

# 多体問題の計算科学

## Computational Science for Many-Body Problems

#10 Linear algebra of large and sparse  
matrices for quantum many-body problems

15:10-16:40 June 21, 2022

Quantum many-body problems and huge sparse matrices

1. Quantum mechanics by linear algebra
2. Linear algebra by computer
3. Quantum many-body problems by linear algebra
4. Eigenvalue problems of large & sparse matrices

# Quantum Mechanics by Linear Algebra

# Quantum Mechanics by Linear Algebra

*Naïvely*, linear partial differential equations are rewritten by Linear equations

Schrödinger equation represented by partial diff. eq.

$$i\hbar \frac{d}{dt} \psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \psi(\vec{r}, t)$$

Stationary solution:  $\psi(\vec{r}, t) = \phi(\vec{r}) e^{-iEt/\hbar}$

$$\left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \phi(\vec{r}) = E \phi(\vec{r})$$

# Quantum Mechanics by Linear Algebra

Schrödinger equation represented by linear eqs.

$$\left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \phi(\vec{r}) = E\phi(\vec{r})$$

Expanded by orthonormal basis

$$\phi(\vec{r}) = \sum_m c_m u_m(\vec{r})$$

$$\begin{aligned} \int d^3r u_\ell^*(\vec{r}) u_m(\vec{r}) &= \delta_{\ell,m} \\ \int d^3r \phi^*(\vec{r}) \phi(\vec{r}) &= \sum_m |c_m|^2 \end{aligned}$$

Matrix representation

$$H_{\ell m} = \int d^3r u_\ell^*(\vec{r}) \left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] u_m(\vec{r})$$

$$\sum_m H_{\ell m} c_m = E c_\ell$$

# Quantum Mechanics by Linear Algebra

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Hermitian matrix  $H_{\ell m} = H_{m\ell}^*$

-Diagonalizable by unitary matrices

-Real eigenvalues

$$\sum_m H_{\ell m} U_{m\alpha} = U_{\ell\alpha} E_\alpha$$

$$\sum_m (U^\dagger)_{\beta m} U_{m\alpha} = \sum_m (U_{m\beta})^* U_{m\alpha} = \delta_{\beta,\alpha}$$

# Quantum Mechanics by Linear Algebra

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Vector representation of expectation value

$$\begin{aligned} \frac{\int d^3r \phi^*(\vec{r}) \hat{O} \phi(\vec{r})}{\int d^3r \phi^*(\vec{r}) \phi(\vec{r})} &= \frac{\sum_{\ell, m} c_\ell^* c_m \int d^3r u_\ell^*(\vec{r}) \hat{O} u_m(\vec{r})}{\sum_n |c_n|^2} \\ &= \frac{\sum_{\ell, m} c_\ell^* O_{\ell m} c_m}{\sum_n |c_n|^2} \end{aligned}$$

# Linear Algebra by Computer

# Linear Algebra by Computer

$$\sum_m H_{\ell m} U_{m\alpha} = U_{\ell\alpha} E_{\alpha}$$

Hermitian matrix  $H_{\ell m} = H_{m\ell}^*$

**LAPACK** (Linear Algebra PACKage)

<http://www.netlib.org/lapack/explore-html/index.html>

zheev

z: double complex

he: hermitian

ev: eigenvalue & eigenvector

```
subroutine zheev ( character JOBZ,  
                  character UPLO,  
                  integer N,  
                  complex*16, dimension( lda, * ) A,  
                  integer LDA,  
                  double precision, dimension( * ) W,  
                  complex*16, dimension( * ) WORK,  
                  integer LWORK,  
                  double precision, dimension( * ) RWORK,  
                  integer INFO  
)
```



# Linear Algebra by Computer

**LAPACK** (Linear Algebra PACKage)

<http://www.netlib.org/lapack/explore-html/index.html>

-Language: Fortran  
C & C++ can call LAPACK

-License:  
Modified BSD license

-Parallelized version:  
ScaLAPACK

cf.) intel MKL  
(commercial library)

-Transformation  
-Eigenvalue  
-Singular value

# Quantum Many-Body Problems by Linear Algebra

# Quantum Many-Body Problem by Linear Algebra

Hamiltonian in 2nd quantization form

Many-body electrons confined in one-body potential

(No spin-orbit coupling)

$$\begin{aligned}\hat{H} = & \sum_{\sigma} \int d^3r \hat{\phi}_{\sigma}^{\dagger}(\vec{r}) \left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \hat{\phi}_{\sigma}(\vec{r}) \\ & + \frac{1}{2} \sum_{\sigma, \sigma'} \int d^3r \int d^3r' \hat{\phi}_{\sigma}^{\dagger}(\vec{r}) \hat{\phi}_{\sigma}(\vec{r}) v(|\vec{r} - \vec{r}'|) \hat{\phi}_{\sigma'}^{\dagger}(\vec{r}') \hat{\phi}_{\sigma'}(\vec{r}')\end{aligned}$$

# Quantum Many-Body Problem by Linear Algebra

Field operator

$$\hat{\phi}_{\sigma}(\vec{r}) = \sum_{\ell} u_{\ell}(\vec{r}) \hat{a}_{\ell\sigma}$$

$$\int d^3r u_{\ell}^*(\vec{r}) u_m(\vec{r}) = \delta_{\ell,m}$$

Fermions

$$\{\hat{a}_{\ell\sigma}, \hat{a}_{m\tau}^{\dagger}\} = \hat{a}_{\ell\sigma} \hat{a}_{m\tau}^{\dagger} + \hat{a}_{m\tau}^{\dagger} \hat{a}_{\ell\sigma} = \delta_{\ell,m} \delta_{\sigma,\tau}$$

$$\{\hat{a}_{\ell\sigma}, \hat{a}_{m\tau}\} = \{\hat{a}_{\ell\sigma}^{\dagger}, \hat{a}_{m\tau}^{\dagger}\} = 0$$

Bosons

$$[\hat{a}_{\ell\sigma}, \hat{a}_{m\tau}^{\dagger}] = \hat{a}_{\ell\sigma} \hat{a}_{m\tau}^{\dagger} - \hat{a}_{m\tau}^{\dagger} \hat{a}_{\ell\sigma} = \delta_{\ell,m} \delta_{\sigma,\tau}$$

$$[\hat{a}_{\ell\sigma}, \hat{a}_{m\tau}] = [\hat{a}_{\ell\sigma}^{\dagger}, \hat{a}_{m\tau}^{\dagger}] = 0$$

# Quantum Many-Body Problem by Linear Algebra

$$\begin{aligned}\hat{H} = & \sum_{\sigma} \int d^3r \hat{\phi}_{\sigma}^{\dagger}(\vec{r}) \left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \hat{\phi}_{\sigma}(\vec{r}) \\ & + \frac{1}{2} \sum_{\sigma, \sigma'} \int d^3r \int d^3r' \hat{\phi}_{\sigma}^{\dagger}(\vec{r}) \hat{\phi}_{\sigma}(\vec{r}) v(|\vec{r} - \vec{r}'|) \hat{\phi}_{\sigma'}^{\dagger}(\vec{r}') \hat{\phi}_{\sigma'}(\vec{r}')\end{aligned}$$

→ General Hamiltonian with two-body interactions

$$\hat{H} = \sum_{\ell, m, \sigma} K_{\ell m} \hat{a}_{\ell \sigma}^{\dagger} \hat{a}_{m \sigma} + \sum_{\ell_1, \ell_2, m_1, m_2} \sum_{\sigma, \sigma'} I_{\ell_1 \ell_2 m_1 m_2} \hat{a}_{\ell_1 \sigma}^{\dagger} \hat{a}_{\ell_2 \sigma} \hat{a}_{m_1 \sigma'}^{\dagger} \hat{a}_{m_2 \sigma'}$$

$$K_{\ell m} = \int d^3r u_{\ell}^*(\vec{r}) \left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] u_m(\vec{r})$$

$$I_{\ell_1 \ell_2 m_1 m_2} = \frac{1}{2} \int d^3r \int d^3r' u_{\ell_1}^*(\vec{r}) u_{\ell_2}(\vec{r}) v(|\vec{r} - \vec{r}'|) u_{m_1}^*(\vec{r}') u_{m_2}(\vec{r}')$$

# Quantum Many-Body Problem by Linear Algebra

*Fock space* of  $N$ -particle fermions expanded by

$$|\Phi\rangle = \sum_{\ell_1, \ell_2, \dots, \ell_N} \sum_{\sigma_1, \sigma_2, \dots, \sigma_N} C_{\ell_1 \ell_2 \dots \ell_N} \hat{a}_{\ell_1 \sigma_1}^\dagger \hat{a}_{\ell_2 \sigma_2}^\dagger \cdots \hat{a}_{\ell_N \sigma_N}^\dagger |\text{vac}\rangle$$

Orthonormalized many-body basis

$$\{\ell_j, \sigma_j\} = \{\ell_1, \sigma_1, \ell_2, \sigma_2, \dots, \ell_N, \sigma_N\}$$

$$|\{\ell_j, \sigma_j\}\rangle = \hat{a}_{\ell_1 \sigma_1}^\dagger \hat{a}_{\ell_2 \sigma_2}^\dagger \cdots \hat{a}_{\ell_N \sigma_N}^\dagger |\text{vac}\rangle$$

$$|\{m_j, \tau_j\}\rangle = \hat{a}_{m_1 \tau_1}^\dagger \hat{a}_{m_2 \tau_2}^\dagger \cdots \hat{a}_{m_N \tau_N}^\dagger |\text{vac}\rangle$$

$$\langle \{m_j, \tau_j\} | \{\ell_j, \sigma_j\} \rangle = \begin{cases} 0 & (\{m_j, \tau_j\} \cup \{\ell_j, \sigma_j\} \neq \{\ell_j, \sigma_j\}) \\ 1 & (\{m_j, \tau_j\} \cup \{\ell_j, \sigma_j\} = \{\ell_j, \sigma_j\}) \end{cases}$$

# Quantum Many-Body Problem by Linear Algebra

Common important formula  
between Hilbert and Fock spaces

Closure by orthonormalized basis

$$1 = \sum_{\mu} |\mu\rangle \langle \mu|$$

$$\langle \mu | \nu \rangle = \delta_{\mu, \nu}$$

$$\begin{aligned} \left( \sum_{\mu} |\mu\rangle \langle \mu| \right) \times |\Phi\rangle &= \left( \sum_{\mu} |\mu\rangle \langle \mu| \right) \times \sum_{\nu} d_{\nu} |\nu\rangle \\ &= \sum_{\nu} d_{\nu} |\nu\rangle \\ &= |\Phi\rangle \end{aligned}$$

# Quantum Many-Body Problem by Linear Algebra

Schrödinger equation  $\hat{H}|\Phi\rangle = E|\Phi\rangle$

Hermitian  $\hat{H}^\dagger = \hat{H}$   $H_{\mu\nu} = H_{\nu\mu}^*$

Many-body orthonormalized basis  $\langle\mu|\nu\rangle = \delta_{\mu,\nu}$

Closure  $1 = \sum_{\mu} |\mu\rangle\langle\mu|$

$$\begin{aligned} \langle\mu| \times \hat{H}|\Phi\rangle &= \langle\mu| \times E|\Phi\rangle \\ \Leftrightarrow \sum_{\nu} \langle\mu|\hat{H}|\nu\rangle\langle\nu|\Phi\rangle &= E\langle\mu|\Phi\rangle \end{aligned}$$

Rewritten Schrödinger equation

$$\sum_{\nu} H_{\mu\nu} d_{\nu} = E d_{\mu}$$

$$H_{\mu\nu} = \langle\mu|\hat{H}|\nu\rangle$$

$$|\Phi\rangle = \sum_{\mu} d_{\mu} |\mu\rangle$$



# Eigenvalue Problems of Large and Sparse Matrices

# Sparse Matrix

- Particle or orbital number:  $N$
  - Fock space dimension:  $\exp[N \times \text{const.}]$
  - # of terms in Hamiltonian: Polynomial of  $N$
- # of matrix elements of Hamiltonian matrix:  
(Polynomial of  $N$ )  $\times \exp[N \times \text{const.}]$

For sufficiently large  $N$ ,  
(Polynomial of  $N$ )  $\times \exp[N \times \text{const.}]$   
 $\ll (\exp[N \times \text{const.}])^2$

Then, the Hamiltonian matrix is **sparse**

# Larger TFIM Revisit

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

-Non-commutative

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

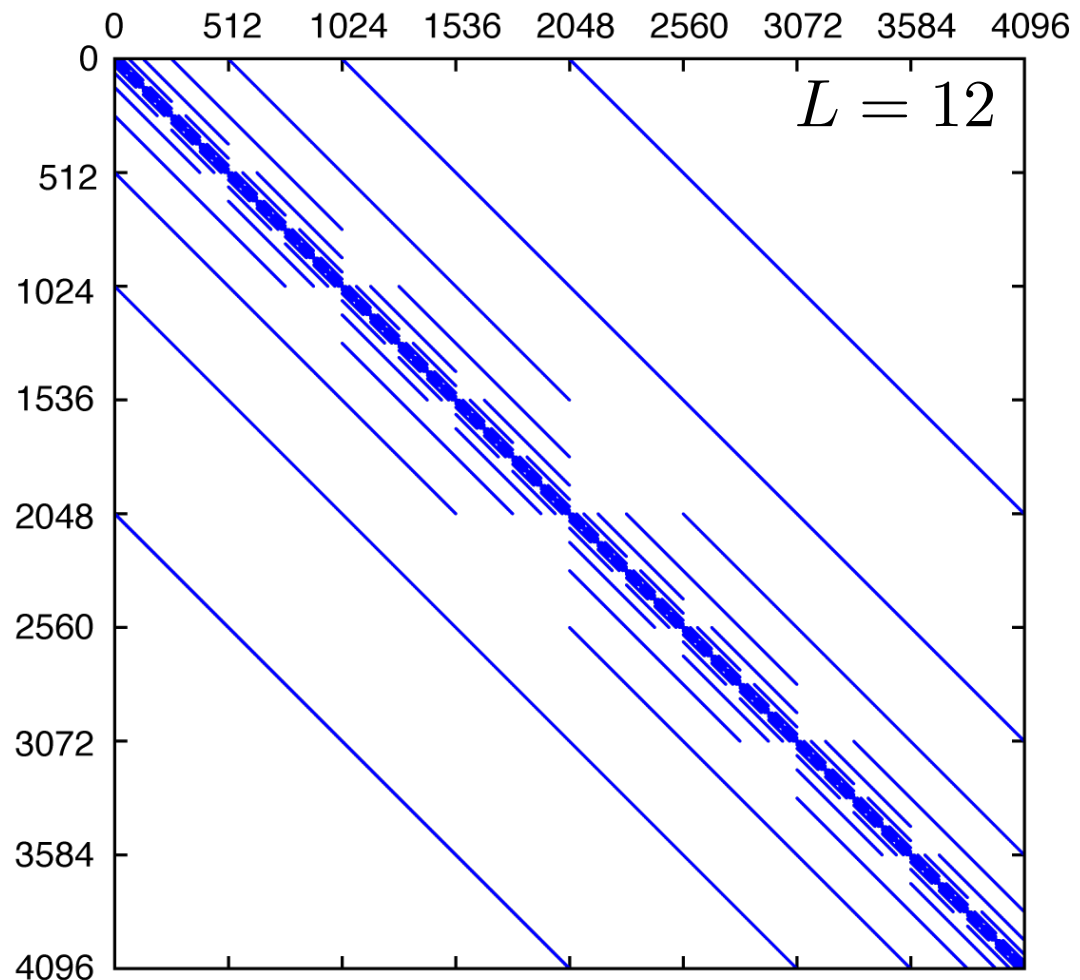
→ Quantum fluctuations  
or Zero point motion

-Sparse

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

-Solvable

-Hierarchical matrix?



# Why Hamiltonian Matrices are Sparse?

Example: TFIM

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

-Diagonal elements

$$\left[ J \sum_{i=0}^{L-1} \hat{S}_i^z \hat{S}_{\text{mod}(i+1,L)}^z \right] |\sigma_0 \sigma_1 \cdots \sigma_{L-1}\rangle = \left[ \frac{J}{4} \sum_{i=0}^{L-1} (-1)^{\sigma_i + \sigma_{\text{mod}(i+1,L)}} \right] |\sigma_0 \sigma_1 \cdots \sigma_{L-1}\rangle$$

-Off diagonal elements

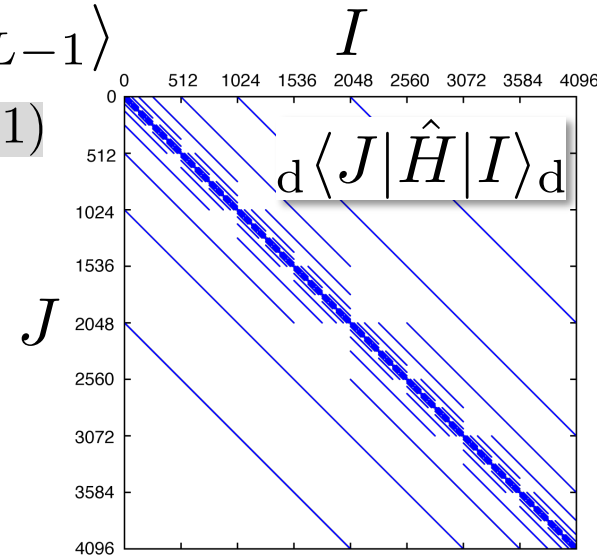
$$\hat{S}_\ell^x |\sigma_0 \sigma_1 \cdots \sigma_\ell \cdots \sigma_{L-1}\rangle = \frac{1}{2} |\sigma_0 \sigma_1 \cdots \bar{\sigma}_\ell \cdots \sigma_{L-1}\rangle$$

ordering of bases

$$\hat{S}_\ell^x |I\rangle_d = \frac{1}{2} |J\rangle_d$$

$$|\sigma_0 \sigma_1 \cdots \sigma_{L-1}\rangle = \left| \sum_{\ell=0}^{L-1} \sigma_\ell \cdot 2^\ell \right\rangle_d$$

$(\sigma_\ell, \bar{\sigma}_\ell) = (1, 0), (0, 1)$



$$I = \sum_{j=0}^{L-1} \sigma_j \cdot 2^j$$

$$J = \sum_{j=0}^{L-1} \sigma_j \cdot 2^j + (1 - 2\sigma_\ell) \cdot 2^\ell$$

Each term in sum of operators maps  $|I\rangle_d$  to  $|J\rangle_d$

→ # of nonzero elements < # of terms in the hamiltonian

# Computational and Memory Costs

Matrix-vector product of dense matrix

$$v_i = \sum_{j=0}^{N_H-1} A_{ij} u_j$$

Computational:  $O(\text{Fock space dimension})^2$

Memory:  $O(\text{Fock space dimension})^2$

Matrix-vector product of  
large and sparse matrix

Computational:  $O(\text{Fock space dimension})$

Memory:  $O(\text{Fock space dimension})$

Hamiltonian is not stored in memory

# Algorithm for Eigenvalue Problems of Large & Sparse Matrix: Power Method

Min. Eigenvalue of hermitian

Initial vector:  $|v_1\rangle = \sum_{n=0} c_n |n\rangle$

Parameter:  $\max_n \{E_n\} \leq \Lambda$

$$\hat{H}|n\rangle = E_n|n\rangle$$

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

$$E_0 \leq E_1 \leq \dots$$

$$\lim_{m \rightarrow +\infty} \frac{(\Lambda - \hat{H})^m |v_1\rangle}{\sqrt{\langle v_1 | (\Lambda - \hat{H})^{2m} | v_1 \rangle}} = |0\rangle$$

$$(\Lambda - \hat{H})^m |v_1\rangle = \sum_n (\Lambda - E_n)^m c_n |n\rangle$$

$$\lim_{m \rightarrow +\infty} \frac{\sum_{n>0} (\Lambda - E_n)^{2m} |c_n|^2}{(\Lambda - E_0)^{2m} |c_0|^2} = 0$$

# Advanced Algorithm: Krylov Subspace Method

Krylov subspace

$$\mathcal{K}_m(\hat{H}, |v_1\rangle) = \text{span}\{|v_1\rangle, \hat{H}|v_1\rangle, \dots, \hat{H}^{m-1}|v_1\rangle\}$$

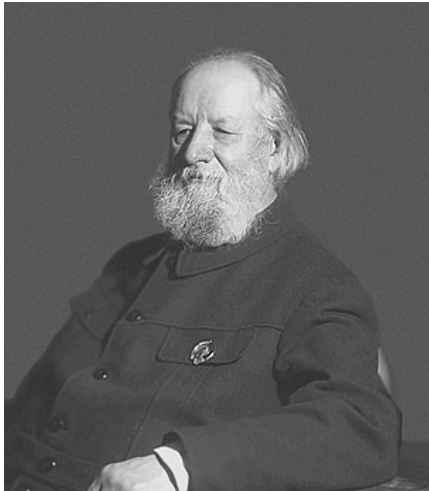
Shift invariance:

$$\mathcal{K}_m(\hat{H}, |v_1\rangle) = \mathcal{K}_m(\hat{H} + z\mathbf{1}, |v_1\rangle)$$

Krylov subspace method:

- Lanczos method (symmetric/hermitian),  
Arnoldi method (general matrix)
- Conjugate gradient method (CG method)  
(many variation)

# 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  $K_n$ :  $\mathcal{O}(\text{nnz}(A) \times n)$

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

Cornelius Lanczos 1950

Walter Edwin Arnoldi 1951

\*nnz: Number of non-zero  
entries/elements



# 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

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

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

Orthogonalization

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

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

# 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

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

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

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

Hamiltonian projected onto  $m$  D Krylov subspace

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

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**

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

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

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

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

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

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

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

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

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

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

# Convergence of Lanczos Method

Yousef Saad,

*Numerical Methods for Large Eigenvalue Problems* (2nd ed)

The Society for Industrial and Applied Mathematics 2011

Assumption:  $\lambda_1 > \lambda_2 > \dots > \lambda_n$

Convergence theorem for the largest eigenvalue

$$0 \leq \lambda_1 - \lambda_1^{(m)} \leq (\lambda_1 - \lambda_n) \left[ \frac{\tan \theta(|v_1\rangle, |0\rangle)}{C_{m-1}(1 + 2\gamma_1)} \right]^2$$
$$\sim 4(\lambda_1 - \lambda_n) [\tan \theta(|v_1\rangle, |0\rangle)]^2 e^{-4\sqrt{\gamma_1}m}$$

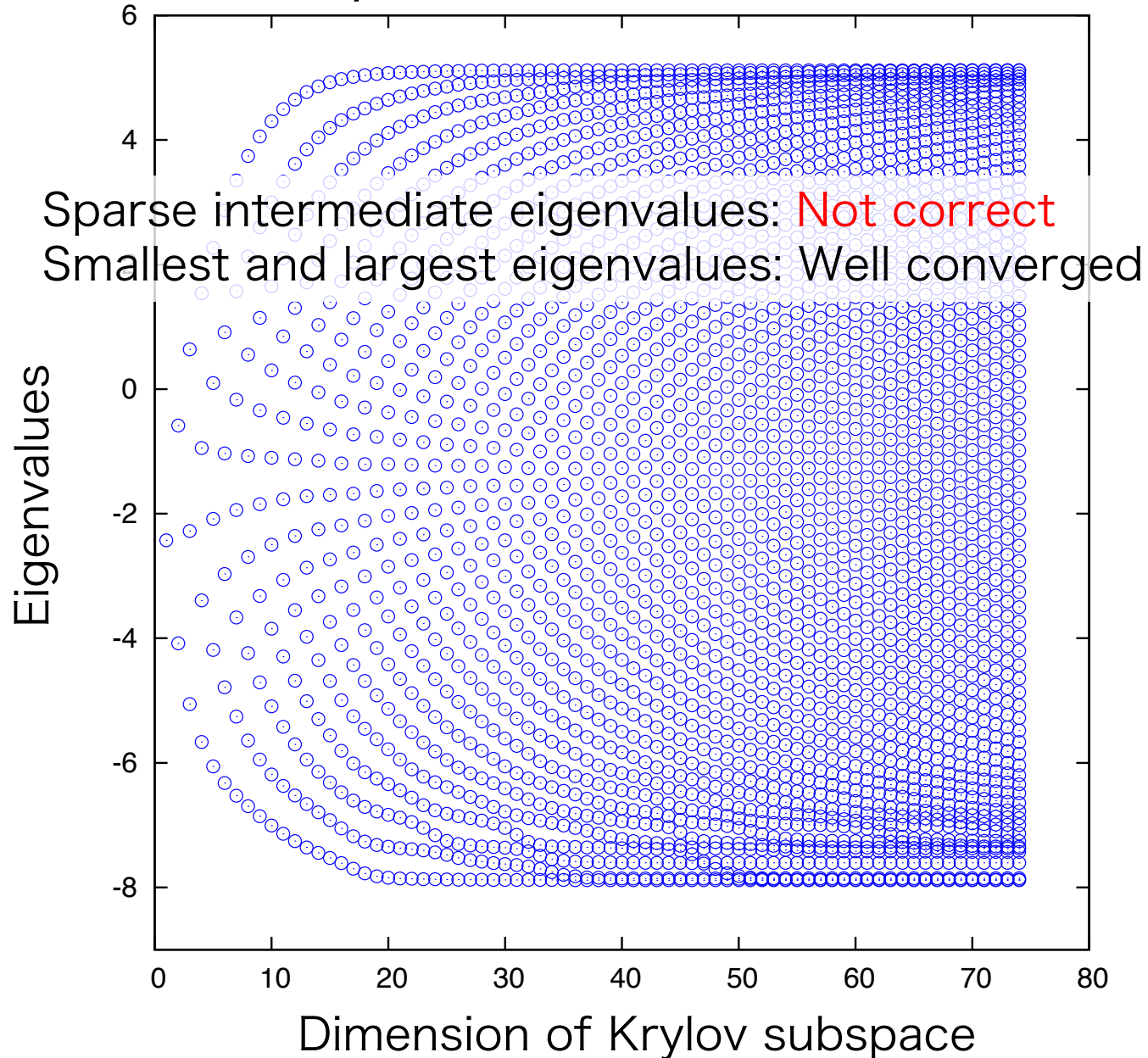
$$\gamma_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

$$C_k(t) = \frac{1}{2} \left[ \left( t + \sqrt{t^2 - 1} \right)^k + \left( t + \sqrt{t^2 - 1} \right)^{-k} \right]$$

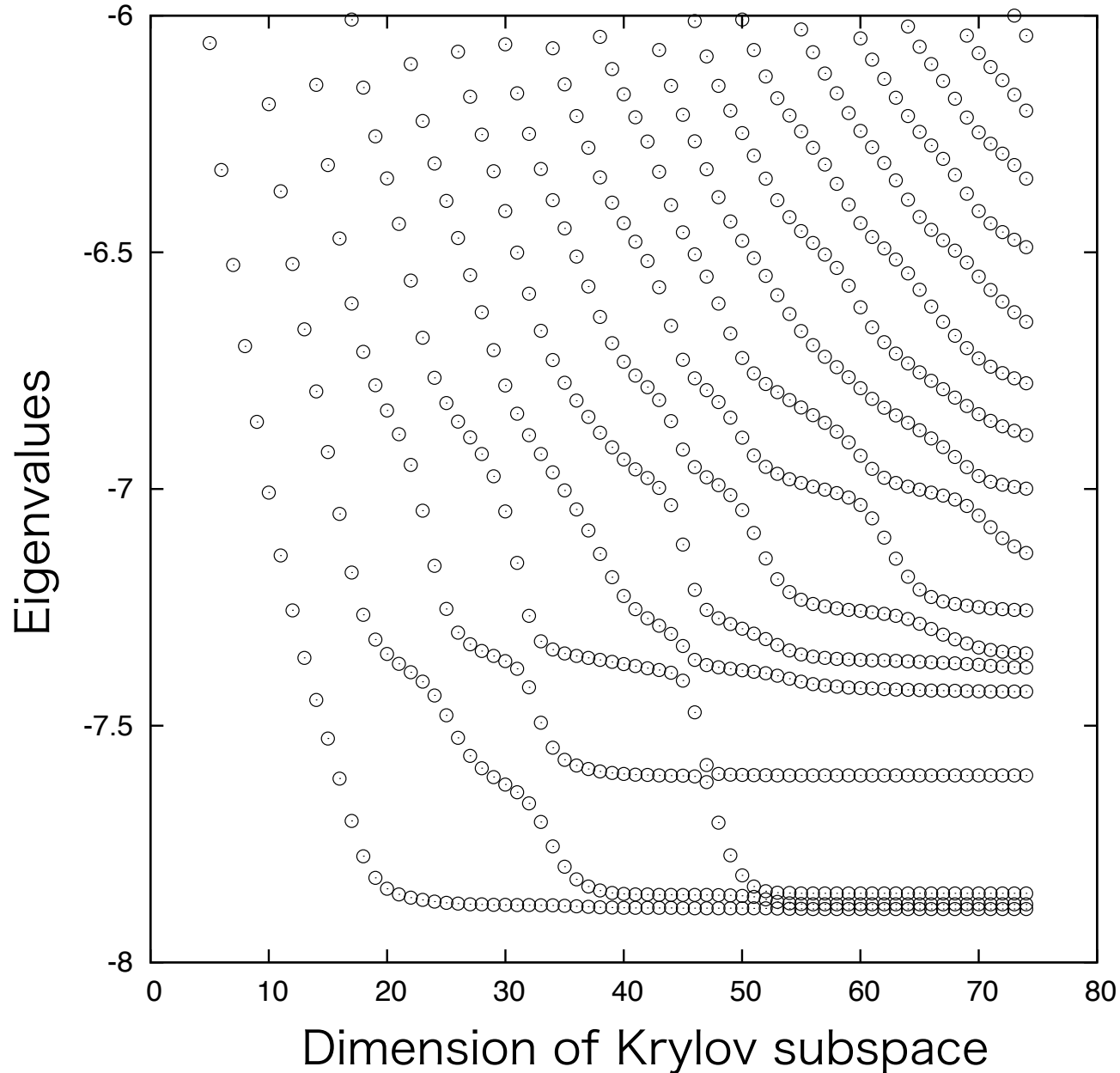
# How Lanczos Method Works



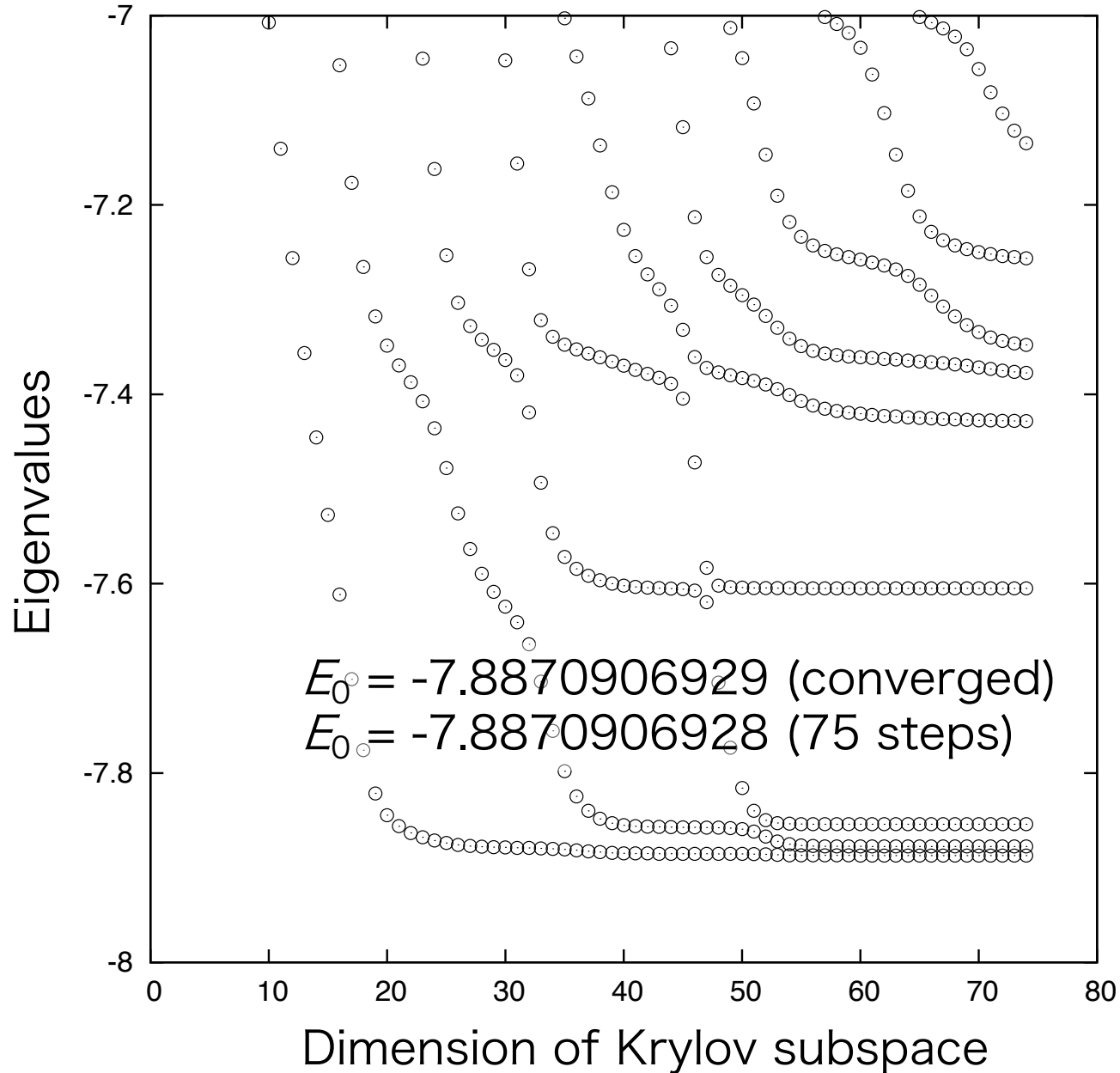
24 site cluster of Kitaev- $\Gamma$  model (frustrated  $S=1/2$  spins)  
Dimension of Fock space:  $2^{24}=16777216$



# How Lanczos Method Works



# How Lanczos Method Works



# Lecture Schedule

## Classical

- #1 Many-body problems in physics and why they are hard to solve
- #2 Classical statistical model and numerical simulation
- #3 Classical Monte Carlo method
- #4 Applications of classical Monte Carlo method
- #5 Molecular dynamics and its application
- #6 Extended ensemble method for Monte Carlo methods
- #7 Quantum lattice models and numerical approaches
- #8 Quantum Monte Carlo methods

## Quantum

- #9 Applications of quantum Monte Carlo methods
- #10 Linear algebra of large and sparse matrices for quantum many-body problems
- #11 Krylov subspace methods and their applications to quantum many-body problems
- #12 Large sparse matrices and quantum statistical mechanics
- #13 Parallelization for many-body problems

# Exercise on Jupyter Notebook

-[https://github.com/compsci-alliance/many-body-problems  
sample\\_Hubbard\\_Helium4\\_v1.ipynb](https://github.com/compsci-alliance/many-body-problems/sample_Hubbard_Helium4_v1.ipynb)

A sample code for small Hubbard models  
and VMC for liquid helium 4