計算物質科学における時空間アップスケーリングと数理手法@電気通信大学

高並列量子多体問題ソルバーがつなぐ物質科学と数理手法

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東京大学大学院工学系研究科附属量子相エレクトロニクス研究センター

1. Quantum many-body problem
2. A numerical solver package: HΦ
3. HΦ as a bridge between condensed matter physics and applied mathematics
4. Summary & discussion

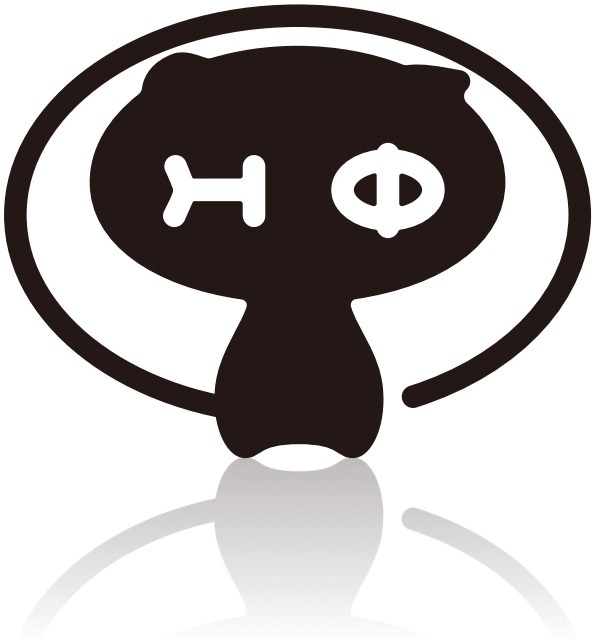
CDMSI

CBSM^2
Post K project

さきがけ PRESTO

MERIT

QPEC Univ. Tokyo

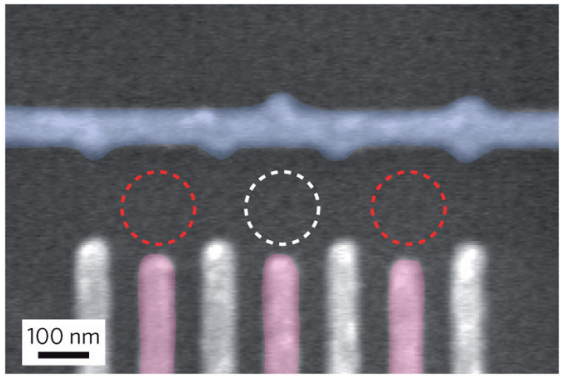


Quantum Many-Body Problem

Quantum Many-Body Problems

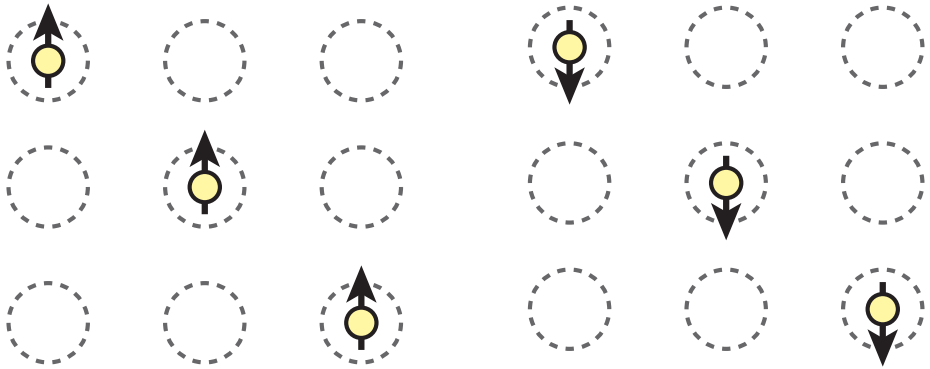
An example: 3 Quantum dots

F. R. Braakman, et al., Nat. Nano. 8, 432 (2013)



Quantum dot:
-A quantum box can confine a single electron
-Utilized for single electron transistor, quantum computers

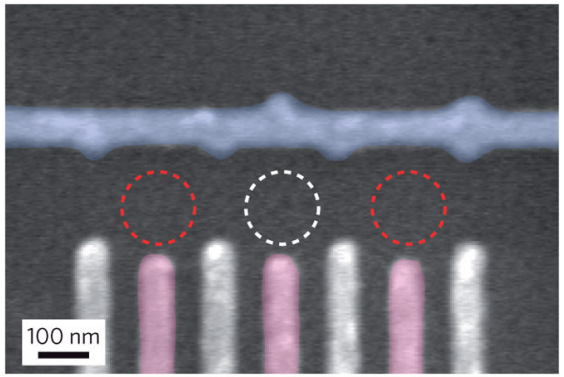
One-body problem:
One electron confined in three quantum dot
→ Number of states = 2×3 (factor 2 from spin)



Quantum Many-Body Problems

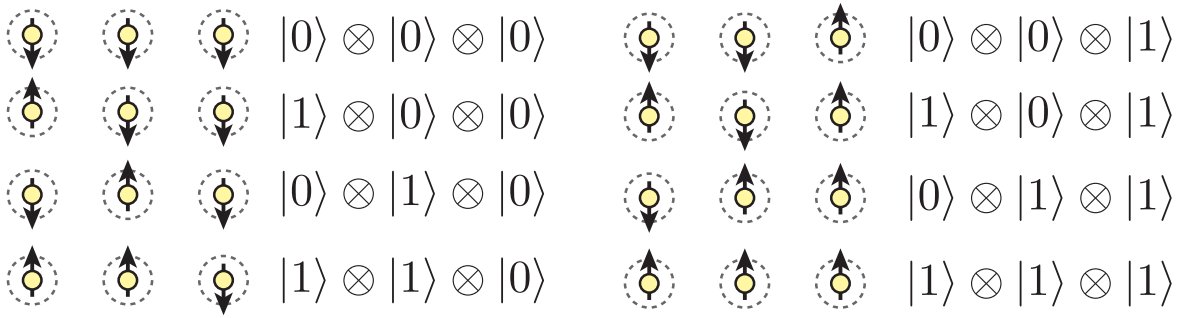
An example: 3 Quantum dots

F. R. Braakman, et al., Nat. Nano. 8, 432 (2013)



Quantum dot:
-A quantum box can confine a single electron
-Utilized for single electron transistor, quantum computers

Three-body problem:
→ Number of states = 2^3 (factor 2 from spin)



States represented by superposition

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \sum_{n_2=0,1} C_{n_0 n_1 n_2} |n_0\rangle \otimes |n_1\rangle \otimes |n_2\rangle : C_{n_0 n_1 n_2} \in \mathbb{C} \}$$

Quantum Many-Body Problems

N Quantum dots

One-body problem:

→ Number of states = $2 \times N$

N-body problem:

→ Number of states = 2^N

Further example: N=12

One-body problem→ Number of states = $2 \times N = 24$

N-body problem→ Number of states = $2^N = 4096$

Extreme example: N=36

One-body→ $2 \times N = 72$

N-body→ $2^N \sim 6.9 \times 10^{10}$

Quantum Many-Body Problems

Mutual Interactions

1. Operators acting on a single qubit

A two dimensional representation of Lie algebra SU(2)

$$[\hat{S}_j^x, \hat{S}_j^y] = i\hat{S}_j^z$$
$$[\hat{S}_j^y, \hat{S}_j^z] = i\hat{S}_j^x$$
$$[\hat{S}_j^z, \hat{S}_j^x] = i\hat{S}_j^y$$

$$\hat{S}_j^x|0\rangle = \frac{1}{2}|1\rangle$$
$$\hat{S}_j^x|1\rangle = \frac{1}{2}|0\rangle$$
$$\hat{S}_j^y|0\rangle = \frac{i}{2}|1\rangle$$
$$\hat{S}_j^y|1\rangle = -\frac{i}{2}|0\rangle$$
$$\hat{S}_j^z|1\rangle = \frac{1}{2}|1\rangle$$
$$\hat{S}_j^z|0\rangle = -\frac{1}{2}|0\rangle$$

Quantum Many-Body Problems

Mutual Interactions

Fock space of N qubits:

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \cdots \sum_{n_{N-1}=0,1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle \}$$

$$(C_{n_0 n_1 \cdots n_{N-1}} \in \mathbb{C})$$

Operators acting on N-quibit Fock space:

$$\hat{S}^a_j, \hat{S}^a_j \hat{S}^a_{j+1} : \mathcal{F} \to \mathcal{F}$$

$$\hat{S}^a_j \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}^a_j \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j}$$

$$\hat{S}^a_j \hat{S}^a_{j+1} \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}^a_j \otimes \hat{S}^a_{j+1} \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j-1}$$

Quantum Many-Body Problems

Quantum entanglement

Example: Two qubits

-Superposition
-Utilized for quantum teleportation
cf.) EPR “paradox”

Mutual interactions between two qubits

$$\hat{H} = J \sum_{a=x,y,z} \hat{S}_0^a \hat{S}_1^a \qquad (J \in \mathbb{R}, J > 0)$$

→Superposition

$$|1\rangle \otimes |0\rangle - |0\rangle \otimes |1\rangle$$

Hamiltonian Matrix

Example: N qubits

N-qubit Fock space:

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \cdots \sum_{n_{N-1}=0,1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle \}$$

$$(C_{n_0 n_1 \cdots n_{N-1}} \in \mathbb{C})$$

Mutual interactions among N qubits:
Hamiltonian operator

$$\hat{H} : \mathcal{F} \to \mathcal{F}$$

$$\hat{H} = J \sum_{j=0}^{N-1} \sum_{a=x,y,z} \hat{S}_j^a \hat{S}_{\mathrm{mod}(j+1,N)}^a$$

Vectors in Fock Space

Correspondence between spin and bit

$$|\uparrow\rangle = |1\rangle$$
$$|\downarrow\rangle = |0\rangle$$

2^N-dimensional Fock space:

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \cdots \sum_{n_{N-1}=0,1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle \}$$
$$(C_{n_0 n_1 \cdots n_{N-1}} \in \mathbb{C})$$

Decimal representation of orthonormalized basis

$$|I\rangle_{\mathrm{d}} = |n_0\rangle \otimes |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_{N-1}\rangle \qquad I = \sum_{\nu=0}^{N-1} n_\nu \cdot 2^\nu$$

Wave function as a vector

$$|\phi\rangle = \sum_{n_0=0}^{1} \sum_{n_1=0}^{1} \cdots \sum_{n_{N-1}=0}^{1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle$$

$$v(I) = C_{n_0 n_1 \cdots n_{N-1}} \qquad v(0 : 2^N - 1)$$

Vectors and Matrices in Fock Space

Inner product of vectors

$$(\langle n_0| \otimes \langle n_1| \otimes \cdots \otimes \langle n_{N-1}|) \times \left(|n'_0\rangle \otimes |n'_1\rangle \otimes \cdots \otimes |n'_{N-1}\rangle\right)$$
$$= \langle n_0|n'_0\rangle \times \langle n_1|n'_1\rangle \times \cdots \times \langle n_{N-1}|n'_{N-1}\rangle$$

$$\langle n| \times |n'\rangle = \langle n|n'\rangle = \delta_{n,n'}$$

$$\langle \phi'|\phi\rangle = \sum_{n_0=0}^{1} \sum_{n_1=0}^{1} \cdots \sum_{n_{N-1}=0}^{1} C'^{*}_{n_0 n_1 \cdots n_{N-1}} C_{n_0 n_1 \cdots n_{N-1}}$$

$$|\phi'\rangle = \sum_{n_0=0}^{1} \sum_{n_1=0}^{1} \cdots \sum_{n_{N-1}=0}^{1} C'_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle$$

$$|\phi\rangle = \sum_{n_0=0}^{1} \sum_{n_1=0}^{1} \cdots \sum_{n_{N-1}=0}^{1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle$$

Hamiltonian matrix

$$H_{II'} = \langle I|\hat{H}|I'\rangle$$

Orthonomalized basis: $|I\rangle, |I'\rangle \in \mathcal{F}$ $\langle I|I'\rangle = \delta_{I,I'}$

Example: Two Spins

Decimal representation of orthonormalized basis

		0 th site		1 st site
$\|0\rangle_{\mathrm{d}}$	$=$	$\|\downarrow\rangle$	$\otimes$	$\|\downarrow\rangle$
$\|1\rangle_{\mathrm{d}}$	$=$	$\|\uparrow\rangle$	$\otimes$	$\|\downarrow\rangle$
$\|2\rangle_{\mathrm{d}}$	$=$	$\|\downarrow\rangle$	$\otimes$	$\|\uparrow\rangle$
$\|3\rangle_{\mathrm{d}}$	$=$	$\|\uparrow\rangle$	$\otimes$	$\|\uparrow\rangle$

Problem: Find 4 by 4 Hamiltonian matrix that describes

$$\hat{H}/J = \hat{S}_0^x \hat{S}_1^x + \hat{S}_0^y \hat{S}_1^y + \hat{S}_0^z \hat{S}_1^z$$

$$= \frac{1}{2}\left(\hat{S}_0^+ \hat{S}_1^- + \hat{S}_0^- \hat{S}_1^+\right) + \hat{S}_0^z \hat{S}_1^z$$

Useful transformation:
Ladder operators

$$\hat{S}_j^+ = \hat{S}_j^x + i\hat{S}_j^y$$
$$\hat{S}_j^- = \hat{S}_j^x - i\hat{S}_j^y$$

$$\hat{S}_j^+|\downarrow\rangle = |\uparrow\rangle$$
$$\hat{S}_j^+|\uparrow\rangle = 0$$
$$\hat{S}_j^-|\downarrow\rangle = 0$$
$$\hat{S}_j^-|\uparrow\rangle = |\downarrow\rangle$$

Answer of the Problem

$$\hat{H} = J\left(\hat{S}_0^x \hat{S}_1^x + \hat{S}_0^y \hat{S}_1^y + \hat{S}_0^z \hat{S}_1^z\right)$$

Matrix element $\quad {}_{\mathrm{d}}\langle I|\hat{H}|J\rangle_{\mathrm{d}} \quad (I, J = 0, 1, 2, 3)$

4 by 4 Hamiltonian matrix

$$\hat{H} \doteq J \begin{bmatrix} +1/4 & 0 & 0 & 0 \\ 0 & -1/4 & +1/2 & 0 \\ 0 & +1/2 & -1/4 & 0 \\ 0 & 0 & 0 & +1/4 \end{bmatrix}$$

total S_z is conserved

$$(\hat{S}_0^z + \hat{S}_1^z)|0\rangle_{\mathrm{d}} = -|0\rangle_{\mathrm{d}}$$
$$(\hat{S}_0^z + \hat{S}_1^z)|1\rangle_{\mathrm{d}} = 0$$
$$(\hat{S}_0^z + \hat{S}_1^z)|2\rangle_{\mathrm{d}} = 0$$
$$(\hat{S}_0^z + \hat{S}_1^z)|3\rangle_{\mathrm{d}} = |3\rangle_{\mathrm{d}}$$

Energy Spectrum of the Two Spins

Problem: Diagonalize 4 by 4 Hamiltonian matrix

$$\hat{H} \doteq J \begin{bmatrix} +1/4 & 0 & 0 & 0 \\ 0 & -1/4 & +1/2 & 0 \\ 0 & +1/2 & -1/4 & 0 \\ 0 & 0 & 0 & +1/4 \end{bmatrix}$$

Answer of the Problem: Energy Spectrum of the Two Spins

$$\hat{H} \doteq J \begin{bmatrix} +1/4 & 0 & 0 & 0 \\ 0 & -1/4 & +1/2 & 0 \\ 0 & +1/2 & -1/4 & 0 \\ 0 & 0 & 0 & +1/4 \end{bmatrix}$$

$$E = -\frac{3J}{4}, +\frac{J}{4}, +\frac{J}{4}, +\frac{J}{4}$$

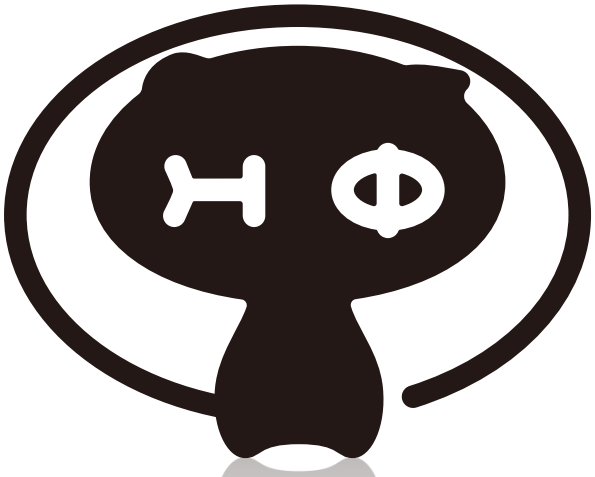
SU(2) symmetry

$$E = -\frac{3J}{4}: \quad \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle)$$

$$E = +J/4: \quad |\downarrow\rangle \otimes |\downarrow\rangle$$

$$E = +J/4: \quad \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\downarrow\rangle + |\downarrow\rangle \otimes |\uparrow\rangle)$$

$$E = +J/4: \quad |\uparrow\rangle \otimes |\uparrow\rangle$$



A Numerical Solver for Quantum Many-Body Problems: HΦ

HΦ developers:
Taka Misawa, Kazu Yoshimi, Mitsu Kawamura,
Naoki Kawashima (ISSP)
Synge Todo (Department of Physics, Utokyo)

Solvers for Quantum Many-Body Problems

TITPACK by Y. Taguchi & H. Nishimori (1985-)
Heisenberg & XXZ model

KOBEPACK by M. Kaburagi, T. Nishino, & T. Tonegawa (1992-)
-S=1 Heisenberg

SPINPACK by J. Schulenburg (1995-)
-MPI & PTHREAD
-XXZ, Hubbard, & t-J model
-Symmetries

ALPS IETL library by P. Dayal, M. Troyer, & R. Villiger

Mainly for fundamental lattice models

HΦ

For direct comparison between experiments and theory and promoting development of other numerical solvers

Numerical diagonalization package for lattice hamiltonian

-For wide range of quantum lattice hamiltonians

Ab initio effective hamiltonians

-Lanczos method [1]:

Ground state and low-lying excited states

Excitation spectra of ground state

-Thermal pure quantum (TPQ) state [2]: Finite temperatures

-Parallelization with MPI and OpenMP

[1] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994) .
[2] S. Sugiura, A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).

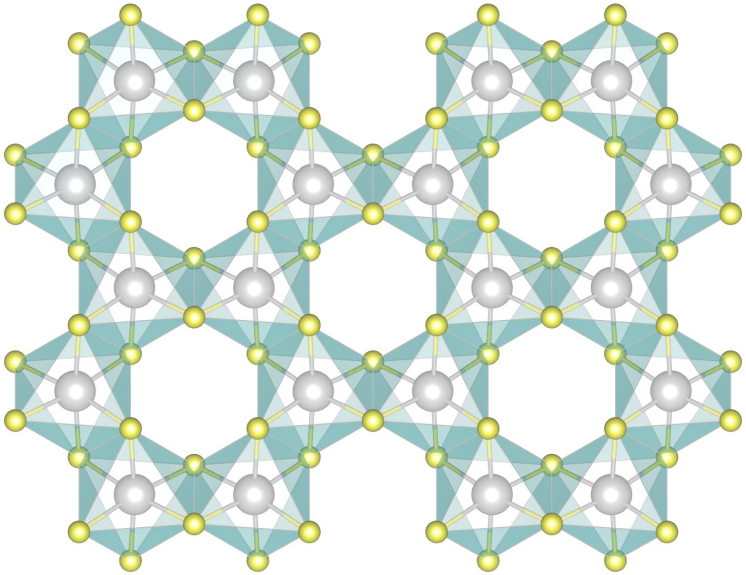
Open source program package (latest release: ver.1.2)

Licence: GNU GPL version3

An Example of *Ab Initio* Hamiltonian: Honeycomb Lattice Iridium Oxides

Na_2IrO_3 J_{eff}=1/2 Mott insulator

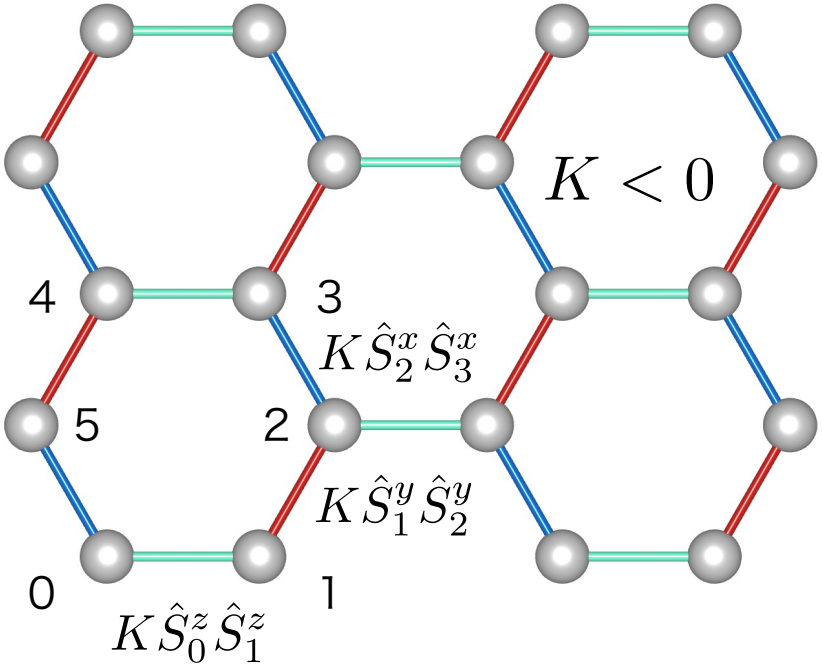
J. Chaloupka, G. Jackeli, and G.Khaliullin,
Phys. Rev. Lett. **105**, 027204 (2010)



(111)
⊙

Kitaev model

Kitaev, Annals Phys. 321, 2 (2006)



-Exactly solvable
-Majorana excitation

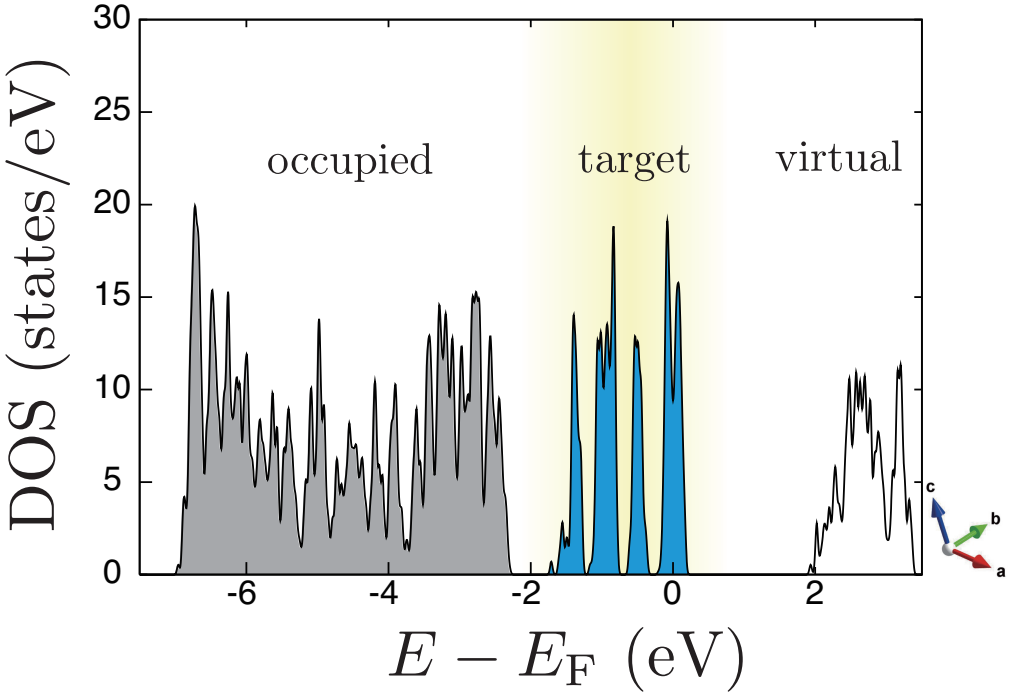
→Topological quantum computing

M. H. Freedman, *et al.*, Commun. Math. Phys. 227, 605 (2002)

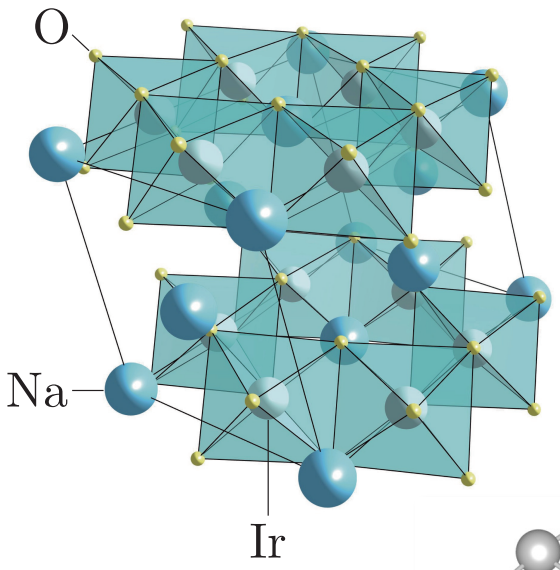
Construct *Ab Initio* Effective Hamiltonians

- Target Hilbert space expanded by localized Wannier orbitals

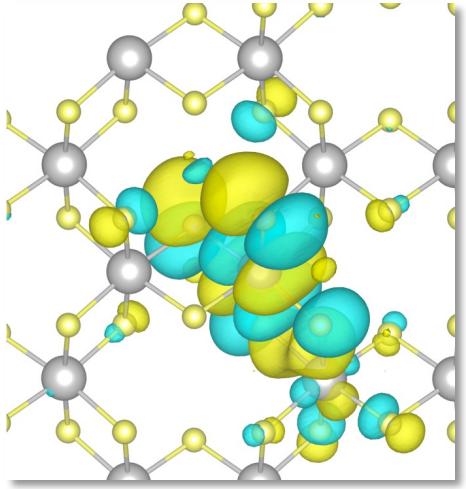
DFT result for energy spectrum



Souza-Marzari-Vanderbilt



Na_2IrO_3



- Effective Coulomb interactions in target space
  Renormalization due to
  infinite virtual particle-hole excitations
  ← Constrained random phase approximation

Imada & Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010)

Ab Initio Hamiltonian

Y. Yamaji, Y. Nomura, M. Kurita, R. Arita, & M. Imada, Phys. Rev. Lett. 113, 107201 (2014).

$$\hat{H} = \sum_{\Gamma=X,Y,Z,Z_{2\mathrm{nd}},3} \sum_{\langle \ell,m\rangle\in\Gamma} \vec{\hat{S}}_\ell^T \mathcal{J}_\Gamma \vec{\hat{S}}_m \qquad \vec{\hat{S}}_\ell^T = (\hat{S}_\ell^x, \hat{S}_\ell^y, \hat{S}_\ell^z)$$

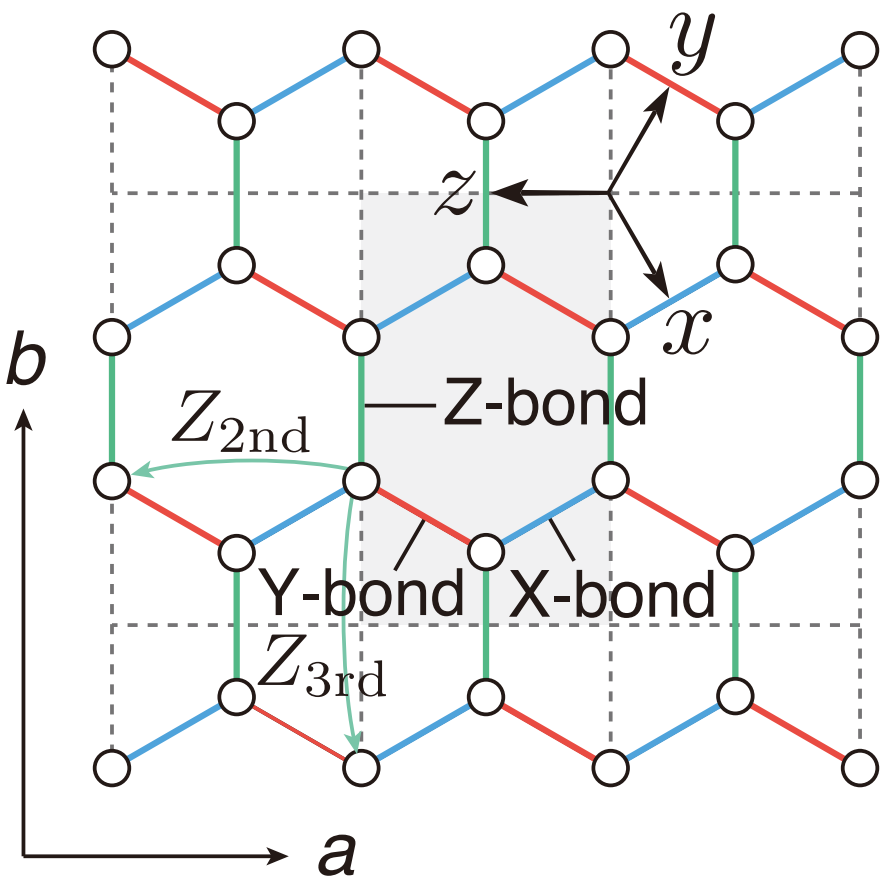
$$\mathcal{J}_X = \begin{bmatrix} \mathbf{-23.9} & -3.1 & -8.4 \\ -3.1 & 3.2 & 1.8 \\ -8.4 & 1.8 & 2.0 \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_Y = \begin{bmatrix} 3.2 & -3.1 & 1.8 \\ -3.1 & \mathbf{-23.9} & -8.4 \\ 1.8 & -8.4 & 2.0 \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_Z = \begin{bmatrix} 4.4 & -0.4 & 1.1 \\ -0.4 & 4.4 & 1.1 \\ 1.1 & 1.1 & \mathbf{-30.7} \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_{Z_{2\mathrm{nd}}} = \begin{bmatrix} -0.8 & 1.0 & -1.4 \\ 1.0 & -0.8 & -1.4 \\ -1.4 & -1.4 & -1.2 \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_3 = \begin{bmatrix} 1.7 & 0.0 & 0.0 \\ 0.0 & 1.7 & 0.0 \\ 0.0 & 0.0 & 1.7 \end{bmatrix} \text{(meV)}$$



HΦ

Solve quantum many-body problems as eigenvalue problems

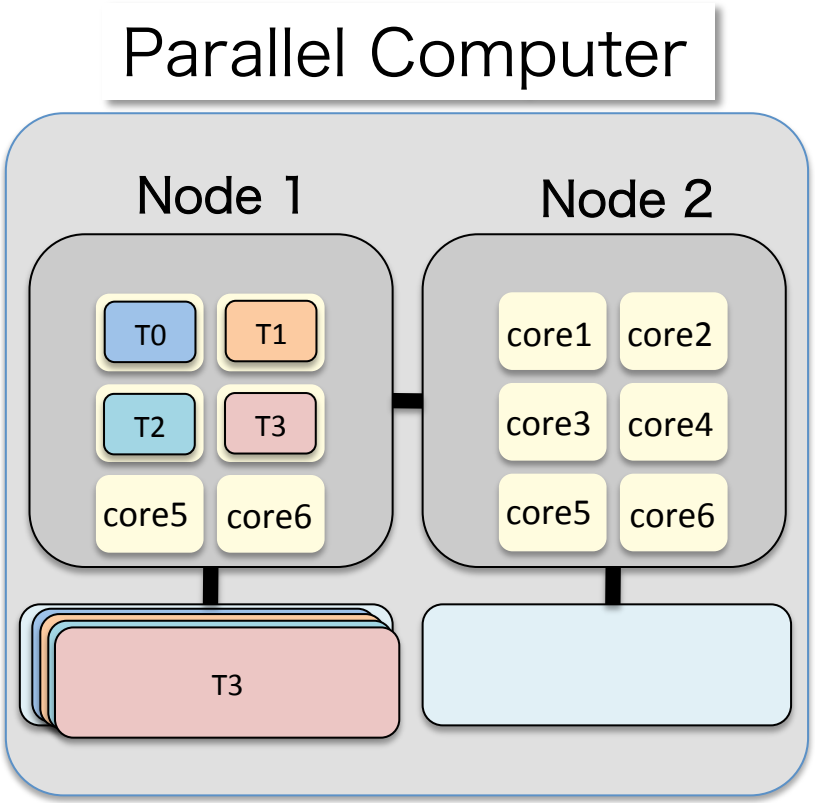
-Input 1: Definition of Hamiltonian & Fock space
-Input 2: Choose algorithm for solving Hamiltonian
○Up to few 10^4 dimensional Hamiltonian matrices
→Generating matrix and calling Lapack
Outputting matrices in Matrix Market form
○Hamiltonian matrices larger than few 10^4 dimension
→Lanczos method or TPQ
(Generating matrix element for each matrix-vector product)

Lanczos method: Up to 6.87×10^{10} dimension
@K computer & ISSP supercomputer
From 4096 32768 cores: Parallelization efficiency 80%

Parallelization

・Hybrid parallel

-Shared memory (OpenMP)
-Distributed memory (MPI)



Parallelization

- Hybrid parallel

-Shared memory (OpenMP)
-Distributed memory (MPI)

Distribution of w.f. : 2 proc.

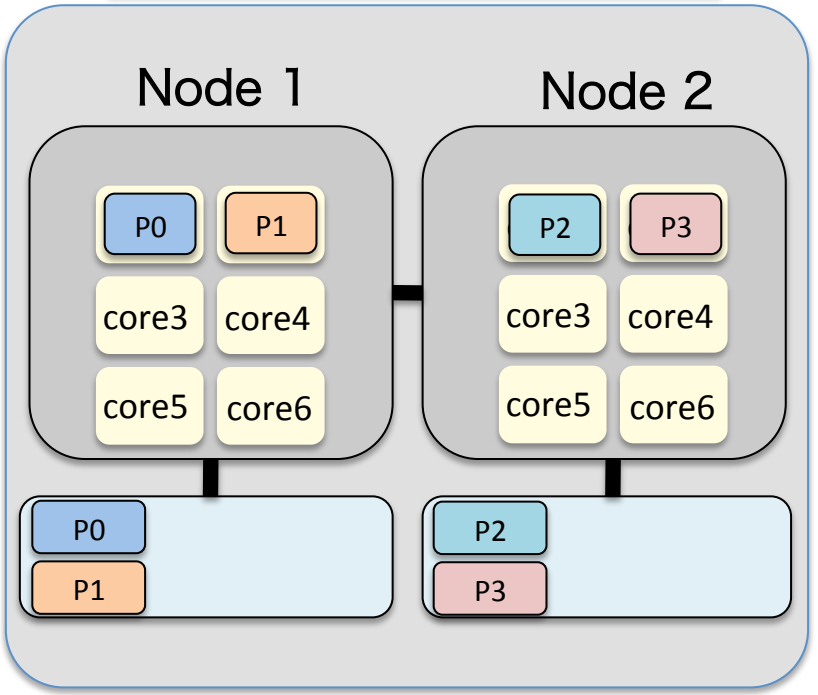
$$
\begin{aligned}
|0\rangle &= |\downarrow\downarrow\ \downarrow\rangle \\
|1\rangle &= |\uparrow\downarrow\ \downarrow\rangle \\
|2\rangle &= |\downarrow\uparrow\ \downarrow\rangle \\
|3\rangle &= |\uparrow\uparrow\ \downarrow\rangle \\
\hline
|4\rangle &= |\downarrow\downarrow\ \uparrow\rangle \\
|5\rangle &= |\uparrow\downarrow\ \uparrow\rangle \\
|6\rangle &= |\downarrow\uparrow\ \uparrow\rangle \\
|7\rangle &= |\uparrow\uparrow\ \uparrow\rangle
\end{aligned}
$$

rank 0

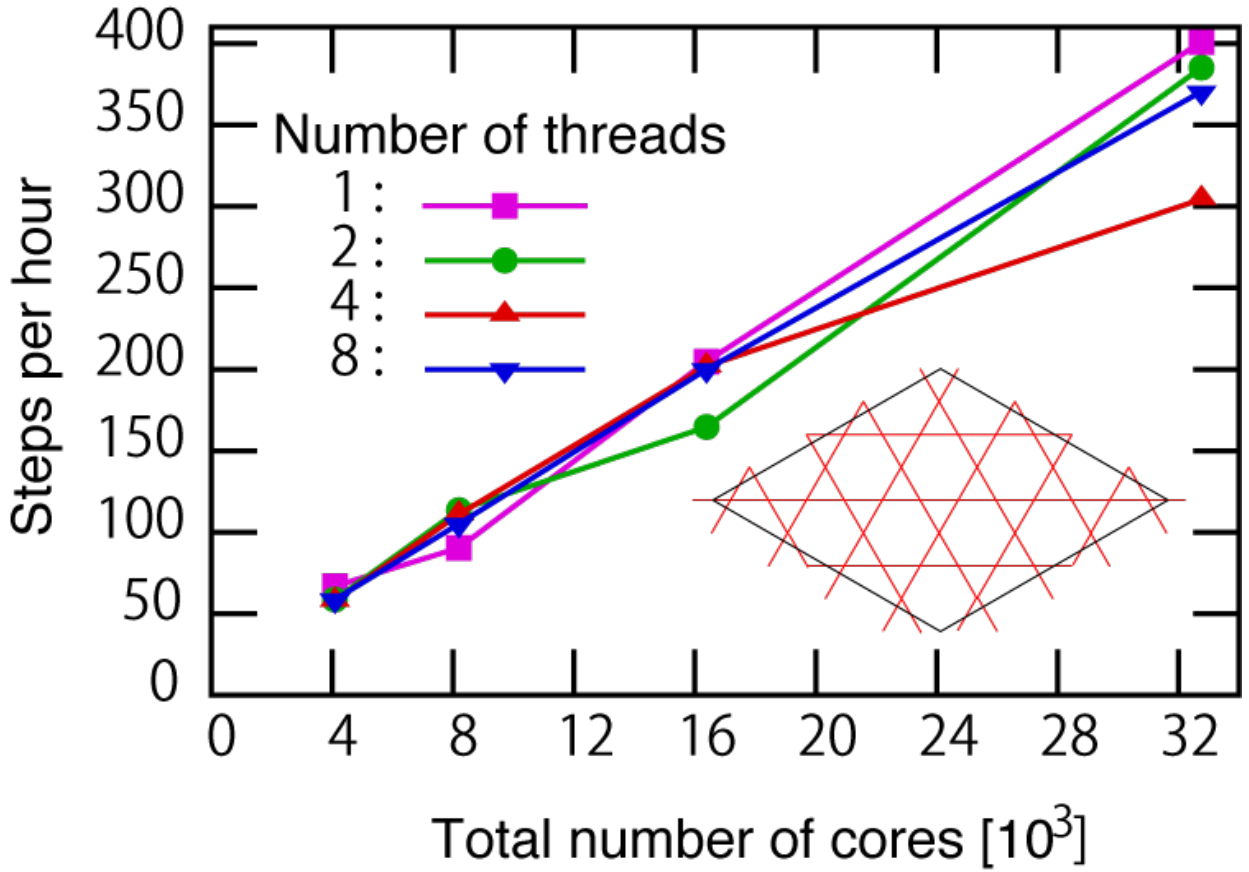
rank 1

- `Hubbard/Kondo Lattice /HubabrdGC`
  →4^n processes
- `Spin/SpinGC`
  →$(2S+1)^n$ processes

Parallel Computer



Speedup



Lanczos method: Up to 6.87×10^{10} dimension

@K computer & ISSP supercomputer

From 4096 32768 cores: Parallelization efficiency 80%

HΦ as a bridge between Many-Body Physics and Applied Mathematics

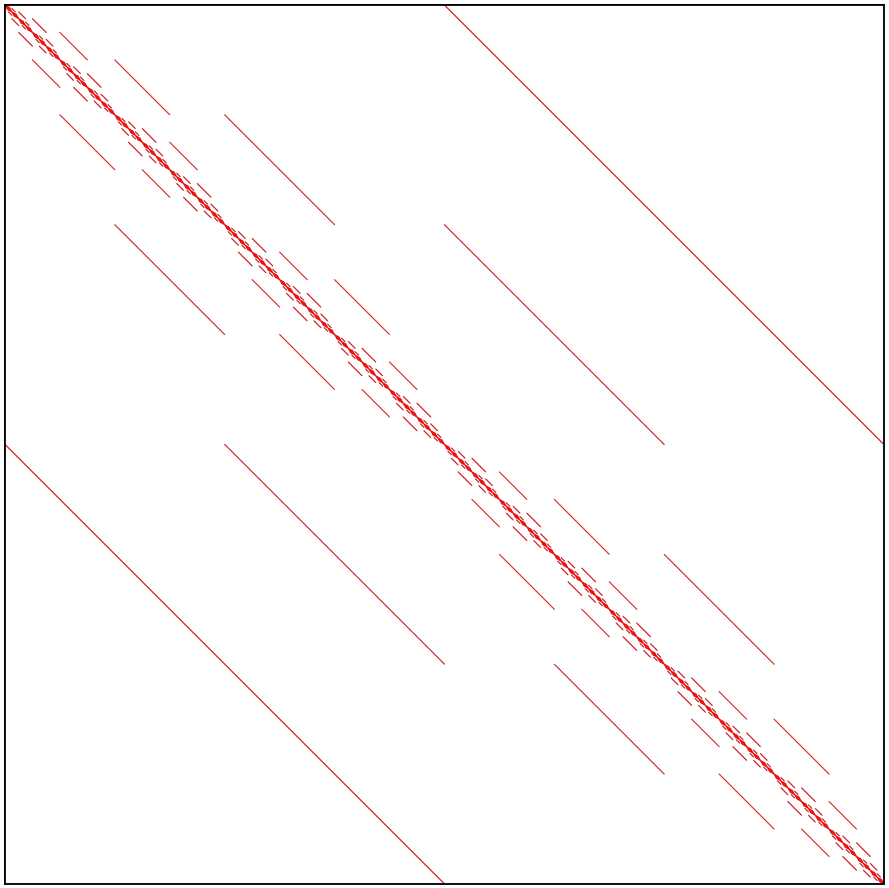
Generating Sparse Matrix

Hamiltonian matrix $H_{II'} = \langle I|\hat{H}|I'\rangle$

N=14 qubits
(1 4 site 1 dimensional Heisenberg)

$$\hat{H} = +J \sum_{j=0}^{N-1} \sum_{a=x,y,z} \hat{S}_j^a \hat{S}_{\mathrm{mod}(j+1,N)}^a$$

-2^{14}=16,384D symmetric
-# of nonzero elements:
73,728

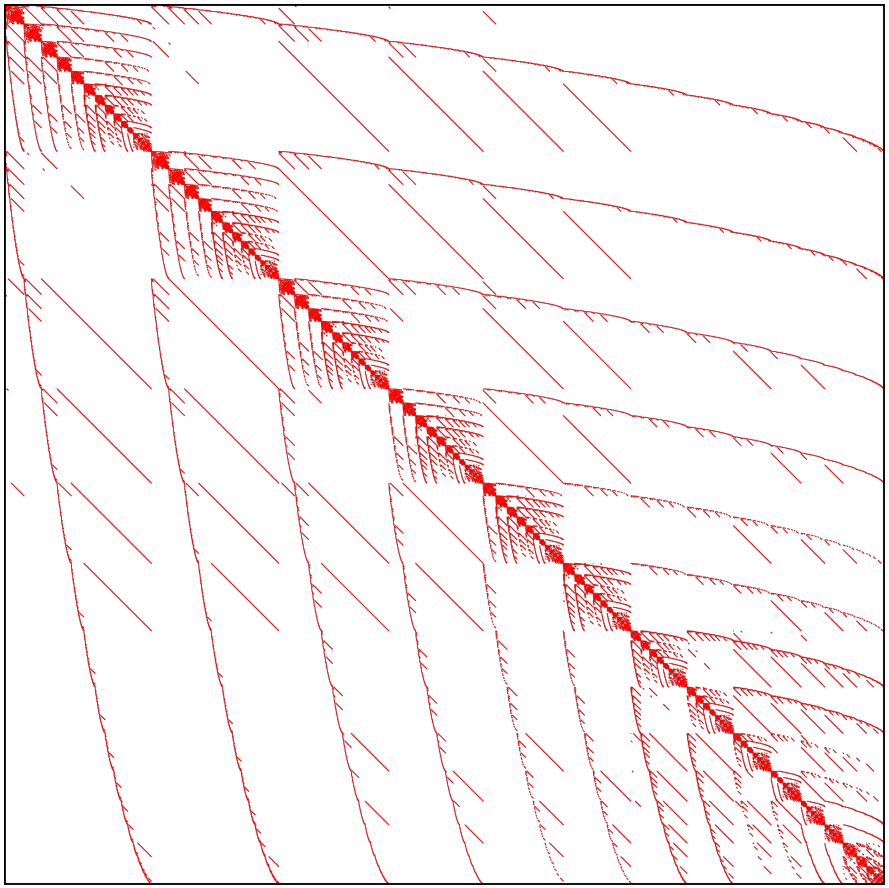


Generating Sparse Matrix

Hamiltonian matrix $H_{II'} = \langle I|\hat{H}|I'\rangle$

Example:
Iridium oxygen cluster
-Hubbard-type model
-Complex elements
due to relativistic SOC

-10,626D Hermitian
-# of nonzero elements:
159,946



Simulating Spectroscopy Measurements

Spectroscopy (分光): 物性物理学の実験手段
対象に振動数ωの電場や磁場などの摂動を
加えることで生じた電流や磁化(応答)を観測する

基底状態(絶対零度の多体状態)の応答

基底状態:
Lanczos法によって求めた最小固有値の固有ベクトル $|\psi\rangle$

Simulating Spectroscopy Measurements

Spectroscopy (分光): 物性物理学の実験手段
対象に振動数ωの電場や磁場などの摂動を
加えることで生じた電流や磁化(応答)を観測する

応答 $$G_{\hat{O}}(z) = \langle\psi|\hat{O}^\dagger(z\mathbf{1} - \hat{H})^{-1}\hat{O}|\psi\rangle$$

$$z \to \omega \quad (z \in \mathbb{C},\ \omega \in \mathbb{R})$$

摂動と応答の例:
量子ビットに磁場を加えた場合の磁化

$$\hat{H}_{\mathrm{ex}} = e^{i\omega t} B_z \left(\frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^z \right) \qquad \hat{O} = \frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^z$$

Excitation Spectra (HΦ ver.1.2)

Lanczos steps with initial vector defined as

$|\phi_0\rangle = \hat{O}|\psi\rangle / \sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle}$ (multiplying excitation operator to g.s.)

Lanczos' tridiagonal matrix

$$z\mathbf{1} - H \doteq z\mathbf{1} - H_{\rm td} = \begin{bmatrix} z-\alpha_0 & -\beta_1 & 0 & 0 & \cdots \\ -\beta_1 & z-\alpha_1 & -\beta_2 & 0 & \cdots \\ 0 & -\beta_2 & z-\alpha_2 & -\beta_3 & \\ 0 & 0 & -\beta_3 & z-\alpha_3 & \\ \vdots & \vdots & & & \ddots \end{bmatrix}$$

→Excitation Spectrum

$$\langle\psi|\hat{O}^\dagger(z\mathbf{1}-\hat{H})^{-1}\hat{O}|\psi\rangle = \sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle}\left\{(z\mathbf{1}-H)^{-1}\right\}_{00}$$

$$= \cfrac{\sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle}}{z-\alpha_0-\cfrac{\beta_1^2}{z-\alpha_1-\cfrac{\beta_2^2}{z-\alpha_2-\cdots}}}$$

Problems: How to estimate truncation errors

Shifted Krylov Subspace Method for Excitation Spectra

Green's function $G_{\hat{O}}(z) = \langle\psi|\hat{O}^\dagger(z\mathbf{1} - \hat{H})^{-1}\hat{O}|\psi\rangle$

$$z \to \omega \quad (z \in \mathbb{C},\ \omega \in \mathbb{R})$$

Liner equations

$$(z\mathbf{1} - H)\vec{x} = \vec{b} \qquad \vec{b} \doteq \hat{O}|\psi\rangle$$

$$\Rightarrow G_{\hat{O}}(z) = \vec{b}^\dagger\vec{x} \qquad \vec{x} \doteq (z\mathbf{1} - \hat{H})^{-1}\hat{O}|\psi\rangle$$

←Solvable by Shifted Krylov subspace method

A. Frommer (1995, 2003)

T. Sogabe, T. Hoshi, S. L. Zhang, and T. Fujiwara, *A numerical method for calculating the Green's function arising from electronic structure theory*, In Frontiers of Computational Science. pp.189-195, 2007.

→Stable and controlled convergence

Shifted Krylov Subspace Method for Excitation Spectra

-Shift invariance of Krylov subspace

-Residual vector

$$(z\mathbf{1} - H)\vec{x} = \vec{b}$$

$$\vec{r}_n = \vec{b} - (z\mathbf{1} - H)\vec{x}_n$$

-Seed switch

S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang, & T. Fujiwara,
J. Phys. Soc. Jpn. 77, 114713 (2008).

Kω library (released) by Dr. Kawamura

Ab Initio Hamiltonian

Y. Yamaji, Y. Nomura, M. Kurita, R. Arita, & M. Imada, Phys. Rev. Lett. 113, 107201 (2014).

$$\hat{H} = \sum_{\Gamma=X,Y,Z,Z_{\rm 2nd},3} \sum_{\langle \ell,m\rangle\in\Gamma} \vec{\hat{S}}_\ell^T \mathcal{J}_\Gamma \vec{\hat{S}}_m \qquad \vec{\hat{S}}_\ell^T = (\hat{S}_\ell^x, \hat{S}_\ell^y, \hat{S}_\ell^z)$$

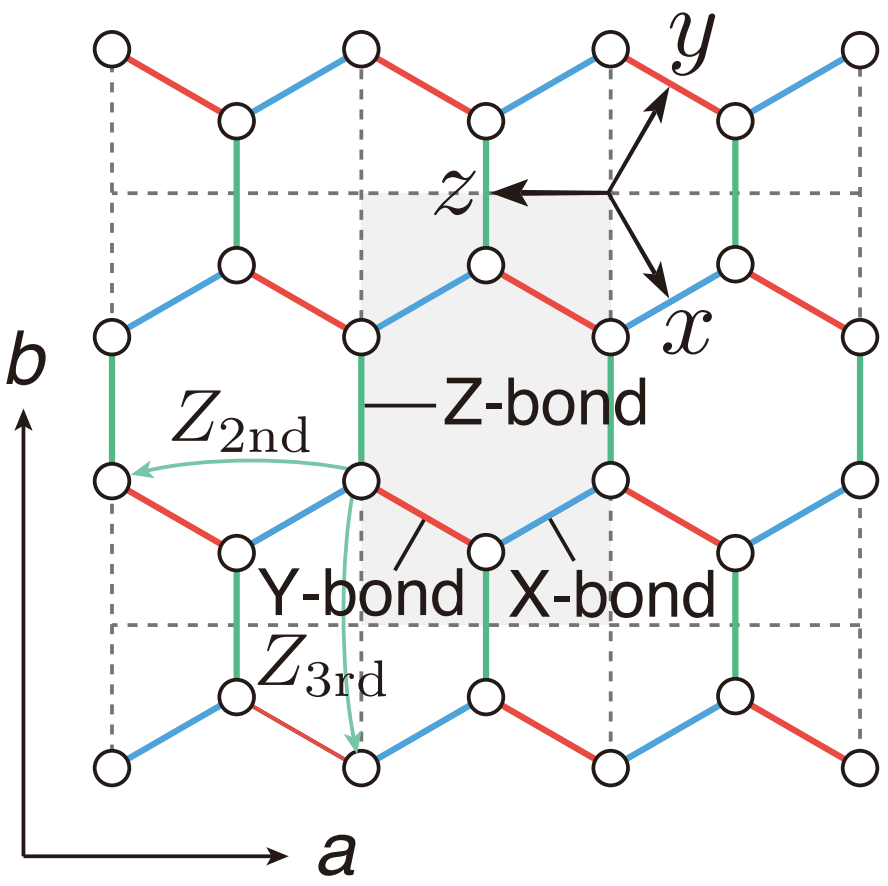
$$\mathcal{J}_X = \begin{bmatrix} \mathbf{-23.9} & -3.1 & -8.4 \\ -3.1 & 3.2 & 1.8 \\ -8.4 & 1.8 & 2.0 \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_Y = \begin{bmatrix} 3.2 & -3.1 & 1.8 \\ -3.1 & \mathbf{-23.9} & -8.4 \\ 1.8 & -8.4 & 2.0 \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_Z = \begin{bmatrix} 4.4 & -0.4 & 1.1 \\ -0.4 & 4.4 & 1.1 \\ 1.1 & 1.1 & \mathbf{-30.7} \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_{Z_{\rm 2nd}} = \begin{bmatrix} -0.8 & 1.0 & -1.4 \\ 1.0 & -0.8 & -1.4 \\ -1.4 & -1.4 & -1.2 \end{bmatrix} \text{(meV)}$$

$$\mathcal{J}_3 = \begin{bmatrix} 1.7 & 0.0 & 0.0 \\ 0.0 & 1.7 & 0.0 \\ 0.0 & 0.0 & 1.7 \end{bmatrix} \text{(meV)}$$



Interpolation between Kitaev and *Ab initio*

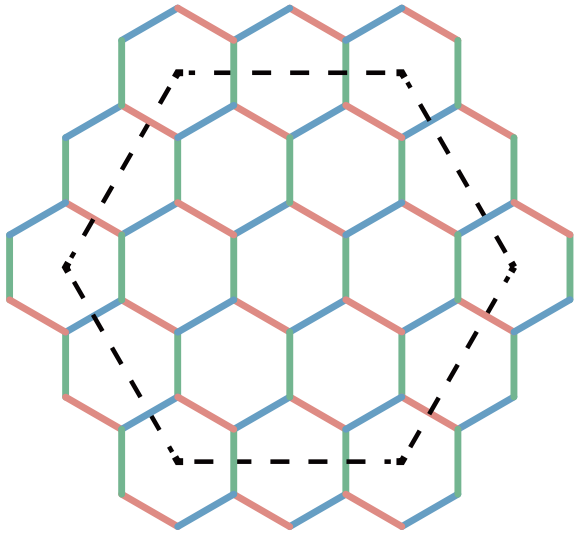
$$\mathcal{J}_X = \begin{bmatrix} K' & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \lambda \begin{bmatrix} 0 & I_2'' & I_2' \\ I_2'' & J'' & I_1' \\ I_2' & I_1' & J' \end{bmatrix}$$

$$\mathcal{J}_Y = \begin{bmatrix} 0 & 0 & 0 \\ 0 & K' & 0 \\ 0 & 0 & 0 \end{bmatrix} + \lambda \begin{bmatrix} J'' & I_2'' & I_1' \\ I_2'' & 0 & I_2' \\ I_1' & I_2' & J' \end{bmatrix}$$

$$\mathcal{J}_Z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & K \end{bmatrix} + \lambda \begin{bmatrix} J & I_1 & I_2 \\ I_1 & J & I_2 \\ I_2 & I_2 & 0 \end{bmatrix}$$

$$\mathcal{J}_2 = \lambda \begin{bmatrix} J^{(2\mathrm{nd})} & I_1^{(2\mathrm{nd})} & I_2^{(2\mathrm{nd})} \\ I_1^{(2\mathrm{nd})} & J^{(2\mathrm{nd})} & I_2^{(2\mathrm{nd})} \\ I_2^{(2\mathrm{nd})} & I_2^{(2\mathrm{nd})} & K^{(2\mathrm{nd})} \end{bmatrix}$$

$$\mathcal{J}_3 = \lambda \begin{bmatrix} J^{(3\mathrm{rd})} & 0 & 0 \\ 0 & J^{(3\mathrm{rd})} & 0 \\ 0 & 0 & J^{(3\mathrm{rd})} \end{bmatrix}$$

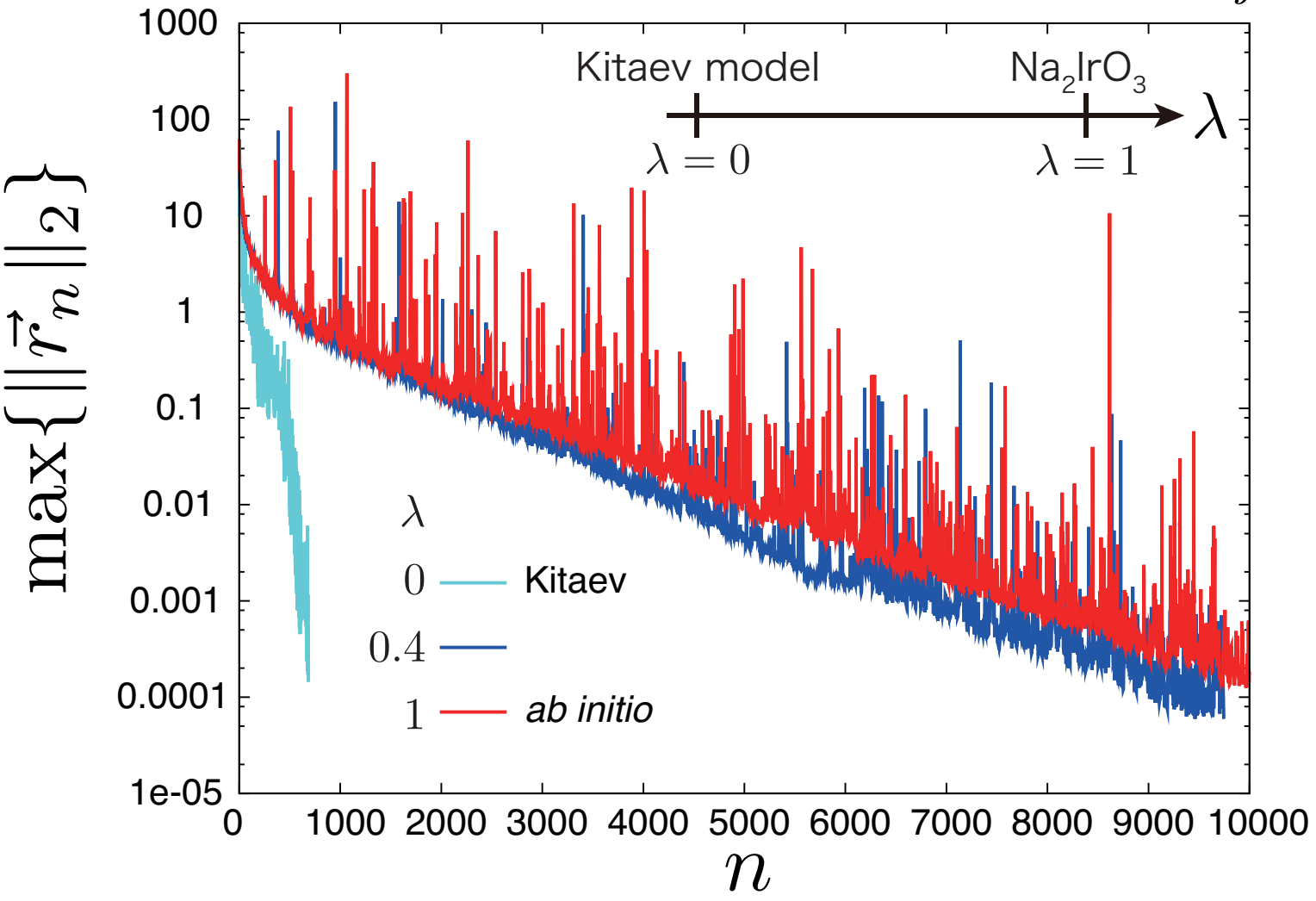


$2^{24} \sim 1.68 \times 10^7$ dimensional

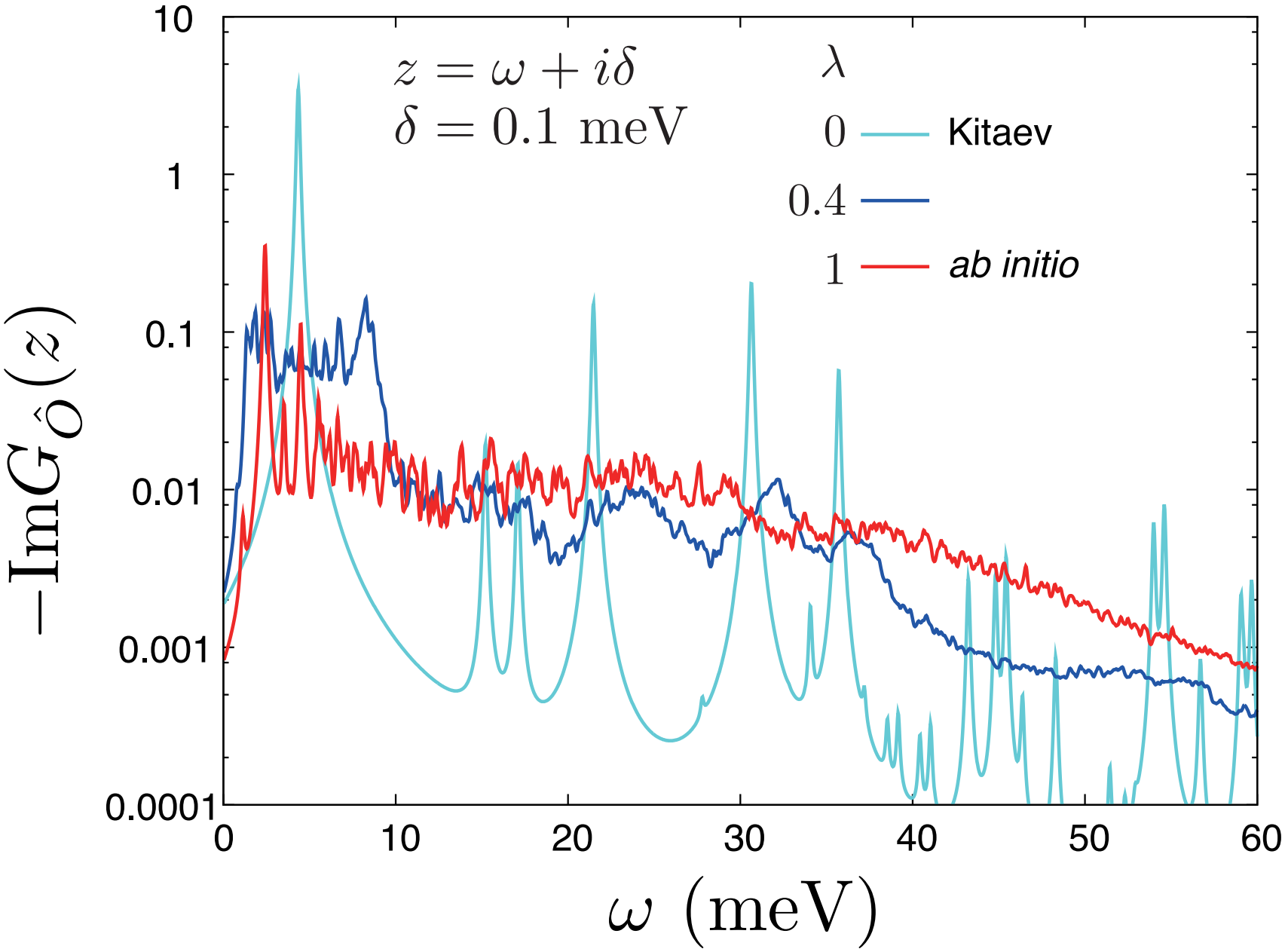
2-Norm of Residual Vector

Strong parameter dependence
in convergence of S(Q,ω) with sBiCG

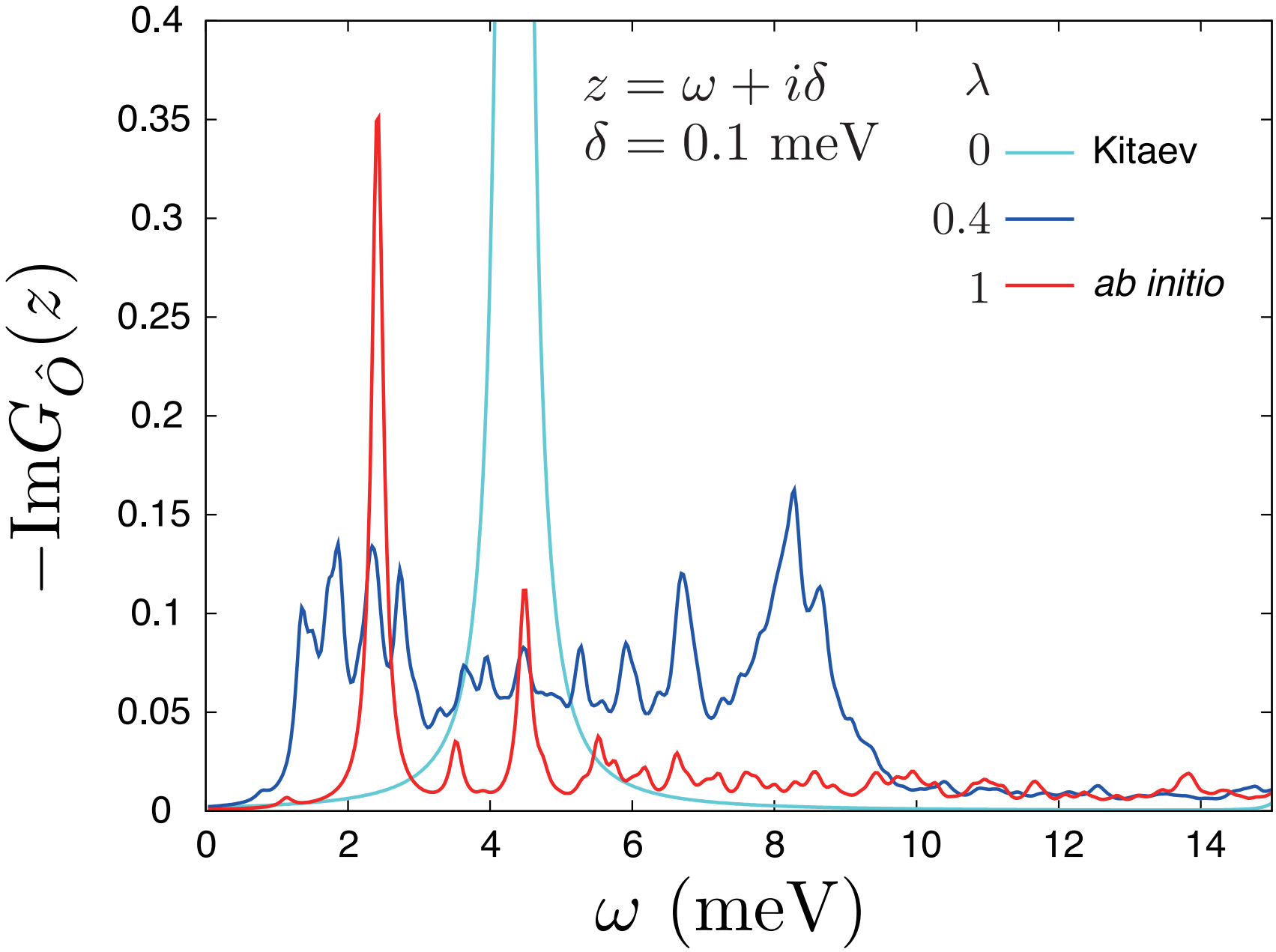
$$\hat{O} = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \hat{S}_j^z$$



Excitation Spectra



Excitation Spectra



Summary & Discussion

-Numerical solver HΦ for quantum lattice Hamiltonian

-HΦ as a bridge between
cond. matt. physics and applied mathematics

HΦ generates sparse Hamiltonian matrices
up to hundreds billion dimensions

HΦ ver.2

- Subroutine `multiply`
- Libraries with RCI

`Input:` $|\Phi\rangle$
`Output:` $\hat{H}|\Phi\rangle$

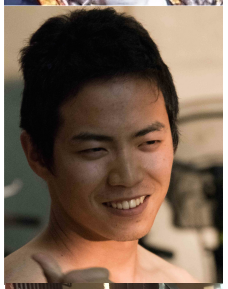
⇄ CMP

⇄ AM

Example: Library for shifted Krylov subspace method
By Dr. Kawamura in collaboration with Prof. Hoshi & Prof. Sogabe

チームHΦ (敬称略、順不同)

三澤貴宏
東京大学物性研究所



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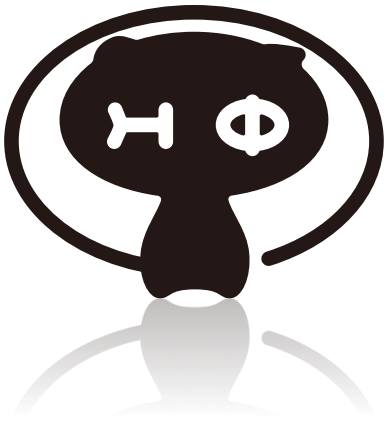
鳥取大学大学院
工学研究科

曽我部知広
名古屋大学大学院
工学研究科



HΦでできること: 計算手法

・計算手法

Imada & Takahashi (1986)
Jaklic & Prelovsek (1994)
Hams & De Raedt (2000)

有限温度計算:
カノニカル平均を典型的な波動関数による期待値で置き換える

Imada & Takahashi (1986)

$$1)\,|\Phi_0\rangle = \frac{1}{\sqrt{Z}}\sum_m |\phi_m\rangle \simeq (\text{random vector})$$

$$(\hat{H}\,|\phi_m\rangle = E_m\,|\phi_m\rangle)$$

$$2)\,|\Phi_T\rangle = e^{-\frac{\beta}{2}\hat{H}}\,|\Phi_0\rangle\,/\sqrt{\langle\Phi_0|\,e^{-\beta\hat{H}}\,|\Phi_0\rangle}$$

$$\Rightarrow\langle\Phi_T|\,\hat{O}\,|\Phi_T\rangle = \sum_m e^{-\beta E_m}\,\langle\phi_m|\,\hat{O}\,|\phi_m\rangle\,/Z$$

$$\text{for } [\hat{H},\hat{O}] = 0$$

HΦでできること: 計算手法

・計算手法

有限温度計算:
カノニカル平均を典型的な波動関数による期待値で置き換える

Replacing canonical ensemble with *typical* wave functions

Thermal Pure Quantum (TPQ) States

Sugiura & Shimizu, PRL 108, 240401 (2012)

Initial state (at $T = +\infty$): $|\Phi_0\rangle = (\mathrm{Random\ vector})$

If possible, taking random average

do k=1,N_{step}

$$|\Phi_k\rangle = (\ell - \hat{H})\,|\Phi_{k-1}\rangle \,/\sqrt{\langle\Phi_{k-1}|\,(\ell - \hat{H})^2\,|\Phi_{k-1}\rangle}$$

$$u_k = \langle\Phi_k|\,\hat{H}\,|\Phi_k\rangle$$

$$\beta = 2(k/N)/(\ell - u_k) \quad (\beta = 1/k_{\mathrm{B}}T)$$

$$\overline{O}(\beta) = \langle\Phi_k|\,\hat{O}\,|\Phi_k\rangle + \mathcal{O}(1/N) \quad \text{even for } [\hat{H},\hat{O}] \neq 0$$

enddo

HΦをどう使うか

・計算モード

-スタンダード・モード

Output

Lanczos	$\langle H \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} c^\dagger_{k\sigma_3} c_{\ell\sigma_4} \rangle$
TPQ	$1/T,\ \langle H \rangle,\ \langle H^2 \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} c^\dagger_{k\sigma_3} c_{\ell\sigma_4} \rangle$
Full Diag	$\langle H \rangle,\ \langle n_{i\uparrow} n_{i\downarrow} \rangle,\ \langle (\sum_i \vec{S}_i)^2 \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} \rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} c^\dagger_{k\sigma_3} c_{\ell\sigma_4} \rangle$

HΦをどう使うか

・計算モード

-エキスパート・モード

$$H = \sum_{i,j} \sum_{\sigma_1,\sigma_2} t_{i\sigma_1 j\sigma_2} c^{\dagger}_{i\sigma_1} c_{j\sigma_2} + \sum_{i,j,k,\ell} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{i\sigma_1 j\sigma_2;k\sigma_3\ell\sigma_4} c^{\dagger}_{i\sigma_1} c_{j\sigma_2} c^{\dagger}_{k\sigma_3} c_{\ell\sigma_4}$$

Keyword & input file name list	`namelist.def`	
Parameter files for definition of model	`zInterAll.def`	$I_{i\sigma_1 j\sigma_2;k\sigma_3\ell\sigma_4}$
	`zTrans.def`	$t_{i\sigma_1 j\sigma_2}$
	`zlocspn.def`	(To specify local spins)
Parameter files for calculation	`modpara.def`	
	`calcmod.def`	
List of Green functions to be output	`greenone.def`	$\langle c^{\dagger}_{i\sigma_1} c_{j\sigma_2} \rangle$
	`greentwo.def`	$\langle c^{\dagger}_{i\sigma_1} c_{j\sigma_2} c^{\dagger}_{k\sigma_3} c_{\ell\sigma_4} \rangle$

計算実行

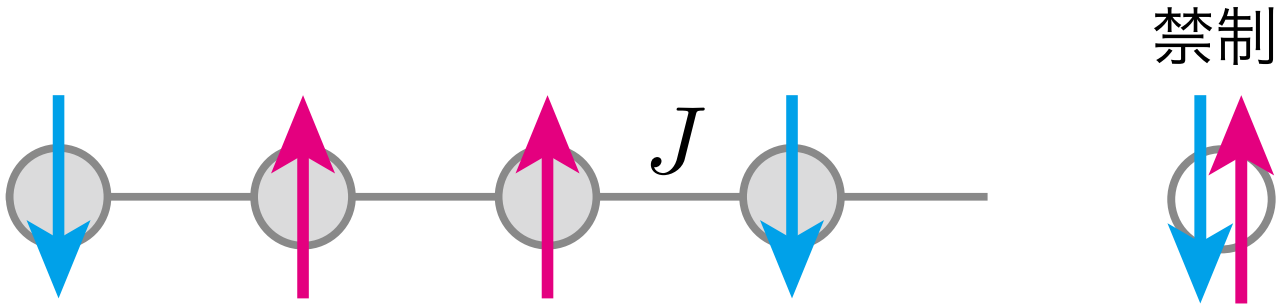
```
PATH/HPhi -e namelist.def
mpirun -np xx PATH/HPhi -e namelist.def
```

HΦでできること: 量子格子模型

・計算できる系

局在スピン系: Heisenberg-type model

$$H = -h\sum_{i=1}^{N} S_i^z + \Gamma\sum_i S_i^x + D\sum_i S_i^z S_i^z + \sum_{i,j}\sum_{\alpha,\beta=x,y,z} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta$$



`Spin:` トータルS_z保存
`SpinGC:` トータルS_z非保存

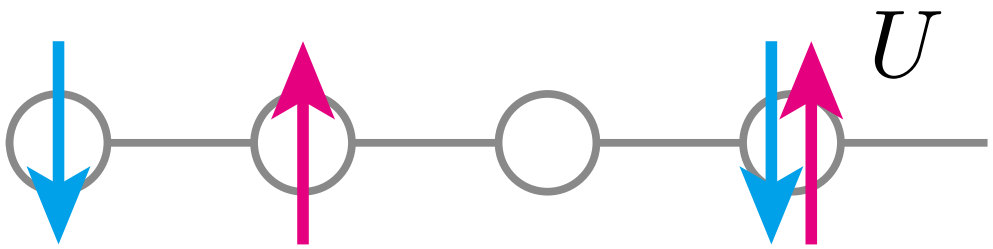
$S > 1/2$にも対応

HΦでできること: 量子格子模型

・計算できる系

遍歴電子系: Hubbard-type model

$$H = -\mu \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{i \neq j} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j} V_{ij} n_i n_j$$



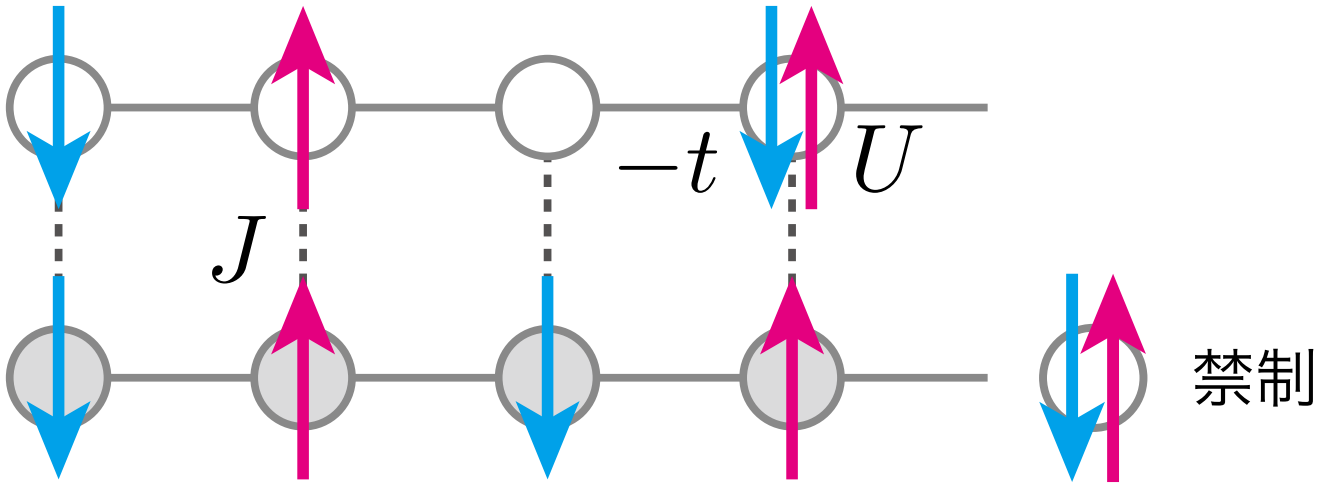
`Fermion Hubbard:` 粒子数・トータルS_z保存
`HubbardNConserved:` 粒子数保存・トータルS_z非保存
`Fermion HubbardGC:` 粒子数・トータルS_z非保存

HΦでできること: 量子格子模型

・計算できる系

局在スピン系: Kondo-lattice-type model

$$H = -\mu \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{J}{2} \sum_{i=1}^{N} \left\{ S_i^{+} c_{i\downarrow}^{\dagger} c_{i\uparrow} + S_i^{-} c_{i\uparrow}^{\dagger} c_{i\downarrow} + S_i^{z} (n_{i\uparrow} - n_{i\downarrow}) \right\}$$



Kondo Lattice: 粒子数・トータルS_z保存

Kondo LatticeGC: 粒子数・トータルS_z非保存

HΦをどう使うか

・計算モード

-エキスパート・モード

$$H = \sum_{i,j} \sum_{\sigma_1,\sigma_2} t_{i\sigma_1 j\sigma_2} c^{\dagger}_{i\sigma_1} c_{j\sigma_2} + \sum_{i,j,k,\ell} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{i\sigma_1 j\sigma_2;k\sigma_3\ell\sigma_4} c^{\dagger}_{i\sigma_1} c_{j\sigma_2} c^{\dagger}_{k\sigma_3} c_{\ell\sigma_4}$$

Keyword & input file name list	`namelist.def`	
Parameter files for definition of model	`zInterAll.def`	$I_{i\sigma_1 j\sigma_2;k\sigma_3\ell\sigma_4}$
	`zTrans.def`	$t_{i\sigma_1 j\sigma_2}$
	`zlocspn.def`	(To specify local spins)
Parameter files for calculation	`modpara.def`	
	`calcmod.def`	
List of Green functions to be output	`greenone.def`	$\langle c^{\dagger}_{i\sigma_1} c_{j\sigma_2} \rangle$
	`greentwo.def`	$\langle c^{\dagger}_{i\sigma_1} c_{j\sigma_2} c^{\dagger}_{k\sigma_3} c_{\ell\sigma_4} \rangle$

計算実行

```
PATH/HPhi -e namelist.def
mpirun -np xx PATH/HPhi -e namelist.def
```

How to Get and Install HΦ

Q. Where can you get HΦ ?
A. Materiapps or Github

http://ma.cms-initiative.jp/en/application-list/hphi?set_language=en
https://github.com/QLMS/HPhi

Q. What does HΦ require?
A. C compiler and Lapack.
If you have MPI library, you can enjoy larger simulation

How to Use HΦ

・We have 2 modes of preparing input files

-Standard mode

`StdFace.def` for 1D S=1/2 Heisenberg model

```
L = 16                          System size
model = "Spin"                  Model
method = "Lanczos"              Method
lattice = "Chain Lattice"       Lattice
J = 1.0                         Exchange coupling
2Sz = 0                         Total Sz
2S = 1                          Size of spin
```

Execution

```
PATH/HPhi -s StdFace.def
mpirun -np xx PATH/HPhi -s StdFace.def (xx: # of process)
```

How to Use HΦ

- Parameters in `StdFace.def`

```
model:
Fermion Hubbard
Fermion HubbardGC
Spin
SpinGC
Kondo Lattice

method:
Lanczos
TPQ
Full Diag

lattice:
Chain Lattice
Square Lattice
Triangular Lattice
Honeycomb Lattice
Kagome Lattice
Ladder
& more
```

Periodic boundary condition!