

HΦの概要

-プログラムとアルゴリズム-

Overview of HΦ: Program & Algorithm

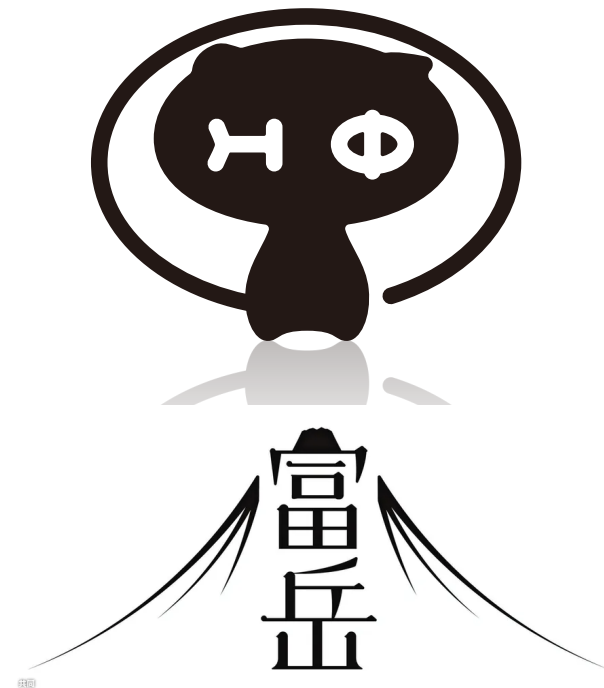
山地 洋平

物質・材料研究機構 エネルギー・環境材料研究拠点

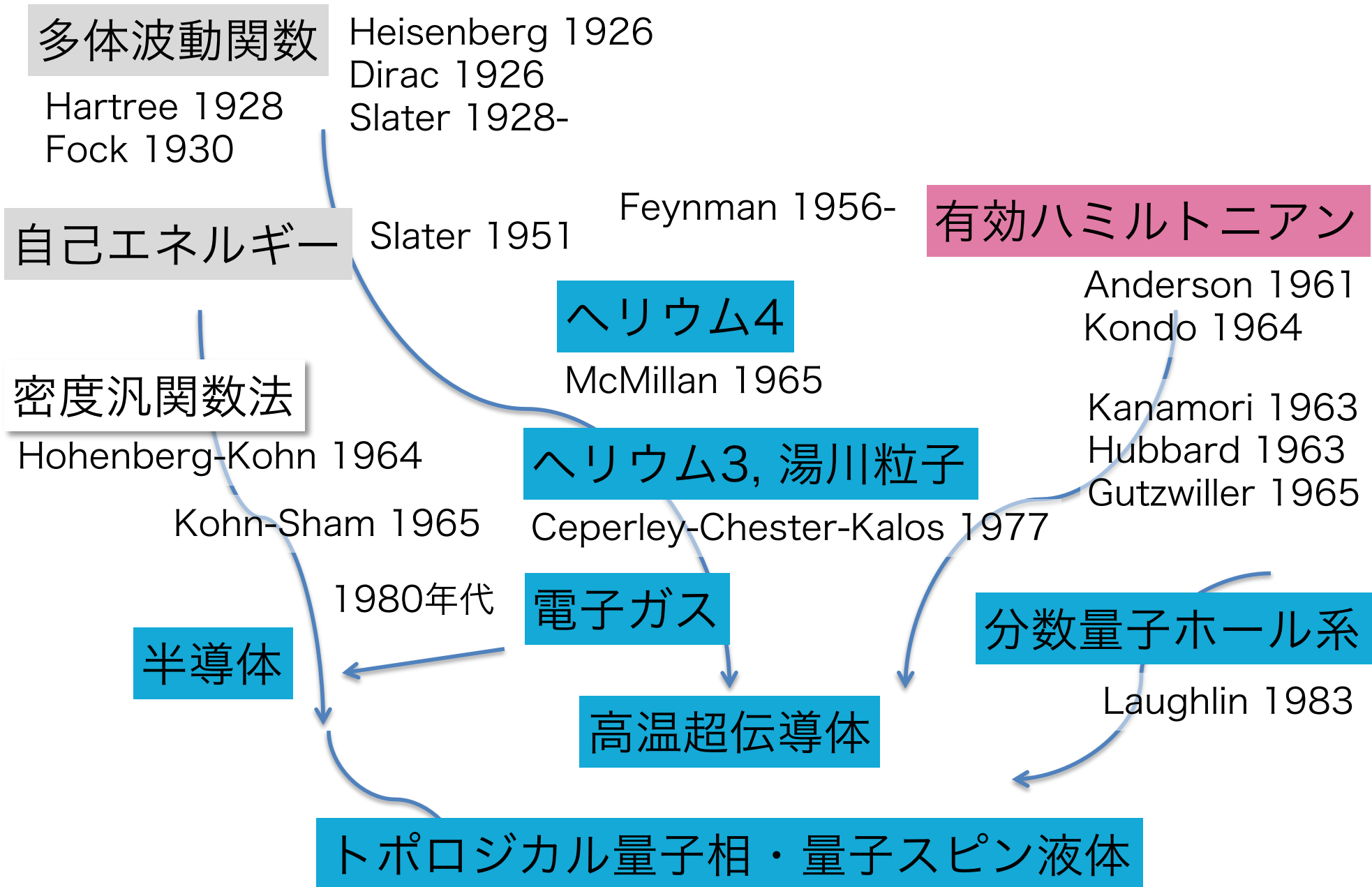
Youhei Yamaji

*Center for Green Research on Energy and Environmental Materials,
National Institute for Materials Science*

1. HΦとは
2. 何故対角化？
3. HΦが扱えるハミルトニアン
4. 並列化
5. アルゴリズム紹介



私見: 多体電子系の研究の流れ



私見: 理論から見た多体電子系研究

多体波動関数

Heisenberg 1926
Dirac 1926
Slater 1928-

Hartree 1928
Fock 1930

自己エネルギー Slater 1951

多体摂動論

Bohm-Pines 1953
Gell-Mann-Brueckner 1957
Hedin 1965

Feynman 1956-

ヘリウム4

McMillan 1965

密度汎関数法

Hohenberg-Kohn 1964
Kohn-Sham 1965

ヘリウム3, 湯川粒子

Ceperley-Chester-Kalos 1977

電子ガス

1980年代

基底の精度とソルバーの精度

基底の精度

有効ハミルトニアンをどう構成するのか

例1) Gaussianの基底セット

例2) 平面波基底のカットオフ

例3) 低エネルギー有効ハミルトニアン導出法

ソルバーの精度

有効ハミルトニアンをどう解くのか

例1) ハートリー-フォック近似

例2) 密度汎関数理論

例3) 多体摂動論

例4) 波動関数法 (CI, CC, モンテカルロ法, …)

2つの観点から精度の収束を図る必要がある

基底の選び方と問題サイズの例

典型的な基底の選び方が分野ごとにある

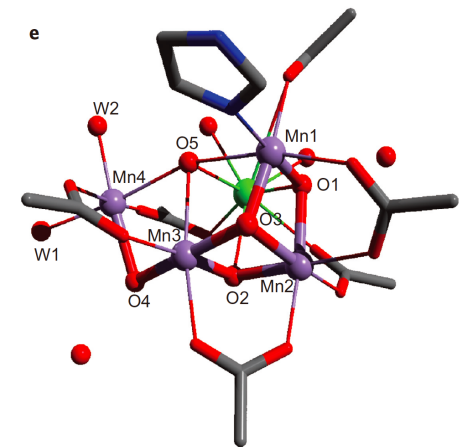
Examples of finite size systems from chemistry

-A H₂O molecule: 5 ↑ & 5 ↓ electrons in 41 orbitals
→ 5.6 x 10¹¹ dimensional (~2³⁹)

G. K.-L. Chan & M. Head-Gordon, J. Chem. Phys. 118, 8551 (2003).

-Manganese cluster in photosystem II:
44 electrons in 35 orbitals
→ 2 x 10¹⁸ dimensional (~2⁶¹)

Y. Kurashige, G. K.-L. Ghan, & T. Yanai, Nat. Chem. 5, 660 (2013).



数値対角化が用いられてきた重要な例

分数量子ホール効果

分数量子ホール効果

D. C. Tsui, *et al.*, Phys. Rev. Lett. 48, 1559 (1982).

R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).

F. D. M. Haldane, Phys. Rev. Lett. 55, 2095 (1985).

ラフリンの波動関数の精度を検証

孤立量子系の熱化

M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008).

孤立量子系の時間発展を長時間追っていった結果

HΦとは

量子格子模型の数値厳密対角化法は、量子多体問題、とくに強相関電子系の数値的研究を行う際の最も基本的な手法です。西森秀稔教授(東京工業大学)が開発された量子スピン模型に対する先駆的な数値対角化パッケージTITPACK[1]は、その公開以来20年以上にわたって幅広いユーザーに利用されてきました。

HΦはTITPACKに代わる並列計算機対応数値対角化パッケージを目指して開発されました。遍歴電子系を含む幅広い量子格子模型に柔軟に適用でき、さらに高並列に対応するソフトウェアです。2015/2016/2017年度東大物性研ソフトウェア開発・高度化支援[2]を受け開発を進めています。

[1] http://www.stat.phys.titech.ac.jp/~nishimori/titpack2_new/index-e.html

[2] <http://www.issp.u-tokyo.ac.jp/supercom/rsayh2/softwea-dev>

定量物性予測から オープンソースソフトウェアへ



量子格子模型ソルバーHΦ

実験と理論の直接比較を目指して

-広汎な多体量子系に対応

第一原理有効ハミルトニアン

-絶対零度[1,2]/有限温度[3]/有限周波数[1]の物理量計算

磁化, 比熱, 非弾性中性子/X線散乱スペクトル, …

-非平衡ダイナミクス

-大規模並列計算機対応

数理的基礎: 応用数理手法による情報圧縮

オープンソースソフトウェア (latest release: ver.3.5.0)

License: GNU GPL version3

Project for advancement of software usability in materials science” by ISSP

[1] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).

[2] A. V. Knyazev, SIAM J. Sci. Comput. 23, 517 (2001).

[3] S. Sugiura, A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).

HΦ開発チーム



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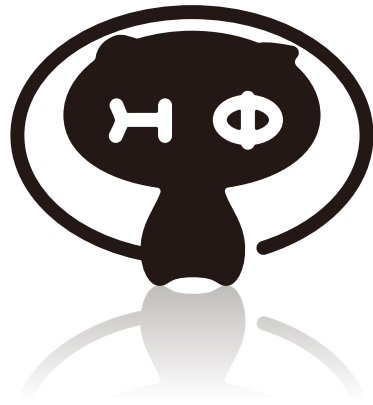
謝辞: 中野義典博士 (同志社大学)
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曾我部智広准教授 (名古屋大学)

“Project for advancement of software usability in materials science” by ISSP



T. Hoshi, M. Kawamura, K. Yoshimi, Y. Motoyama, T. Misawa, Y. Yamaji,
S. Todo, N. Kawashima, and T. Sogabe,
“Kw—Open-source library for the shifted Krylov subspace method,” CPC 2021

HΦの普及状況



- 通算**2,500**ダウンロード以上
- HΦが使われた研究論文(**2020**年)

-H. Zhang, *et al.*, Phys. Rev. RESEARCH 2, 013214 (2020).
-H. Araki, *et al.*, Phys. Rev. RESEARCH 2, 012009(R) (2020).
-J. Yoshitake, *et al.*, Phys. Rev. B 101, 100408(R) (2020).
-P. Laurell and S. Okamoto, npj Quantum Mat. 5, 2 (2020).
-R. Martinazzo and E. Pollakc, PNAS 117, 16181 (2020).
-Y. Nomura, arXiv:2009.14777.
-Y. Nomura and M. Imada, arXiv:2005.14142.
-T. Nakamura, Sci. Rep. 10, 14201 (2020).
-A. S. Patri, et al., Phys. Rev. RESEARCH 2, 023253 (2020).
-M. Charlebois and M. Imada, Phys. Rev. X 10, 041023 (2020).
-N. Aiba and K. Nomura, Phys. Rev. B 102, 134435 (2020).
-S. H. Jang, et al., Phys. Rev. Mat. 4, 104420 (2020).
-H. Kobayashi, et al., arXiv:2011.04303.
-G. Sala, *et al.*, arXiv:2003.01754.
-T. Yamada, T. Suzuki, and S. Suga, arXiv:2004.09622.

- 全国10のスパコンに
プリンストール



北海道大学
HOKKAIDO UNIVERSITY



JCAHPC



東京大学 物性研究所
THE INSTITUTE FOR SOLID STATE PHYSICS
THE UNIVERSITY OF TOKYO



東京大学
THE UNIVERSITY OF TOKYO



名古屋大学



京都大学
KYOTO UNIVERSITY



大阪大学
OSAKA UNIVERSITY



東北大学



東京工業大学



九州大学
KYUSHU UNIVERSITY

厳密対角化に基づく量子格子模型ソルバー

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

主に量子統計力学の標準的な模型
(Heisenberg, Hubbard)向け
cf.) Quspin, Quany (不純物向け)

How Useful in Condensed Matter Physics

Exact diagonalization/full CI

- Lanczos/Arnoldi or CG-type algorithm
- Applicable to finite-size clusters
 - $N (< 30)$ orbital systems
 - $N (< 50)$ *spin* systems

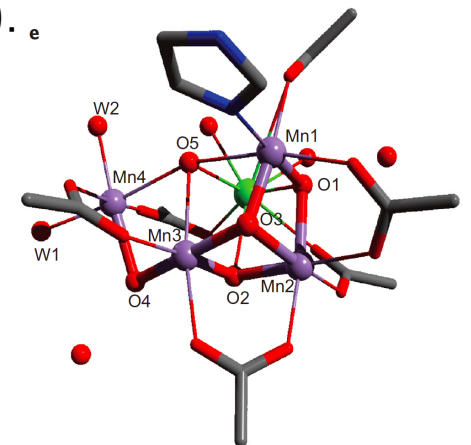
DMRG in chemistry

- A H₂O molecule: 5 \uparrow & 5 \downarrow electrons in 41 orbitals
 - 5.6×10^{11} dimensional

G. K.-L. Chan & M. Head-Gordon, J. Chem. Phys. 118, 8551 (2003).

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How Useful in Condensed Matter Physics

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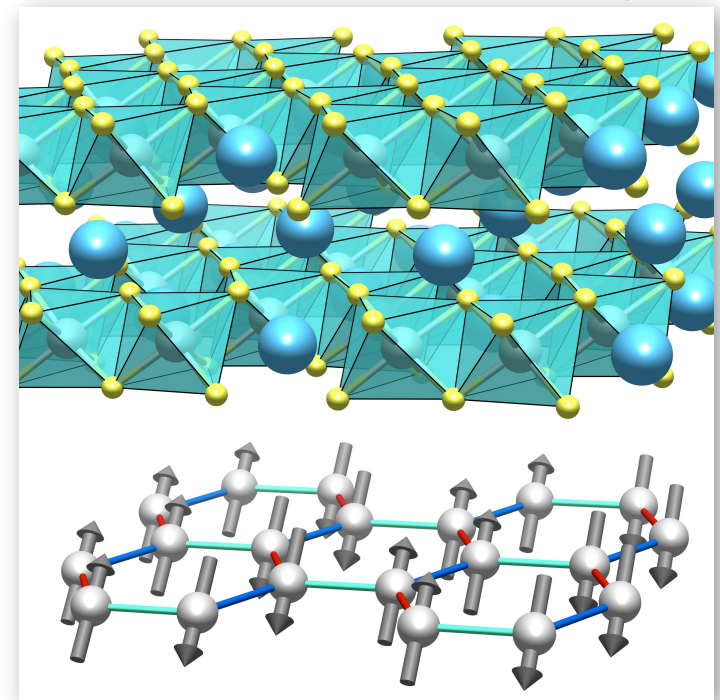
Application to crystalline lattice (with periodic boundary)

- Emergent phenomena beyond perturbation theory
- Finite-temperature thermodynamic quantities and spectra

cf.) Nearsightedness

W. Kohn, Phys. Rev. Lett. 76, 3168 (1996).

lower temperature, larger size



Basis of Hamiltonians in HΦ: Spin-1/2 Fermions

Hamiltonian in 2nd quantization form

$$\hat{H} = \hat{H}_K + \hat{H}_I$$

$$\hat{H}_K = - \sum_{\ell_1, \ell_2} \sum_{\sigma_1, \sigma_2} t_{\ell_1 \ell_2}^{\sigma_1 \sigma_2} \hat{c}_{\ell_1 \sigma_1}^\dagger \hat{c}_{\ell_2 \sigma_2}$$

$$\hat{H}_I = \sum_{\ell_1, \ell_2, \ell_3, \ell_4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} I_{\ell_1 \ell_2 \ell_3 \ell_4}^{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \hat{c}_{\ell_1 \sigma_1}^\dagger \hat{c}_{\ell_2 \sigma_2} \hat{c}_{\ell_3 \sigma_3}^\dagger \hat{c}_{\ell_4 \sigma_4}$$

Numerically exact eigenvalues and eigenvectors

$$\hat{H}|\phi\rangle = E|\phi\rangle$$

$$|\phi\rangle = \sum_{\{I_j, \bar{I}_j\}} C_{I_0 \bar{I}_0 I_1 \bar{I}_1 \dots I_{N-1} \bar{I}_{N-1}} \left[\prod_{j=0}^{N-1} (\hat{c}_{\ell_j \uparrow}^\dagger)^{I_j} (\hat{c}_{\ell_j \downarrow}^\dagger)^{\bar{I}_j} \right] |0\rangle$$

CI coefficients

Pauli principle: $I_j, \bar{I}_j \in \{0, 1\}$

Variety of Hamiltonian

Periodic (Standard or Expert)

-Hubbard model

- $S=1/2$ Heisenberg model with anisotropy

-Kondo lattice model

- $S=1, 3/2, 2, \dots$ Heisenberg model

(Standard or Expert)

-*Ab initio* hamiltonian

Aperiodic (Expert)

-Molecules/qubits

Example of Hamiltonian: 1D Hubbard model

$$\hat{H} = -t \sum_{i=0}^{L-1} \sum_{\sigma=\uparrow,\downarrow} \left[\hat{c}_{i\sigma}^\dagger \hat{c}_{\text{mod}(i+1,L)\sigma} + \hat{c}_{\text{mod}(i+1,L)\sigma}^\dagger \hat{c}_{i\sigma} \right] \\ + U \sum_{i=0}^{L-1} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}$$

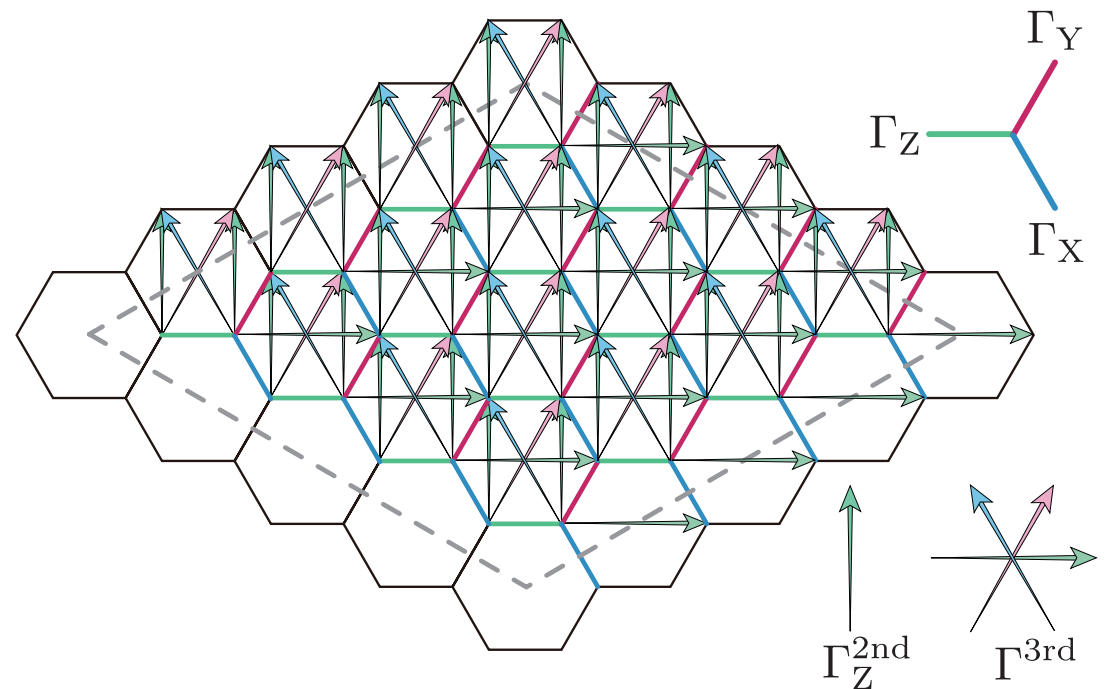
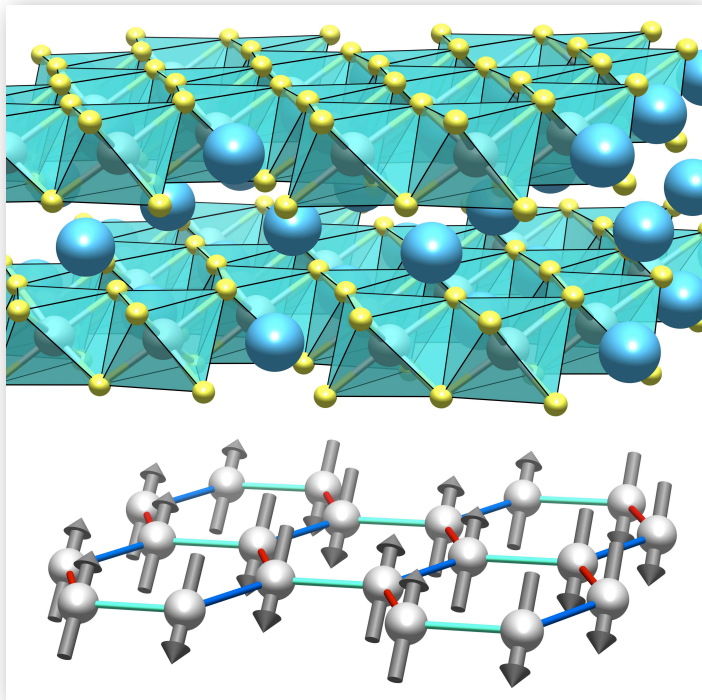
Standard input

```
model = "Hubbard"  
method = "CG"  
lattice = "chain"  
L = 8  
t = 1.0  
U = 8.0  
nelec = 8  
2Sz = 0  
exct = 1
```


An Example of Complicated Hamiltonian: *Ab Initio* Spin Hamiltonian

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

An example: Frustrated magnet Na_2IrO_3

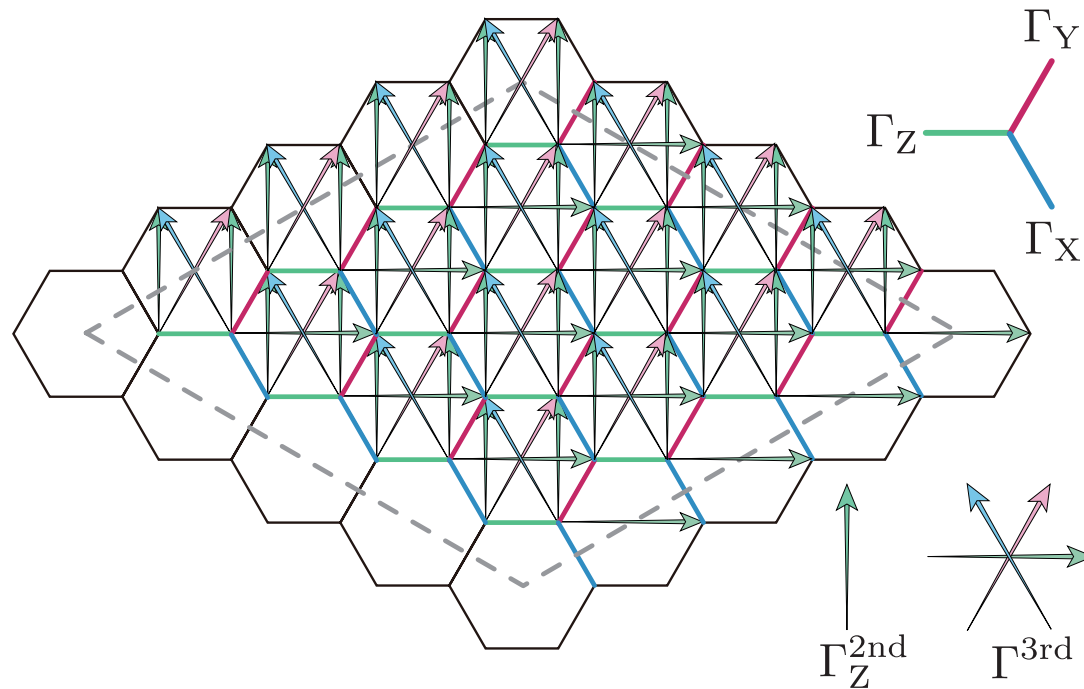


An Example of Complicated Hamiltonian: *Ab Initio* Spin Hamiltonian

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

$$\hat{H} = \sum_{\Gamma=X,Y,Z,Z_{2\text{nd}},3} \sum_{\langle \ell, m \rangle \in \Gamma} \vec{\hat{S}}_{\ell}^T \mathcal{J}_{\Gamma} \vec{\hat{S}}_m$$

$$\vec{\hat{S}}_{\ell}^T = (\hat{S}_{\ell}^x, \hat{S}_{\ell}^y, \hat{S}_{\ell}^z)$$



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

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

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

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

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

cf.) RESPACK

Overview of Software HΦ

- Language: C
- Compiler: C & Fortran compiler
- Library: BLAS, LAPACK, $K\omega$ (distributed with HΦ)
(optional: MPI, Scalapack, MAGMA)
- Parallelization: OpenMP & MPI

For installation, `cmake` is useful

Standard input

```
W = 4
L = 4
model = "Hubbard"
method = "TPQ"
lattice = "Square"
t = 1.0
t' = 0.5
U = 8.0
nelec = 16
2Sz = 0
```

Flow of Simulation

Standard interface

Making input files
from scratch

Expert input

```
Def. files for Hamiltonian
Def. files for controlling simulation
```

Expert interface

```
Subroutines:
-Lanczos
-CG
-TPQ
-TimeEvolution
-Full diag.
(LAPACK, Scalapack, MAGMA)
```

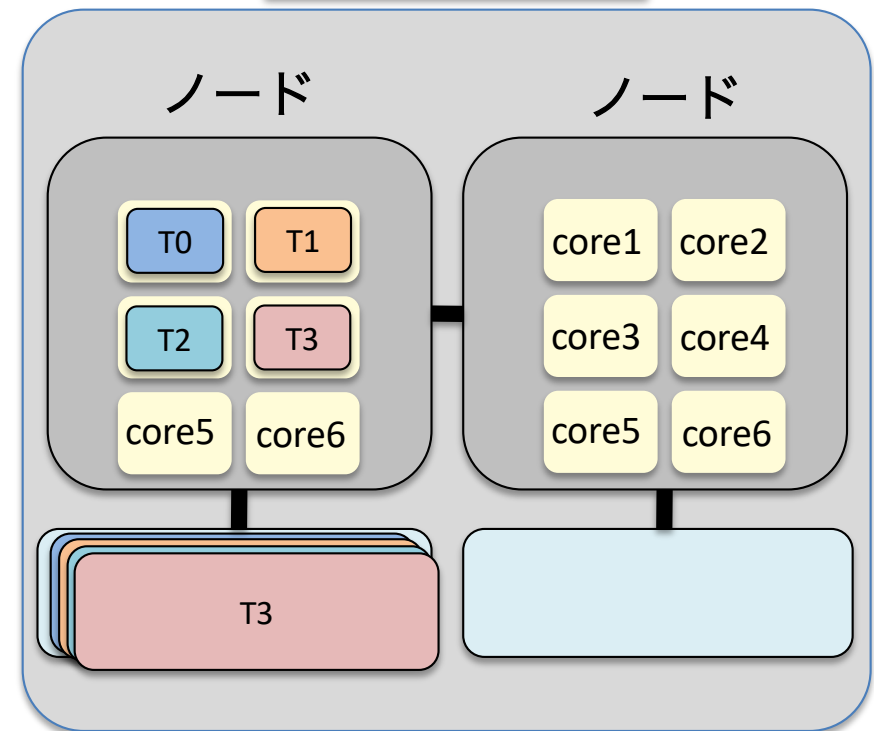
Standard output
Output files

HΦ Automatically Performs Parallelized Simulation

- Hybrid parallelization

-共有メモリ並列(OpenMP) スレッド
-分散メモリ並列(MPI) プロセス

並列計算機



HΦ Automatically Performs Parallelized Simulation

- Hybrid parallelization

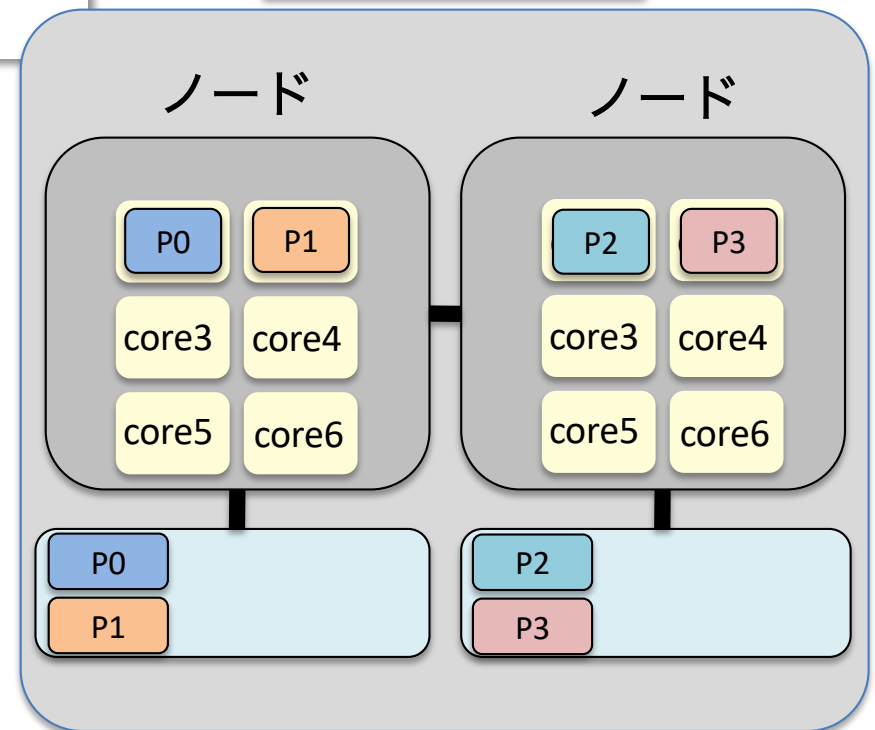
-共有メモリ並列(OpenMP) スレッド
 -分散メモリ並列(MPI) プロセス

- Hubbard/Kondo Lattice /HubabrdGC
 → 4^n プロセス
- Spin/SpinGC
 → $(2S+1)^n$ プロセス

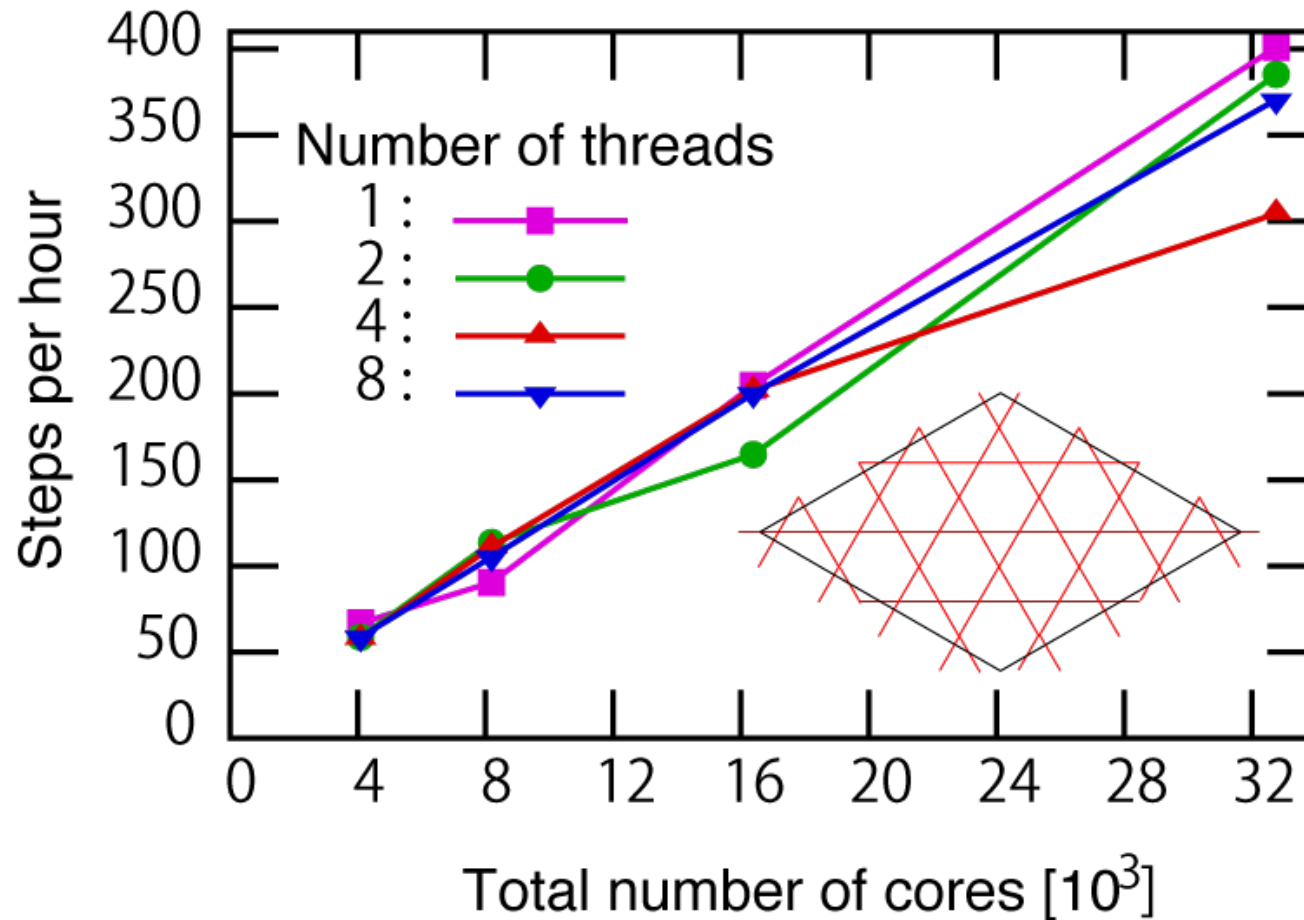
Decomposition of wave function by 2 processes

$ 0\rangle$	=	$ \downarrow\downarrow\downarrow\rangle$	rank 0
$ 1\rangle$	=	$ \uparrow\downarrow\downarrow\rangle$	
$ 2\rangle$	=	$ \downarrow\uparrow\downarrow\rangle$	
$ 3\rangle$	=	$ \uparrow\uparrow\downarrow\rangle$	
<hr/>			
$ 4\rangle$	=	$ \downarrow\downarrow\uparrow\rangle$	rank 1
$ 5\rangle$	=	$ \uparrow\downarrow\uparrow\rangle$	
$ 6\rangle$	=	$ \downarrow\uparrow\uparrow\rangle$	
$ 7\rangle$	=	$ \uparrow\uparrow\uparrow\rangle$	

並列計算機

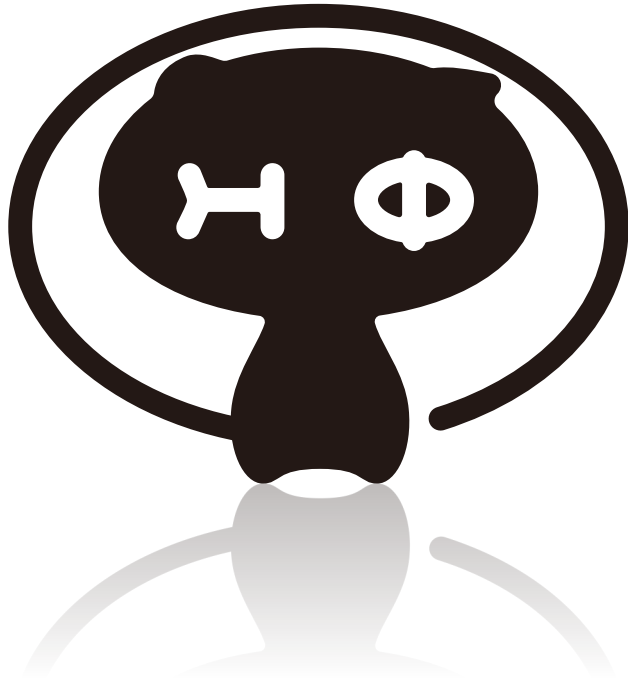


Speedup



Lanczos method: Up to 6.87×10^{10} dimension
@K computer & ISSP supercomputer

From 4096 32768 cores: Parallelization efficiency 80%



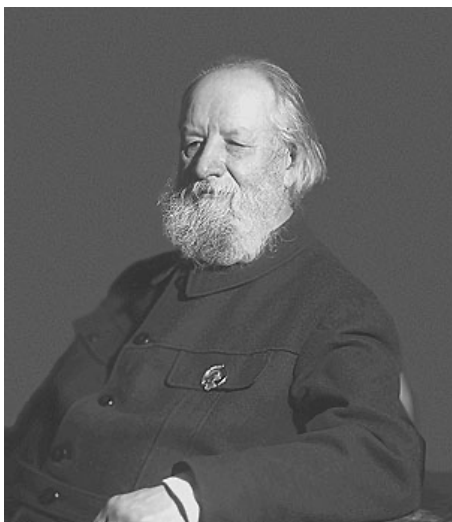
アルゴリズム紹介

1. Zero temperature
2. Finite temperatures
3. Real-time evolution
4. Dynamical properties (linear response)



Algorithm Implemented in $H\Phi$
1. Zero Temperature:
Lanczos & LOBCG

Krylov Subspace Method for Sparse and Huge Matrices



Alexey Krylov

Aleksey Nikolaevich Krylov

1863-1945

Russian naval engineer and applied mathematician

Krylov subspace

$$A \in \mathbb{C}^{L \times L}$$

$$\mathcal{K}_n(A, \vec{b}) = \text{span}\{\vec{b}, A\vec{b}, \dots, A^{n-1}\vec{b}\}$$

Numerical cost to construct \mathcal{K}_n : $\mathcal{O}(\text{nnz}(A) \times n)$

Numerical cost to orthogonalize \mathcal{K}_n : $\mathcal{O}(L \times n^2)$

Cornelius Lanczos 1950

Walter Edwin Arnoldi 1951

*nnz: Number of non-zero
entries/elements

An Example of Sparse Matrix: TFIM

$$\hat{H} = J \sum_{i=0}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z - \Gamma \sum_{i=0}^{L-1} \hat{S}_i^x$$

-Non-commutative

$$\left[\sum_{i=0}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z, \sum_{i=0}^{L-1} \hat{S}_i^x \right] \neq 0$$

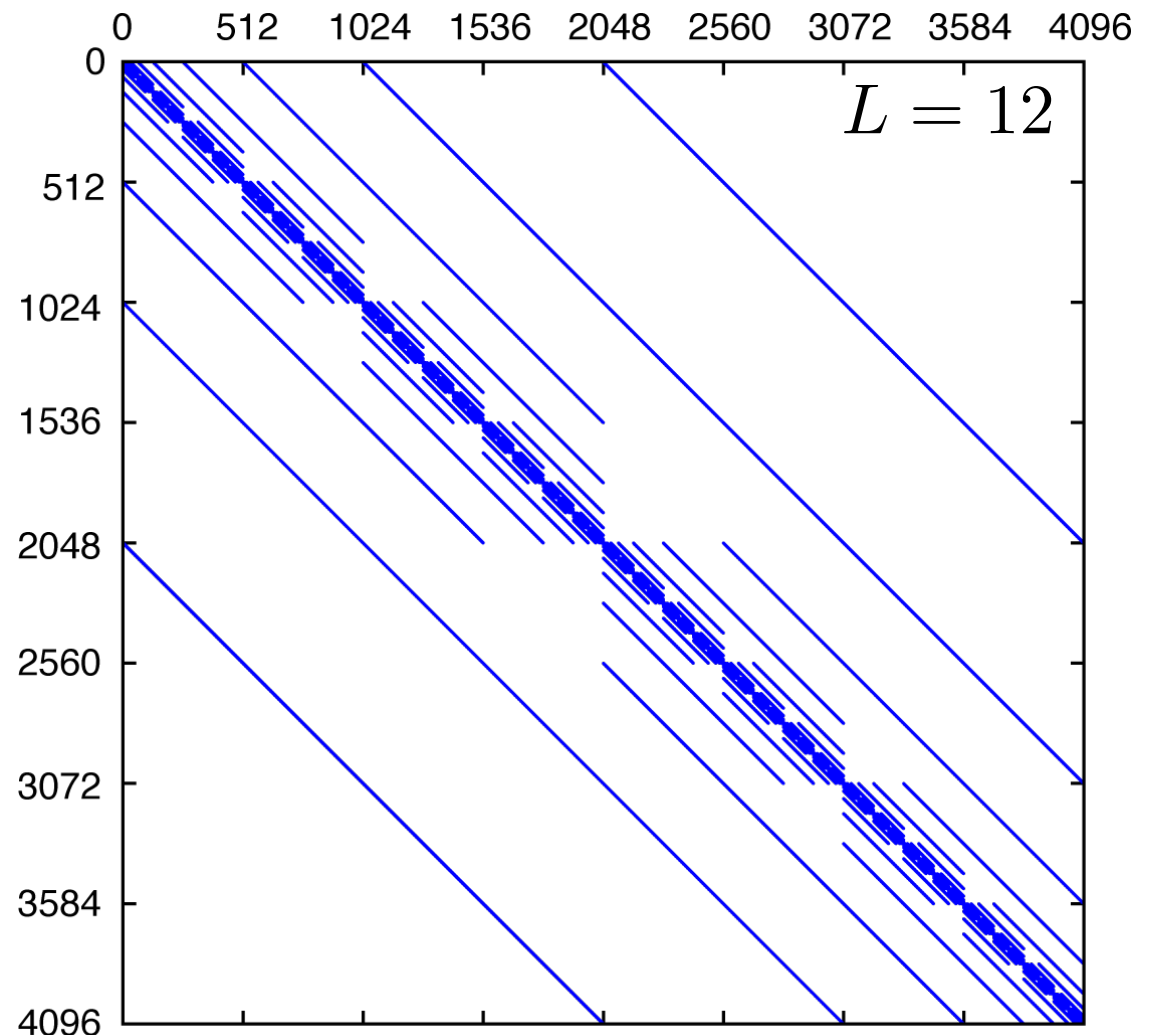
→ Quantum fluctuations
or Zero point motion

-Sparse

of elements $\propto O(2^L)$

-Solvable

-Hierarchical matrix?



Krylov Subspace Method

from *SIAM News*, Volume 33, Number 4

The Best of the 20th Century: Editors Name Top 10 Algorithms

By Barry A. Cipra

1950: Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of **Krylov subspace iteration methods**.

These algorithms address the seemingly simple task of solving equations of the form $Ax = b$. The catch, of course, is that A is a huge $n \times n$ matrix, so that the algebraic answer $x = b/A$ is not so easy to compute. (Indeed, matrix “division” is not a particularly useful concept.) Iterative methods—such as solving equations of the form $Kx_{i+1} = Kx_i + b - Ax_i$ with a simpler matrix K that’s ideally “close” to A —lead to the study of Krylov subspaces. Named for the Russian mathematician Nikolai Krylov, Krylov subspaces are spanned by powers of a matrix applied to an initial “remainder” vector $r_0 = b - Ax_0$. Lanczos found a nifty way to generate an orthogonal basis for such a subspace when the matrix is symmetric. Hestenes and Stiefel proposed an even niftier method, known as the conjugate gradient method, for systems that are both symmetric and positive definite. Over the last 50 years, numerous researchers have improved and extended these algorithms. The current suite includes techniques for non-symmetric systems, with acronyms like GMRES and Bi-CGSTAB. (GMRES and Bi-CGSTAB premiered in *SIAM Journal on Scientific and Statistical Computing*, in 1986 and 1992, respectively.)

Lanczos Method

Initial : $\beta_1 = 0, |v_0\rangle = 0$

for $j = 1, 2, \dots, m$ **do**

$$|w_j\rangle = \hat{H}|v_j\rangle - \beta_j|v_{j-1}\rangle$$

$$\alpha_j = \langle w_j | v_j \rangle$$

$$|w_j\rangle \leftarrow |w_j\rangle - \alpha_j|v_j\rangle$$

$$\beta_{j+1} = \sqrt{\langle w_j | w_j \rangle}$$

$$|v_{j+1}\rangle = |w_j\rangle / \beta_{j+1}$$

Lanczos Method

$$\alpha_j = \langle v_j | \hat{H} | v_j \rangle$$

$$\beta_j = \langle v_{j-1} | \hat{H} | v_j \rangle = \langle v_j | \hat{H} | v_{j-1} \rangle$$

Orthogonalization

$$|v_j\rangle = \frac{\hat{H}|v_{j-1}\rangle - \sum_{\ell=1}^{j-1} |v_\ell\rangle \langle v_\ell | \hat{H} | v_{j-1} \rangle}{\langle v_j | \hat{H} | v_{j-1} \rangle}$$

$$\langle v_\ell | \hat{H} | v_{j-1} \rangle = \begin{cases} 0 & (\ell \leq j-3) \\ \beta_{j-1} & (\ell = j-2) \\ \alpha_{j-1} & (\ell = j-1) \end{cases}$$

Lanczos Method

$$\alpha_j = \langle v_j | \hat{H} | v_j \rangle$$

$$\langle v_j | v_k \rangle = \delta_{j,k}$$

$$\beta_j = \langle v_{j-1} | \hat{H} | v_j \rangle = \langle v_j | \hat{H} | v_{j-1} \rangle$$

Hamiltonian projected onto m D Krylov subspace

$$H_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & & \\ & \beta_3 & \alpha_3 & \ddots & & & \\ & & \ddots & \ddots & & & \\ & & & \ddots & \beta_{m-1} & & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m & \\ 0 & & & & \beta_m & \alpha_m & \end{pmatrix}$$

Eigenvalues of projected Hamiltonian

→ Approximate eigenvalues of original Hamiltonian

Lanczos Method: # of Vectors Required

Initial : $\beta_1 = 0, |v_0\rangle = 0$

for $j = 1, 2, \dots, m$ **do**

$$|w_j\rangle \leftarrow \hat{H}|v_j\rangle - \beta_j|v_{j-1}\rangle$$

$$\alpha_j = \langle w_j | v_j \rangle$$

$$|w_j\rangle \leftarrow |w_j\rangle - \alpha_j|v_j\rangle$$

$$\beta_{j+1} = \sqrt{\langle w_j | w_j \rangle}$$

$$|v_{j+1}\rangle = |w_j\rangle / \beta_{j+1}$$

$$|v_{j-1}\rangle \rightarrow |w_j\rangle, |v_j\rangle$$

$$|w_j\rangle, |v_j\rangle$$

$$|w_j\rangle, |v_j\rangle$$

$$|w_j\rangle, |v_j\rangle$$

$$|w_j\rangle \rightarrow |v_{j+1}\rangle, |v_j\rangle$$

注意

Lanczos法

良い点

- 実装が簡単
- メモリ・コストが少ない

悪い点

- 固有ベクトルが直接求まらない

固有ベクトルはCG法で求められる:

$$\text{逆反復法 } (\hat{H} - E_m)\vec{v}_{k+1} = \vec{v}_k$$

$$\vec{v}_k \rightarrow |m\rangle$$

固有値・固有ベクトルを同時に求める方法

Locally optimal block CG (LOBCG):

A. V. Knyazev,

SIAM journal on scientific computing **23**, 517 (2001).

LOB(P)CG

A. V. Knyazev, SIAM journal on scientific computing **23**, 517 (2001).

Algorithm of LOBCG: m lowest eigenstates

Initial condition: m orthogonal initial vectors $\mathbf{x}_0^{(i)}$
 $\mathbf{p}_0^{(i)} = \mathbf{0}$ ($i = 1, \dots, m$)

for ($k = 0; k < k_{\max}; k++$)

$$\mu_k^{(i)} = \frac{(\mathbf{x}_k^{(i)} A \mathbf{x}_k^{(i)})}{(\mathbf{x}_k^{(i)}, \mathbf{x}_k^{(i)})}$$

← approximation of i th smallest eigenvalue

$$\mathbf{w}_k^{(i)} = A \mathbf{x}_k^{(i)} - \mu_k^{(i)} \mathbf{x}_k^{(i)}$$

$$S_A = \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}^T A \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}$$

$$S_B = \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}^T \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}$$

Obtain i th smallest eigenstate of $S_A \mathbf{v}^{(i)} = \mu^{(i)} S_B \mathbf{v}^{(i)}$, $\mathbf{v}^{(i)} = (\alpha_1^{(i)}, \dots, \alpha_m^{(i)}, \beta_1^{(i)}, \dots, \beta_m^{(i)}, \gamma_1^{(i)}, \dots, \gamma_m^{(i)})^T$
($i = 1, \dots, m$)

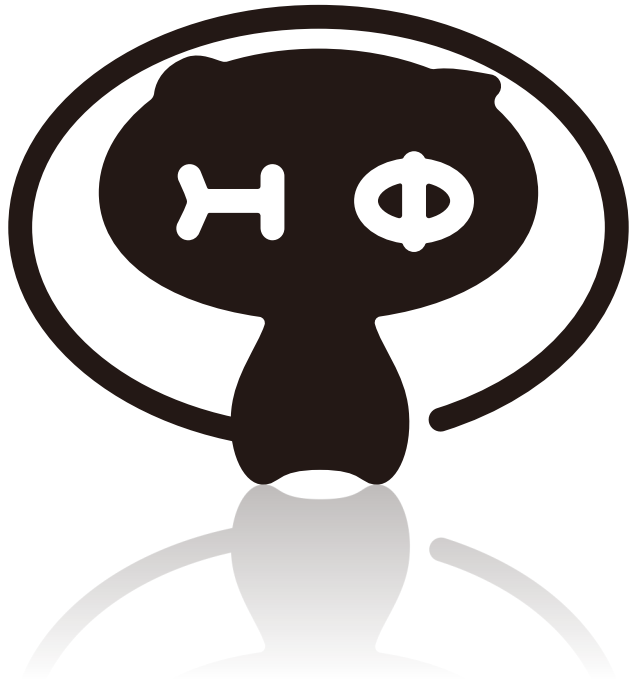
← m smallest eigenstates are chosen from $3m$ states

$$\mathbf{x}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{w}_k^{(j)} + \beta_j^{(i)} \mathbf{x}_k^{(j)} + \gamma_j^{(i)} \mathbf{p}_k^{(j)} \right)$$

$$\mathbf{p}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{w}_k^{(j)} + \gamma_j^{(i)} \mathbf{p}_k^{(j)} \right)$$

Until convergence

解説と発展: 山田進, 今村俊幸, 町田昌彦,
日本計算工学会論文集**2006**, 20060027 (2006).



Algorithm Implemented in $H\Phi$
2. Finite Temperatures
TPQ

Finite-Temperature Physical Quantity: Heat Capacity

Spread of energy distribution

$$C = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{k_B T^2}$$

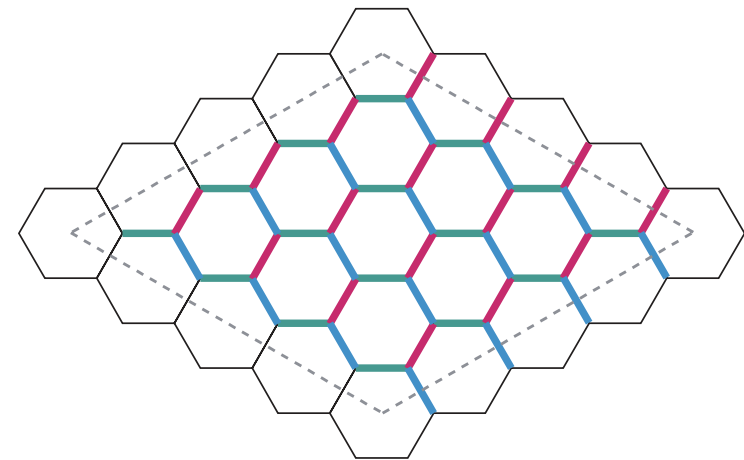
-Average with Boltzmann distribution

$$\langle \hat{O}_\beta^{\text{ens}} \rangle = \frac{\sum_n e^{-E_n/k_B T} \langle n | \hat{O} | n \rangle}{\sum_n e^{-E_n/k_B T}}$$

Complexity $\mathcal{O}(N_H^3)$

Memory $\mathcal{O}(N_H^2)$

32 site cluster of $S=1/2$ spin



$$N_H = 2^{32}$$

Hamiltonian
 $\sim 3 \times 10^8$ TB!

$|n\rangle \sim 69$ GB

Typical Pure State Approach

Complexity $\mathcal{O}(N_H)$
 Memory

Imada-Takahashi (1986)
 Lloyd (1988)
 Jacklic-Prelovsek (1994)
 Hams-De Raedt (2000)
 Sugiura-Shimizu (2012, 2013)

M. Imada & M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).

$\beta = 0$ ($T \rightarrow +\infty$) Typical state: Random vector

$$|\phi_0\rangle = \sum_x c_x |x\rangle \quad \left(\sum_x |c_x|^2 = 1 \right)$$

$$\langle \hat{O} \rangle_{\beta=0}^{\text{ens}} = \mathbb{E}[\langle \phi_0 | \hat{O} | \phi_0 \rangle]$$

At finite temperature

$$|\phi_\beta\rangle = e^{-\beta \hat{H}/2} |\phi_0\rangle$$

N. Ullah, Nucl. Phys. 58, 65 (1964).

-Uniform distribution on unit sphere in \mathbb{R}^{2N_H}

$$\mathbb{E}[|c_x|^{2n}] = \frac{\Gamma(N_H)\Gamma(n+1)}{\Gamma(N_H+n)}$$

Average over the distribution

How large is the standard deviation?

$$\sigma_O^2 = \mathbb{E} \left[\left(\frac{\langle \phi_\beta | \hat{O} | \phi_\beta \rangle}{\langle \phi_\beta | \phi_\beta \rangle} - \langle \hat{O} \rangle_\beta^{\text{ens}} \right)^2 \right]$$

Typical Pure State Approach

Seth Lloyd, Ph.D. Thesis, Rockefeller University (1988); arXiv:1307.0378.

A. Hams & H. De Raedt, Phys. Rev. E 62, 4365 (2000).

A. Sugita, RIMS Kokyuroku (Kyoto) 1507, 147 (2006).

P. Reimann, Phys. Rev. Lett. 99, 160404 (2007).

S. Sugiura & A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).

S. Sugiura & A. Shimizu, Phys. Rev. Lett. 111, 010401 (2013).

$$\sigma_O^2 \leq \frac{\langle (\Delta O)^2 \rangle_{2\beta}^{\text{ens}} + (\langle O \rangle_{2\beta}^{\text{ens}} - \langle O \rangle_{\beta}^{\text{ens}})^2}{\exp[2\beta\{F(2\beta) - F(\beta)\}]} \\ \propto \exp[-S(\beta^*)/2] \quad (\beta < \beta^* < 2\beta)$$

Exponentially small when system size increases

Construction of Typical Pure State: *Microcanonical* TPQ

Thermal Pure Quantum (TPQ) States $|\phi_\beta\rangle = |\Phi_k\rangle$

Sugiura & Shimizu, Phys. Rev. Lett. 108, 240401 (2012)

Initial state (at $T = +\infty$): $|\Phi_0\rangle =$ (Random vector)
do $k=1, N_{\text{step}}$ If possible, taking random average
 $|\Phi_k\rangle = (\ell - \hat{H}/N) |\Phi_{k-1}\rangle / \sqrt{\langle \Phi_{k-1} | (\ell - \hat{H}/N)^2 | \Phi_{k-1} \rangle}$
 $u_k = \langle \Phi_k | \hat{H}/N | \Phi_k \rangle$
 $\beta = 2(k/N) / (\ell - u_k)$ ($\beta = 1/k_B T$)
 $\bar{O}(\beta) = \langle \Phi_k | \hat{O} | \Phi_k \rangle + \mathcal{O}(1/N)$
enddo

Hamiltonian-wave function product is essential

Construction of Typical Pure State: Canonical TPQ

Seth Lloyd, Ph.D. Thesis, Rockefeller University (1988); arXiv:1307.0378.

A. Hams & H. De Raedt, Phys. Rev. E 62, 4365 (2000).

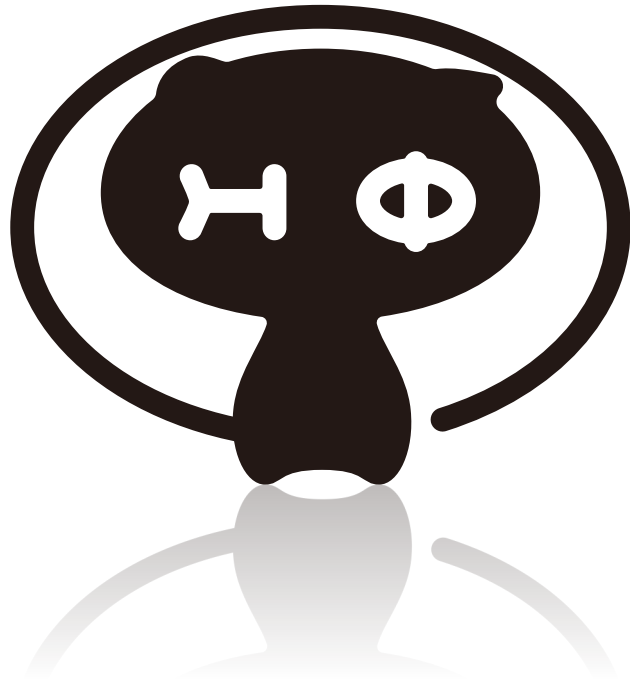
S. Sugiura & A. Shimizu, Phys. Rev. Lett. 111, 010401 (2013).

$$\beta_k = k\Delta\tau$$

$$\begin{aligned} |\phi_{\beta_k}\rangle &= e^{-\beta_k \hat{H}/2} |\phi_0\rangle \\ &= \left[e^{-\Delta\tau \hat{H}/2} \right]^k |\phi_0\rangle \\ &\simeq \left[\sum_{n=0}^{n_{\max}} \frac{1}{n!} \left(-\Delta\tau \hat{H}/2 \right)^n \right]^k |\phi_0\rangle \end{aligned}$$

$$\langle \hat{O} \rangle_{\beta_k} = \frac{\mathbb{E}[\langle \phi_{\beta_k} | \hat{O} | \phi_{\beta_k} \rangle]}{\mathbb{E}[\langle \phi_{\beta_k} | \phi_{\beta_k} \rangle]}$$

See Tutorial Sec. 2,
especially 2.1.4



Algorithm Implemented in $H\Phi$

3. Real Time Evolution

4. Dynamical Properties

3. Real-Time Evolution

Real time evolution by Taylor expansion

$$e^{-i\mathcal{H}(t_n)\Delta t} \approx \sum_{l=0}^M \frac{1}{l!} (-i\mathcal{H}(t_n)\Delta t)^l$$

$$|\psi(t_{n+1})\rangle = e^{-i\mathcal{H}(t_n)\Delta t} |\psi(t_n)\rangle$$

Time dependent Hamiltonian

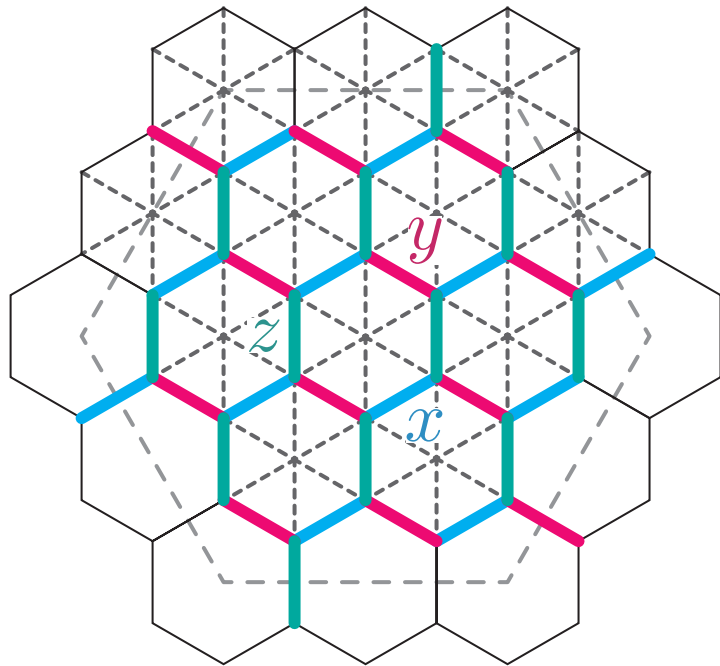
- Standard: Interaction quench or laser (pulse, AC, DC)
- Expert: Time dependent 1-body and 2-body terms

→ Tutorial Sec. 3

Example of Excitation Spectra: Effective Hamiltonian of α -RuCl₃, K - Γ - J_3 Model

$$\hat{H} = \sum_{\Gamma=X,Y,Z,3} \sum_{\langle \ell, m \rangle \in \Gamma} \vec{\hat{S}}_\ell^T \mathcal{J}_\Gamma \vec{\hat{S}}_m$$

$$\vec{\hat{S}}_\ell^T = (\hat{S}_\ell^x, \hat{S}_\ell^y, \hat{S}_\ell^z)$$



$$\mathcal{J}_X = \begin{bmatrix} -\cos \phi & 0 & 0 \\ 0 & 0 & \sin \phi \\ 0 & \sin \phi & 0 \end{bmatrix}$$

$$\mathcal{J}_Y = \begin{bmatrix} 0 & 0 & \sin \phi \\ 0 & -\cos \phi & 0 \\ \sin \phi & 0 & 0 \end{bmatrix}$$

$$\mathcal{J}_Z = \begin{bmatrix} 0 & \sin \phi & 0 \\ \sin \phi & 0 & 0 \\ 0 & 0 & -\cos \phi \end{bmatrix}$$

Nearest neighbor

$$\mathcal{J}_3 = \begin{bmatrix} J_3 & 0 & 0 \\ 0 & J_3 & 0 \\ 0 & 0 & J_3 \end{bmatrix}$$

3rd neighbor

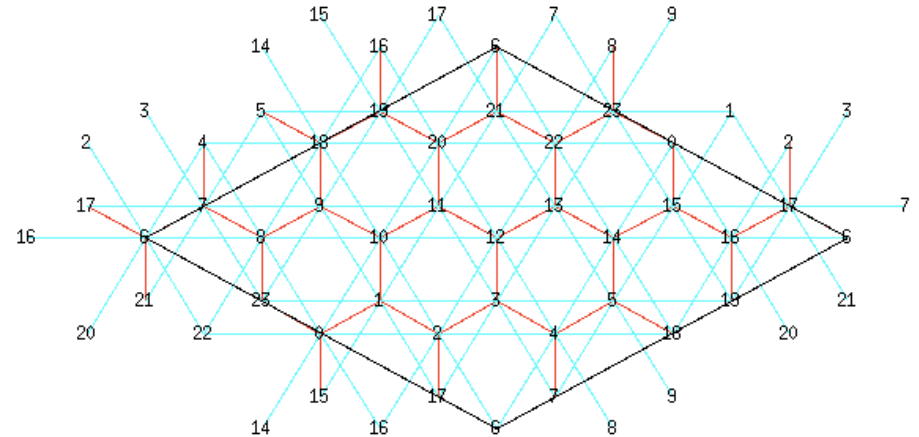
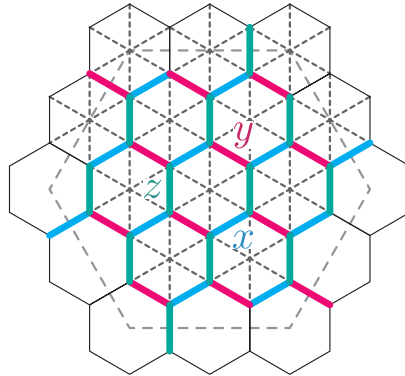
$$J_3 [\hat{S}_\ell^x \hat{S}_m^x + \hat{S}_\ell^y \hat{S}_m^y + \hat{S}_\ell^z \hat{S}_m^z]$$

Excitation Spectra: K - Γ - J_3 Model

$$\phi/\pi = 0.2$$

```

model = "SpinGC"
method = "TPQ"
lattice = "Honeycomb"
a0w = 2
a0l = 2
a1w = 4
a1l = -2
J0x = -0.80901699437
J0yz = 0.58778525229
J0zy = 0.58778525229
J1zx = 0.58778525229
J1y = -0.80901699437
J1xz = 0.58778525229
J2xy = 0.58778525229
J2yx = 0.58778525229
J2z = -0.80901699437
J'' = 0.05
h = 0.07071067811
Gamma = -0.07071067811
2S=1
    
```



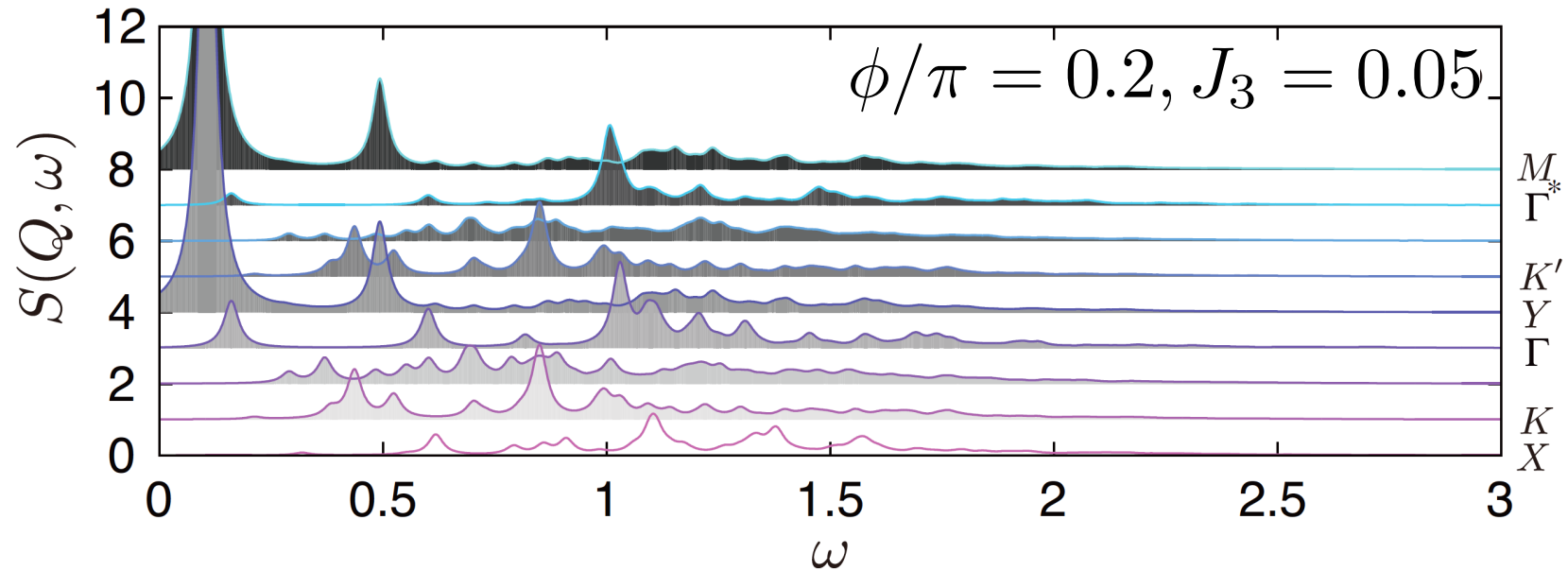
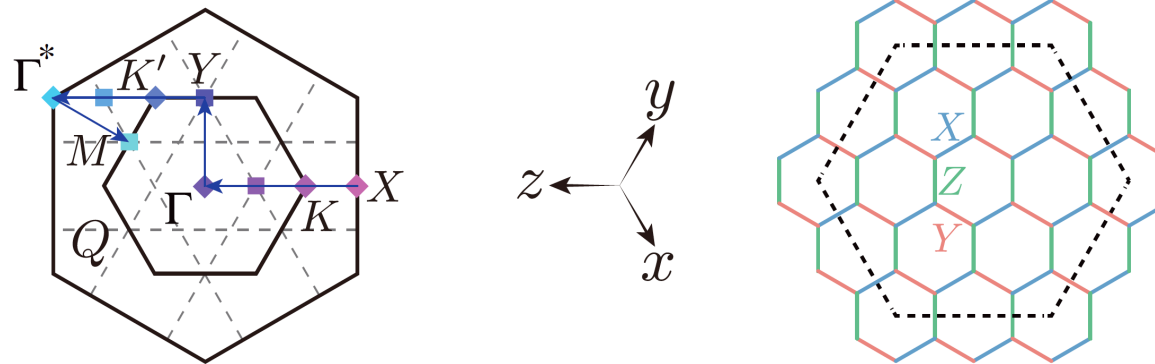
$$\mathcal{J}_X = \begin{bmatrix} -\cos \phi & 0 & 0 \\ 0 & 0 & \sin \phi \\ 0 & \sin \phi & 0 \end{bmatrix}$$

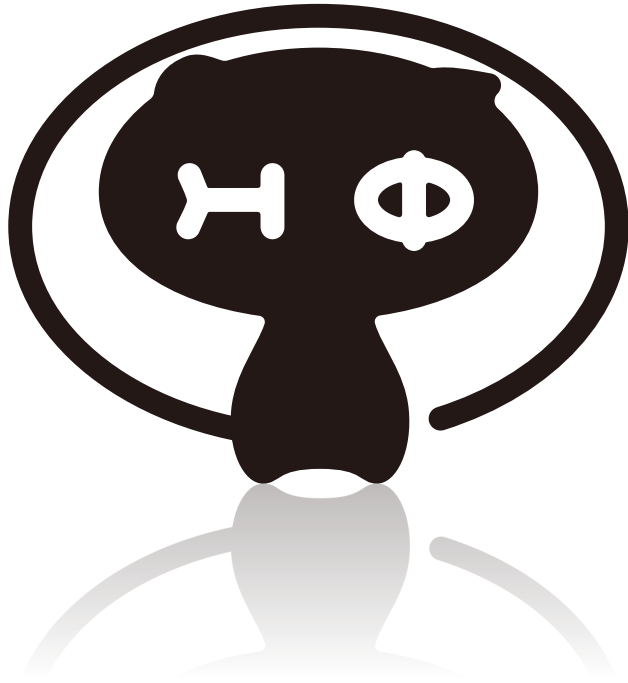
$$\mathcal{J}_Y = \begin{bmatrix} 0 & 0 & \sin \phi \\ 0 & -\cos \phi & 0 \\ \sin \phi & 0 & 0 \end{bmatrix}$$

$$\mathcal{J}_Z = \begin{bmatrix} 0 & \sin \phi & 0 \\ \sin \phi & 0 & 0 \\ 0 & 0 & -\cos \phi \end{bmatrix}$$

$$\vec{B} \propto (1, 0, -1)$$

Excitation Spectra: K - Γ - J_3 Model





チュートリアルをお楽しみください!

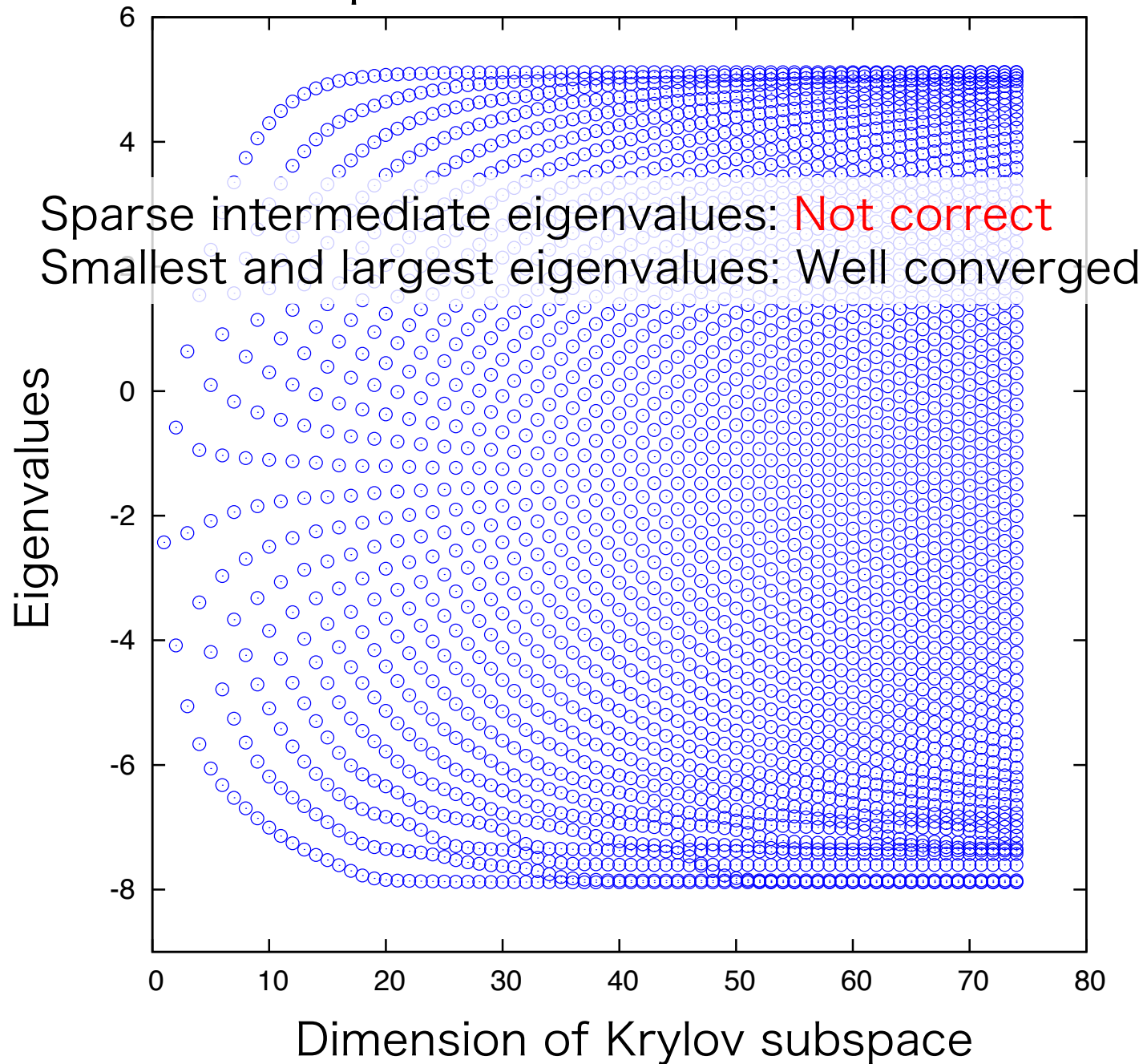
1. Zero temperature
2. Finite temperatures
3. Real-time evolution
4. Dynamical properties (linear response)

<https://issp-center-dev.github.io/HPhi/manual/develop/tutorial/en/html/index.html>

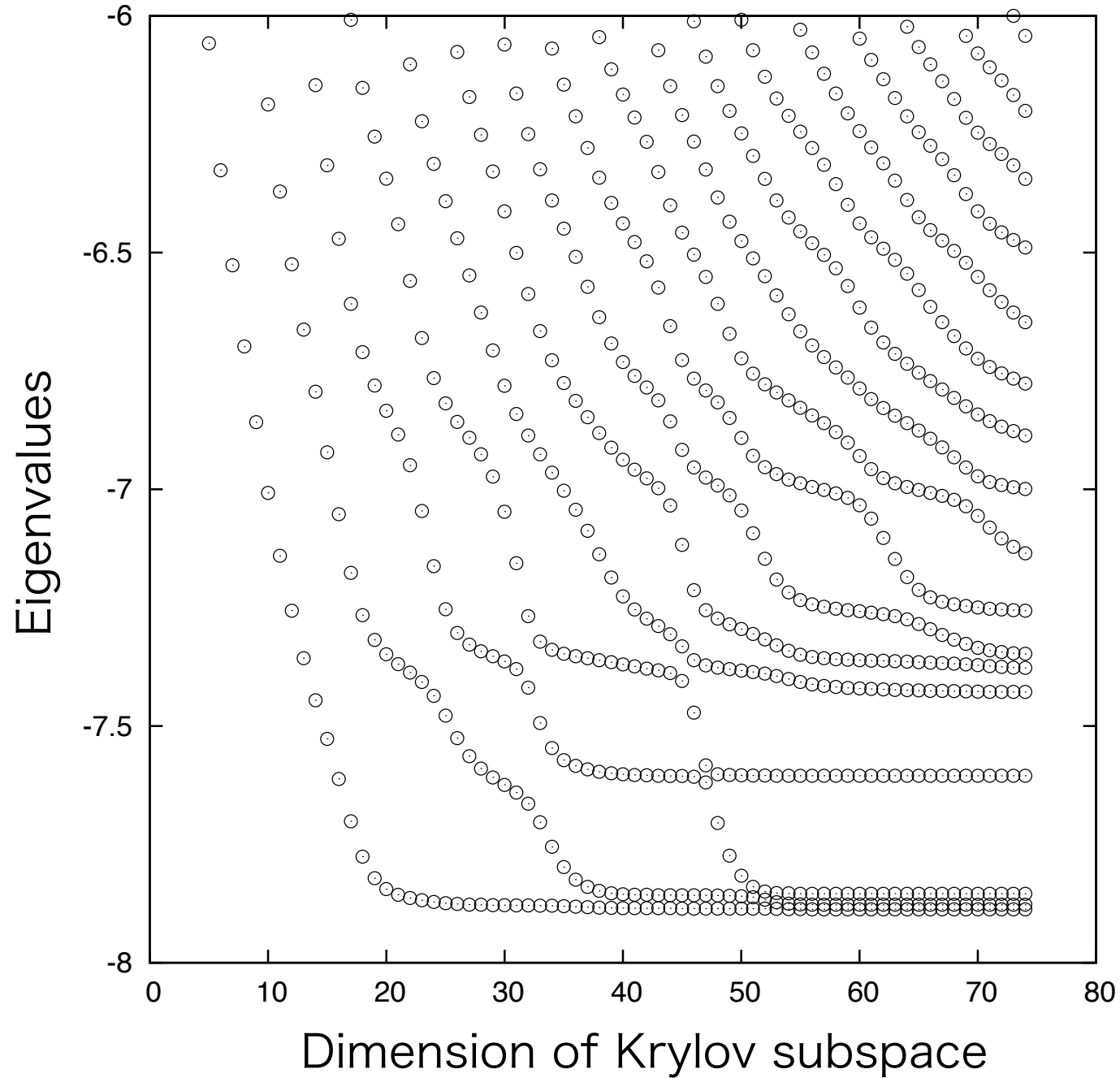
補足: ランチヨス法がどう働くか

24 site cluster of Kitaev- Γ model (frustrated $S=1/2$ spins)

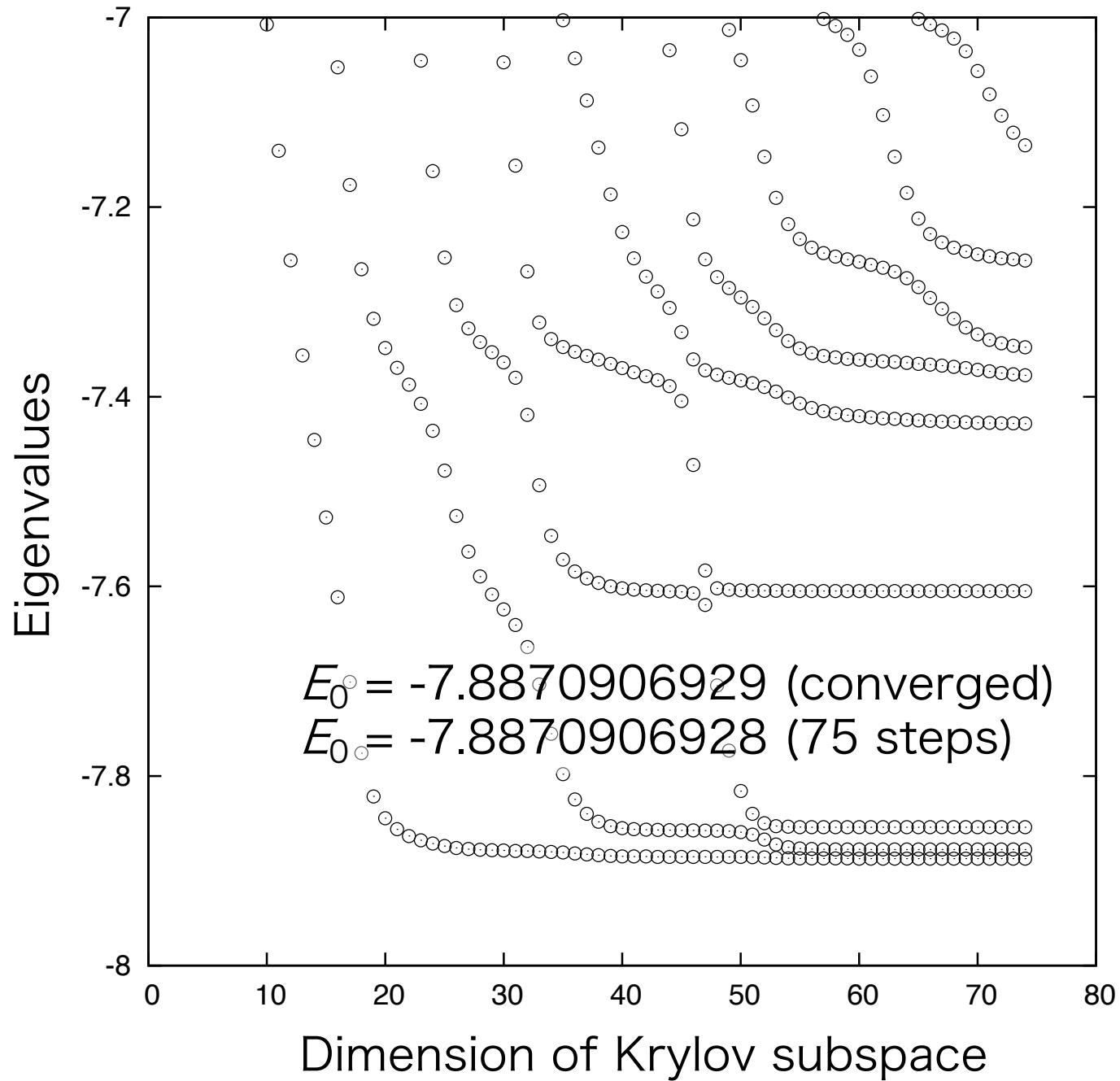
Dimension of Fock space: $2^{24}=16777216$



How Lanczos Method Works



How Lanczos Method Works



How Lanczos Method Works

注意点:

- Lanczos法における正規直交化の数値誤差の蓄積
→ゴースト状態
- 固有値の縮退数は要注意

*どちらも回避にはLOBCGが有効