

# Information Compression #9

## Data compression: Application of Krylov subspace method

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1. Application of Krylov subspace  
SVD, eigenvalue problems, excitation spectra,  
density of states
2. Appendix



The University of Tokyo

# Application of Krylov Subspace Method

*Small # of extreme/intermediate eigenvalues*

- Electronic states of DFT Hamiltonian (one-body)
- Ground state and excited states of (cluster of) lattice model (many-body)

Excitation spectra

- Linear responses describing inelastic neutron scattering, X-ray scattering, electric/thermal transport, ...

Memory cost

- Matrices can/cannot be stored
- Vectors can/cannot be stored

# Krylov Subspace Method

from *SIAM News*, Volume 33, Number 4

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

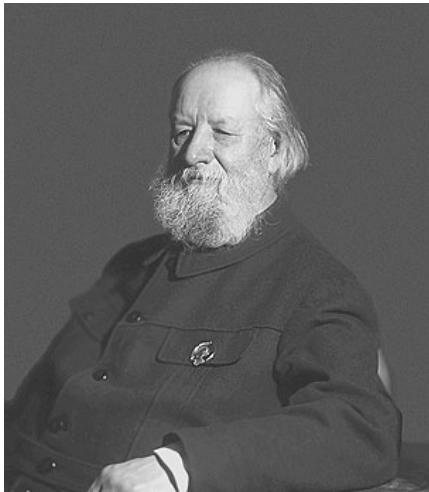
By Barry A. Cipra

**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.)

# 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

# Approximate SVD by Krylov Subspace Method

## Low-rank approximation by *block* Krylov subspace

C. Musco & C. Musco,

NIPS'15 Proceedings of 28th International Conference on  
Neural Information Processing Systems 1, 1396 (2015)

$$\|A - ZZ^T A\|_2 \leq (1 + \epsilon) \|A - A_k\|_2 \quad \begin{matrix} \text{Operator norm defined by 2-norm} \\ (\text{Spectral norm}) \end{matrix}$$

$$A \in \mathbb{R}^{L \times M} \quad Z \in \mathbb{R}^{L \times k} \quad \text{rank } k \leq L, M$$

$$q = \mathcal{O}(\ln d / \sqrt{\epsilon})$$

random matrix  $\Pi \in \mathbb{R}^{M \times k}$

$$\mathcal{K}_{q+1} = \text{span}\{A\Pi, (AA^T)A\Pi, \dots, (AA^T)^q A\Pi\}$$

$Q \in \mathbb{R}^{N \times qk}$  Orthogonalized basis set of the block Krylov subspace

$$M = Q^T AA^T Q \in \mathbb{R}^{qk \times qk}$$

$U_k$  : the top  $k$ singular vectors of  $M$

$$Z = QU_k$$

$(\Pi)_{ij}$  : Random number generated by  $e^{-x^2/2} / \sqrt{\pi}$

# Lanczos Method

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

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

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

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

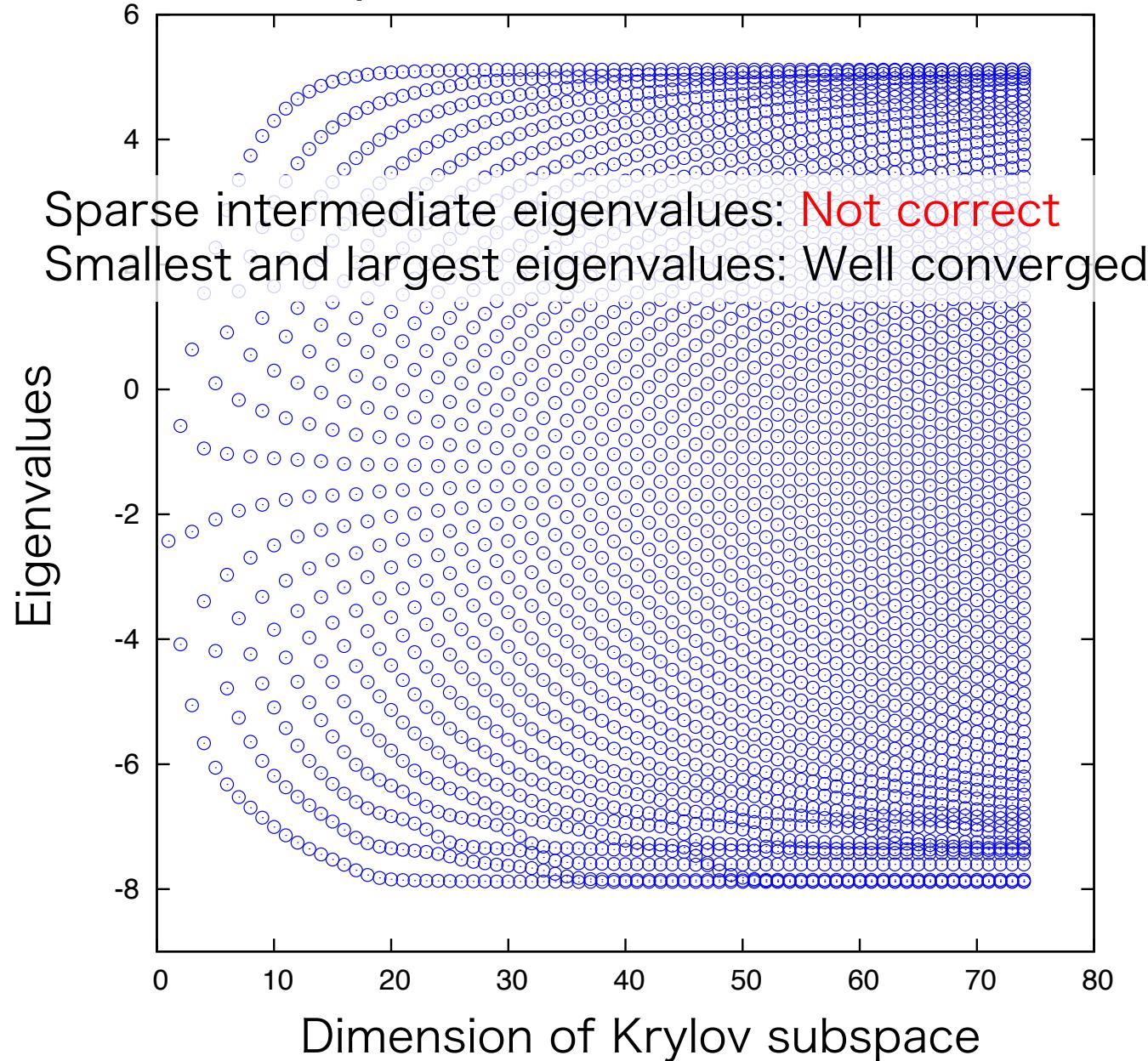
$$|w_j\rangle \leftarrow |w_j\rangle - \alpha_j|v_j\rangle$$

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

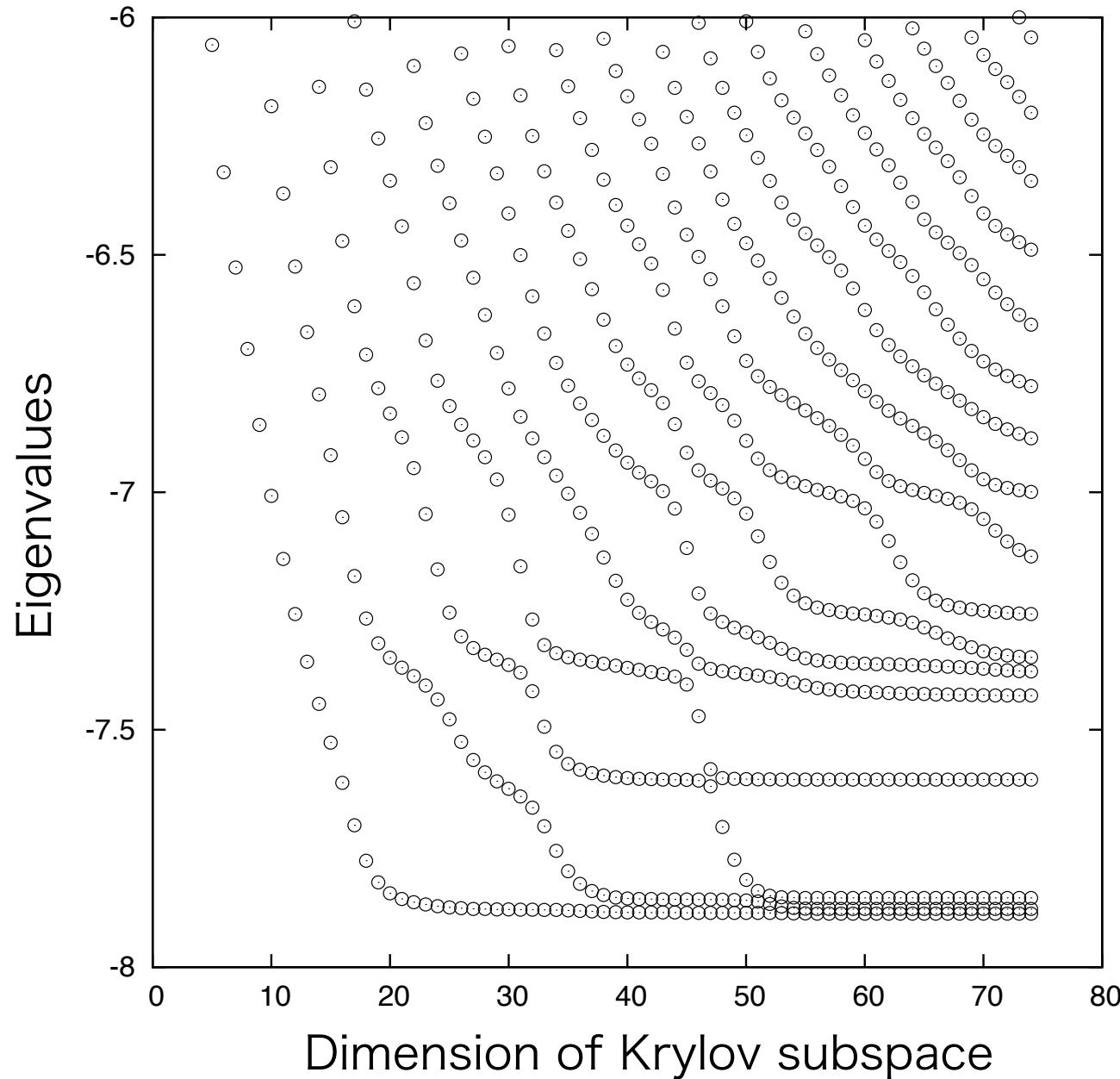
$$|v_{j+1}\rangle = |w_j\rangle / \beta_{j+1}$$

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

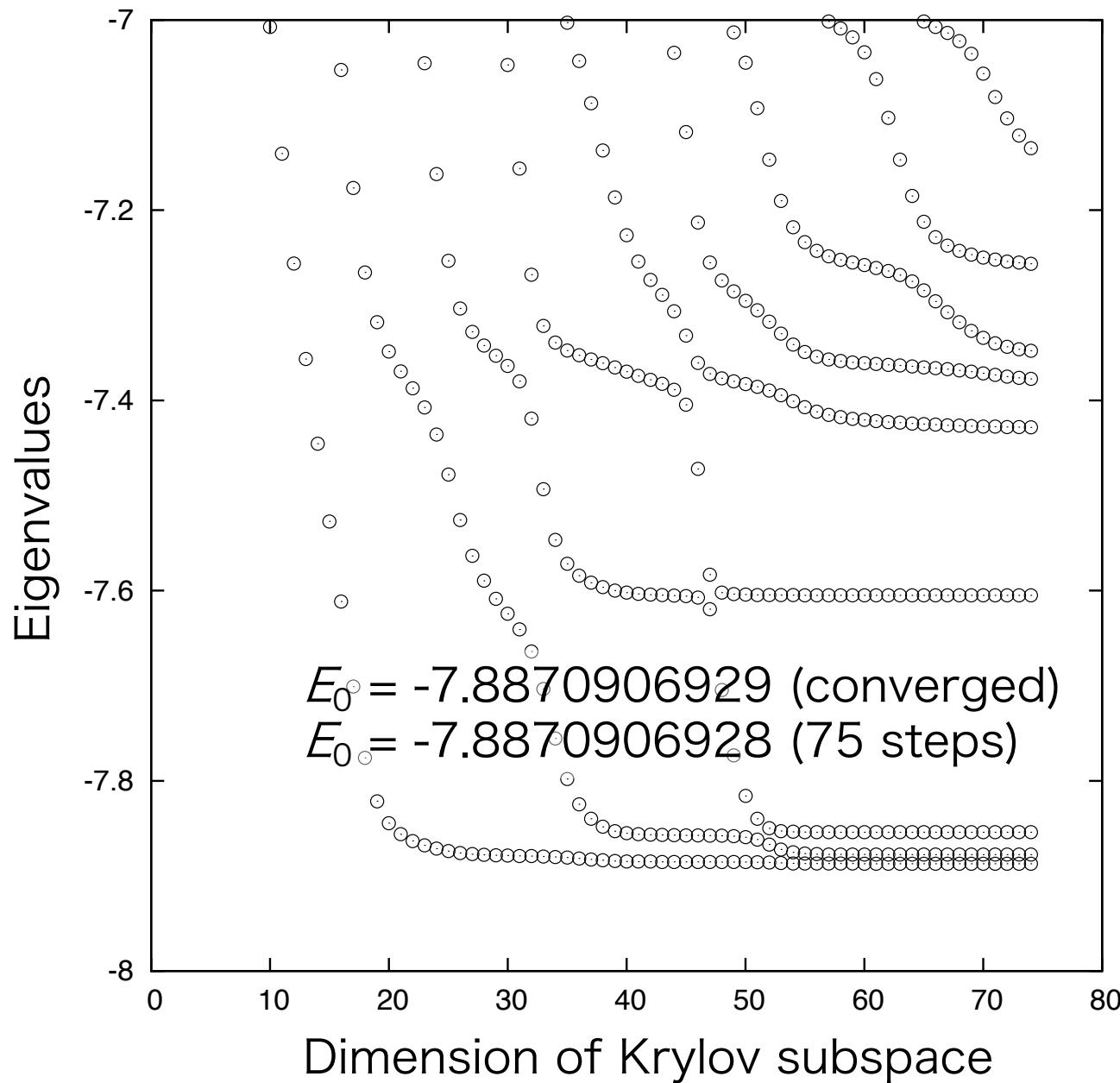
Dimension of Fock space:  $2^{24}=16777216$



# How Lanczos Method Works



# How Lanczos Method Works



# An Example of Important Eigenvalue Problems Where Low-Lying Eigenstates Matter

One-body Schrödinger equation from Hartree-Fock/DFT

$$\left[ -\frac{1}{2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V[\{\phi\}](x, y, z) \right] \phi_n(x, y, z) = E_n \phi_n(x, y, z)$$

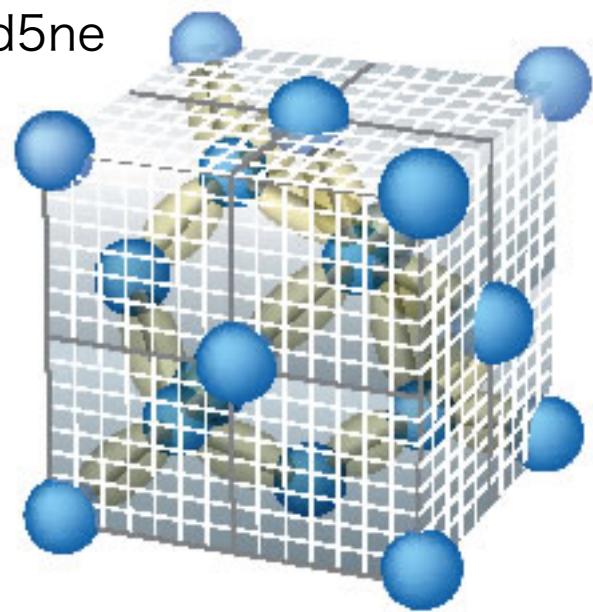
-DFT (density functional theory)

P. Hohenberg & W. Kohn, Phys. Rev. 136, B864 (1964).  
W. Kohn, Rev. Mod. Phys. 71, 1253 (1999).

$$V[\{\phi\}](x, y, z) = V[\rho](x, y, z)$$

$$\rho(x, y, z) = \sum_{n \leq N_e} |\phi_n(x, y, z)|^2 \quad N_e : \text{Number of electrons}$$
$$\int |\phi_n(x, y, z)|^2 dx dy dz = 1$$

We need to solve self-consistently  
(自己無撞着)



## 1D example: Finite difference

$$-\frac{1}{2} \frac{\phi(x + h) + \phi(x - h) - 2\phi(x)}{h^2} + V(x)\phi(x) = E\phi(x)$$

$$\vec{\phi} = -(\phi(0), \phi(h), \phi(2h), \dots, \phi((N-1)h))^T$$

$$H\vec{\phi} = E\vec{\phi}$$

We only need occupied eigenstates for electronic structure calculations, for example,  $O(10^2)$  out of  $O(10^4)$ .

# Intermediate Eigenstates

In addition to the Largest  
and Smallest

# Excitation Spectra by Krylov Subspace Method

## Excitation spectrum

$$\begin{aligned} S_O(\omega) &= \sum_n |\langle n | \hat{O} | 0 \rangle|^2 \delta(\omega - E_n + E_0) \\ &= - \lim_{\delta \rightarrow +0} \frac{1}{\pi} \text{Im} G(\omega + i\delta) \\ \\ G(z) &= \langle 0 | \hat{O}^\dagger (z \hat{I} - \hat{H})^{-1} \hat{O} | 0 \rangle \\ &= \sum_n \frac{\langle 0 | \hat{O}^\dagger | n \rangle \langle n | \hat{O} | 0 \rangle}{z - E_n + E_0} \\ \\ \delta(\omega - E_n + E_0) &= - \lim_{\delta \rightarrow +0} \frac{1}{\pi} \text{Im} \frac{1}{\omega + i\delta - E_n + E_0} \end{aligned}$$

# Excitation Spectra

Fermi's golden rule gives probability of transition (per unit time) from the ground state to excited states with energy  $\omega = E_n - E_0$

$$\begin{aligned} S_O(\omega) &= \sum_n |\langle n | \hat{O} | 0 \rangle|^2 \delta(\omega - E_n + E_0) \\ &= - \lim_{\delta \rightarrow +0} \frac{1}{\pi} \text{Im} G(\omega + i\delta) \end{aligned}$$

# Corresponding Experiment: Neutron Scattering

$$S(\vec{Q}, \omega) = \sum_{\alpha=x,y,z} \sum_n |\langle n | \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle|^2 \delta(\omega - E_n + E_0)$$

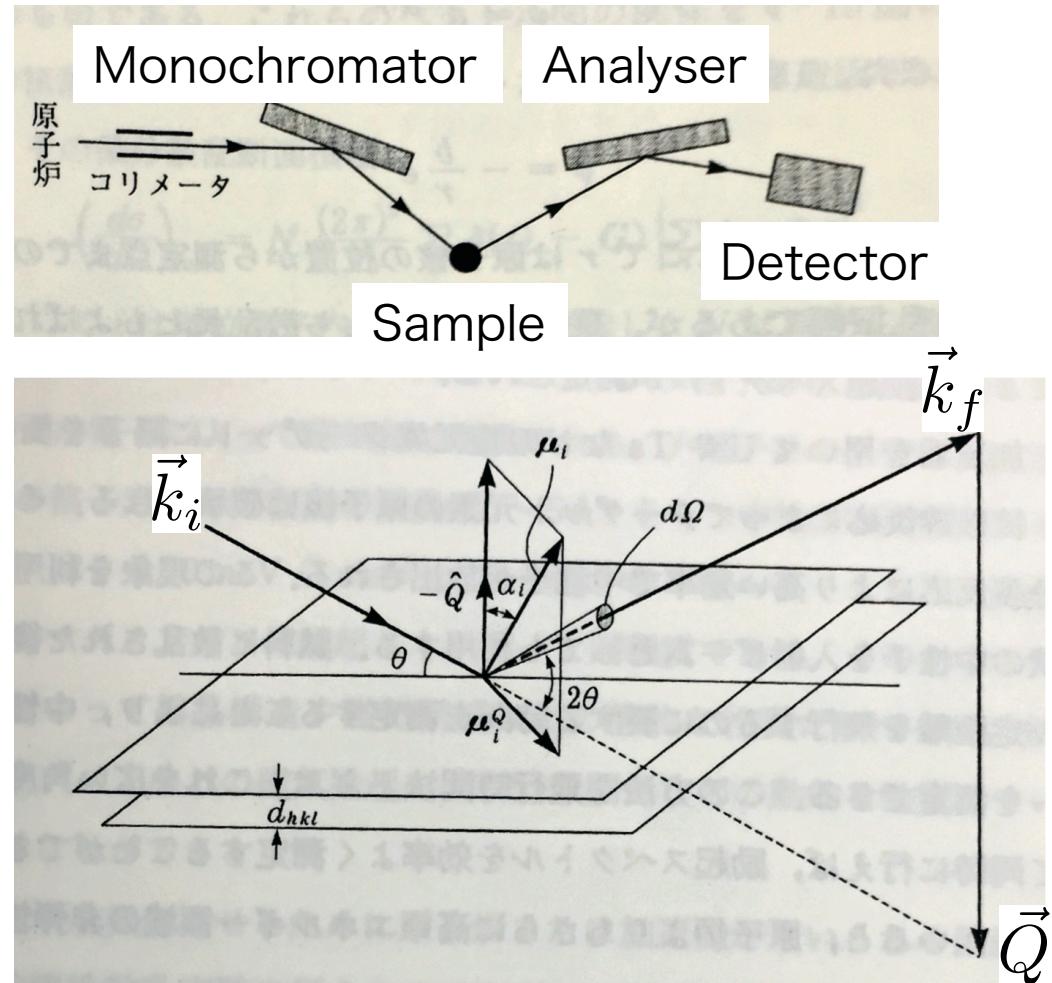
Nuclear reactor

$$\vec{k}_i - \vec{k}_f = \vec{Q}$$

$$E_i - E_f = \omega$$

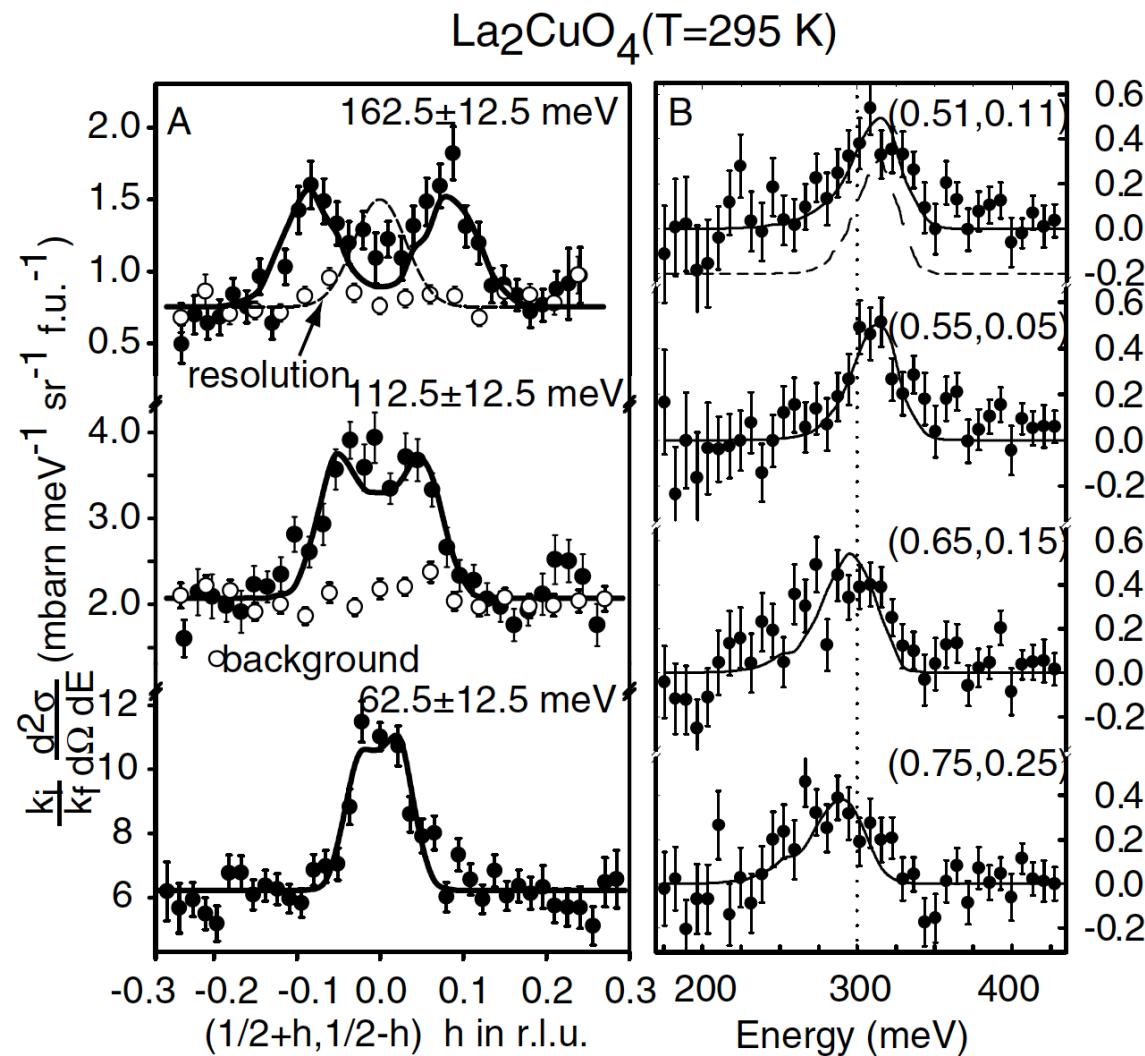
$$\hat{O} = \hat{S}_{\vec{Q}}^\alpha$$

$$= \frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^\alpha e^{+i\vec{Q}\cdot\vec{r}_j}$$



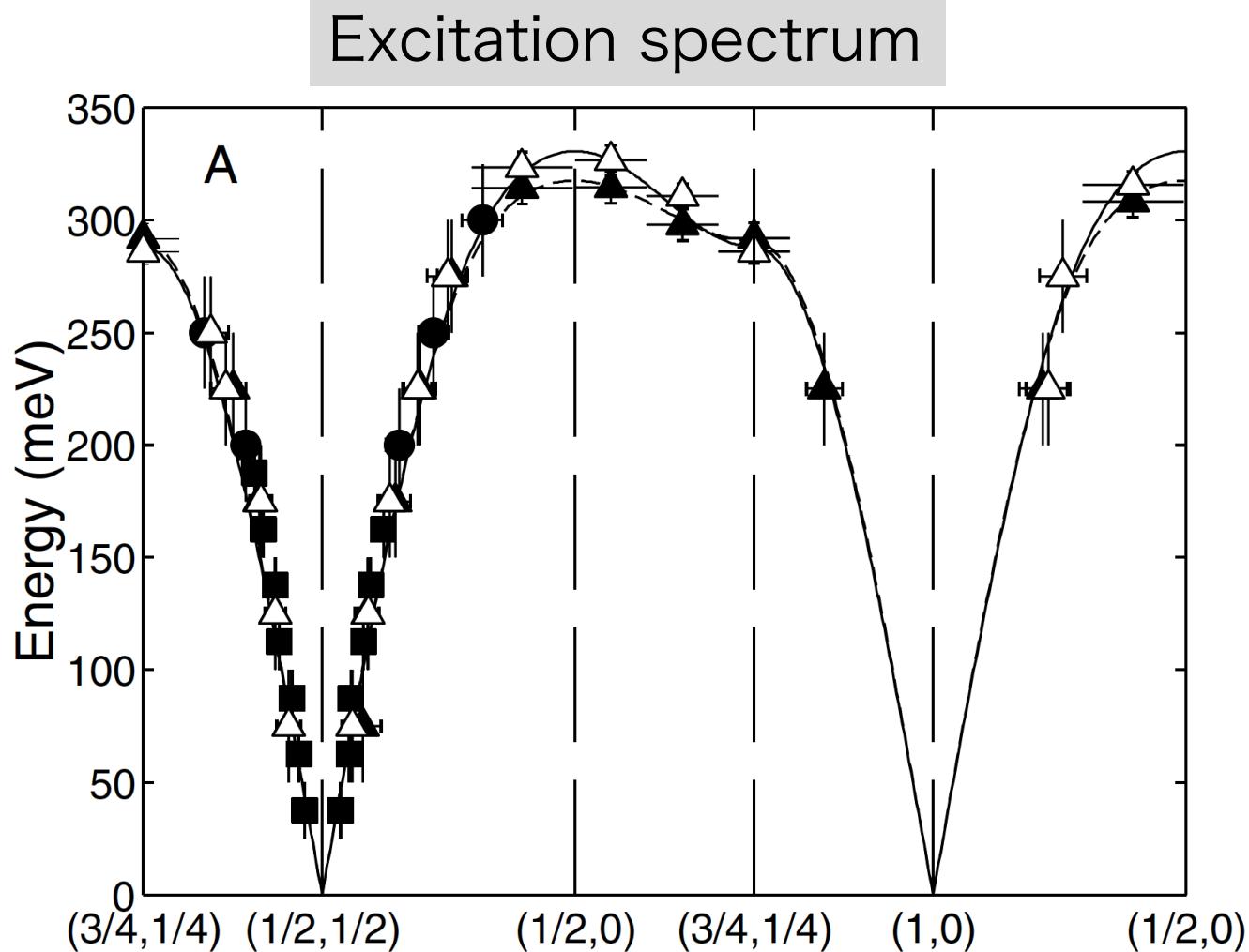
# Inelastic Neutron Scattering Measurement of $\text{La}_2\text{CuO}_4$

R. Coldea, *et al.*,  
Phys. Rev. Lett. 86, 5377 (2001).



# Inelastic Neutron Scattering Measurement of $\text{La}_2\text{CuO}_4$

R. Coldea, *et al.*,  
Phys. Rev. Lett. 86, 5377 (2001).



# Green's Function

## Green's function

$$G(z) = \langle \phi | (z\hat{I} - \hat{H})^{-1} | \phi \rangle$$

$$|v_1\rangle = |\phi\rangle / \sqrt{\langle \phi | \phi \rangle}$$

$$G(z) = \langle \phi | \phi \rangle \langle v_1 | (z\hat{I} - \hat{H})^{-1} | v_1 \rangle$$

→ Lanczos method can accurately approximate  
the multiplication of inverse of  $(z - H)$

# Lanczos Method

Making tridiagonal symmetric matrix

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

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

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

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

# Resolvent by Lanczos Method

$$z\hat{I} - \hat{H} \simeq \sum_{j,k=1}^m (z\mathbf{1}_m - H_m)_{jk} |v_j\rangle\langle v_k|$$

$$(z\hat{I} - \hat{H})^{-1} \simeq \sum_{j,k=1}^m (z\mathbf{1}_m - H_m)^{-1}_{jk} |v_j\rangle\langle v_k|$$

$$\hat{I} \simeq \sum_{j=1}^m |v_j\rangle\langle v_j| \quad \text{Closure in the Krylov subspace}$$

$$G(z) = \langle \phi | \phi \rangle \langle v_1 | (z\hat{I} - \hat{H})^{-1} | v_1 \rangle$$

$$\langle v_1 | (z\hat{I} - \hat{H})^{-1} | v_1 \rangle \simeq (z\mathbf{1}_m - H_m)^{-1}_{11}$$

$$z = \omega + i\delta + E_0$$

# Useful Formula for Calculating Inverse

Assume  $A$  and  $E$  has their inverse

$$A = \begin{pmatrix} B & C \\ D & E \end{pmatrix}$$

$$\begin{aligned} A &\in \mathbb{C}^{N \times N} \\ B &\in \mathbb{C}^{L \times L} \\ E &\in \mathbb{C}^{M \times M} \\ C &\in \mathbb{C}^{L \times M} \\ D &\in \mathbb{C}^{M \times L} \\ N &= L + M \end{aligned}$$

$$1 \leq \ell, m \leq L$$

$$(A^{-1})_{\ell m} = (B - CE^{-1}D)_{\ell m}^{-1}$$

Schur complement

# Resolvent by Lanczos & Continued Fraction (連分数)

$$(z \mathbf{1}_m - H_m)^{-1}_{11} = \frac{1}{z - \alpha_1 - \Sigma_2(z)}$$

E. R. Gagliano and C. A. Balseiro,  
Phys. Rev. Lett. 59, 2999 (1987).

$$\Sigma_\ell(z) = \frac{\beta_\ell^2}{z - \alpha_\ell - \Sigma_{\ell+1}(z)}$$

$$\Sigma_{m+1}(z) = 0$$

$$(z \mathbf{1}_m - H_m)^{-1}_{11} = \cfrac{1}{z - \alpha_1 - \cfrac{\beta_2^2}{z - \alpha_2 - \cfrac{\beta_3^2}{z - \alpha_3 - \dots}}}$$

$$G(z) = \cfrac{\langle \phi | \phi \rangle}{z - \alpha_1 - \cfrac{\beta_2^2}{z - \alpha_2 - \cfrac{\beta_3^2}{z - \alpha_3 - \dots}}}$$

# Another Method: Conjugate Gradient

Rewrite the Green's function to generate  
Linear equations

$$G(z) = \langle 0 | \hat{O} | \chi(z) \rangle$$

$$| \chi(z) \rangle = (z \hat{I} - \hat{H})^{-1} \hat{O} | 0 \rangle$$

$$(z \hat{I} - \hat{H}) | \chi(z) \rangle = \hat{O} | 0 \rangle$$

$$A \vec{x} = \vec{b}$$

$A$  is non-hermitian

Calculating unknown  $x$  for given  $b$

*Biorthogonal Conjugate Gradient (BiCG)*

C. Lanczos,

J. Res. Nat. Bur. Standards 45, 255 (1950).

Recent formulation: Andreas Frommer, Computing 70, 87 (2003).

# Algorithm: Conjugate Gradient

$$A\vec{x} = \vec{b}$$

$$\vec{p}_0 = \vec{r}_0 = \vec{b} - A\vec{x}_0$$

For  $k = 0, 1, \dots, m$

$$\alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k}$$

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$$

$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$

$$\beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$

$$\vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$$

Not BiCG!

# Other Algorithm

## Variation of Krylov subspace method

-LOBCG

(Locally Optimal Block Conjugate Gradient)

A. V. Knyazev,

SIAM J. Sci. Comput. 23, 517 (2001)

-Shifted Krylov subspace method

A. Frommer,

Computing 70, 87 (2003).

-Sakurai-Sugiura & FEAST

T. Sakurai & H. Sugiura,

J. Comput. Appl. Math. 159, 119 (2003).

T. Ikegami, T. Sakurai, & U. Nagashima.

J. Comput. Appl. Math. 233, 1927 (2010).

E. Polizzi, Phys. Rev. B 79, 115112 (2009).

## Non-Krylov subspace: Jacobi-Davidson

<http://www.netlib.org/utk/people/JackDongarra/etemplates/node136.html>

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

$$\mu_k^{(i)} = \frac{(\mathbf{x}_k^{(i)}, A\mathbf{x}_k^{(i)})}{(\mathbf{x}_k^{(i)}, \mathbf{x}_k^{(i)})} \quad \leftarrow \text{approximation of } i\text{th smallest eigenvalue}$$

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

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

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

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

$\leftarrow m$  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).

# Nature of Random Vector

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

## Random wave function

$$|\phi_0\rangle = \sum_x c_x |x\rangle \quad \sum_x |c_x|^2 = 1$$
$$|x\rangle = |\sigma_0 \sigma_1 \cdots \sigma_{N-1}\rangle$$

## Infinite-temperature result

$$\mathbb{E}[\langle\phi_0|\hat{O}|\phi_0\rangle] = N_{\text{H}}^{-1} \sum_n \langle n|\hat{O}|n\rangle = \langle\hat{O}\rangle_{\beta=0}^{\text{ens}}$$

$$\mathbb{E}[|c_x|^2] = N_{\text{H}}^{-1}$$
$$|n\rangle = \sum_x U_{xn} |x\rangle$$

Complexity  
Memory

$$\mathcal{O}(N_{\text{H}})$$

N. Ullah, Nucl. Phys. 58, 65 (1964).  
-Uniform distribution on  
unit sphere in  $\mathbb{R}^{2N_{\text{H}}}$

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

# Approximate Spectral Projection

$$\hat{P}_{\gamma,\rho} = \frac{1}{2\pi i} \oint_{C_{\gamma,\rho}} \frac{dz}{z - \hat{H}}$$

T. Kato, Progress of Theoretical Physics 4, 514 (1949).  
 $z = \rho e^{i\theta} + \gamma$

$$|\phi\rangle = \sum_n d_n |n\rangle$$
$$\hat{P}_{\gamma,\rho} |\phi\rangle = \sum_{E_n \in (\gamma-\rho, \gamma+\rho)} d_n |n\rangle$$

Discretized by Riemann sum

$$\hat{P}_{\gamma,\rho,M} = \frac{1}{M} \sum_{j=1}^M \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}}$$

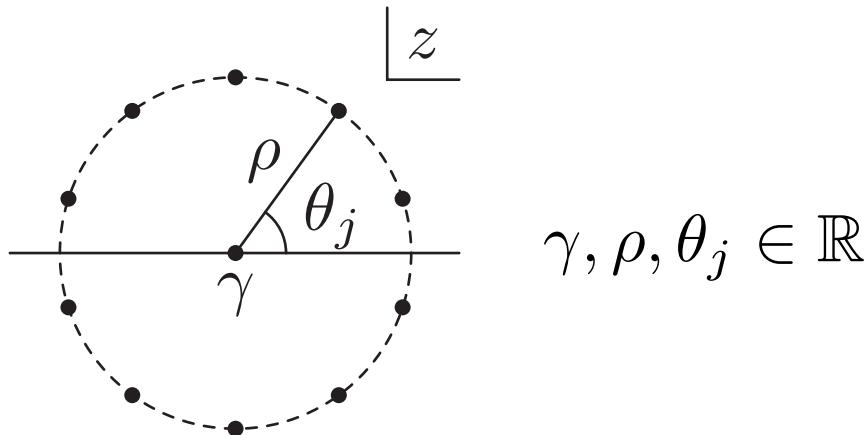
T. Sakurai and H. Sugiura,  
J. Comput. Appl. Math. 159, 119 (2003).  
T. Ikegami, T. Sakurai, and U. Nagashima,  
J. Comput. Appl. Math. 233, 1927 (2010).

$$\theta_j = 2\pi(j - 1/2)/M$$

# Projected Wave Function

$$\hat{P}_{\gamma, \rho, M} |\phi\rangle = \sum_{j=1}^M |\phi_j\rangle$$

$$|\phi_j\rangle = \frac{1}{M} \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}} |\phi\rangle$$

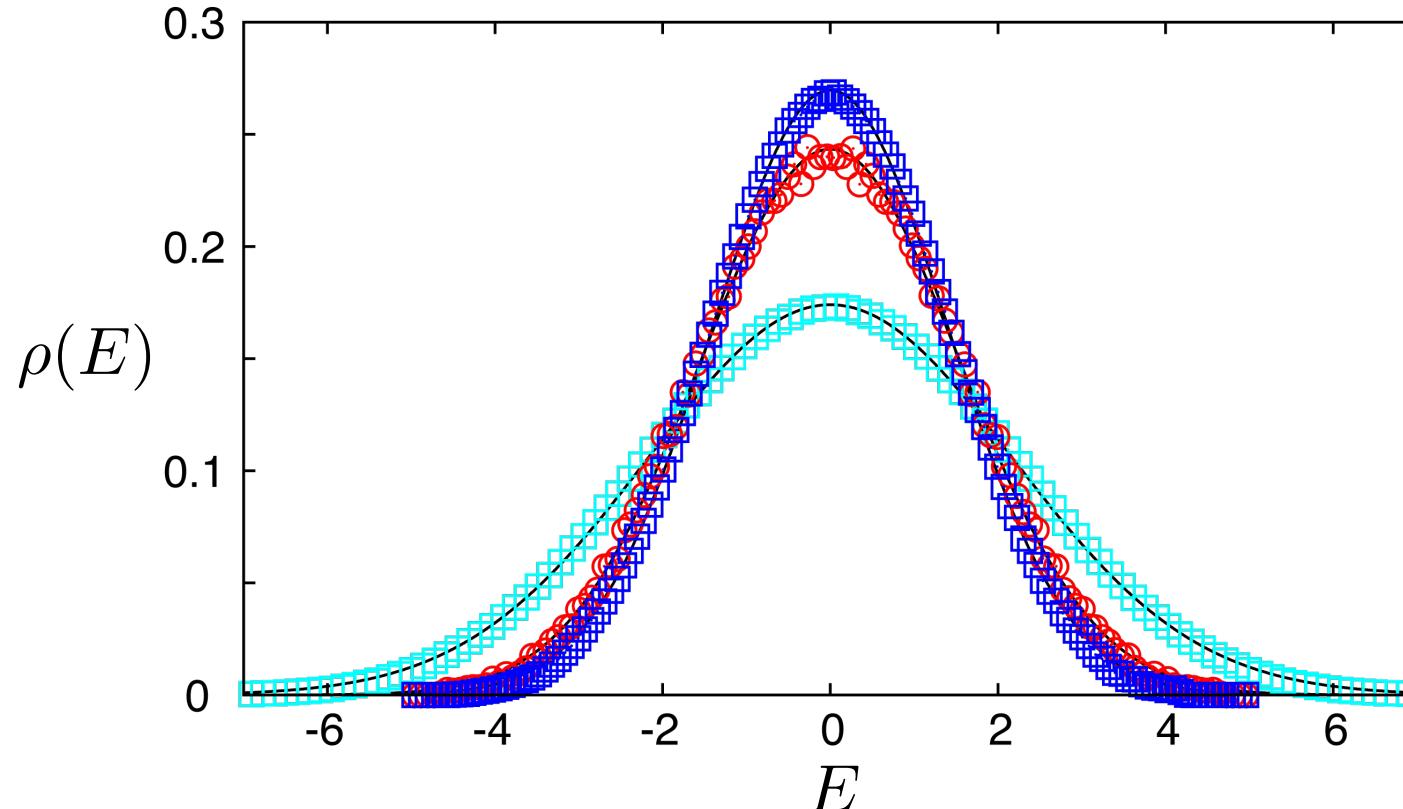


$$\gamma, \rho, \theta_j \in \mathbb{R}$$

# Density of States by Krylov Subspace Method

Density of states included in random vectors

Kitaev model, Kitaev-Heisenberg model,  $\Gamma$  model



# Summary: Classification of Information Compression by Memory Costs

(1) A matrix can be stored

- SVD for dense matrix
- Compressed sensing

(2) Although a matrix cannot be stored, vectors can be stored

- SVD for sparse matrix
- Krylov subspace method

(3) A vector cannot be stored

- MPS/Tensor network states

# Appendix: Krylov subspace and application of random vectors to statistical mechanics

## *Statistical mechanics 2.0*

E. T. Jaynes, “Information Theory and Statistical Mechanics,”  
Phys. Rev. 106, 620 (1957).

Maximum entropy (Shannon entropy) estimate of probability distribution for given energy spectra and expectation value of energy  $\langle E \rangle$

→ Boltzmann distribution/statistical mechanics

# Statistical mechanics from Krylov Subspace Method

## *Statistical mechanics 3.0*

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

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

J. Skilling, Maximum entropy and bayesian methods: Cambridge, England, 1988," (Springer Science & Business Media, 2013) p. 455.

P. de Vries and H. De Raedt, Phys. Rev. B 47, 7929 (1993).

J. Jaklic and P. Prelovsek, Phys. Rev. B 49, 5065 (1994).

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

A. Sugita, Nonl. Phen. Compl. Sys. 10, 192 (2007).

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

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

Krylov subspace initiated by a random vector

→ Typical pure state that replaces canonical ensemble

# Construction of Typical Pure State

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

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

Initial state ( at  $T = +\infty$  ):  $|\Phi_0\rangle = (\text{Random vector})$   
do  $k=1, N_{\text{step}}$  If possible, taking random average

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

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

$$\beta = 2(k/N)/(\ell - u_k) \quad (\beta = 1/k_B T)$$

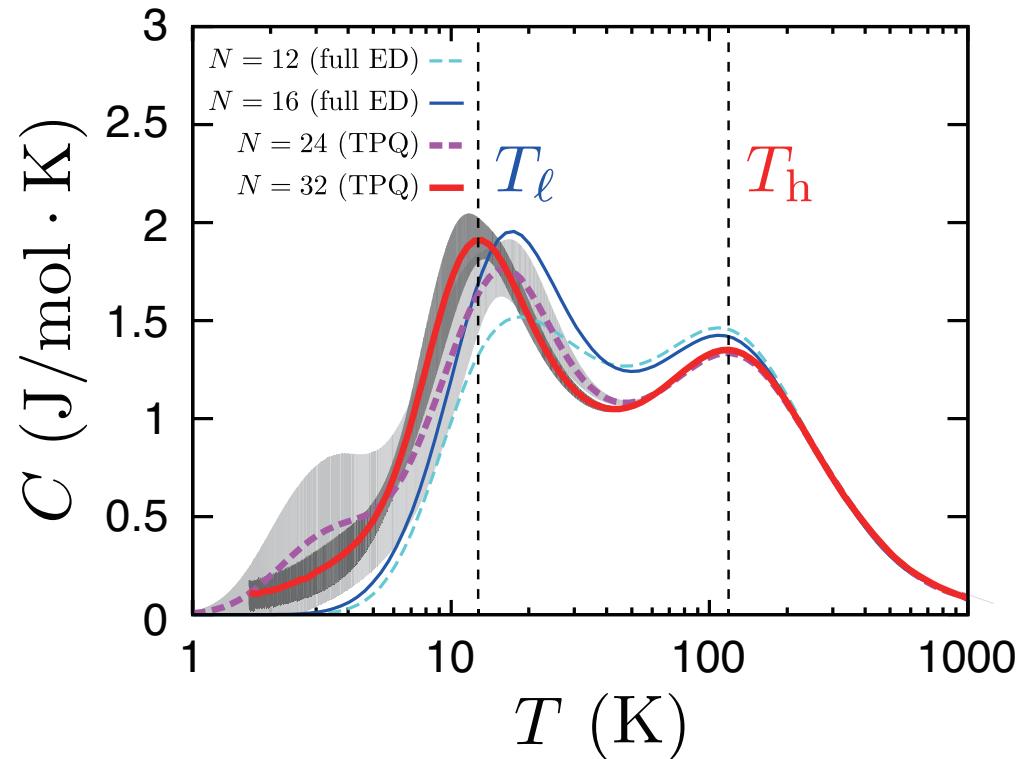
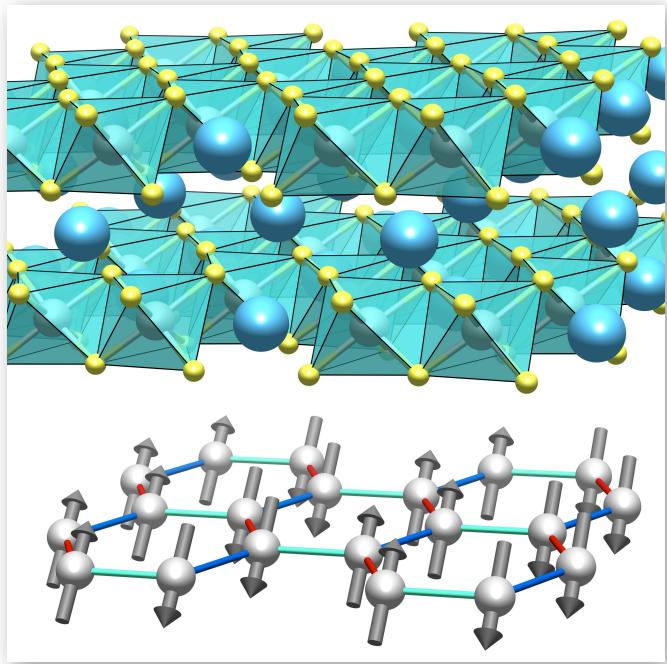
$$\overline{O}(\beta) = \langle \Phi_k | \hat{O} | \Phi_k \rangle + \mathcal{O}(1/N)$$

enddo

Hamiltonian-wave function product is essential

# Application of Typical Pure State

An example: Frustrated magnet  $\text{Na}_2\text{IrO}_3$



Y. Yamaji, *et al.*, Phys. Rev. Lett. 113, 107201 (2014).  
Y. Yamaji *et al.*, Phys. Rev. B 93, 174425 (2016).

# References

-Application of Lanczos method for excited states

E. Dagotto,

“Correlated electrons in high-temperature superconductors,”  
Rev. Mod. Phys. 66, 763 (1994)



-Software for Krylov subspace method  
(for interacting qubits)

M. Kawamura, K. Yoshimi, T. Misawa, Y. Yamaji, S. Todo, and N. Kawashima,  
“Quantum lattice model solver  $H\Phi$ ,”  
Compt. Phys. Commun. 217, 180 (2017).



-Numerical library for Shifted Krylov subspace method

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,”  
Compt. Phys. Commun. 258, 107536 (2021).

# Next Week

- 1st: Huge data in modern physics
- 2nd: Information compression in modern physics
- 3rd: Review of linear algebra
- 4th: Singular value decomposition and low rank approximation
- 5th: Basics of sparse modeling
- 6th: Basics of Krylov subspace methods
- 7th: Information compression in materials science
- 8th: Accelerating data analysis: Application of sparse modeling
- 9th: Data compression: Application of Krylov subspace method
- 10th: Entanglement of information and  
matrix product states**
- 11th: Application of MPS to eigenvalue problems
- 12th: Tensor network representation
- 13th: Information compression by tensor network renormalization