Quantum dynamics simulation towards Fugaku

The 2nd R-CCS International Symposium

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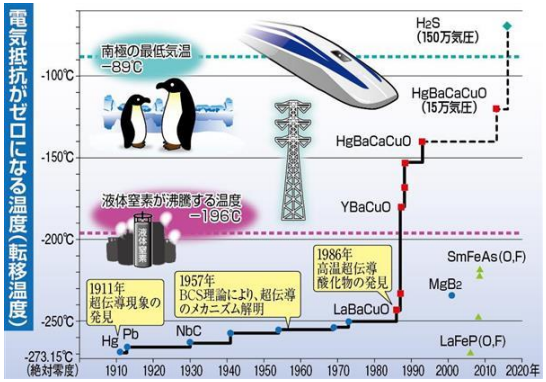
Quantum many-body systems

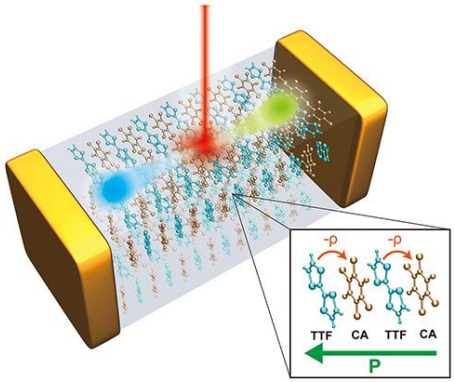
- **Applications of quantum many-body systems**
  - High-T_c superconductors
  - Solar battery
  - Artificial photosynthesis
  - Spintronic
  - Optical devices
  - Multiferroic materials
  - Quantum computer

  ⋮



Superconducting transition temperature

https://www.sankei.com/west/news/171124/wst1711240006-n1.html



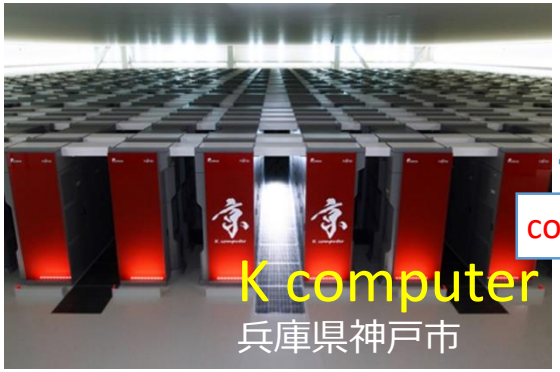
Solar battery by strongly correlated materials

https://www.cems.riken.jp/jp/laboratory/scirg

Next-generation fundamental technologies

- **Study of quantum many-body systems**

Theory：



collaboration

Experiment：

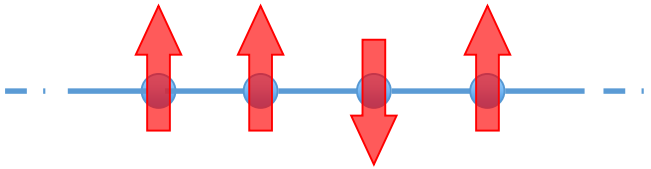
Numerical method

- Quantum many-body system

(time independent) Schrödinger equation : $\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$ (Eigenvalue equation)

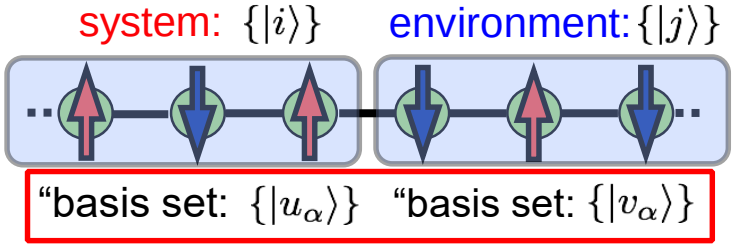
N spin-½ system: degree of freedom is not N but 2^N !!

E.g. N=100 ➔ $2^N \approx 10^{31}$



up-spin
or
down-spin

- Density matrix renormalization group (DMRG) method S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).



Optimized to describe target state.

target state:

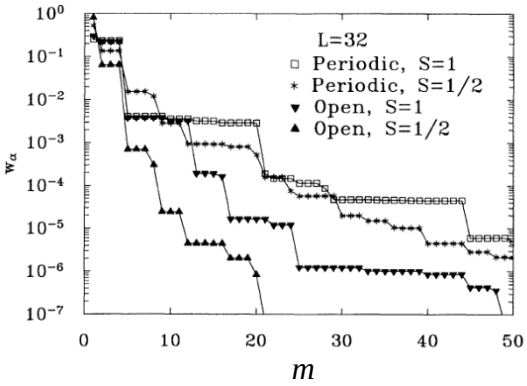
$$|\Psi\rangle = \sum_{i,j} \Psi_{ij}|i\rangle|j\rangle \approx \sum_{\alpha} \lambda_\alpha |u_\alpha\rangle|v_\alpha\rangle$$

Singular value decomposition

$$\Psi_{ij} = \sum_{\alpha=1}^{D_s} U_{i\alpha}\lambda_\alpha (V^\dagger)_{\alpha j}$$

$$|\Psi\rangle = \sum_{\alpha=1}^{D_s} \lambda_\alpha |u_\alpha\rangle|v_\alpha\rangle \approx \sum_{\alpha=1}^{m} \lambda_\alpha |u_\alpha\rangle|v_\alpha\rangle$$

m singular vectors with largest singular values: λ_α $(m << D_s)$



Numerical error of ground state calculation by DMRG

S. R. White, PRB **48**, 10345(1993).

Practical calculations by DMRG

(computing resource)

(※Size of optimized Hilbert space: $O(m^2)$)

P C
(100~1000GFLOPS)

Cluster machine
(few TFLOPS)

HPC (Univ. etc.)
(~ 1PFLOPS)

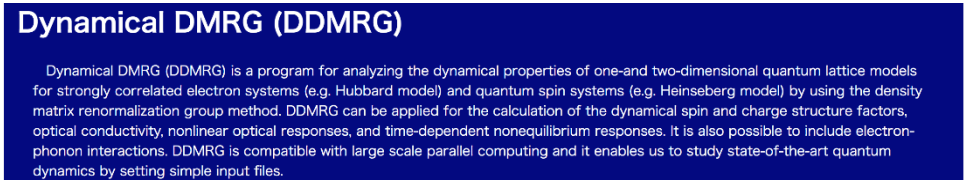
K computer
(10PFLOPS)

Fugaku
(~ 1EFLOPS)

- Ground state calculations on one-dimensional (1-D) systems
  (DMRG truncation number : $m < 500$)
- Quantum dynamics on 1-D systems (DDMRG, tDMRG)
- Finite temperature calculations on 1-D systems (FT-DMRG)
  ($m < 1{,}000$)
- Quantum dynamics on 1-D systems including electron-phonon interaction
- Ground state calculations on two-dimensional (2-D) systems
- Quantum dynamics on 2-D systems ($m < 20{,}000$)
- Finite temperature calculations on 2-D systems
- Quantum dynamics on 2-D systems including electron-phonon interaction
- 3-D systems (ground state, quantum dynamics)

Developed Massively parallel DMRG

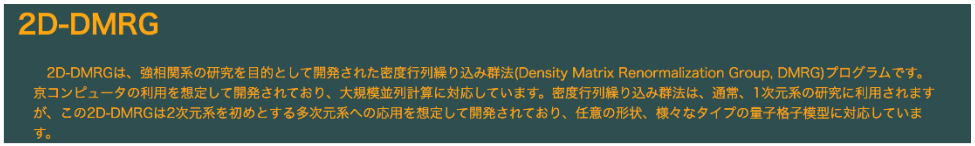
- Dynamical DMRG (SS, H. Matsueda, K. Morita, S. Yunoki, T. Tohyama)



Target:
Quantum dynamics

https://www.r-ccs.riken.jp/labs/cms/DMRG/Dynamical_DMRG.html

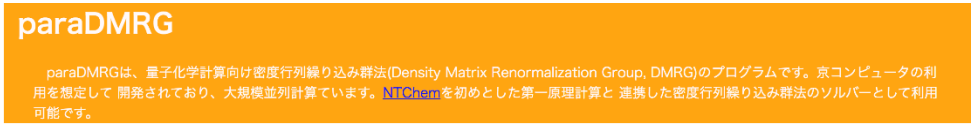
- 2D-DMRG (SS, T. Tohyama, S. Yunoki)



Target:
Two- (higher-) dimensional systems

https://www.r-ccs.riken.jp/labs/cms/DMRG/2D_DMRG.html

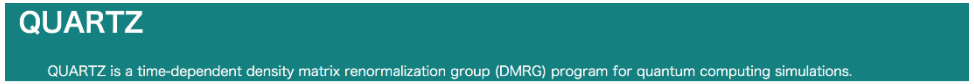
- paraDMRG (SS, Y. Imamura, T. Tohyama, T. Nakajima, S. Yunoki)



Target:
Quantum chemistry (Ab initio DMRG)

https://www.r-ccs.riken.jp/labs/cms/DMRG/paraDMRG.html

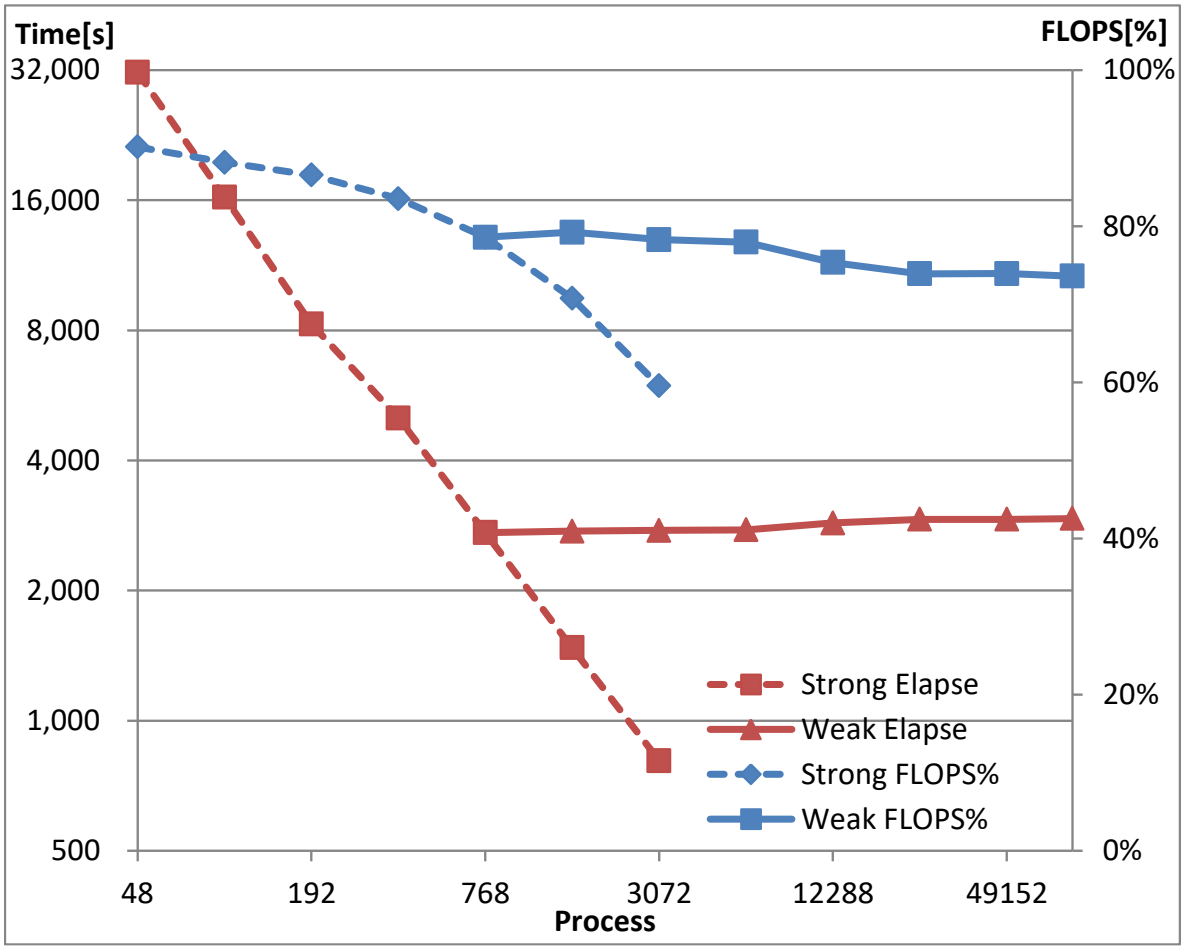
- QUARTZ (SS, S. Yunoki)



Target:
Quantum computing simulator
(quantum annealing, quantum logic gate)

https://www.r-ccs.riken.jp/labs/cms/DMRG/QUARTZ.html

Performance of developed DMRG



7.8 PFLOPS on K computer

SS, S. Yunoki, T. Tohyama, A. Kuroda,Y. Kitazawa, K. Minami, and F. Shoji

Quantum dynamics simulation towards Fugaku

◆ Optimization of our massively parallel DMRG programs for Fugaku

Dynamical DMRG (DDMRG)

Dynamical DMRG (DDMRG) is a program for analyzing the dynamical properties of one-and two-dimensional quantum lattice models for strongly correlated electron systems (e.g. Hubbard model) and quantum spin systems (e.g. Heinseberg model) by using the density matrix renormalization group method. DDMRG can be applied for the calculation of the dynamical spin and charge structure factors, optical conductivity, nonlinear optical responses, and time-dependent nonequilibrium responses. It is also possible to include electron-phonon interactions. DDMRG is compatible with large scale parallel computing and it enables us to study state-of-the-art quantum dynamics by setting simple input files.

QUARTZ

QUARTZ is a time-dependent density matrix renormalization group (DMRG) program for quantum computing simulations.

2D-DMRG

2D-DMRGは、強相関系の研究を目的として開発された密度行列繰り込み群法(Density Matrix Renormalization Group, DMRG)プログラムです。京コンピュータの利用を想定して開発されており、大規模並列計算に対応しています。密度行列繰り込み群法は、通常、1次元系の研究に利用されますが、この2D-DMRGは2次元系を初めとする多次元系への応用を想定して開発されており、任意の形状、様々なタイプの量子格子模型に対応しています。

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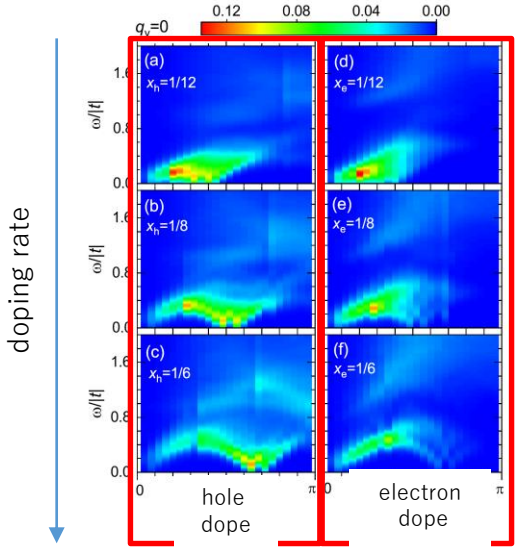
◆ Quantum dynamics simulation using DDMRG

"Dynamical density matrix renormalization group study of spin and charge excitations in the four-leg t-t'-J ladder" T. Tohyama, M. Mori, S. Sota, PRB **97**, 235137 (2018).

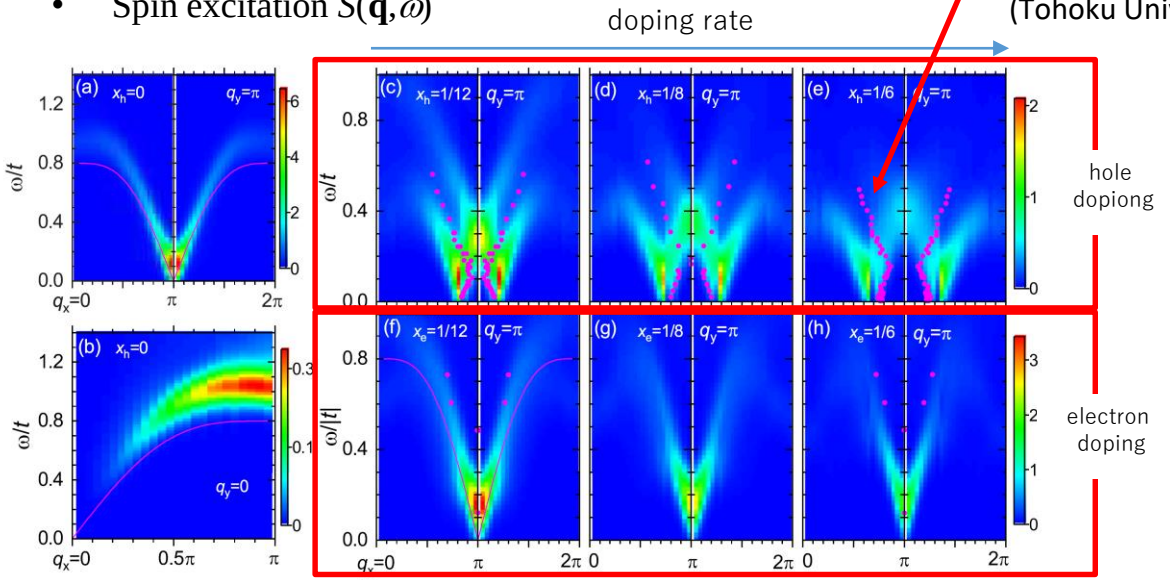
Hamiltonian: $H = -t\sum_{\mathbf{l},\delta,\sigma}\left(\tilde{c}^{\dagger}_{\mathbf{l}+\delta,\sigma}\tilde{c}_{\mathbf{l},\sigma}+\tilde{c}^{\dagger}_{\mathbf{l}-\delta,\sigma}\tilde{c}_{\mathbf{l},\sigma}\right)-t'\sum_{\mathbf{l},\delta',\sigma}\left(\tilde{c}^{\dagger}_{\mathbf{l}+\delta',\sigma}\tilde{c}_{\mathbf{l},\sigma}+\tilde{c}^{\dagger}_{\mathbf{l}-\delta',\sigma}\tilde{c}_{\mathbf{l},\sigma}\right)+J\sum_{\mathbf{l},\delta}\left(\mathbf{S}_{\mathbf{l}+\delta}\mathbf{S}_{\mathbf{l}}-\frac{1}{4}n_{\mathbf{l}+\delta}n_{\mathbf{l}}\right)$

Fujita group (Tohoku Univ.)

- Charge excitation $N(\mathbf{q},\omega)$



- Spin excitation $S(\mathbf{q},\omega)$



Real time simulation of quantum many-body systems

- Newly developed time-dependent DMRG for higher dimensional systems

Time-dependent DMRG:

Dual optimized Hilbert spaces

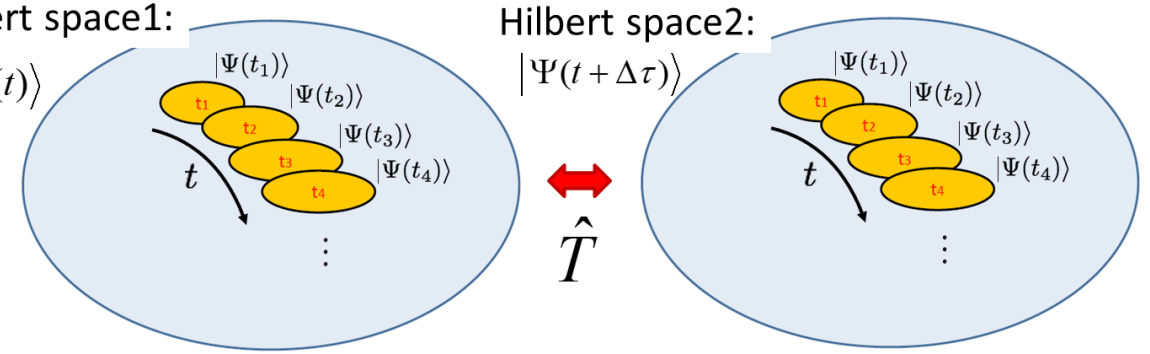
+ (original)

Time evolution:

Kernel polynomial method

Hilbert space1: $|\Psi(t)\rangle$

Hilbert space2: $|\Psi(t+\Delta\tau)\rangle$



$$|\Psi(t+\Delta\tau)\rangle = e^{-i\hat{H}\Delta\tau}|\Psi(t)\rangle$$

$$= \sum_{l=0}^{\infty}(-i)^l(2l+1)j_l(\Delta\tau)P_l(\hat{H})|\Psi(t)\rangle$$

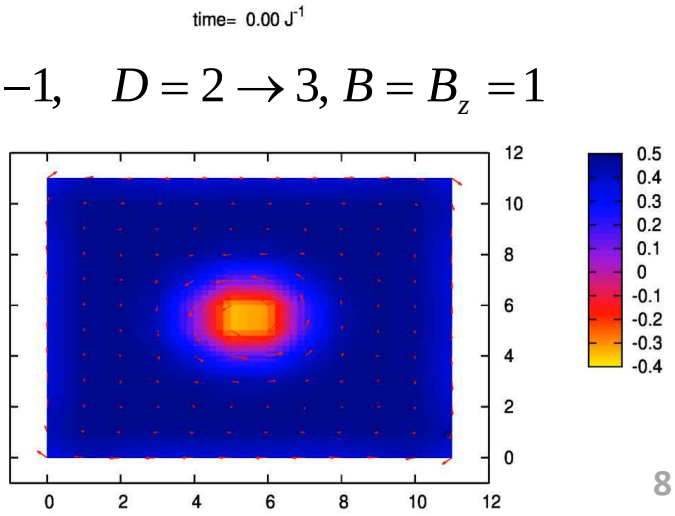
- Real time simulation of quantum skyrmion

$$H = J\sum_{<i,j>}\mathbf{S}_i\cdot\mathbf{S}_j \quad (\textit{Heisenberg spin exchange})$$

$$+D\sum_i\left\{(\mathbf{S}_i\times\mathbf{S}_{i+e_x})\cdot\mathbf{e}_x+(\mathbf{S}_i\times\mathbf{S}_{i+e_y})\cdot\mathbf{e}_y\right\}$$

(*Dzyaloshinskii–Moriya interaction*)

$$+\mathbf{B}\cdot\sum_i\mathbf{S}_i \quad (\textit{Magnetic field to z-direction})$$



Quantum computing simulation using Fugaku

D-Wave (quantum annealing)

http://dwavejapan.com/system/

◆ Quantum computing simulation

- Developed software: QUARTZ

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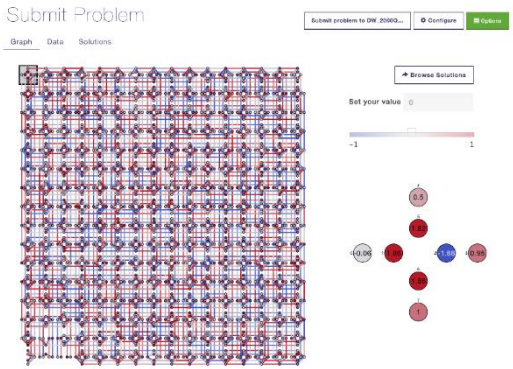
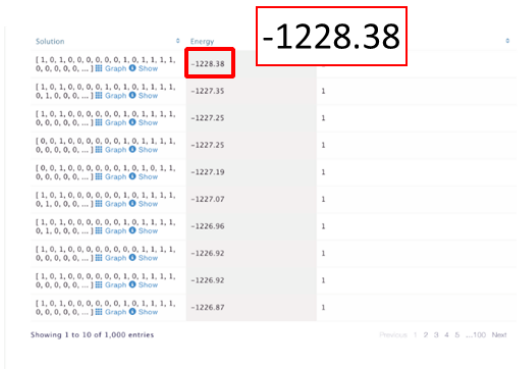
"quantum annealing" and "quantum logic gate"

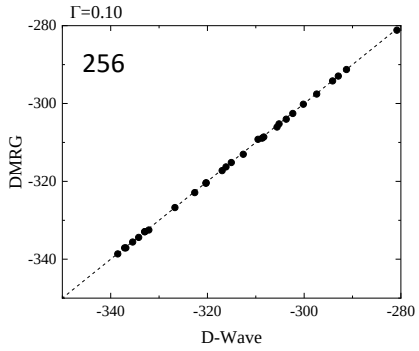
- Quantum annealing by D-Wave

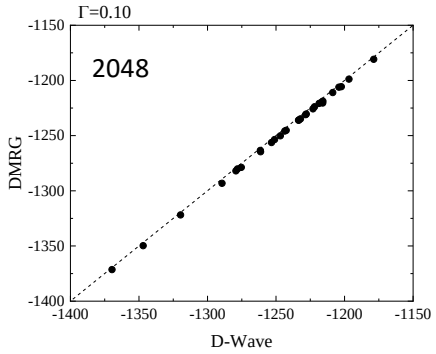


Hamiltonian is given by random number.



- Energy



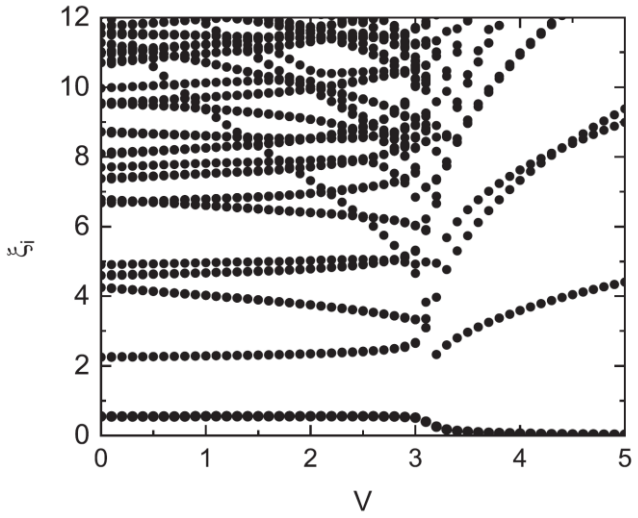


Increasing the number of Qubit

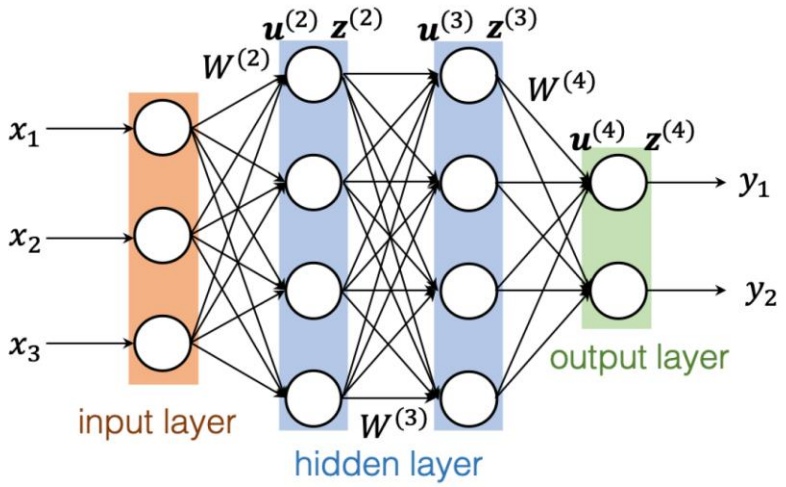
How to stabilize quantum annealing?

Machine learning for quantum many-body systems

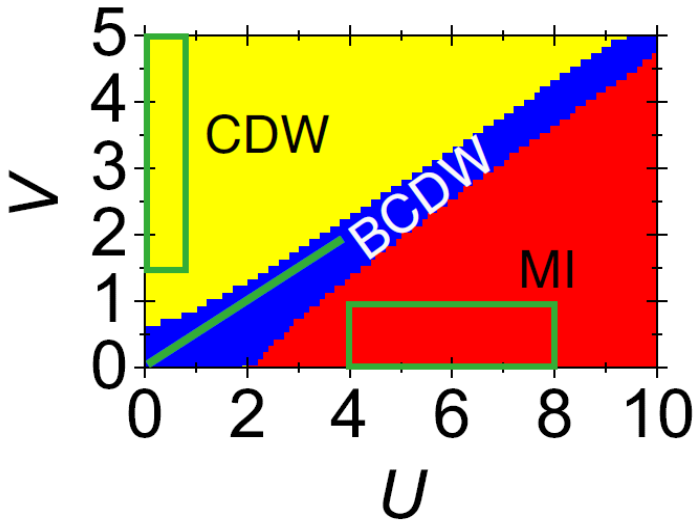
- Entanglement spectrum



- Neural network



- Phase diagram



Future work:

- Quantum dynamics (arXiv:1901.07900)
- Appling to different systems
- Data assimilation (arXiv:1908.09335)
- Effective model

Summary

◆ Past and current works

- Development of massively parallel DMRG programs

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◆ Future works for Fugaku

- Massively parallel DMRG for Fugaku

  “Quantum dynamics of quantum many-body system”

- New method to study quantum many-body systems
  - ✓ Machine learning
  - ✓ Quantum computer
  - ✓ New numerical method

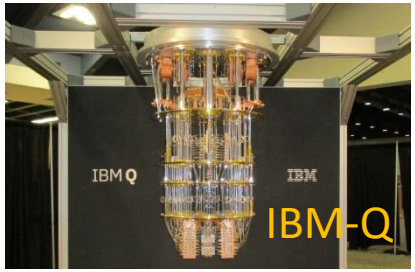
  ⋮

→ “Quantum many-body systems”

http://rsc.riken.jp/synchrotron/third.html

https://www.tohoku-epco.co.jp/seven/slit-j/

http://dwavejapan.com/system/



https://www.sbbit.jp/article/cont1/36729