多体問題の計算科学

Computational Science for Many-Body Problems

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

14:55-16:40 June 27, 2023

0. Applications of QMC

Quantum many-body problems and huge sparse matrices

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

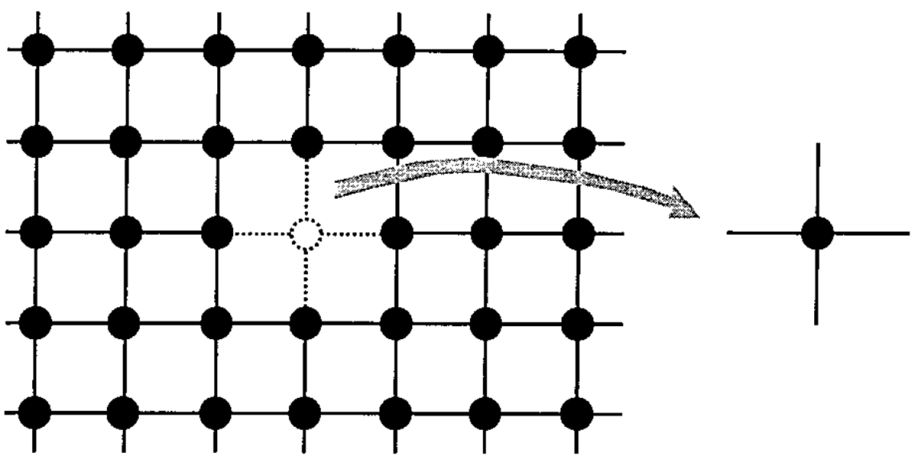
Applications of QMC

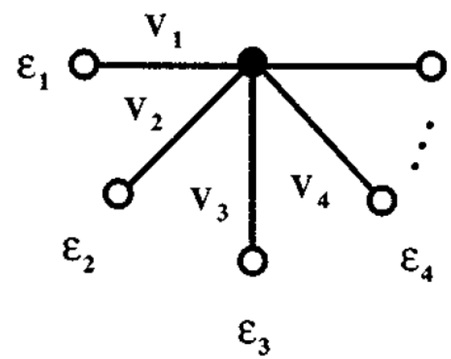
Dynamical Mean Field and Impurity Model

As a review, A. Georges, G. Kotliar, W. Krauth, and Marcelo J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).

Mapping from lattice model to impurity model

$$\hat{H} = \sum_{\langle i,j \rangle,\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}) + U\sum_{i} \hat{c}^{\dagger}_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^{\dagger}_{i\downarrow}\hat{c}_{i\downarrow}$$





$$\hat{H} = \sum_{j,\sigma} \epsilon_j \hat{c}^{\dagger}_{j\sigma}\hat{c}_{j\sigma} + \sum_{j,\sigma} v_j(\hat{c}^{\dagger}_{j\sigma}\hat{d}_{\sigma} + \hat{d}^{\dagger}_{\sigma}\hat{c}_{j\sigma}) + U\hat{d}^{\dagger}_{\uparrow}\hat{d}_{\uparrow}\hat{d}^{\dagger}_{\downarrow}\hat{d}_{\downarrow}$$

Dynamical Mean Field and Impurity Model

As a review, A. Georges, G. Kotliar, W. Krauth, and Marcelo J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).

Self-consistent impurity model

$$\hat{H} = \sum_{j,\sigma} \epsilon_j \hat{c}^\dagger_{j\sigma} \hat{c}_{j\sigma} + \sum_{j,\sigma} v_j (\hat{c}^\dagger_{j\sigma} \hat{d}_\sigma + \hat{d}^\dagger_\sigma \hat{c}_{j\sigma}) + U \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$$

-Green's function of impurity model

$$G^{\mathrm{imp}}(\omega) = \frac{1}{\omega + i\delta + \mu - \Sigma^{\mathrm{imp}}(\omega) - \Delta(\omega)}$$

-Dynamical mean-field

$$\Delta(\omega) = \omega + i\delta + \mu - \Sigma^{\mathrm{imp}}(\omega) - \left[\frac{1}{N} \sum_{\vec{k}} \frac{1}{\omega + i\delta + \mu - \epsilon(\vec{k}) - \Sigma^{\mathrm{imp}}(\omega)} \right]^{-1}$$

$$= \sum_j \frac{|v_j|^2}{\omega + i\delta - \epsilon_j}$$

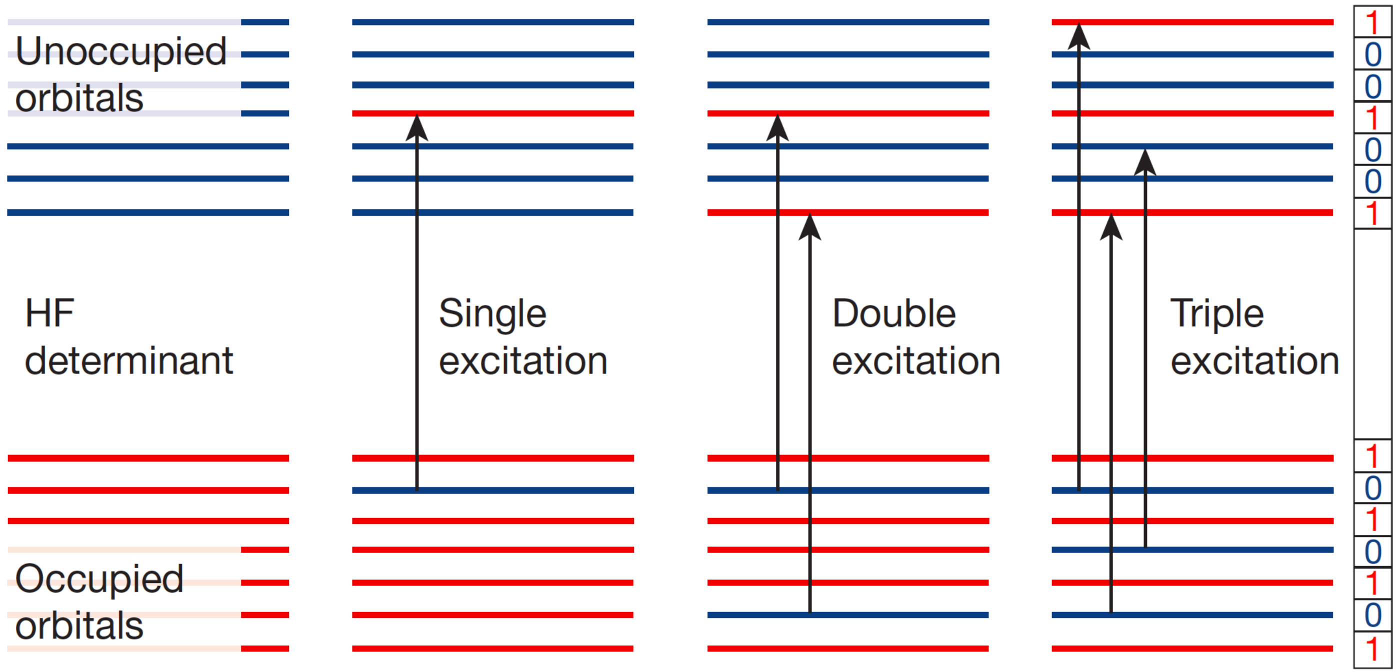
You can find applications of DMFT in G. Kotliar, *et al.*, Rev. Mod. Phys. 78, 865 (2006).

Configuration Interaction Monte Carlo

G. H. Booth, A. Grüneis, G. Kresse, A. Alavi, Nature 493, 365 (2013).

Sampling basis set

$$|\Psi\rangle = \sum_m C_m \left[\prod_\lambda \left(\hat{c}_\lambda^\dagger \right)^{\nu_\lambda^{(m)}} \right] |0\rangle$$

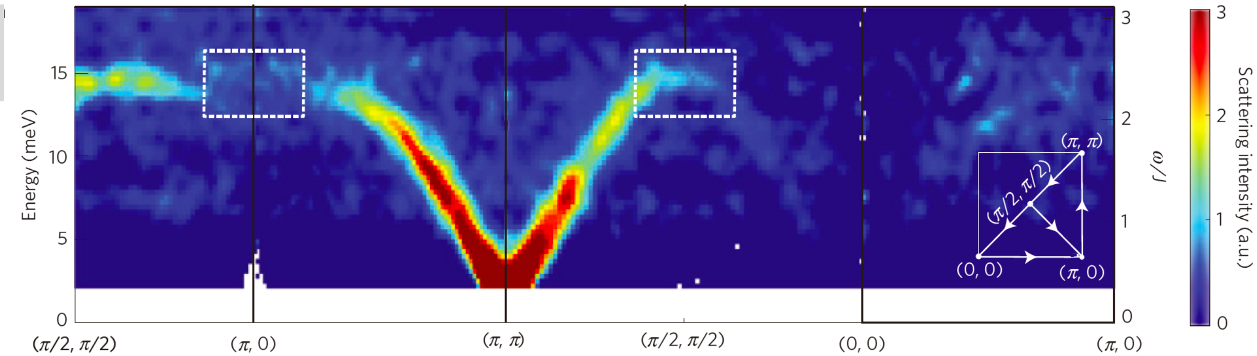


$$\{\nu_\lambda\}$$

$$\left[\prod_\lambda \left(\hat{c}_\lambda^\dagger \right)^{\nu_\lambda} \right] |0\rangle$$

Example of Applications: Spin Excitations in Square Lattice Heisenberg model

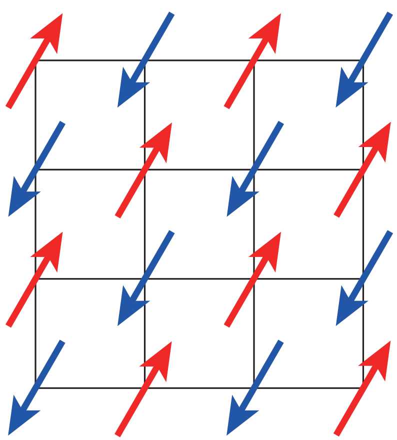
$Cu(DCOO)_2 \cdot 4D_2O$

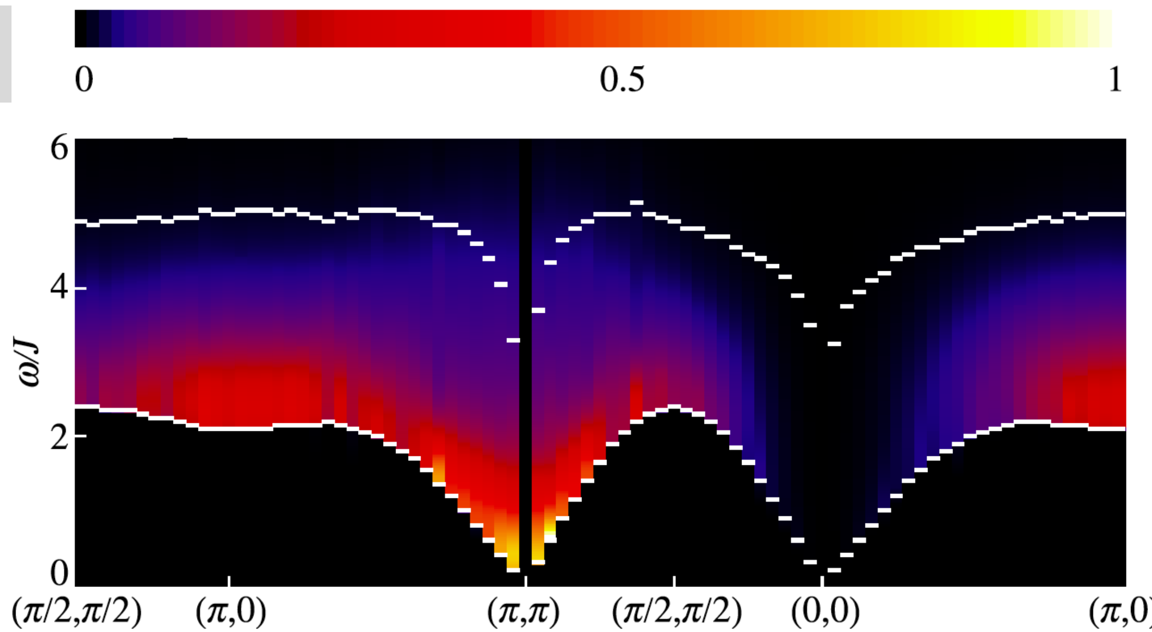


B. Dalla Piazza, *et al.*, Nat. Phys. 11, 62 (2015)

S=1/2 Heisenberg

Ground state





H. Shao, *et al.*, Phys, Rev, X 7, 041072 (2017)

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.

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

Expanded by orthonormal basis

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

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

$$\int d^3r\phi^*(\vec{r})\phi(\vec{r}) = \sum_m |c_m|^2$$

Matrix representation

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

$$\boxed{\sum_m H_{\ell m}c_m = Ec_\ell}$$

Quantum Mechanics by Linear Algebra

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

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

-Diagonalizable by unitary matrices
-Real eigenvalues

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

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

Quantum Mechanics by Linear Algebra

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

Vector representation of expectation value

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

$$= \frac{\sum_{\ell,m} c_\ell^* O_{\ell m} c_m}{\sum_n |c_n|^2}$$

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)

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

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

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

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

Bosons

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

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

Quantum Many-Body Problem by Linear Algebra

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

→ General Hamiltonian with two-body interactions

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

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

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

Quantum Many-Body Problem by Linear Algebra

Fock space of *N*-particle fermions expanded by

$$|\Phi\rangle = \sum_{\ell_1,\ell_2,\ldots,\ell_N} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_N} C_{\ell_1\ell_2\cdots\ell_N} \hat{a}^\dagger_{\ell_1\sigma_1} \hat{a}^\dagger_{\ell_2\sigma_2} \cdots \hat{a}^\dagger_{\ell_N\sigma_N} |\mathrm{vac}\rangle$$

Orthonormalized many-body basis

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

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

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

$$\langle\{m_j, \tau_j\}|\{\ell_j, \sigma_j\}\rangle = \left\{ \begin{array}{ll} 0 & (\{m_j, \tau_j\} \cup \{\ell_j, \sigma_j\} \neq \{\ell_j, \sigma_j\}) \\ 1 & (\{m_j, \tau_j\} \cup \{\ell_j, \sigma_j\} = \{\ell_j, \sigma_j\}) \end{array} \right.$$

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

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

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

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

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 x const.]

■ # of terms in Hamiltonian: Polynomial of N

→ # of matrix elements of Hamiltonian matrix:
(Polynomial of N) x exp[N x const.]

For sufficiently large N,
(Polynomial of N) x exp[N x const.]
<< (exp[N x 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

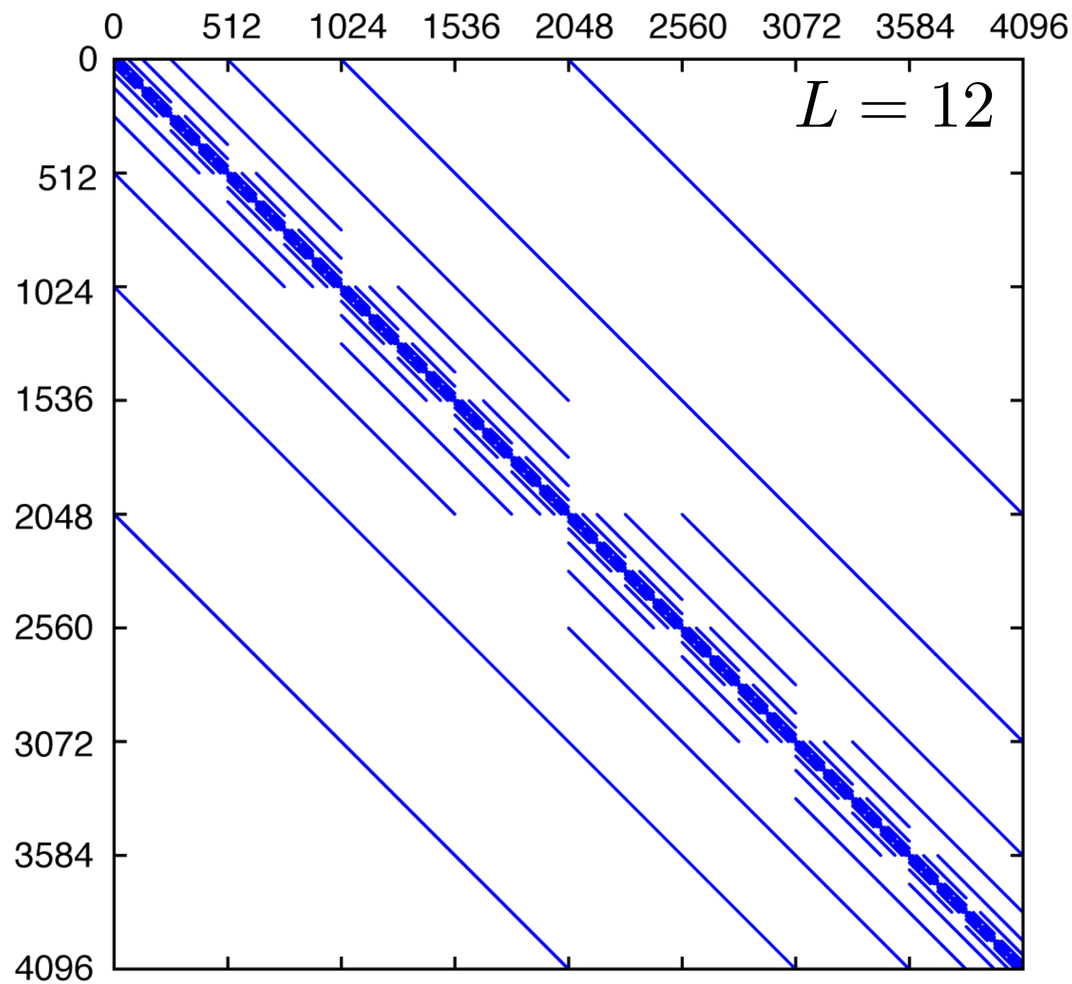
$$\left[\sum_{i=0}^{L-1}\hat{S}_i^z\hat{S}_{i+1}^z, \sum_{i=0}^{L-1}\hat{S}_i^x\right] \neq 0$$

→Quantum fluctuations
or Zero point motion

-Sparse
\# of elements ∝ $O(2^L)$

-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

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

-Off diagonal elements

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

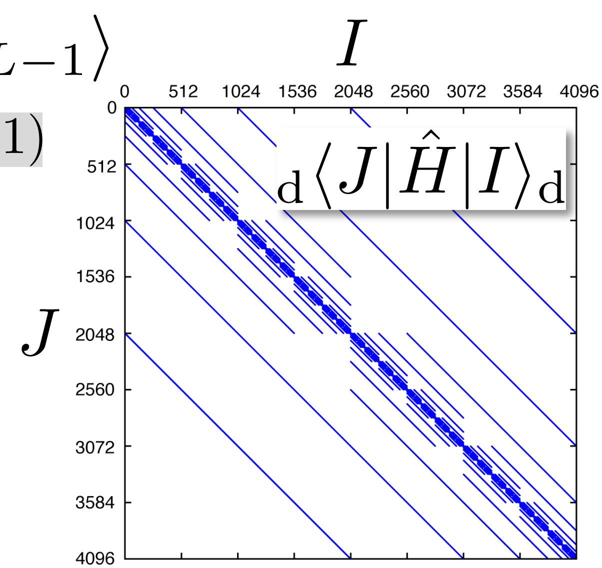
$$(\sigma_\ell,\overline{\sigma_\ell}) = (1,0),(0,1)$$

ordering of bases

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

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

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



Each term in sum of operators maps $|I\rangle_{\mathrm{d}}$ to $|J\rangle_{\mathrm{d}}$

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

Computational and Memory Costs

Matrix-vector product of dense matrix

$$v_i = \sum_{j=0}^{N_{\mathrm{H}}-1} A_{ij} u_j$$

Computational: O((Fock space dimension)^2)
Memory: O((Fock space dimension)^2)

Matrix-vector product of large and sparse matrix

Computational: O(Fock space dimension)
Memory: O(Fock space dimension)
Hamiltonian is not stored in memory

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

Min. Eigenvalue of hermitian

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

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

$$E_0 \leq E_1 \leq \cdots$$

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

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

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

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

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

Advanced Algorithm: Krylov Subspace Method

Krylov subspace

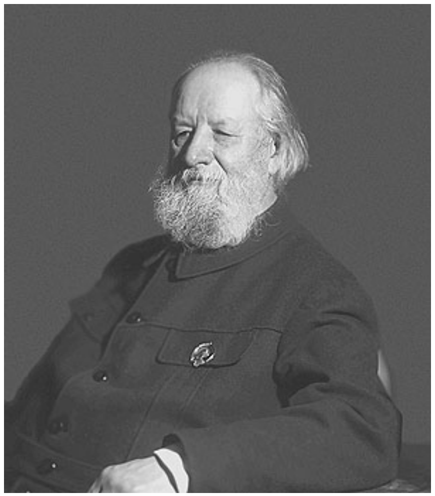
$$\mathcal{K}_m(\hat{H}, |v_1\rangle) = \mathrm{span}\{|v_1\rangle, \hat{H}|v_1\rangle, \dots, \hat{H}^{m-1}|v_1\rangle\}$$

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

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

Numerical cost to construct K_n: $\mathcal{O}(\mathrm{nnz}(A) \times n)$

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

$$\textbf{Initial}: \beta_1 = 0,\ |v_0\rangle = 0$$

$$\textbf{for } j = 1, 2, \ldots, m \textbf{ do}$$

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

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

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

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

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

Lanczos Method

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

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

Orthogonalization

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

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

Lanczos Method

$$\textbf{Initial}:\ \beta_1 = 0,\ \ |v_0\rangle = 0$$

$$\textbf{for}\ j = 1, 2, \ldots, m\ \textbf{do}$$

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

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

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

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

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

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 subsace

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

Eigenvalues of projected Hamiltonian
$\rightarrow$ Approximate eigenvalues of original Hamiltonian

Lanczos Method: # of Vectors Required

$$\textbf{Initial}: \beta_1 = 0,\ |v_0\rangle = 0$$

$$\textbf{for } j = 1, 2, \ldots, m \textbf{ do}$$

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

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

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

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

$$|v_{j+1}\rangle = |w_j\rangle/\beta_{j+1} \qquad |w_j\rangle \to |v_{j+1}\rangle,\ |v_j\rangle$$

Convergence of Lanczos Method

Yousef Saad,
Numerical Methods for Large Eigenvalue Problems (2nd ed)
The Society for Industrial and Applied Mathematics 2011

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

Convergence theorem for the largest eigenvalue

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

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

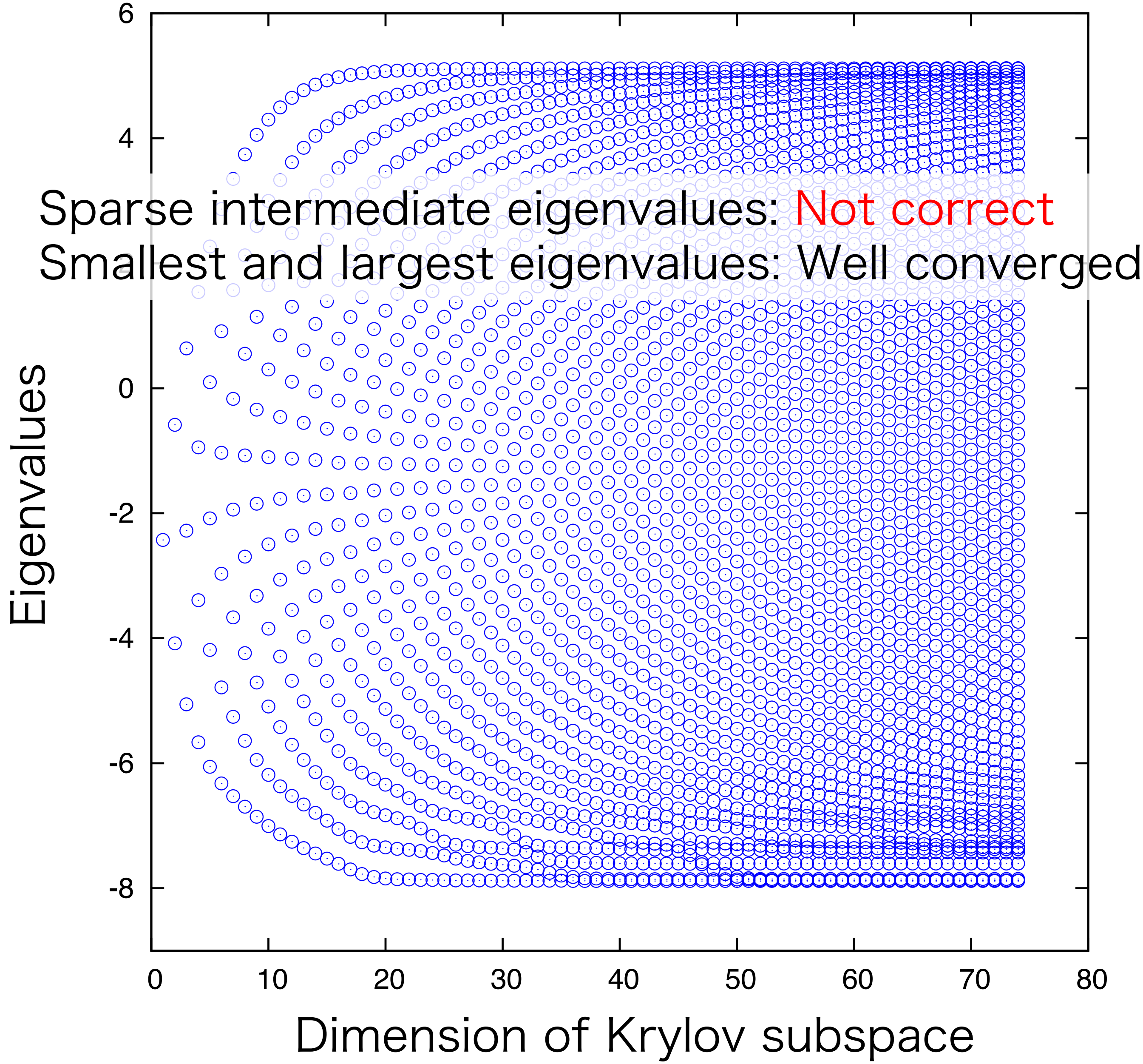
$$\gamma_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

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

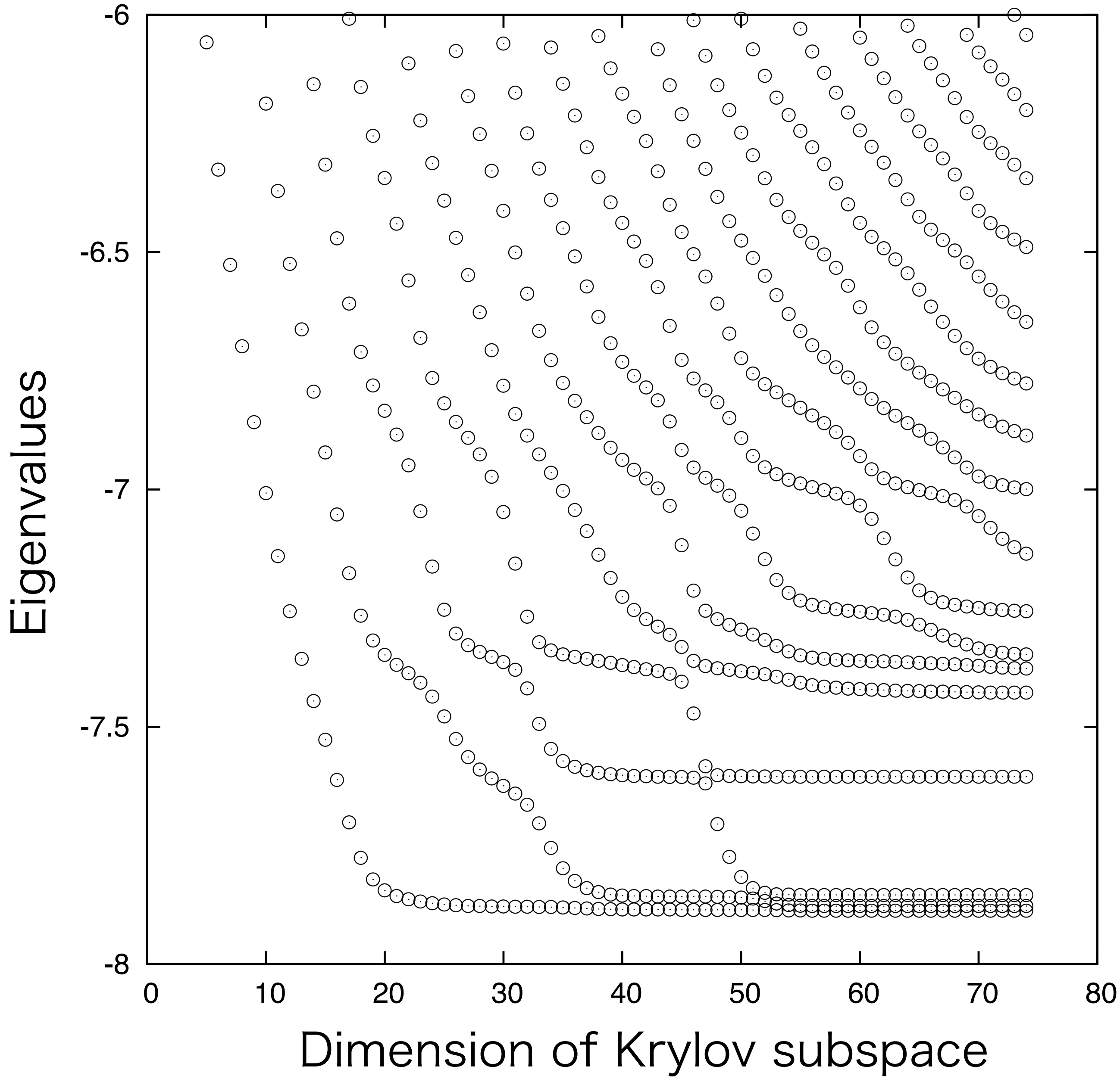
How Lanczos Method Works

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

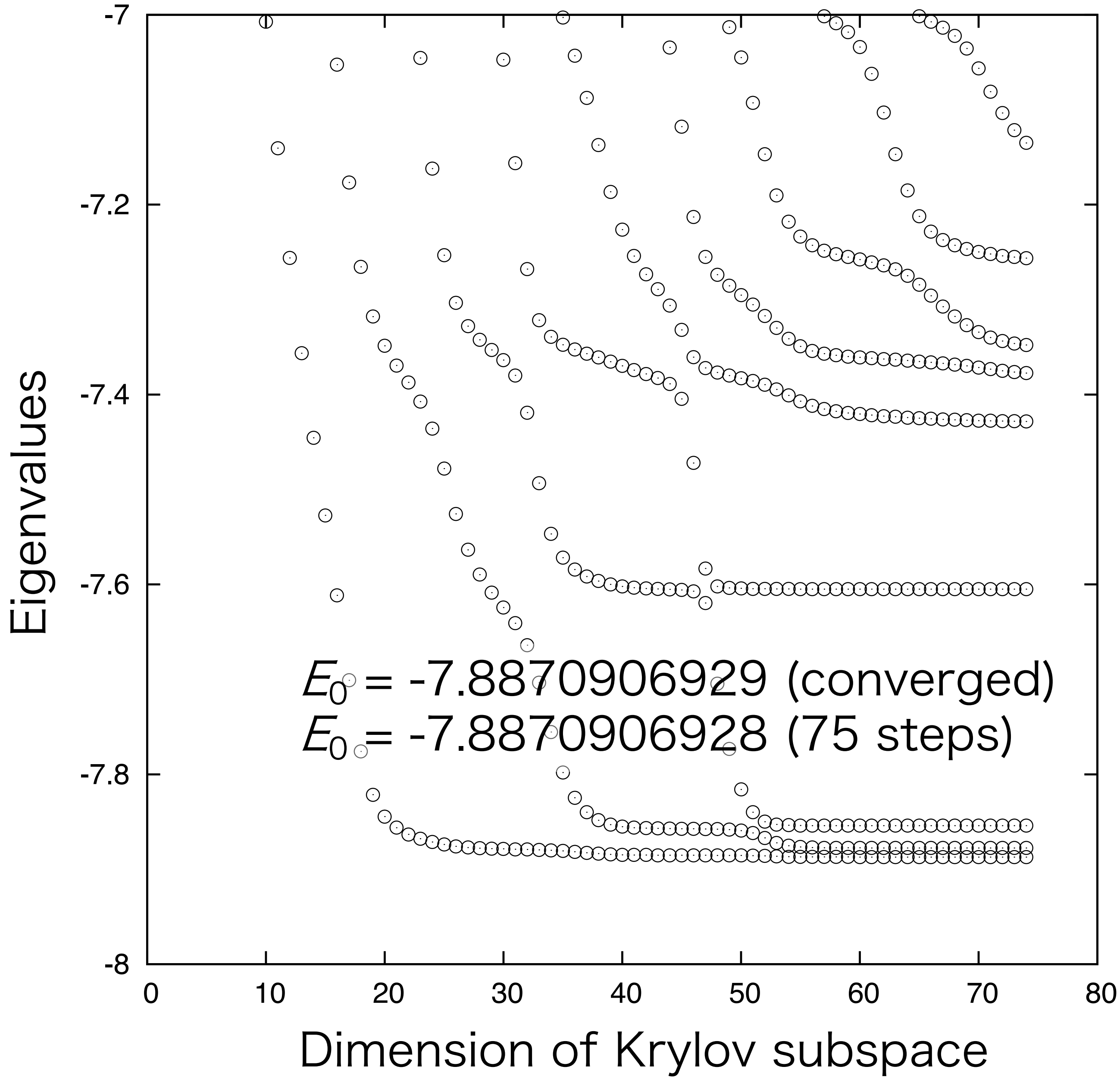
Dimension of Fock space: 2^{24}=16777216



How Lanczos Method Works



How Lanczos Method Works



Lecture Schedule

Quantum

#8 Quantum lattice models and numerical approaches
#9 Quantum Monte Carlo methods
#10 Applications of quantum Monte Carlo methods
#11 Linear algebra of large and sparse matrices for quantum many-body problems
#12 Large sparse matrices and quantum statistical mechanics
#13 Modern algorithms for quantum many-body problems

7/4 12th
7/11 13th
7/18 No lecture!!
7/31 will be the deadline for Report 2

If you are interested in QMC, open source softwares
-ALF F. F. Assaad, *et al.*, SciPost Physics Codebases 1 (2022)
-DSQSS https://github.com/issp-center-dev/dsqss
would be worth trying.