Massively parallel density matrix renormalization group method algorithm for two-dimensional strongly correlated systems and its applications

1st R-CCS Symposium (Kobe)

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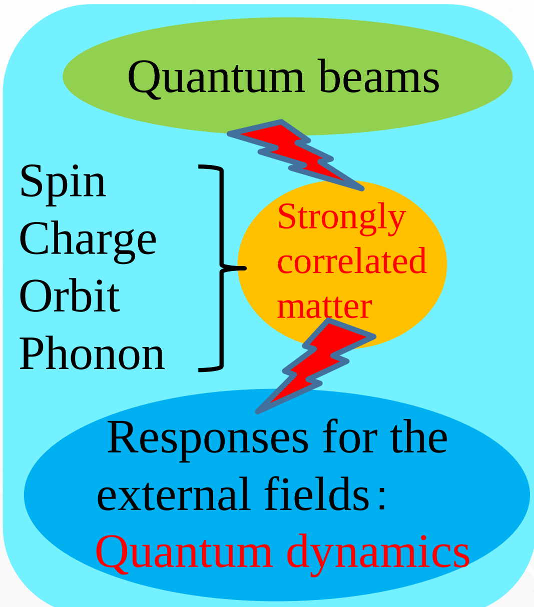
Collaboration with large scale quantum beam experiments



Large scale quantum beam facilities

Collaboration between theoretical and experimental researchers

K/Post-K computer

Quantum fluctuation and excitation dynamics of quantum many-body system

☑ Constructions of theory and computation to accurately understand complex experiment results

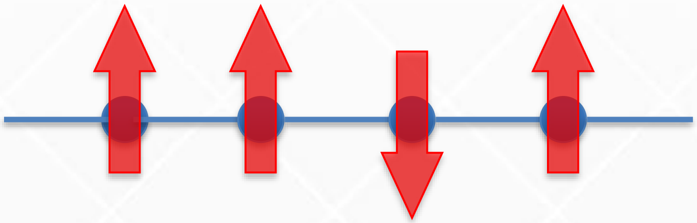
☑ Predicting characteristics from the numerical calculations and proposing experiments for large quantum beam facilities

Introduction

➢ Quantum many-body systems

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

E.g. N=100 ➔ $2^{100} \approx 10^{31}$



$$\bar{H}|\Psi\rangle = E|\Psi\rangle$$

$2^N \times 2^N$ matrix

2^N vector

➢ Physical quantities

$2^N \times 2^N$ matrix

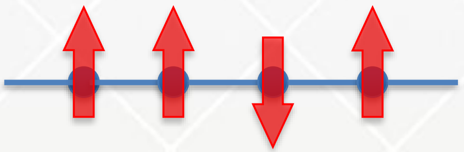
$$\langle Q\rangle = \langle\Psi|\bar{Q}|\Psi\rangle$$

Introduction

➢ The spirit of density matrix renormalization (DMRG)

- Optimize the basis set to describe the state to be calculated
- Use only m^2 bases instead of 2^N bases （$m^2 \ll 2^N$）

$$|\Psi\rangle = \sum_{n=1}^{2^N} c_n |n\rangle \approx \sum_{n'=1}^{m^2} \phi_{n'} |n'\rangle$$

$$|i_n\rangle = |$$  $$\rangle$$

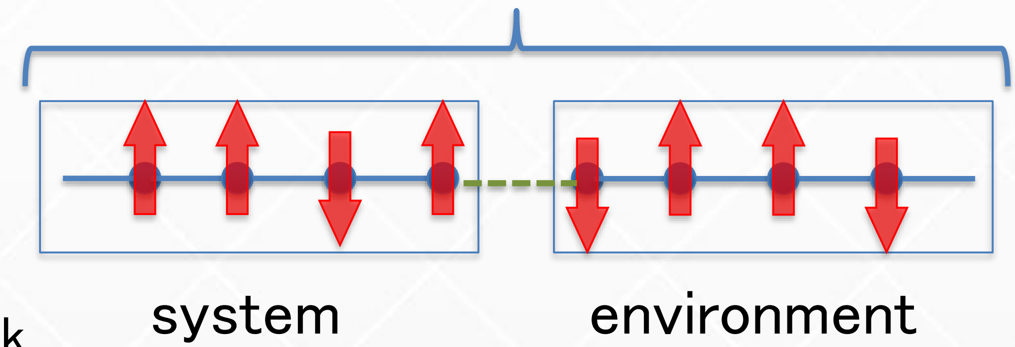
S. R. White, PRL **69**, 2863 (1992).

Introduction

Computer simulations create the future

- How to choose the optimized bases

- *m* eigenstates with largest eigenvalues of the reduced density matrix of the superblock ground state



- Ground state of the superblock

$$|\Psi^{\mathrm{SB}}\rangle = \sum_{ij} \psi_{ij}^{\mathrm{SB}} |i^{(\mathrm{sys})}\rangle |j^{(\mathrm{env})}\rangle$$

- Reduced density matrix

$$\rho_{i,i'} = \sum_{j} \psi_{ij}^{\mathrm{SB}} \psi_{i'j}^{\mathrm{SB}}$$

- *m* eigenstates with largest eigenvalues: $\left|\Phi_i^{(\mathrm{sys})}\right\rangle$

$$\boxed{\begin{aligned} |\Psi\rangle &= \sum_{n=1}^{2^N} c_n |n\rangle \approx \sum_{n'=1}^{m^2} \phi_{n'} |n'\rangle \\ &= \sum_{i'=1}^{m} \sum_{j'=1}^{m} a_{i',j'} |i'\rangle |j'\rangle \end{aligned}}$$

Dynamical DMRG method

Computer simulations create the future

E. Jeckelmann, Phys. Rev. B **66**, 045114 (2002)

- Dynamical Correlation function

$$\chi_A(\omega) \equiv \frac{1}{2\pi N} \mathrm{Im} \langle 0 | \hat{A}^\dagger \frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A} | 0 \rangle$$

$\hat{A}$: arbitrary operator

$|0\rangle$: ground state $\hat{H}|0\rangle = \varepsilon_0 |0\rangle$

- Target state

$$\underbrace{|0\rangle, \quad \hat{A}|0\rangle, \quad \boxed{\frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A} | 0 \rangle}}$$

Basis set is optimized to describe these states

Multi target procedure

Kernel polynomial method

$$\frac{1}{\omega - \hat{H} \pm i\gamma} \hat{A}|0\rangle$$

$$= \mp \sum_{l=0}^{\infty} w_l^{-1} \{2Q_l(\omega) + iP_l(\omega)\} P_l(\hat{H}) \hat{A} |0\rangle$$

SS, M. Ito, J. Phys. Soc. Jpn. **76**, 054004 (2007).
SS , T. Tohyama, PRB **82**, 195130 (2010).

Massively parallel Dynamical DMRG

Dynamical DMRG (https://www.r-ccs.riken.jp/labs/cms/DMRG/Dynamical_DMRG_en.html)

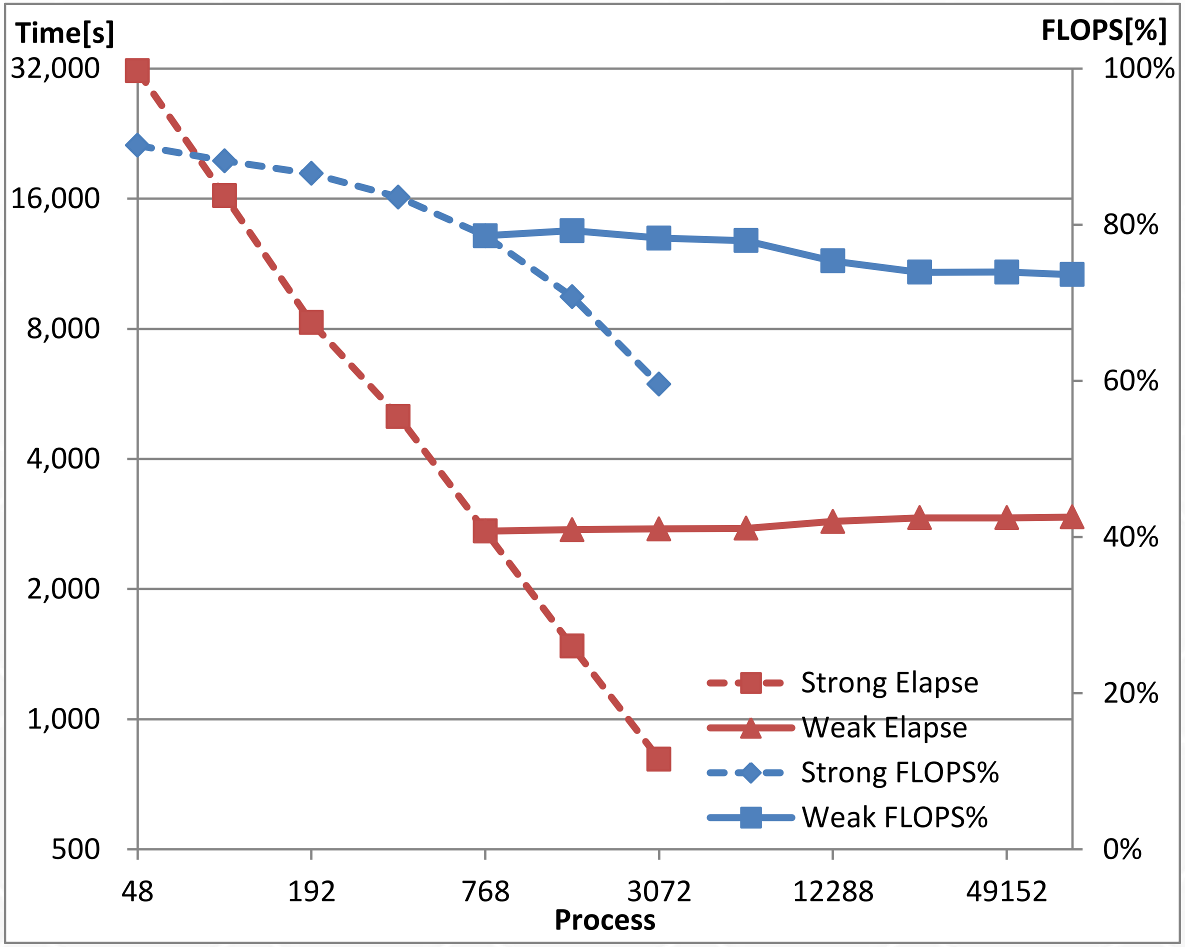
Density Matrix Renormalization Group (DMRG)

Kernel Polynomial method (KPM)

Massively Parallelization

Quantum Dynamics of strongly correlated quantum systems

Efficiency

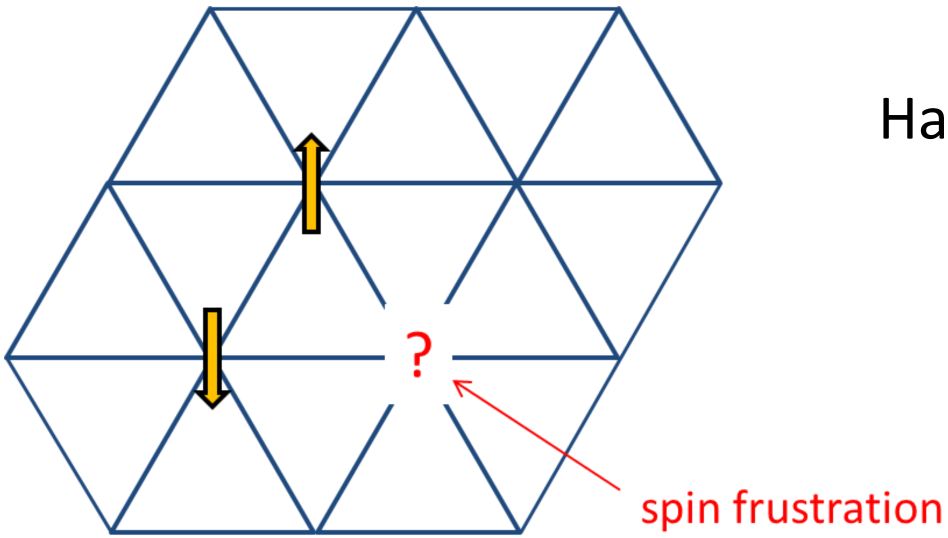


7.8 PFLOPS on K computer

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

Spin excitation dynamics on spin frustrated system

◆ S=1/2 triangular lattice Heisenberg antiferromagnet



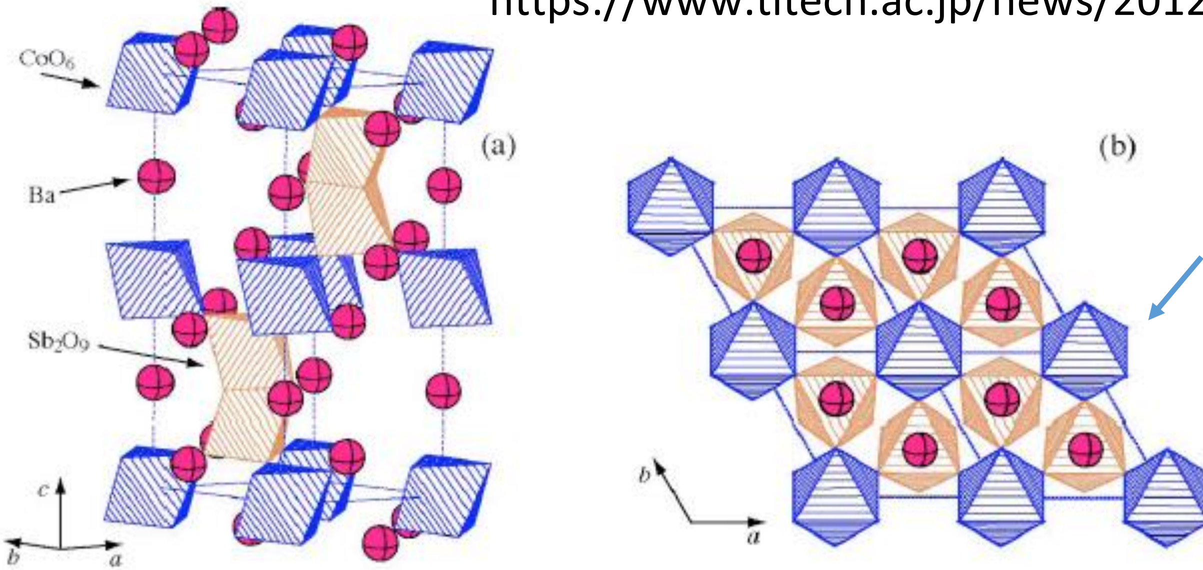
Hamiltonian:

$$H = \sum_{<i,j>} J_{i,j}\, \mathbf{S}_i \cdot \mathbf{S}_j$$

- Typical spin frustrated system.
- Ground state properties have been already well known.
    - ➢ i.e. uniform triangular lattice: three-sublattice 120° Néel ordered state.
- The magnetic excitations are less well understood.

$Ba_3CoSb_2O_9$

https://www.titech.ac.jp/news/2012/025500.html



Co^{2+} ion is located at the center of octahedra.

The effective magnetic moment of Co^{2+} ions with an octahedral environment can be described by the pseudospin-1/2.

→ Magnetic Co^{2+} ions forms a uniform triangular lattice.

- Spin-1/2 XXZ model with small easy-plane anisotropy

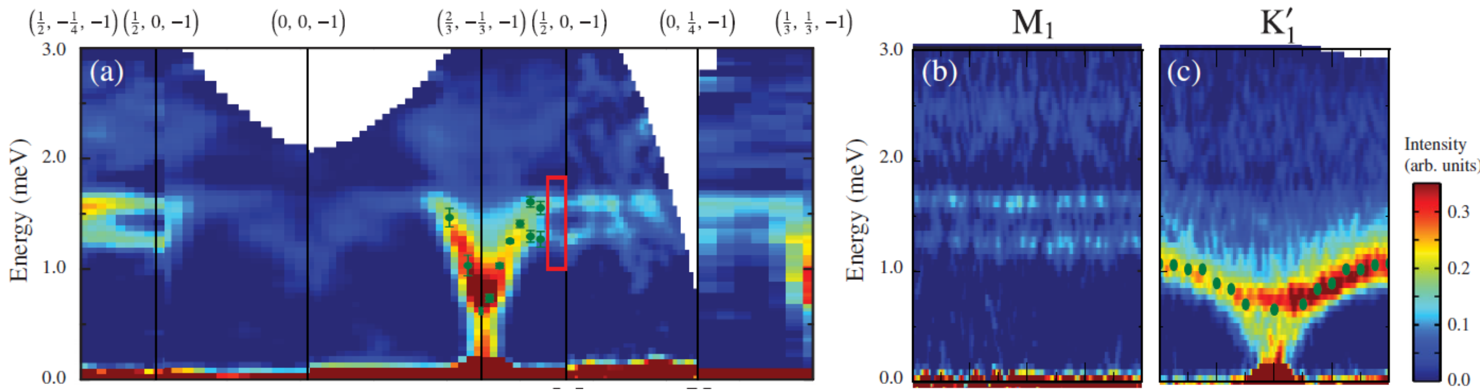
$$H = \sum_{<i,j>}^{\text{layer}} J(\mathbf{S}_i \cdot \mathbf{S}_j - \Delta S_i^z S_j^z) + \sum_{<l,m>}^{\text{interlayer}} J' \mathbf{S}_l \cdot \mathbf{S}_m$$

J=1.67meV, Δ=0.046, and J'=0.12meV

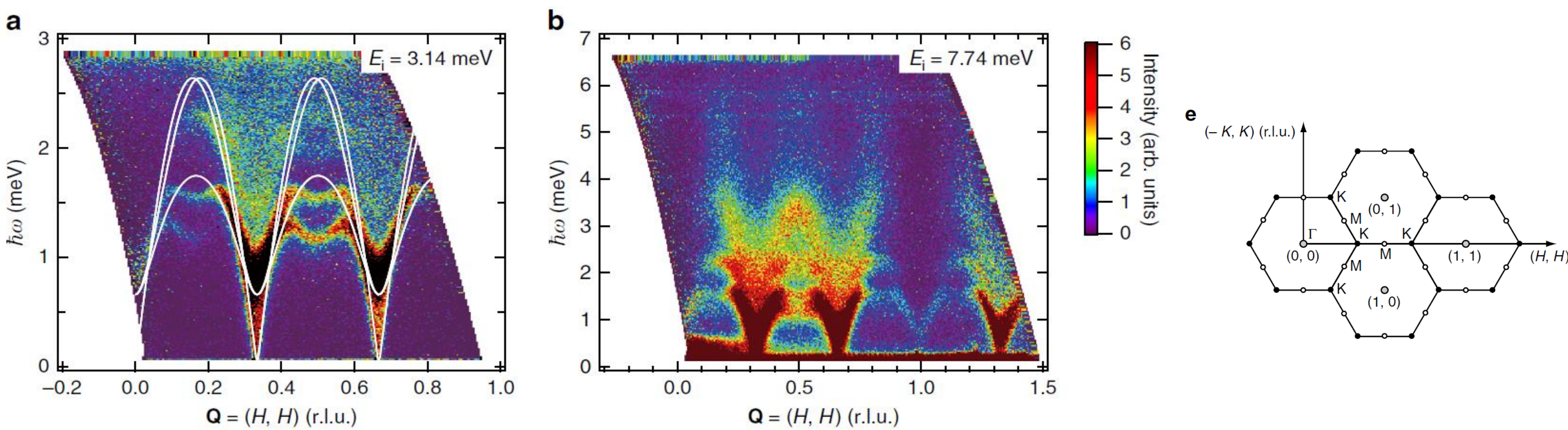
T. Suzuki, et al. Phys. Rev. Lett **110**, 267201 (2013).

Magnetic Excitations (1)

- Inelastic neutron scattering spectra of $Ba_3CoSb_2O_9$



J. Ma, et. al., Phys. Rev. Lett. **116**, 087201 (2016).

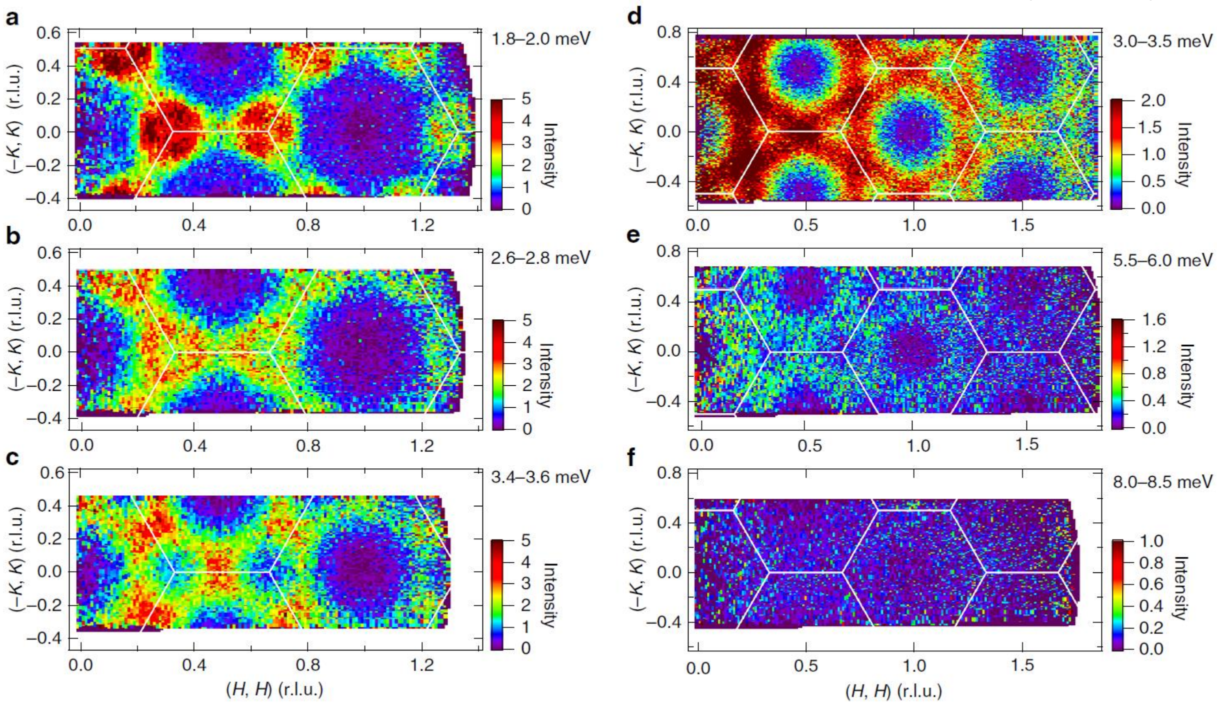


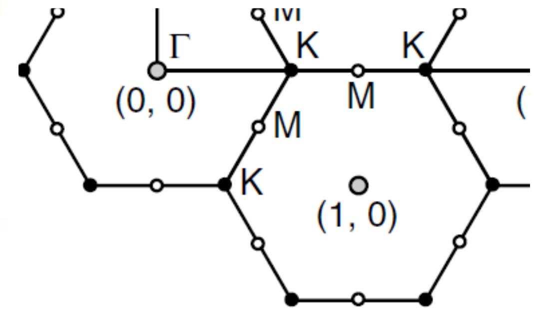
S. Ito, et. al, Nat. Communi. **8**, 235 (2017).

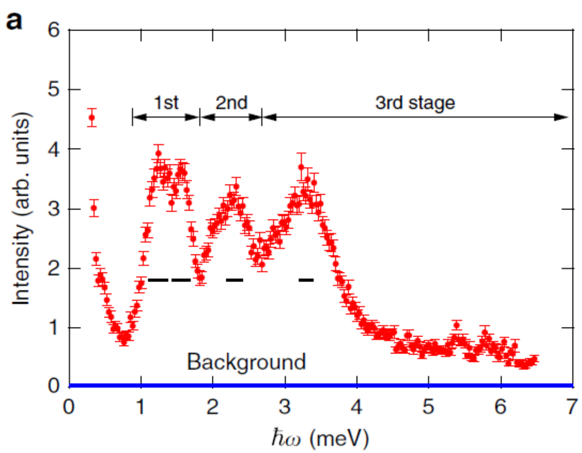
Magnetic excitations cannot be understood by linear spin wave theory.

Magnetic excitation (2)

S. Ito, et. al, Nat. Communi. **8**, 235 (2017)







At present, theory cannot explain the high energy excitations continua observed in $Ba_3CoSb_2O_9$.

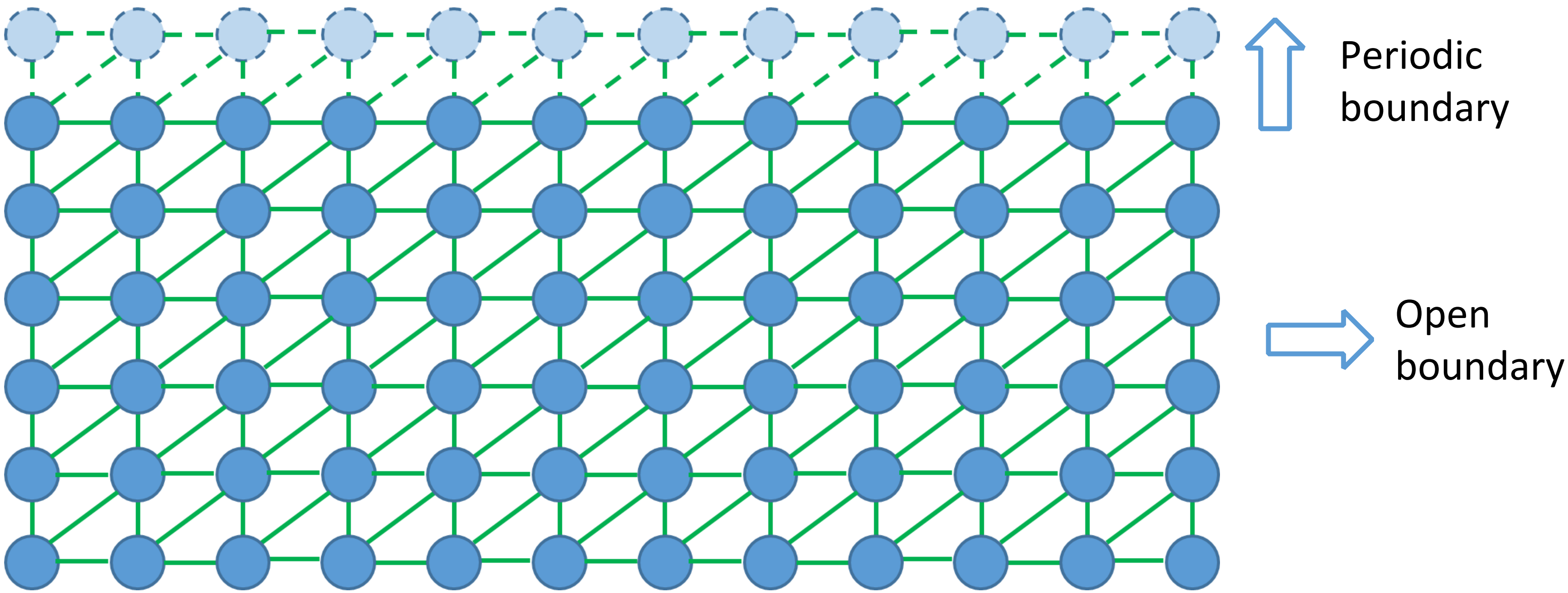
We investigate the magnetic excitations by the Dynamical DMRG.

Model and computational conditions

- Hamiltonian: $H = J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$ (We assume $J = 1.67\mathrm{meV}$.)

  S. Ito, et. al, Nat. Communi. **8**, 235 (2017)

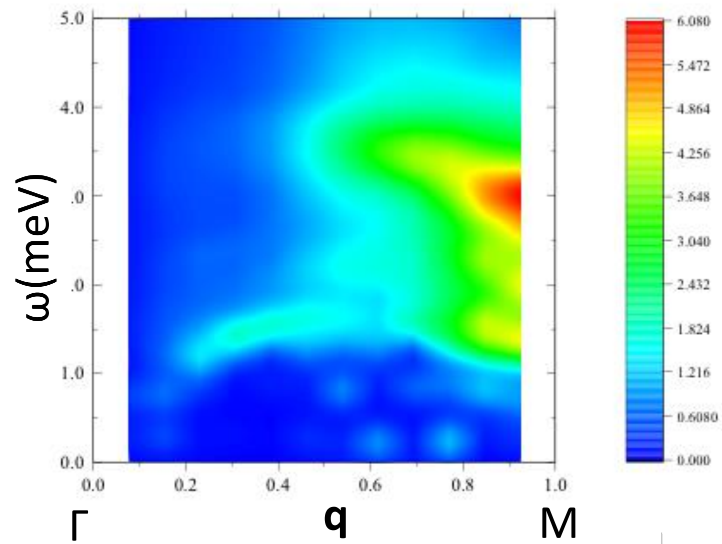
- lattice: 12×6 triangular lattice (cylindrical boundary condition)

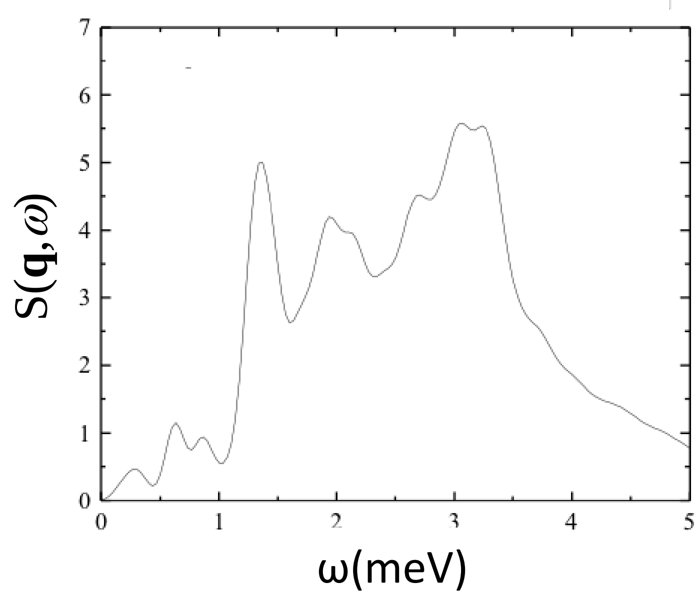


- DMRG truncation number m=6000.
- Half width at half maximum is $0.1J$. (Kernel polynomial method)

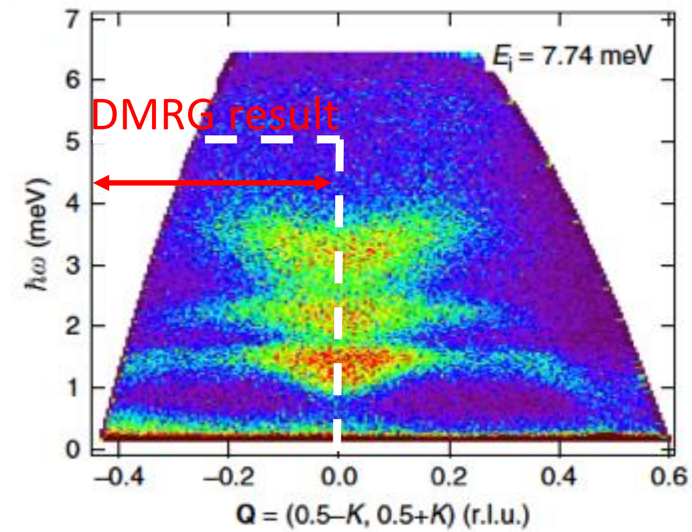
Dynamical spin structure factor S($\mathbf{q}$,ω) along Γ→M

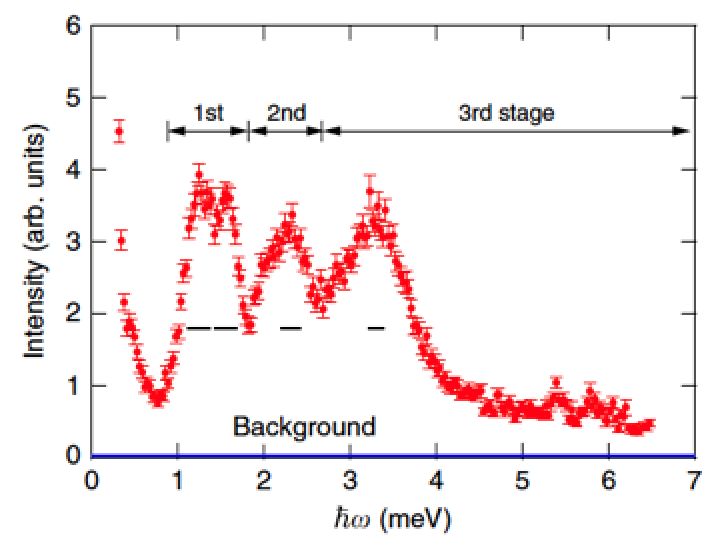
DMRG (J=1.67meV)





Experiment Ito, et al, Nat. Commun. **8**, 235 ('17)

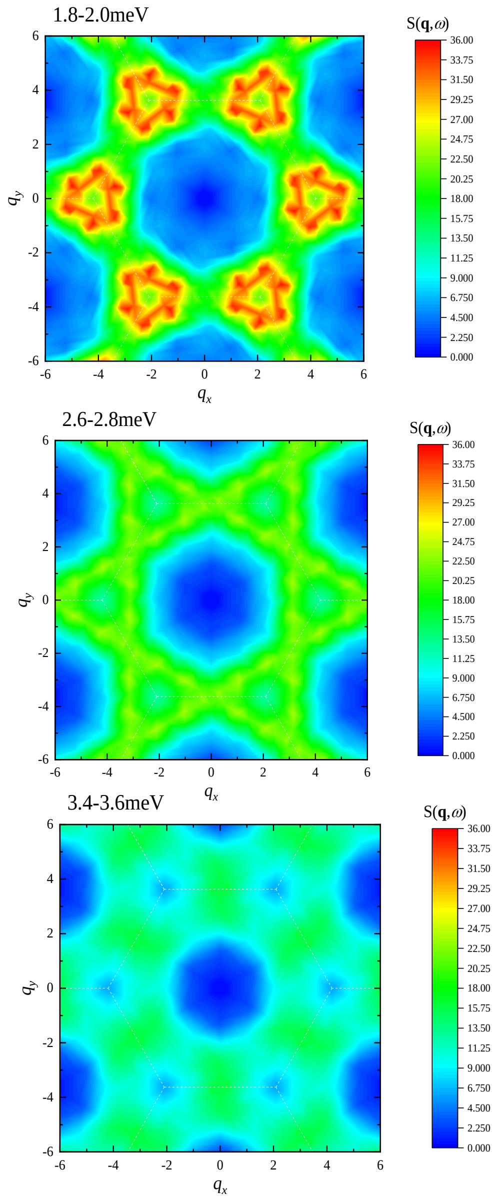




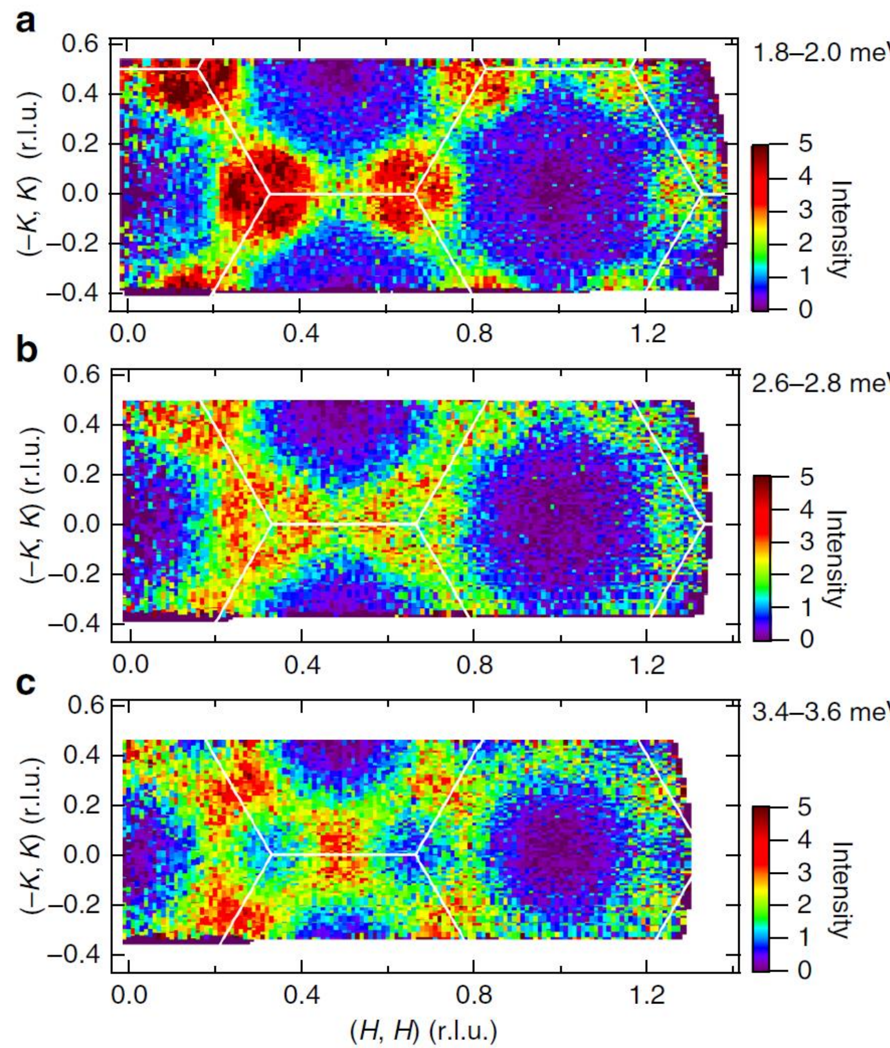
S($\mathbf{q}$,ω): constant energy map

Computer simulations create the future

DMRG (J=1.67meV)



Experiment Ito, et al, Nat. Commun. **8**, 235 ('17)



Summary

- **Our developed massively parallel dynamical DMRG shows high performance on K computer**

Japanese/English

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.

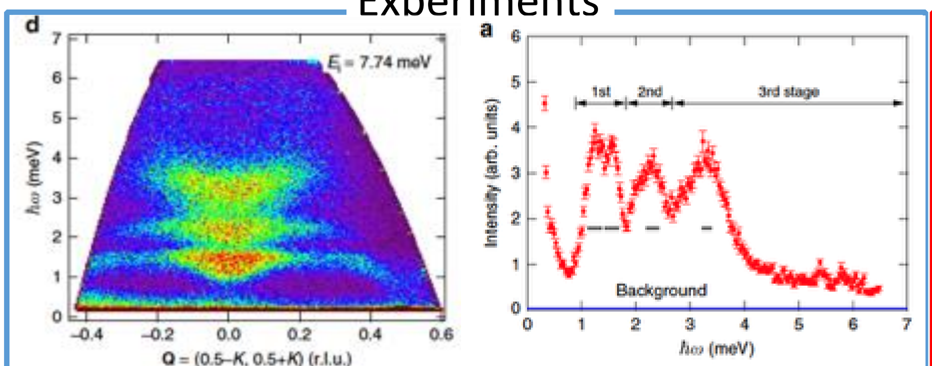
- Information

DDMRG version 2.0.0 (released 2018/9/29)

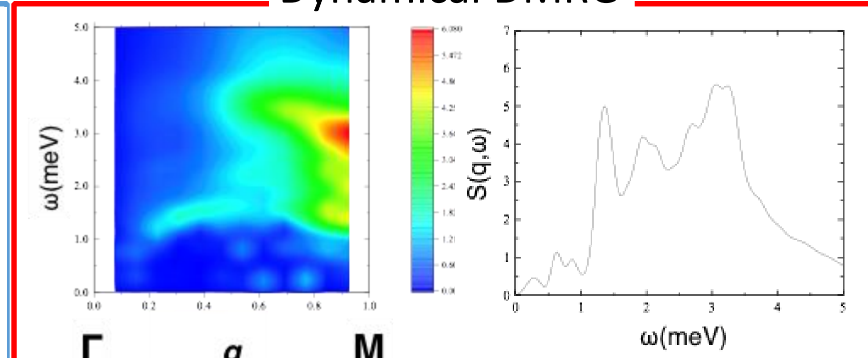
https://www.r-ccs.riken.jp/labs/cms/DMRG/Dynamical_DMRG_en.html

- **Spin dynamics of S=1/2 AFMHM on triangular lattice**
  - In good qualitative agreement with experiments

Experiments



Dynamical DMRG



  - What is the nature of high energy excitations??