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

- Study of quantum many-body systems
  - Theory:
  - Experiment:
    - Superconducting transition temperature
    - Solar battery by strongly correlated materials
      - https://www.cems.riken.jp/jp/laboratory/scirg

Next-generation fundamental technologies
**Numerical method**

- Quantum many-body system
  
  (time independent) Schrödinger equation: \( \hat{H} \ket{\Psi_n} = E_n \ket{\Psi_n} \) (Eigenvalue equation)

  \( N \) spin-\( \frac{1}{2} \) system: degree of freedom is not \( N \) but \( 2^N \)!!

  E.g. \( N=100 \Rightarrow 2^N \approx 10^{31} \)

- Density matrix renormalization group (DMRG) method

  **system**: \( \{|i\}\)  
  **environment**: \( \{|j\}\)  
  "basis set": \( \{|u_\alpha\}\)  
  "basis set": \( \{|v_\alpha\}\)  

  Target state:

  \[
  \ket{\Psi} = \sum_{i,j} \Psi_{ij} \ket{i} \ket{j} \\ \approx \sum_{\alpha} \lambda_\alpha \ket{u_\alpha} \ket{v_\alpha}
  \]

  Optimized to describe target state.

  **Singular value decomposition**

  \[
  \ket{\Psi} = \sum_{\alpha=1}^{D_s} \lambda_\alpha \ket{u_\alpha} \ket{v_\alpha} \approx \sum_{\alpha=1}^{m} \lambda_\alpha \ket{u_\alpha} \ket{v_\alpha}
  \]

  \( m \) singular vectors with largest singular values: \( \lambda_\alpha \) \( (m << D_s) \)

  Numerical error of ground state calculation by DMRG

Practical calculations by DMRG

(computing resource)

- 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)**
  
  **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. Heisenberg 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.

  [https://www.r-ccs.riken.jp/labs/cms/DMRG/Dynamical_DMRG.html](https://www.r-ccs.riken.jp/labs/cms/DMRG/Dynamical_DMRG.html)

  **Target:**
  Quantum dynamics

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

  **2D-DMRG**

  2D-DMRG is a program developed for two-dimensional quantum systems. It is designed to handle systems with periodic boundary conditions and can be applied to various types of two-dimensional quantum systems, including those with exact diagonalization. 2D-DMRG is particularly useful for simulating quantum many-body systems and has been successfully applied to a wide range of problems, from condensed matter physics to quantum chemistry.

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

  **Target:**
  Two- (higher-) dimensional systems

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

  **paraDMRG**

  paraDMRG is a program for quantum chemistry that is specifically designed to handle large systems. It employs the density matrix renormalization group (DMRG) method to efficiently simulate the ground state of quantum systems. paraDMRG is particularly useful for systems with strong electron-electron correlations, such as those found in strongly correlated electronic systems.


  **Target:**
  Quantum chemistry (Ab initio DMRG)

• **QUARTZ (SS, S. Yunoki)**

  **QUARTZ**

  QUARTZ is a time-dependent density matrix renormalization group (DMRG) program for quantum computing simulations. It is designed to simulate the dynamics of quantum systems with high accuracy and efficiency.


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

DDMRG (Dynamical DMRG) 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., Heisenberg model) by using the density matrix renormalization group method. DDRG can be applied to 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. DDRG 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.

◆ 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: $H = -t \sum_{\langle \mathbf{1}, \mathbf{1}' \rangle, \omega} \left( \tilde{c}_{1 \uparrow \omega} \tilde{c}_{\mathbf{1} \uparrow \omega} \tilde{c}_{1 \downarrow \omega} \tilde{c}_{\mathbf{1} \downarrow \omega} + \tilde{c}_{1 \downarrow \omega} \tilde{c}_{\mathbf{1} \downarrow \omega} \tilde{c}_{1 \uparrow \omega} \tilde{c}_{\mathbf{1} \uparrow \omega} \right) - t' \sum_{\langle \mathbf{1}, \mathbf{1}' \rangle, \omega} \left( \tilde{c}_{1 \uparrow \omega} \tilde{c}_{\mathbf{1} \downarrow \omega} + \tilde{c}_{1 \downarrow \omega} \tilde{c}_{\mathbf{1} \uparrow \omega} \right) + J \sum_{\langle \mathbf{1}, \mathbf{1}' \rangle} \left( \mathbf{S}_{1 \uparrow \omega} \mathbf{S}_{\mathbf{1} \downarrow \omega} - \frac{1}{4} n_{1 \uparrow \omega} n_{1 \downarrow \omega} \right)$

- 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

Time evolution:

Kernel polynomial method

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

• Real time simulation of quantum skyrmion

\[ H = J \sum_{<i,j>} S_i \cdot S_j \quad (\text{Heisenberg spin exchange}) \]
\[ + D \sum_i \left\{ (S_i \times S_{i+e_x}) \cdot e_x + (S_i \times S_{i+e_y}) \cdot e_y \right\} \quad (\text{Dzyaloshinskii–Moriya interaction}) \]
\[ + B \sum_i S_i \quad (\text{Magnetic field to z-direction}) \]

\[ J = -1, \quad D = 2 \rightarrow 3, \quad B = B_z = 1 \]

Heisenberg spin exchange

Dzyaloshinskii–Moriya interaction

Magnetic field to z-direction
Quantum computing simulation using Fugaku

◆ Quantum computing simulation
  • Developed software: QUARTZ

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

“quantum annealing” and “quantum logic gate”

• Quantum annealing by D-Wave

• Energy

Hamiltonian is given by random number.

Increasing the number of Qubit

How to stabilize quantum annealing?

D-Wave (quantum annealing)

http://dwavejapan.com/system/
Machine learning for quantum many-body systems

- Entanglement spectrum
- Phase diagram
- Neural network

Future work:
- Quantum dynamics (arXiv:1901.07900)
- Applying to different systems
- Data assimilation (arXiv:1908.09335)
- Effective model
Summary

◆ Past and current works
  • Development of massively parallel DMRG programs

Dynamical DMRG (DDMRG)

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QUARTZ

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

◆ 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”

2D-DMRG

2D-DMRG is a program developed to study quantum many-body systems by Density Matrix Renormalization Group (DMRG) method. 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.

paraDMRG

paraDMRG is a program developed to study quantum many-body systems by Density Matrix Renormalization Group (DMRG) method. 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.

Spring-8

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

SACLA

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

Drogo

http://dwavejapan.com/system/

Sendai

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

D-Wave 2000Q

https://www.ibm.jp/