition

- Consider Suzuki-Trotter decomposition, e.g., $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$

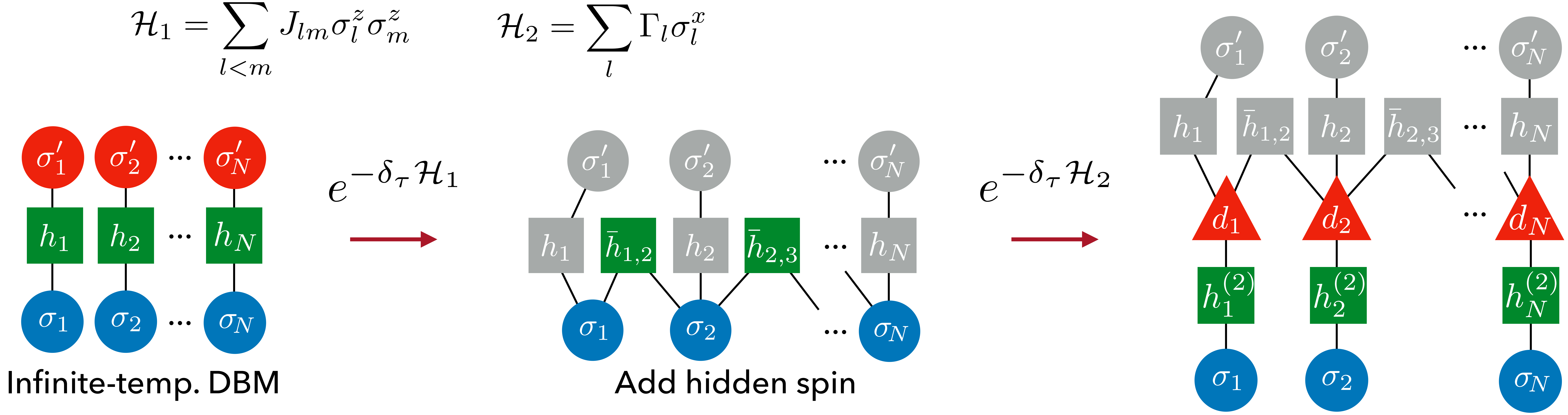
$$|\Psi_T\rangle := \left(\left[e^{-\delta_\tau \mathcal{H}_2} e^{-\delta_\tau \mathcal{H}_1}\right]^{N_\tau} \otimes \mathbb{1}'\right) |\Psi_{T=\infty}\rangle, \quad \text{where} \quad |\Psi_{T=\infty}\rangle = \bigotimes_i \frac{\left(|\uparrow\downarrow'\rangle + |\downarrow\uparrow'\rangle\right)_i}{\sqrt{2}}$$

- Find DBM that exactly encodes propagator

$$|\Psi'_{\mathrm{DBM}}\rangle \propto e^{-\delta_\tau \mathcal{H}_\nu} |\Psi_{\mathrm{DBM}}\rangle$$

<u>e.g. Transverse-field Ising model</u>

$$\mathcal{H}_1 = \sum_{l<m} J_{lm} \sigma_l^z \sigma_m^z \qquad \mathcal{H}_2 = \sum_l \Gamma_l \sigma_l^x$$

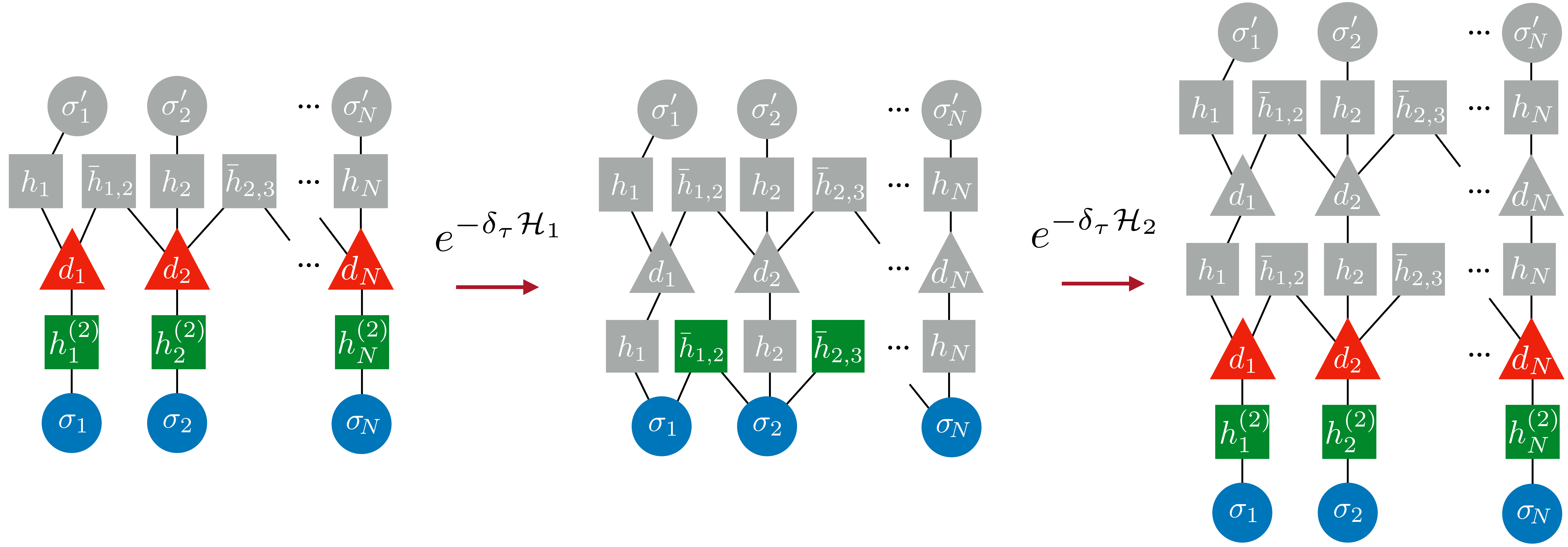


Method (I): Exact Gibbs DBM

Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

e.g. Transverse-field Ising model

$$\mathcal{H}_1 = \sum_{l<m} J_{lm}\sigma_l^z \sigma_m^z \qquad \mathcal{H}_2 = \sum_l \Gamma_l \sigma_l^x$$

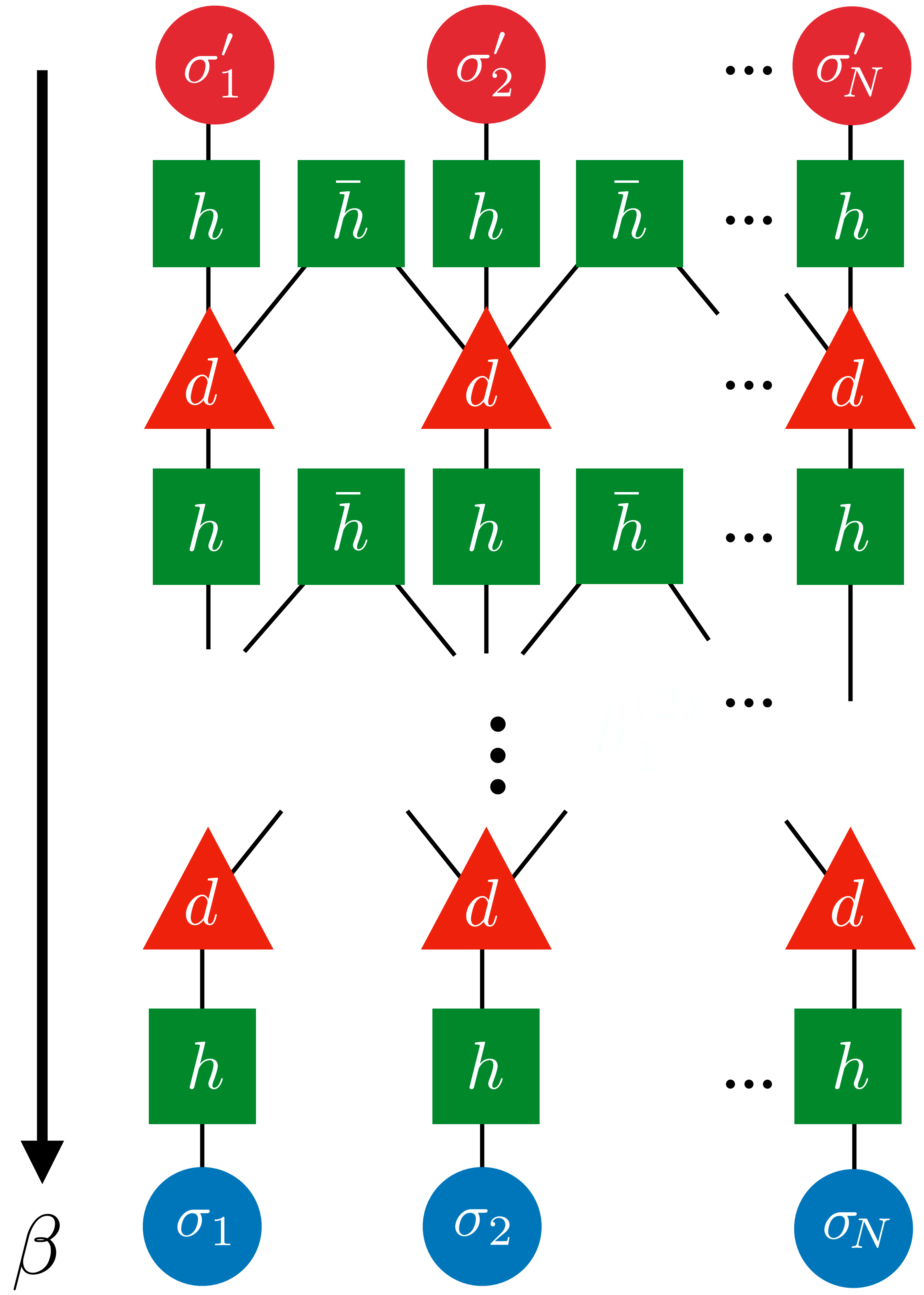


Method (I): Exact Gibbs DBM

Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

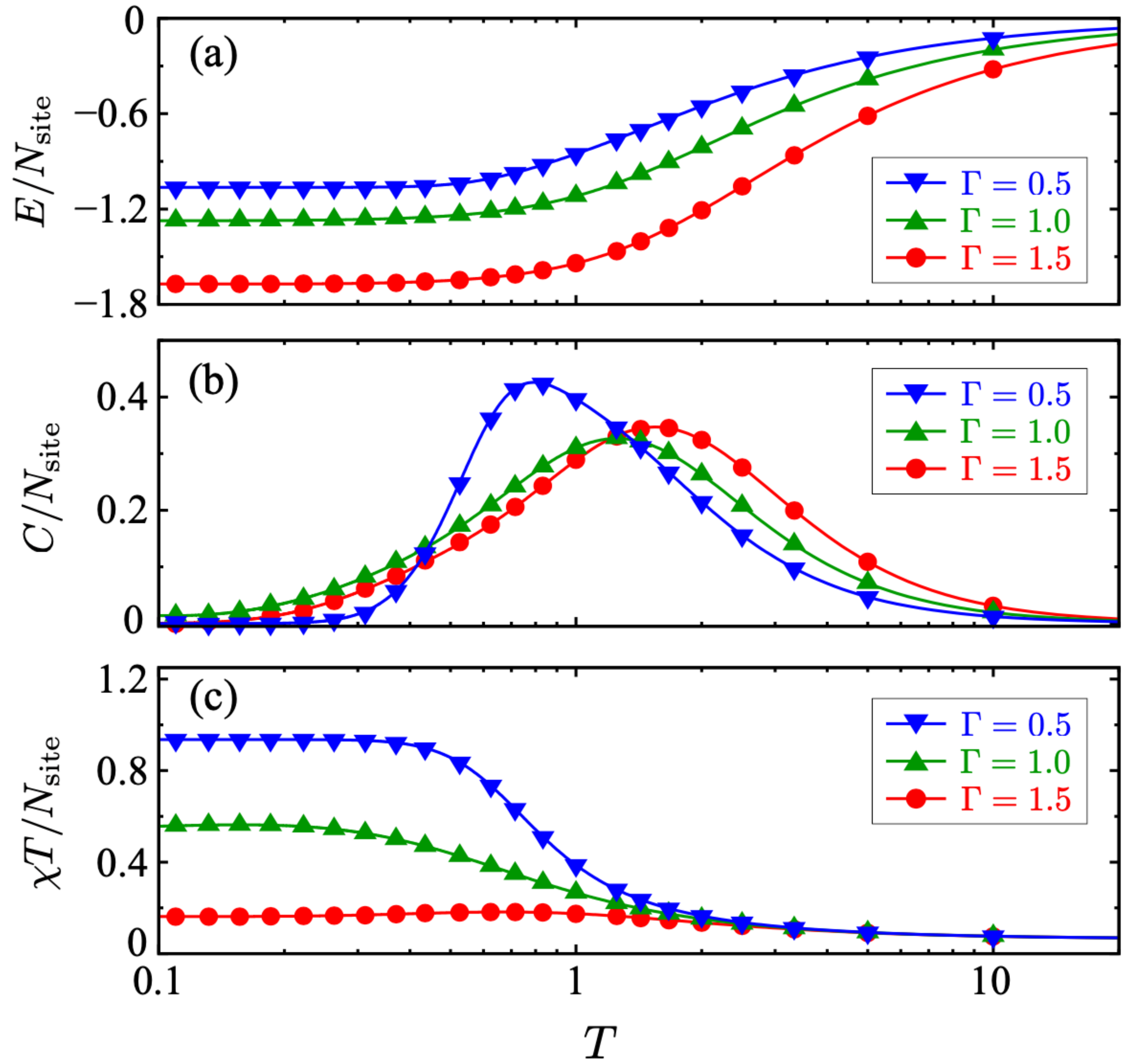
e.g. Transverse-field Ising model

$$\mathcal{H}_1 = \sum_{l<m} J_{lm}\sigma_l^z \sigma_m^z \qquad \mathcal{H}_2 = \sum_l \Gamma_l \sigma_l^x$$



DBM-based calculation for 1D TFI (16 sites)

symbols: DBM solid curves: ED



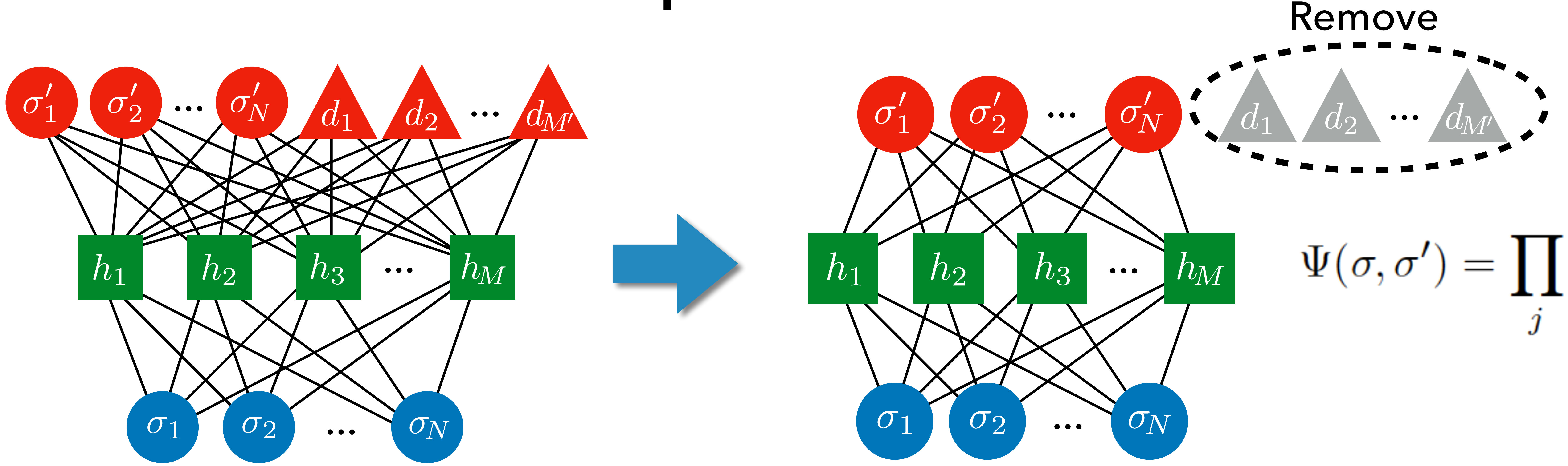
Path-integral formalism for certain class of Hamiltonian completely mapped into DBM

(Cannot not avoid negative sign problem)

Method (II): Approximate Gibbs DBM

Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

DBM wave function without d spins



$$\Psi(\sigma, \sigma') = \prod_j 2\cosh\left[b_j + \sum_i (W_{ji}\sigma_i + W'_{ji}\sigma'_i)\right]$$

Approximate imaginary-time evolution

- Stochastic reconfiguration: use of Fubini-Study metic Sorella, PRB ('01)

$$\delta\mathcal{W} = \arg\min_{\delta\mathcal{W}} \left(\mathcal{F}\left(e^{-\delta_\tau \mathcal{H}} |\Psi_\mathcal{W}\rangle, |\Psi_{\mathcal{W}+\delta\mathcal{W}}\rangle\right)\right)$$

$\delta\mathcal{W}$: network parameter

$e^{-\delta_\tau \mathcal{H}} |\Psi_\mathcal{W}\rangle$: Exact

$|\Psi_{\mathcal{W}+\delta\mathcal{W}}\rangle$: Approximate

$\mathcal{F}$: Fubini-Study metric

$$= -\delta_\tau S^{-1} g$$

S : quantum Fisher matrix

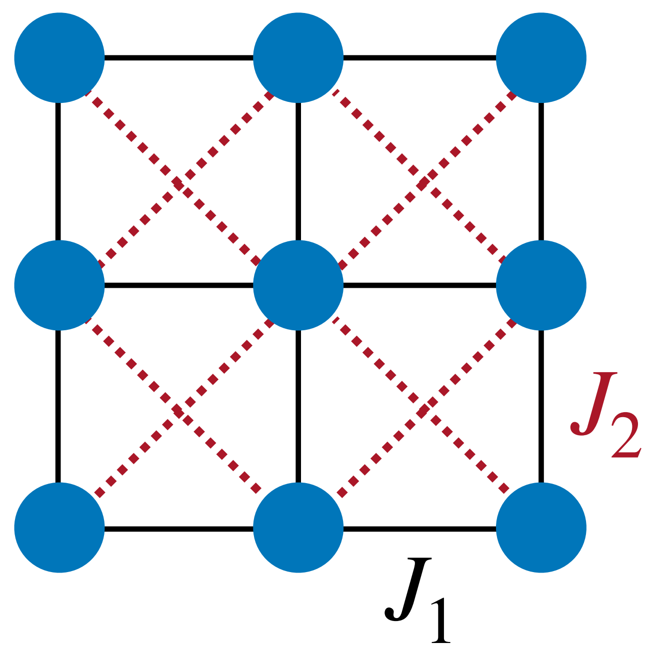
g: generalized force

Estimated by MC sampling

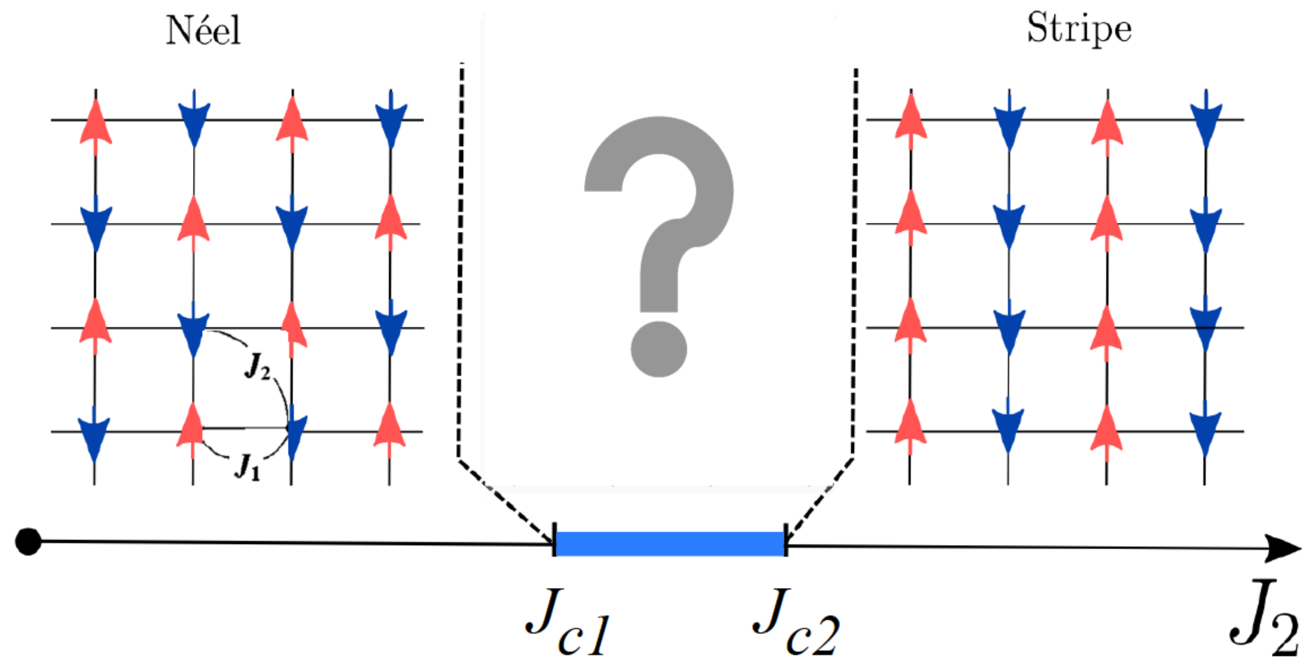
Method (II): Approximate Gibbs DBM

Y. Nomura*, **NY***, and F. Nori, arXiv:2103.04791

Demonstration in 2d J_1-J_2 Heisenberg model

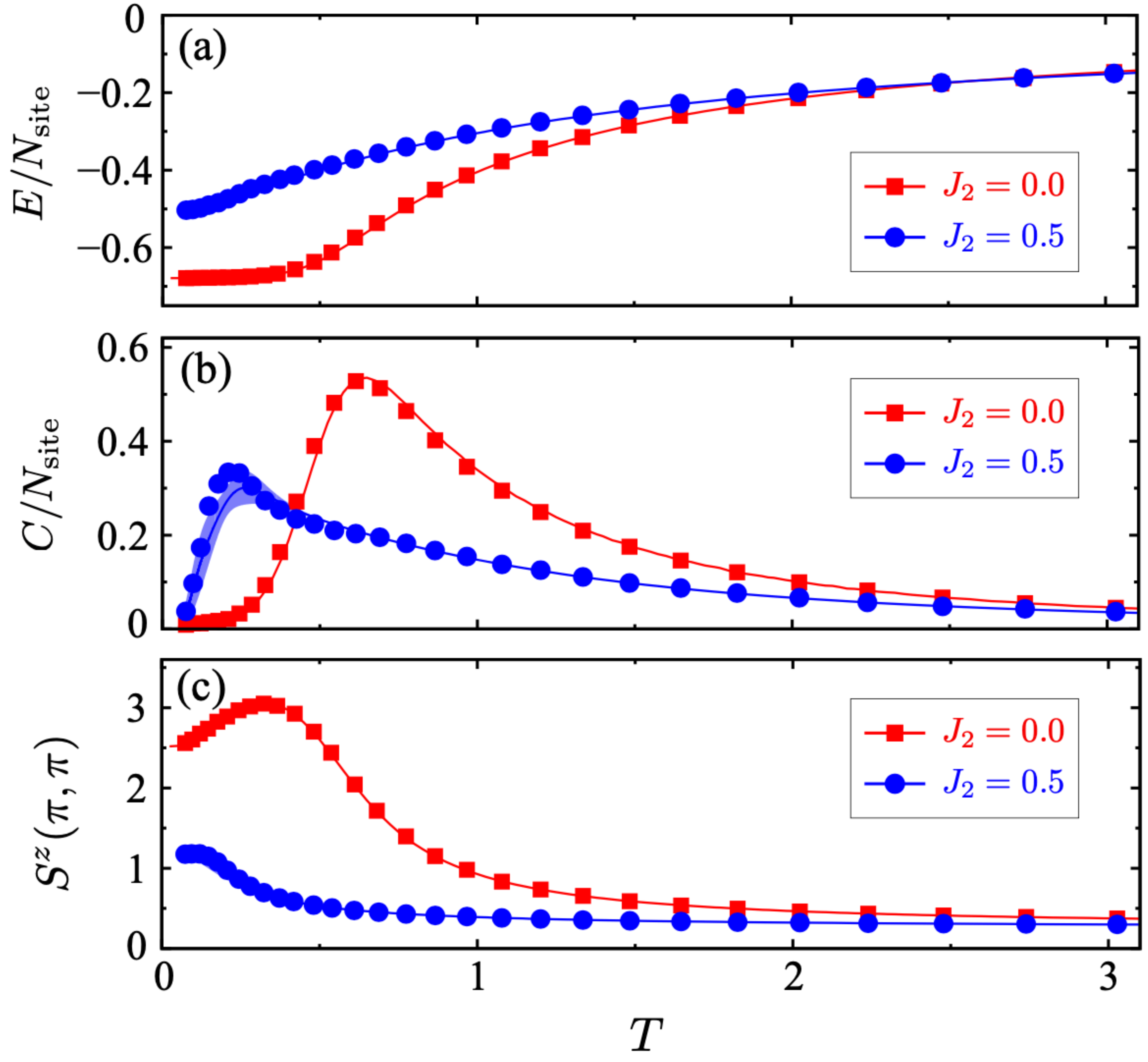


Quantum spin liquid in GS?



6x6 lattice, total Sz=0

symbols: Method(II) solid curves: Method(I) (J_2=0), TPQ (J_2=0.5)



- Excellent match with TPQ (J2=0.5) , also with QMC at J2=0

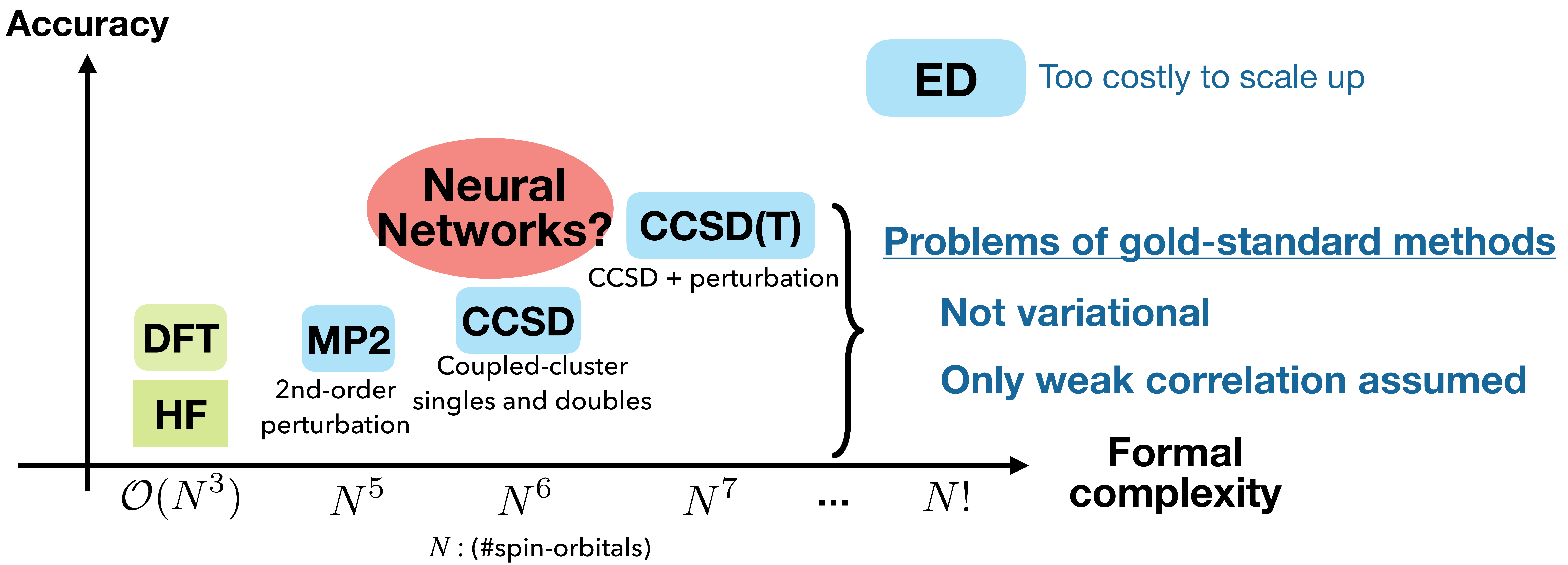
- $O(N_h N^2)$ observed as computational scaling

  where N:#sites, N_h : (#hidden spins)

- Strongly advancing NN-calculations for exploring exotic physics

Ab-initio calculation methods for electronic structure

Yoshioka, Mizukami, & Nori, Commun. Phys. 4, 106 (2021).



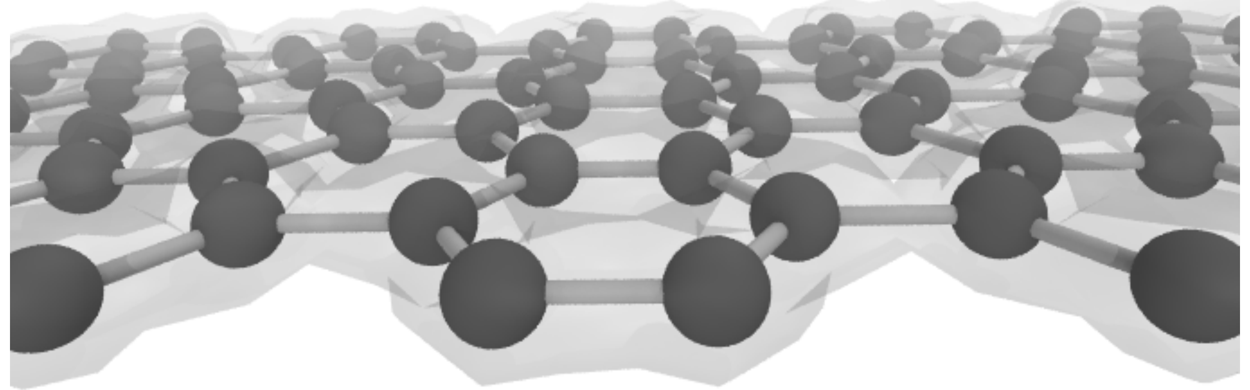
Small molecules: Choo, Mezzacapo, Carleo, Nat. Commun. ('20)
Hermann, Schaetzle, Noe, Nat. Chem. ('20)
Peng-Jian et al., arXiv ('19)
Pfau et al., Phys. Rev. Research ('20)

Electronic structure calculation

NY, Mizukami, & Nori, Commun. Phys. 4, 106 (2021).

1. Determine lattice geometry

Fix atomic coordinates (energy scale separation)



First-quantized Hamiltonian

$$H_{\mathrm{QC}} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_{i,A}\frac{Z_A}{|\mathbf{r}_i - \mathbf{R}_A|} + \sum_{i<j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

2. Derive second quantized Hamiltonian

- Optimize the finite basis set $\{\phi_{\mathbf{k},p}\}$, solve HF equation
- All-to-all interacting fermonic Hubbard Hamiltonian

$$H_{\mathrm{QC}} = \sum_{pq}\sum_{\mathbf{k}} h^{\mathbf{k}}_{pq} a^\dagger_{p\mathbf{k}} a_{q\mathbf{k}}$$

1-body term

$$+ \sum_{pqrs}\sum_{\mathbf{k}_p\mathbf{k}_q\mathbf{k}_r\mathbf{k}_s}{}' h^{\mathbf{k}_p\mathbf{k}_q\mathbf{k}_r\mathbf{k}_s}_{pqrs} a^\dagger_{p\mathbf{k}_p} a^\dagger_{q\mathbf{k}_q} a_{r\mathbf{k}_r} a_{s\mathbf{k}_s}$$

2-body term

3. GS calculation by VMC

: encoding into RBM state

(4. Band structure as quasi-particle excitation)

- Construct truncated Hilbert space $\mathscr{H} = \mathrm{Span}\{O_\mu|\Psi_{\mathrm{GS}}\rangle\}$, where O_μ is 1-particle excitation

$$H'C = SCE$$

eigenvec eigenvalues

$$H'_{\mu\nu} = \langle\Psi_\theta|O^\dagger_\mu H O_\nu|\Psi_\theta\rangle$$: Excited-state Hamiltonian

$$S_{\mu\nu} = \langle\Psi_\theta|O^\dagger_\mu O_\nu|\Psi_\theta\rangle$$: Overlap between nonorthogonal basis

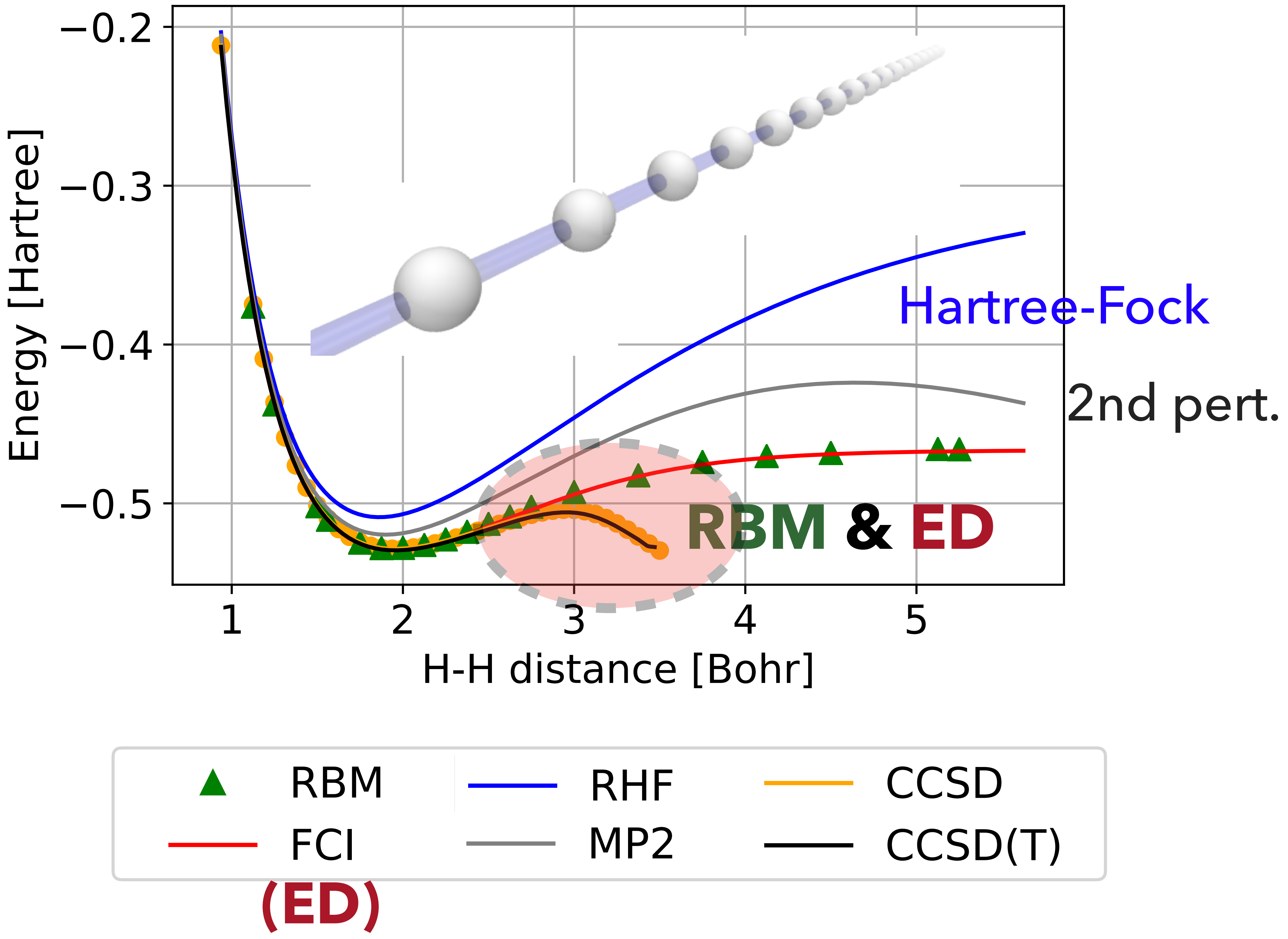
Ground states in solid-systems

Yoshioka, Mizukami, & Nori, Commun. Phys. 4, 106 (2021).

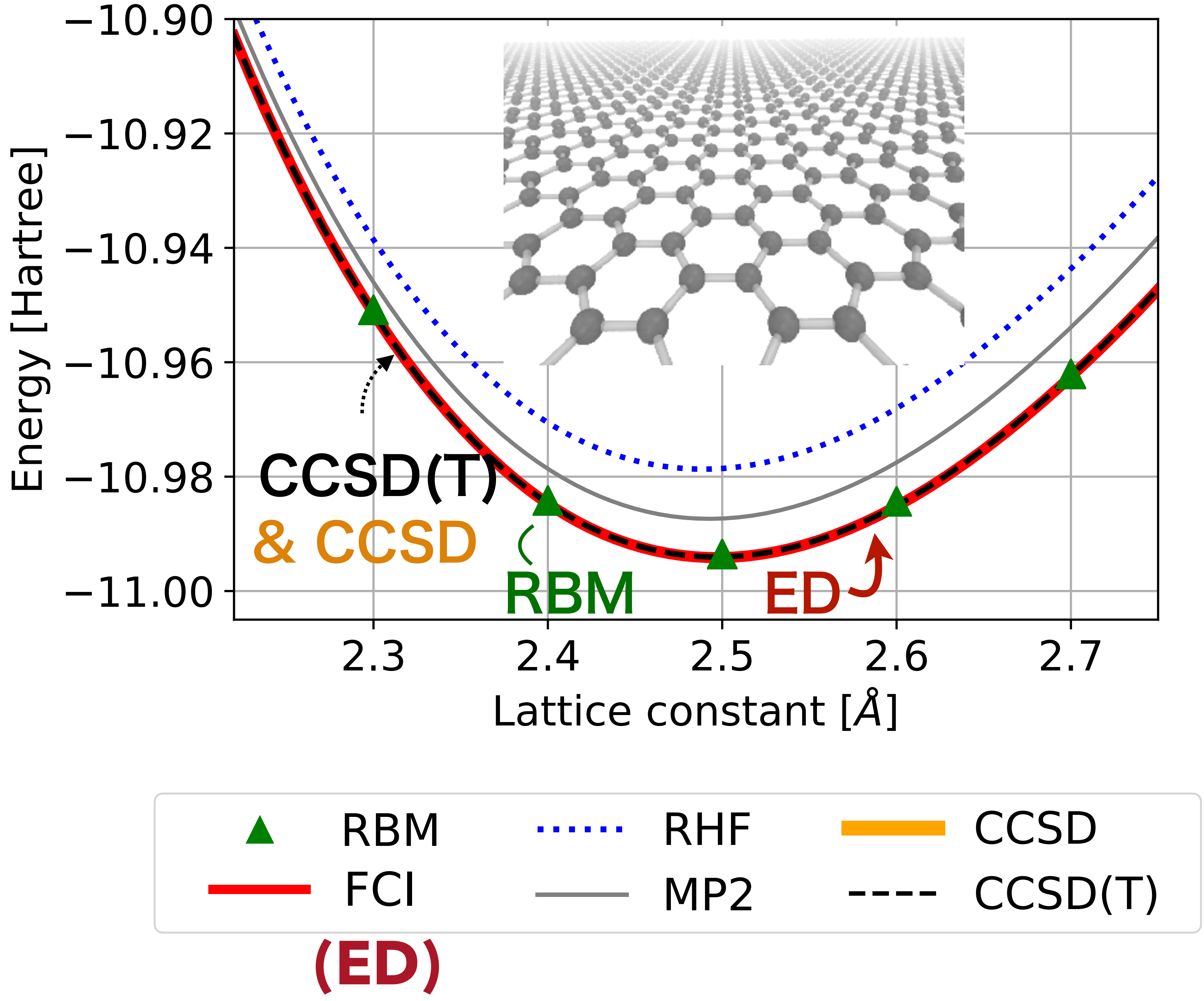
Ground-state simulation

- Demonstration in 1, 2, 3d systems
- Both in weakly/strongly-correlated region

e.g. hydrogen chain (metal-to-Mott transition)



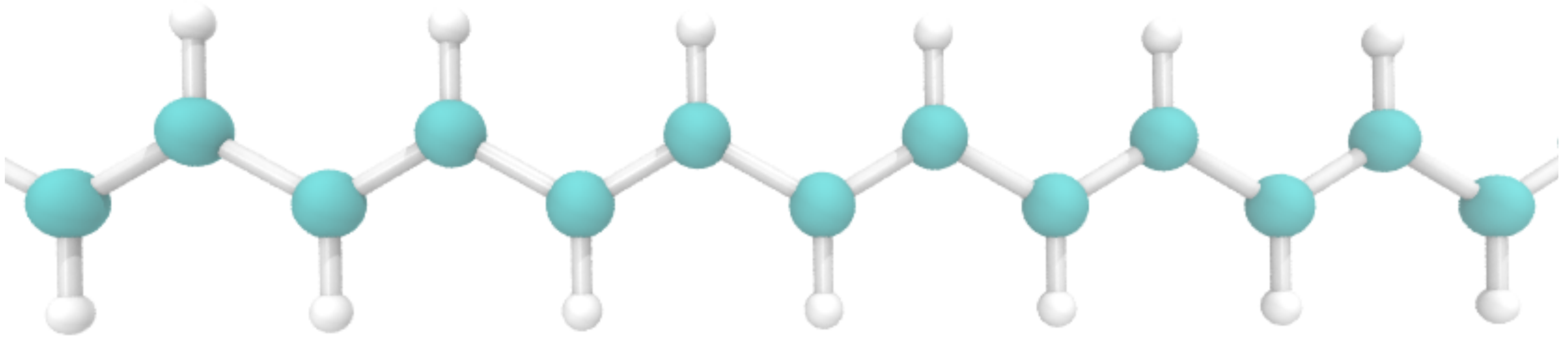
e.g. graphene (weakly correlated)

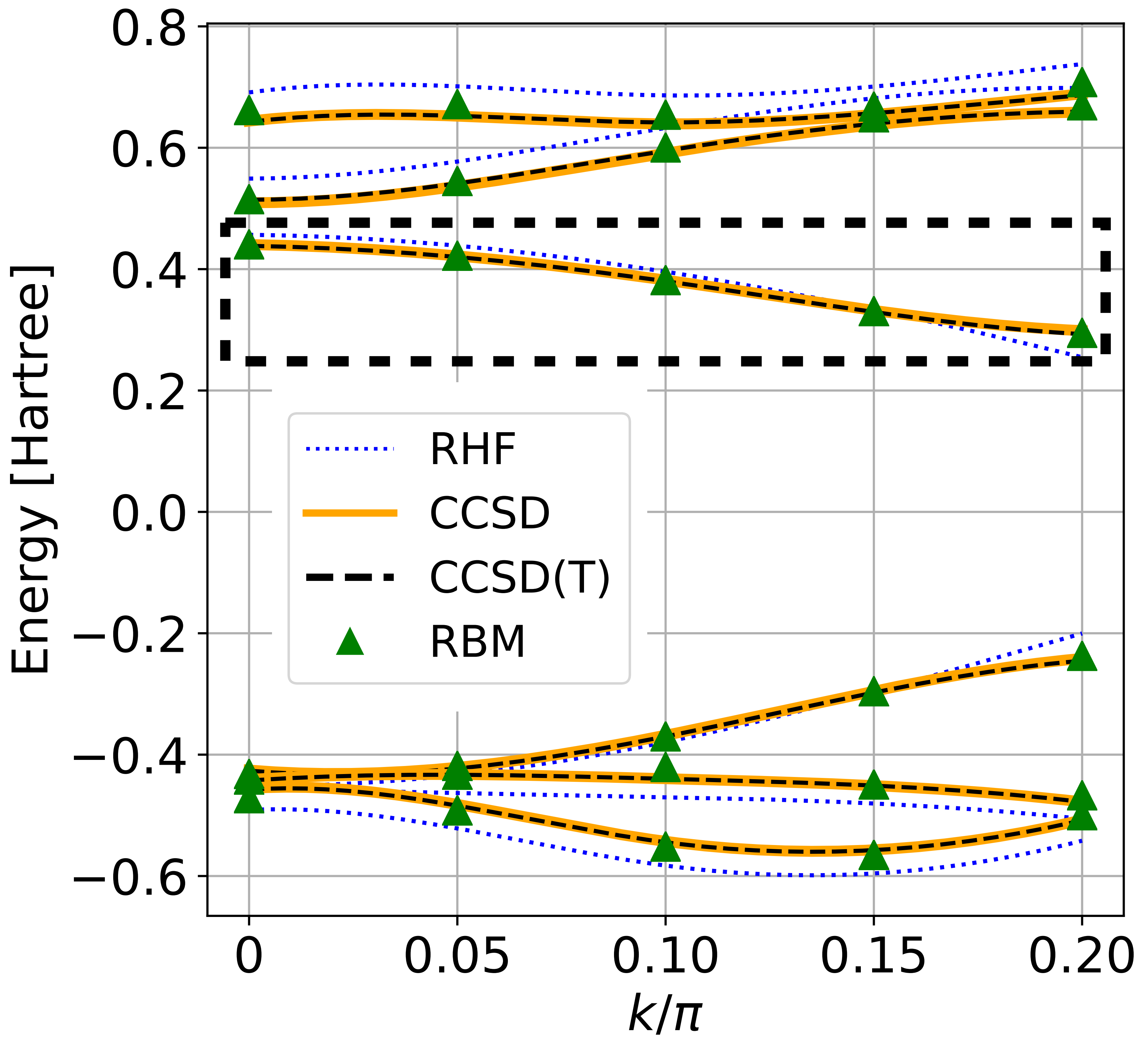


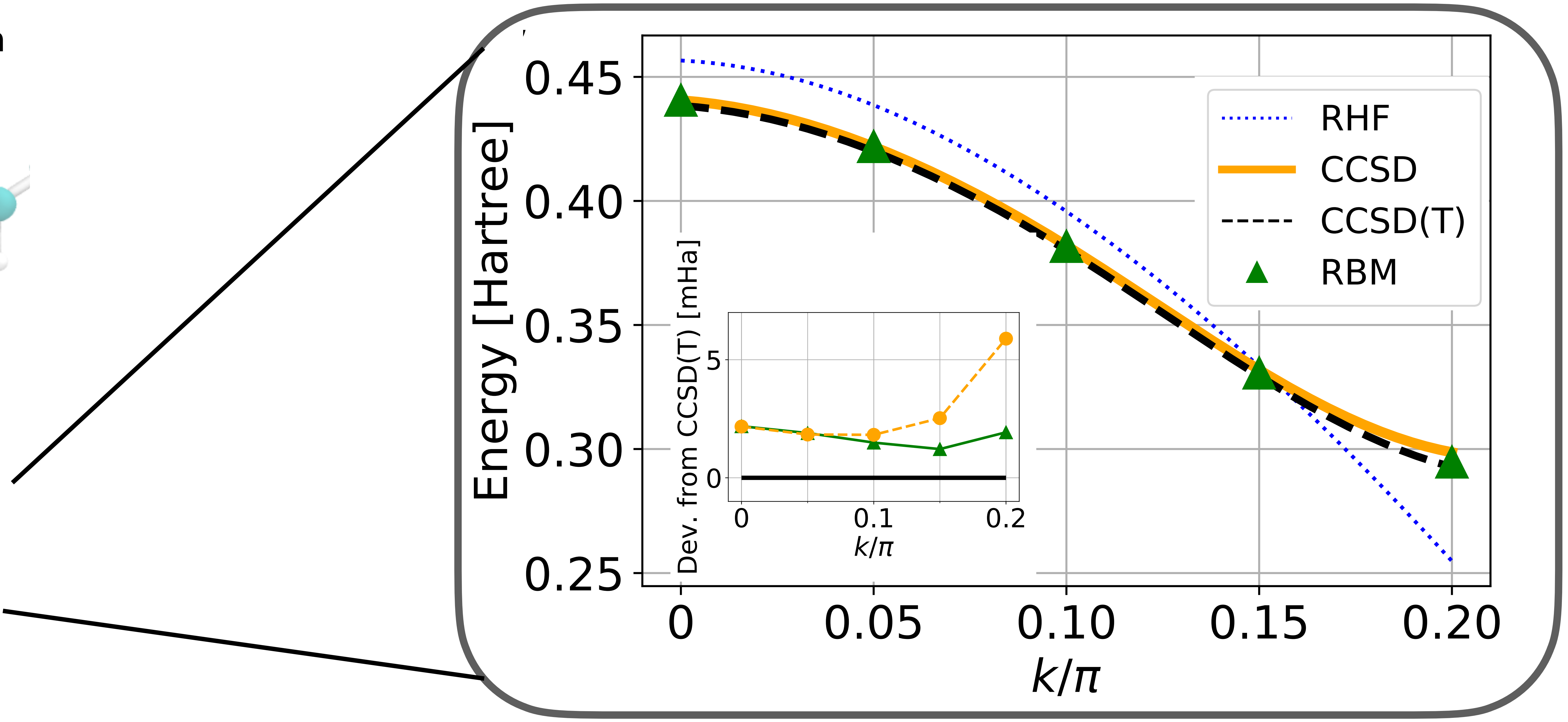
Band-structure simulation

Yoshioka, Mizukami, & Nori, Commun. Phys. 4, 106 (2021).

Bands in trans-polyacetylene $(C_2H_2)_n$







- First multiple excited-states simulation in NN ever

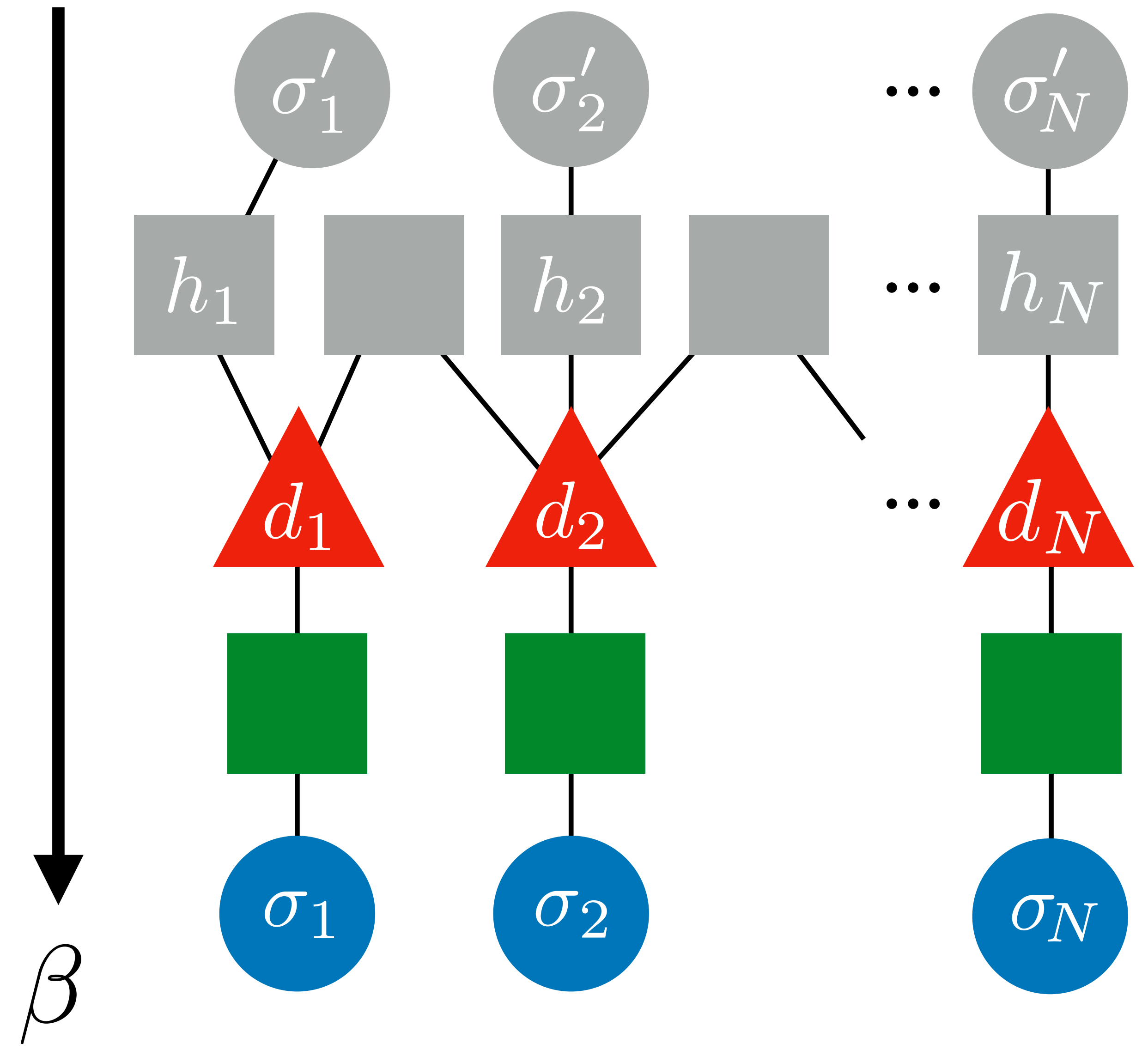
- Valence/conduction bands within chemical acc.

- Worse for higher excitation due to insufficient QSE dim.
  (cf. 2h-1e or 2e-1h for CCSD, CCSD(T))

Summary

Neural network as quantum many-body states

- Ansatz for *physics-agnostic* simulation
- Benchmarks in 200+ qubits, capable of volume-law entanglement



Novel algorithms beyond GS problems

1. Gibbs states as purified DBM Nomura*, **NY***, Nori, arXiv:2103.04791
   - Exact mapping of Trotterized ITE using quantum-to-classical mapping
   - Approximation by variational simulation

2. Ab-initio calculation of GS/band structure in solids **NY**, Mizukami, & Nori, Commun. Phys. 4, 106 (2021).
   - Applicable to strongly-correlated regime, where "gold-standard" methods fail
   - Band structure from multiple quasiparticle excitations