HΦの概要
-プログラムとアルゴリズム-
Overview of HΦ: Program & Algorithm

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1. Introduction to HΦ
2. Algorithm: Lanczos & LOBCG
3. Algorithm: TPQ

Appendix:
Formulation of many-body quantum systems in a nutshell

Computational
Science
Alliance
The University of Tokyo

HΦ

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

Numerical diagonalization package for lattice hamiltonian

-For wide range of quantum lattice hamiltonians

Ab initio effective hamiltonians

-Lanczos method [1] and LOB(P)CG [2]:

Ground state and low-lying excited states

Excitation spectra of ground state

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

-Real-time evolution

-Parallelization with MPI and OpenMP

[1] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994) .
[2] A. V. Knyazev, SIAM J. Sci. Cumput. 23, 517 (2001).
[3] S. Sugiura, A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).

Open source program package (latest release: ver.3.1.2)

License: GNU GPL version3

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

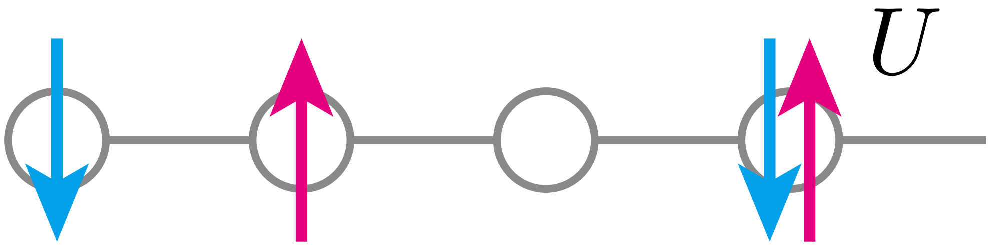
Target Hamiltonian

- Standard Hamiltonian 1

Itinerant electrons: Hubbard-type model

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

N



Fermion Hubbard: Particle # & total S_z conserved

HubbardNConserved: Particle # conserved & total S_z not

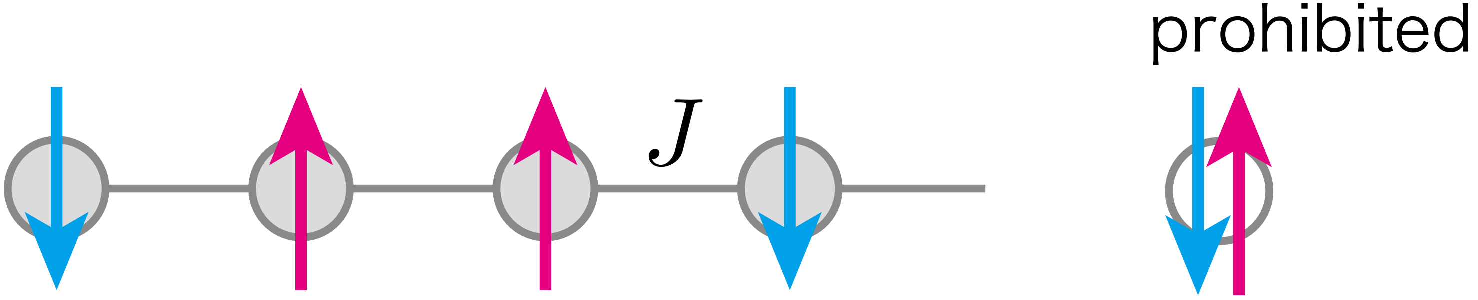
Fermion HubbardGC: Particle # & total S_z not conserved

Target Hamiltonian

- Standard Hamiltonian 2

Localized spin: Heisenberg-type model

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



Spin: total S_z conserved

SpinGC: total S_z not conserved

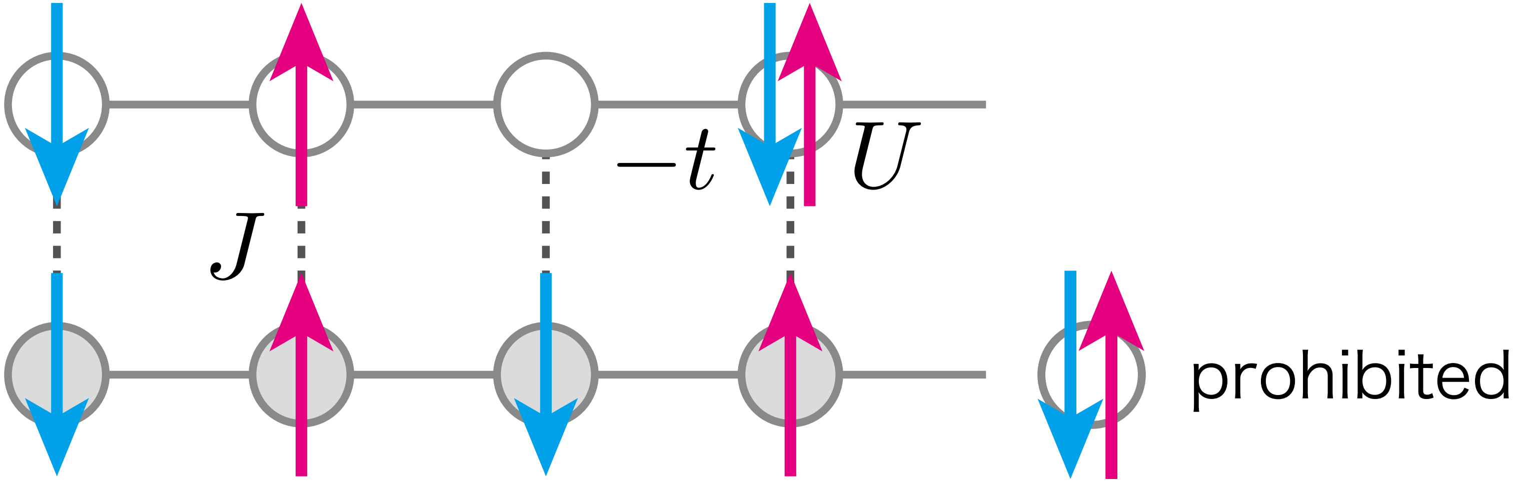
S > 1/2 can be simulated
if your memory is enough large

Target Hamiltonian

- Standard Hamiltonian 3

Mixture: Kondo-lattice-type model

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



`Kondo Lattice:` Particle # & total S_z conserved

`Kondo LatticeGC:` Particle # & total S_z not conserved

Standard input: Simplified input for typical lattice models

Hubbard

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

Quantum spins

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

Kondo lattice

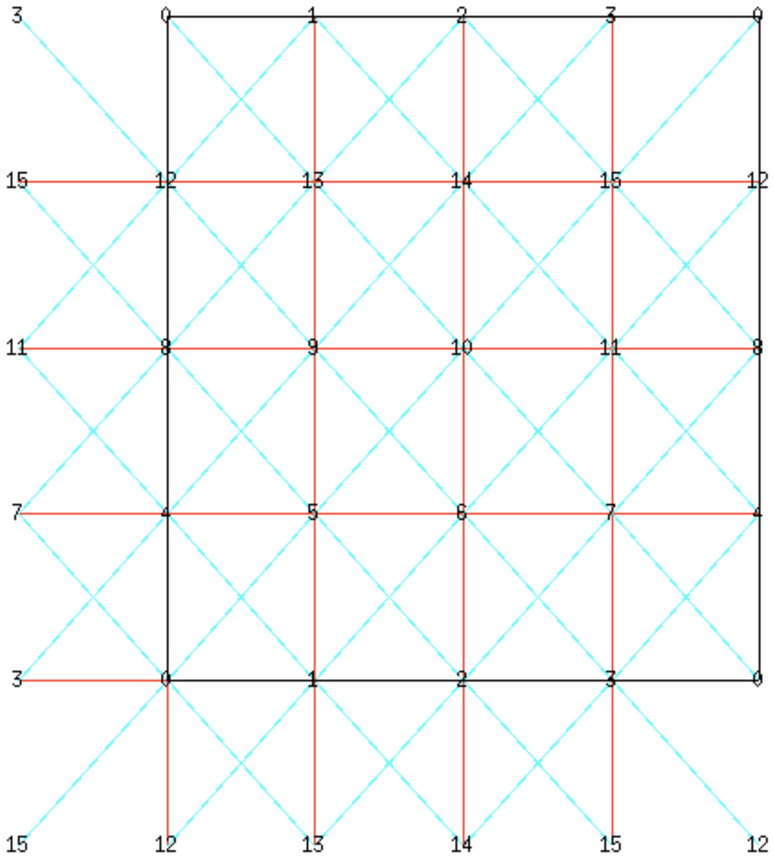
$$H = -\mu \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle i,j\rangle} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{J}{2} \sum_{i=1}^{N} \left\{ S_i^{+} c_{i\downarrow}^{\dagger} c_{i\uparrow} + S_i^{-} c_{i\uparrow}^{\dagger}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

Expert input: Flexible input for any one- and two-body hamiltonian

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

Primitive Standard Input File

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



Output

Ground-state/finite-temperature/time-evolution of
-Energy
-Square of energy
-One-body equal time Green’s function
-Two-body equal time Green’s/correlation function

$$\langle H\rangle,\ \langle H^2\rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2}\rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} c^\dagger_{k\sigma_3} c_{\ell\sigma_4}\rangle$$

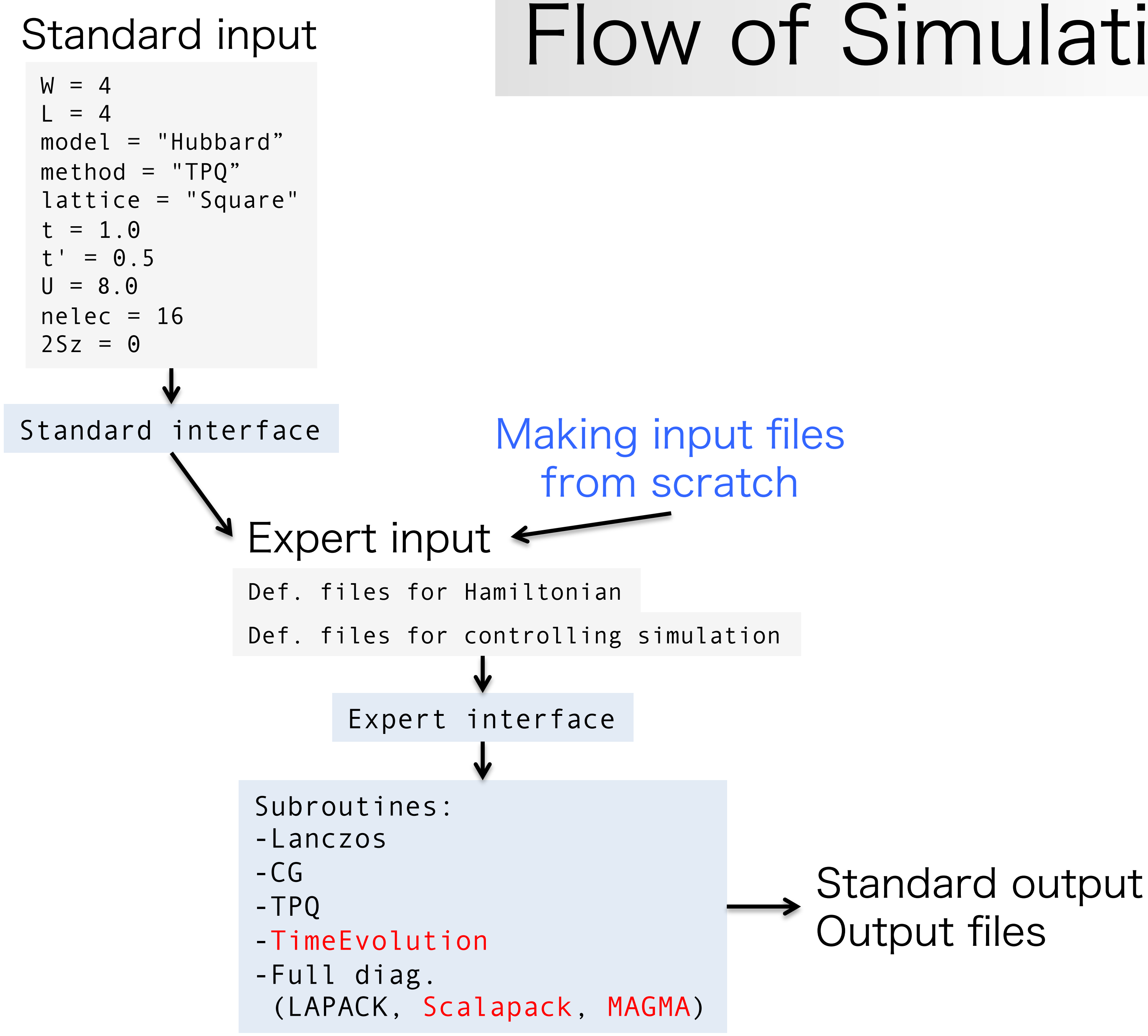
-Dynamical Green’s function is also available

Overview of Software HΦ

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

For installation, cmake is required

Flow of Simulation



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
```

Standard interface

Making input files from scratch

Expert input

Def. files for Hamiltonian

Def. files for controlling simulation

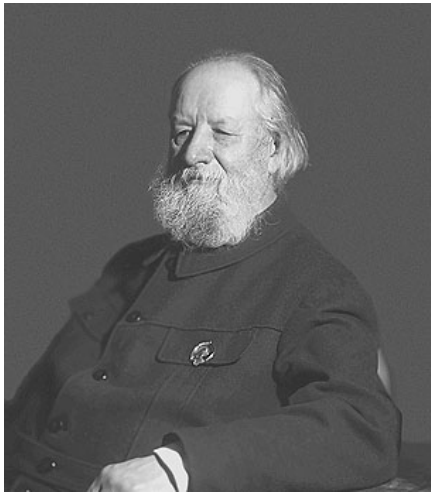
Expert interface

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

Standard output
Output files

Algorithm Implemented in HΦ:
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 $A \in \mathbb{C}^{L \times L}$

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

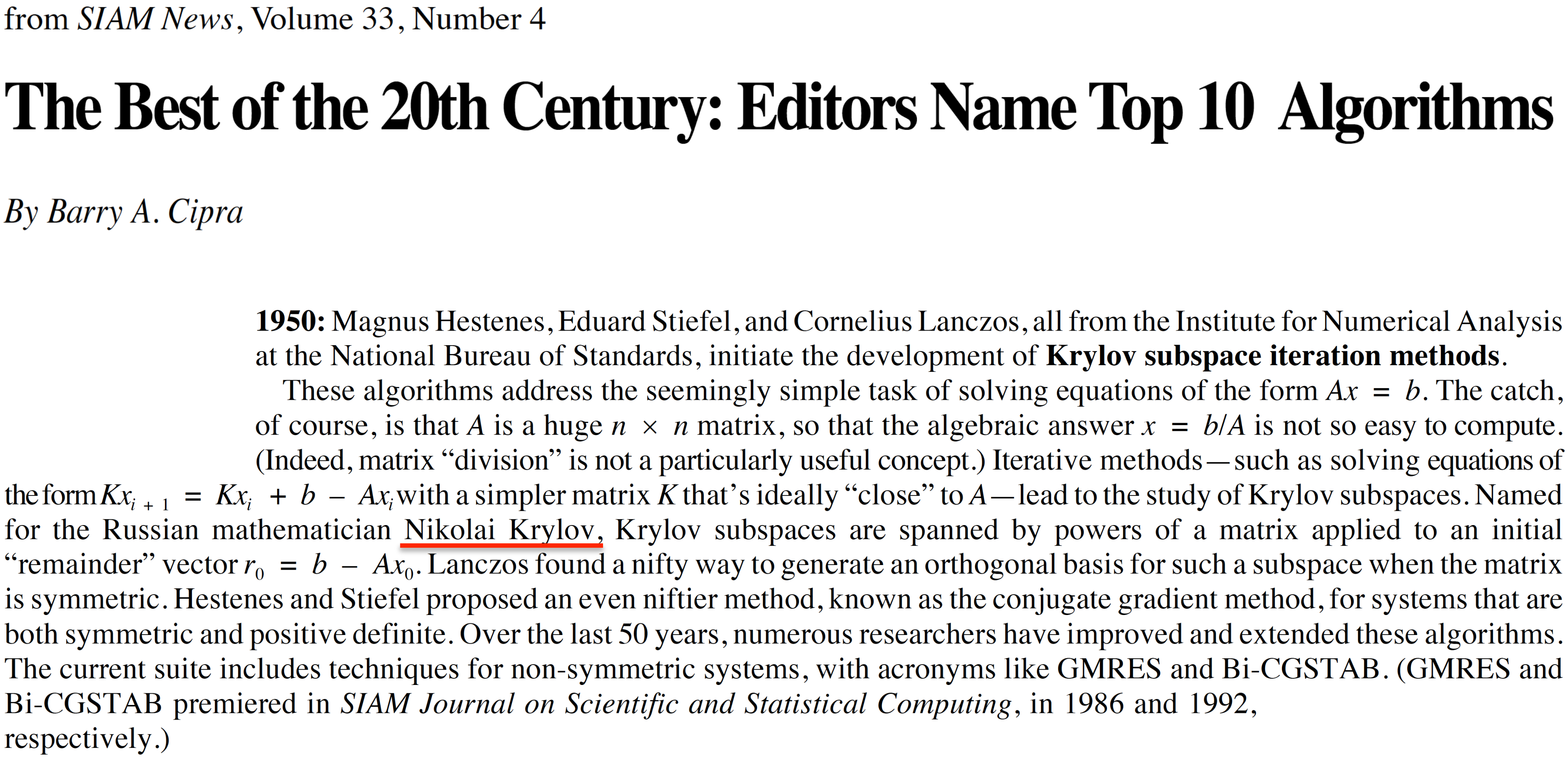
Numerical cost to construct K_n: $\mathcal{O}(\mathrm{nnz}(A) \times n)$

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

```
Initial : $\beta_1 = 0,\ |v_0\rangle = 0$
for $j = 1, 2, \ldots, m$ 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 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
→ Approximate eigenvalues of original Hamiltonian

Lanczos Method: # of Vectors Required

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

**for** $j = 1, 2, \ldots, m$ **do**
    $|w_j\rangle \leftarrow \hat{H}|v_j\rangle - \beta_j|v_{j-1}\rangle$        $|v_{j-1}\rangle \rightarrow |w_j\rangle,\ |v_j\rangle$
    $\alpha_j = \langle w_j|v_j\rangle$                                     $|w_j\rangle,\ |v_j\rangle$
    $|w_j\rangle \leftarrow |w_j\rangle - \alpha_j|v_j\rangle$                    $|w_j\rangle,\ |v_j\rangle$
    $\beta_{j+1} = \sqrt{\langle w_j|w_j\rangle}$                           $|w_j\rangle,\ |v_j\rangle$
    $|v_{j+1}\rangle = |w_j\rangle/\beta_{j+1}$                        $|w_j\rangle \rightarrow |v_{j+1}\rangle,\ |v_j\rangle$
```

Convergence of Lanczos Method

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

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

Convergence theorem for the largest eigenvalue

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

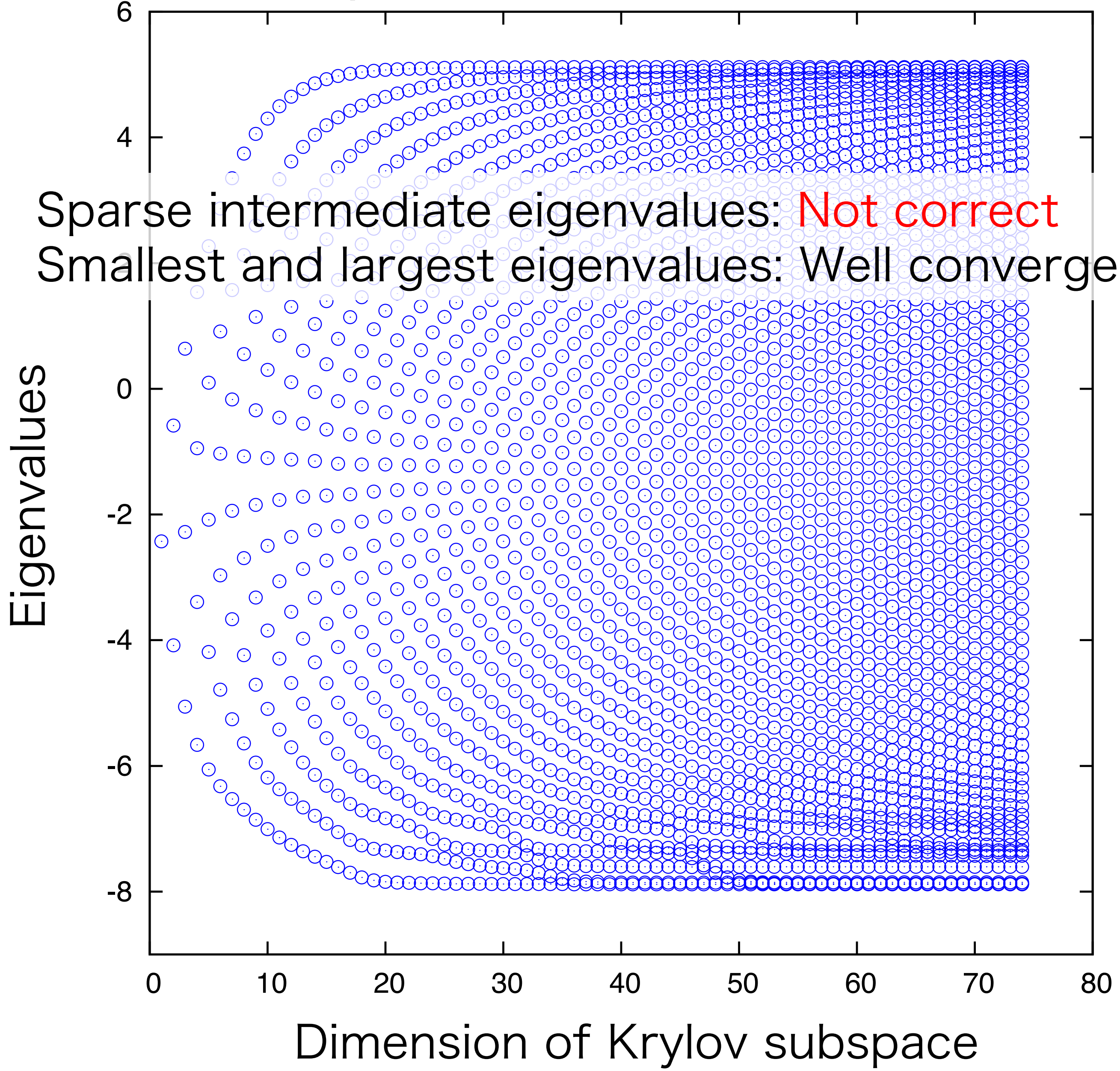
$$\sim 4(\lambda_1 - \lambda_n) \left[\tan\theta(|v_1\rangle, |1\rangle)\right]^2 e^{-4\sqrt{\gamma_1} m}$$

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

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

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

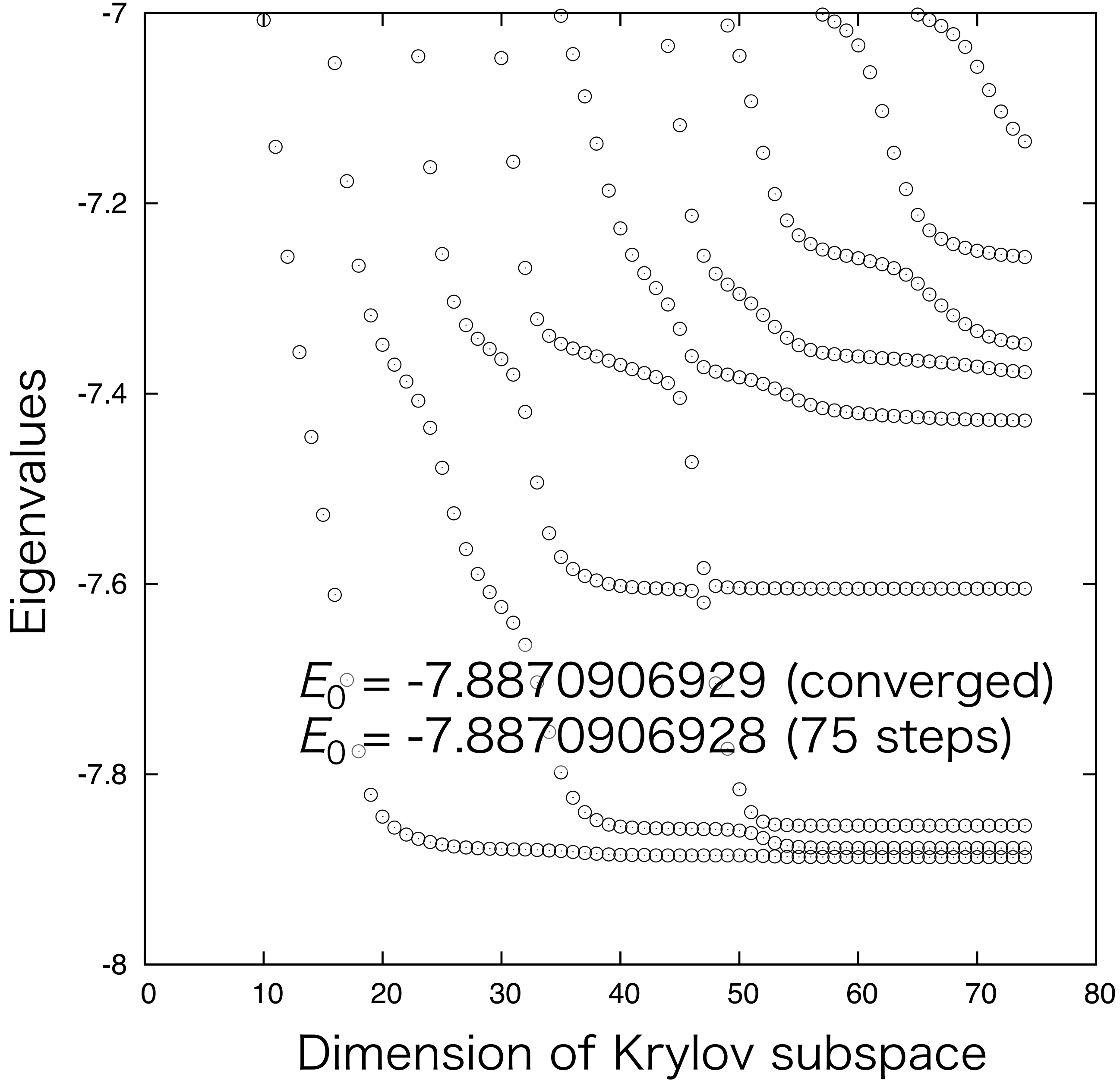
Dimension of Fock space: 2^{24}=16777216



Sparse intermediate eigenvalues: Not correct

Smallest and largest eigenvalues: Well converged

How Lanczos Method Works



E_0 = -7.8870906929 (converged)

E_0 = -7.8870906928 (75 steps)

LOB(P)CG

Algorithm of LOBCG: *m* lowest eigenstates

Initial condition: m orthogonal initial vectors $\boldsymbol{x}_0^{(i)}$

$\boldsymbol{p}_0^{(i)} = \boldsymbol{0} \ (i = 1, \ldots, m)$

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

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

←approximation of *i* th smallest eigenvalue

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

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

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

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

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

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

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

Until convergence

Algorithm Implemented in HΦ: TPQ

(Finite-Temperature Simulation)

Finite-Temperature Physical Quantity: Heat Capacity

Spread of energy distribution

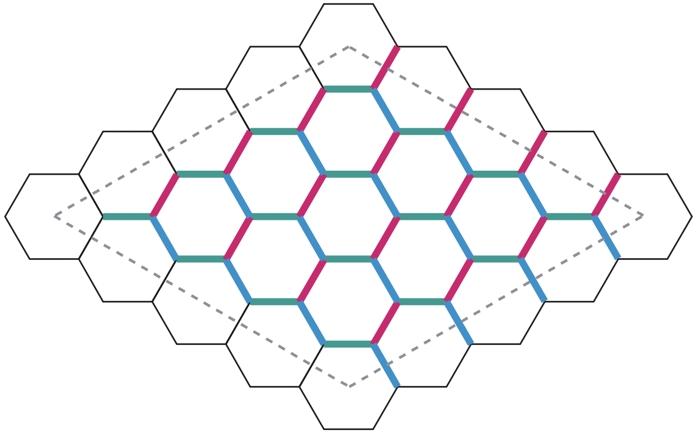
$$C = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{k_\mathrm{B} T^2}$$

-Average with Boltzmann distribution

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

Complexity	$\mathcal{O}(N_\mathrm{H}^3)$
Memory	$\mathcal{O}(N_\mathrm{H}^2)$

32 site cluster of S=1/2 spin



$$N_\mathrm{H} = 2^{32}$$

Hamiltonian
∼3x10⁸TB!

$|n\rangle$ ∼69GB

Typical Pure State Approach

Complexity

Memory

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

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).

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

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

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

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

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

At finite temperature

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

Average over the distribution

How large is the standard deviation?

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

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).

$$\boxed{\sigma_O^2 \le \frac{\langle(\Delta O)^2\rangle_{2\beta}^{\mathrm{ens}} + (\langle O\rangle_{2\beta}^{\mathrm{ens}} - \langle O\rangle_{\beta}^{\mathrm{ens}})^2}{\exp[2\beta\{F(2\beta) - F(\beta)\}]}}$$

$$\propto \exp[-S(\beta^*)/2] \ (\beta < \beta^* < 2\beta)$$

Exponetially small when system size increases

Construction of Typical Pure State

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

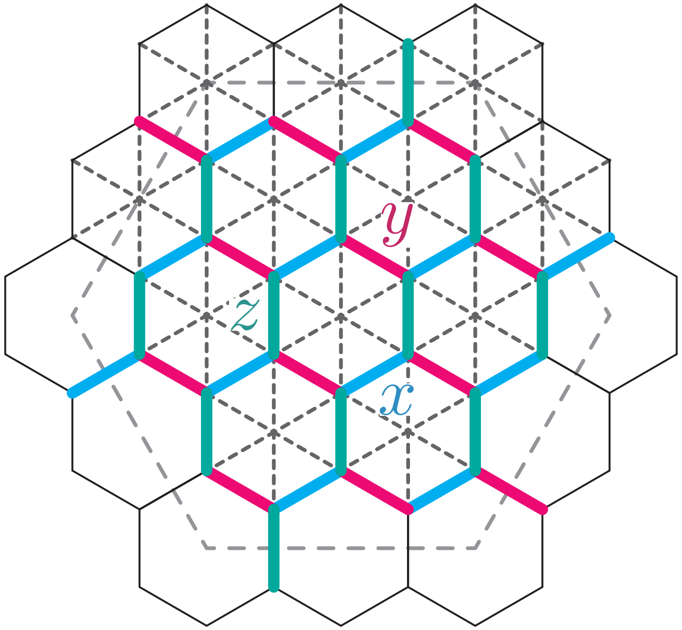
Sugiura & Shimizu, Phys. Rev. Lett. 108, 240401 (2012)

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

Hamiltonian-wave function product is essential

Example of TPQ: K-Γ-J_3 Model

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



$$\left.\begin{array}{l}
\mathcal{J}_X = \begin{bmatrix} -\cos\phi & 0 & 0 \\ 0 & 0 & \sin\phi \\ 0 & \sin\phi & 0 \end{bmatrix} \\
\mathcal{J}_Y = \begin{bmatrix} 0 & 0 & \sin\phi \\ 0 & -\cos\phi & 0 \\ \sin\phi & 0 & 0 \end{bmatrix} \\
\mathcal{J}_Z = \begin{bmatrix} 0 & \sin\phi & 0 \\ \sin\phi & 0 & 0 \\ 0 & 0 & -\cos\phi \end{bmatrix}
\end{array}\right\}$$

Nearest neighbor

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

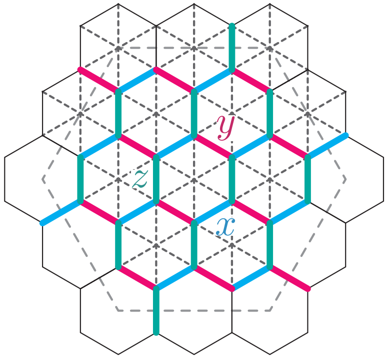
3rd neighbor

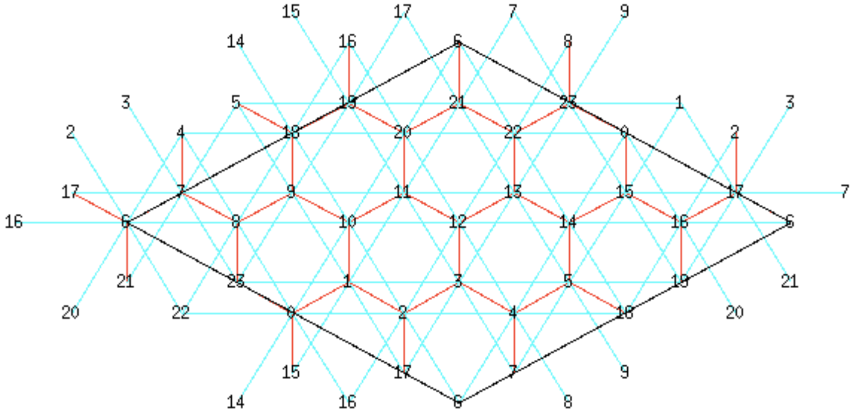
$$J_3[\hat{S}_\ell^x \hat{S}_m^x + \hat{S}_\ell^y \hat{S}_m^y + \hat{S}_\ell^z \hat{S}_m^z]$$

How to Simulate 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
h = 0.07071067811
Gamma = -0.07071067811
2S=1
```





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

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

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

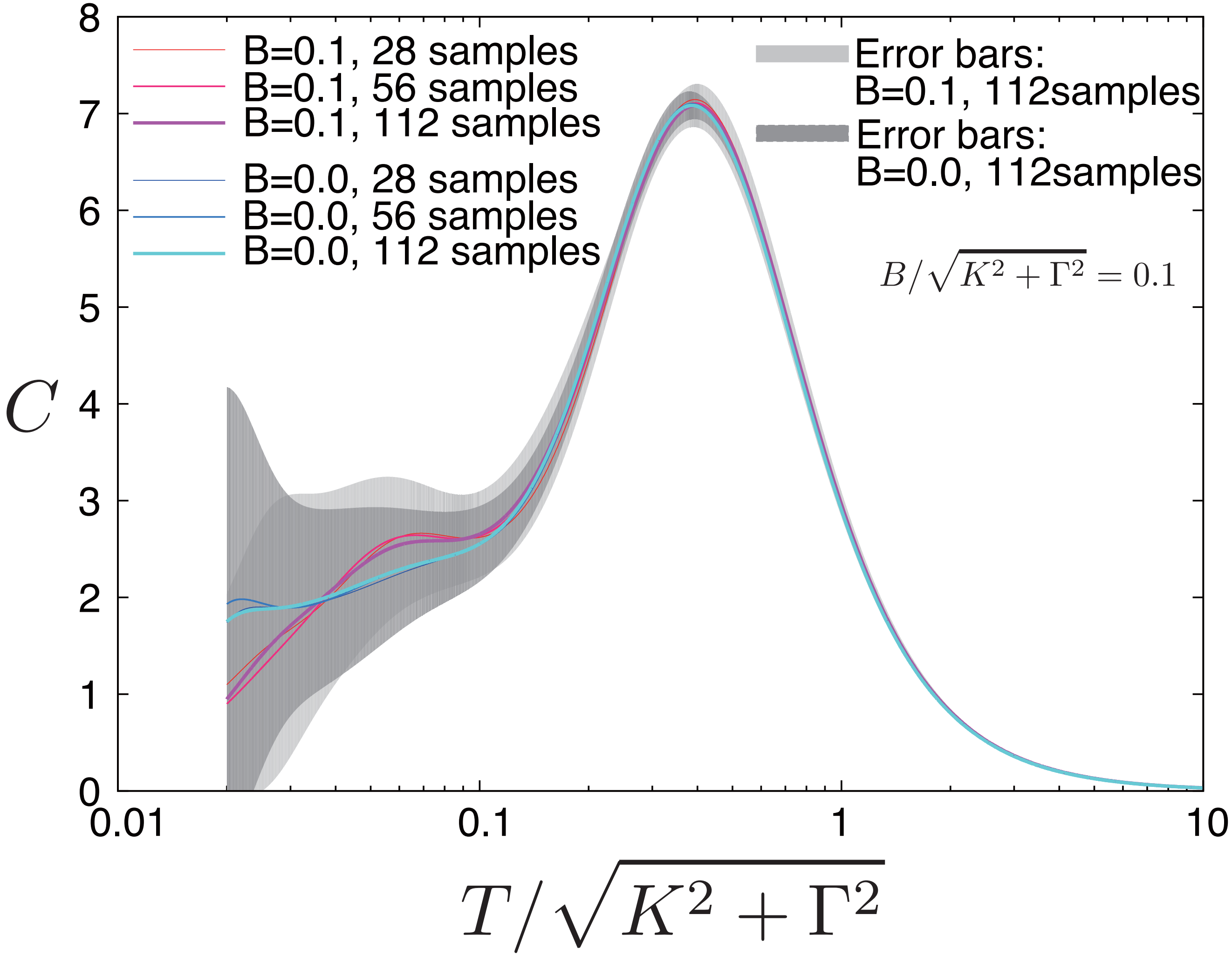
$$\vec{B} \propto (1, 0, -1)$$

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

Add `Exchange` and `Ising` by Expert mode

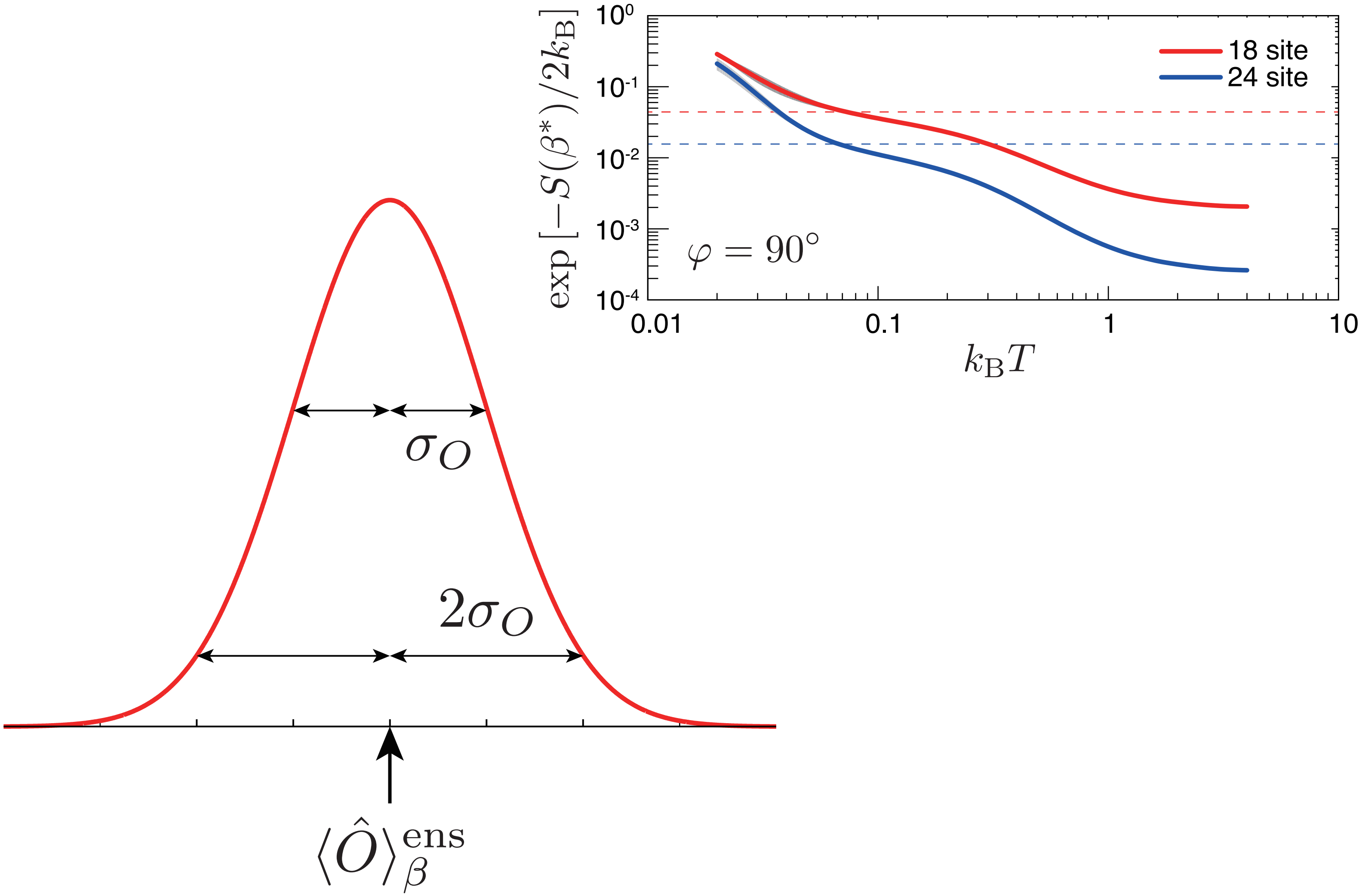
Heat Capacity of K-Γ-J_3 Model

$$\phi/\pi = 0.2,\ \ J_3/\sqrt{K^2+\Gamma^2} = 0.05$$



Standard Deviation

Standard deviation in TPQ



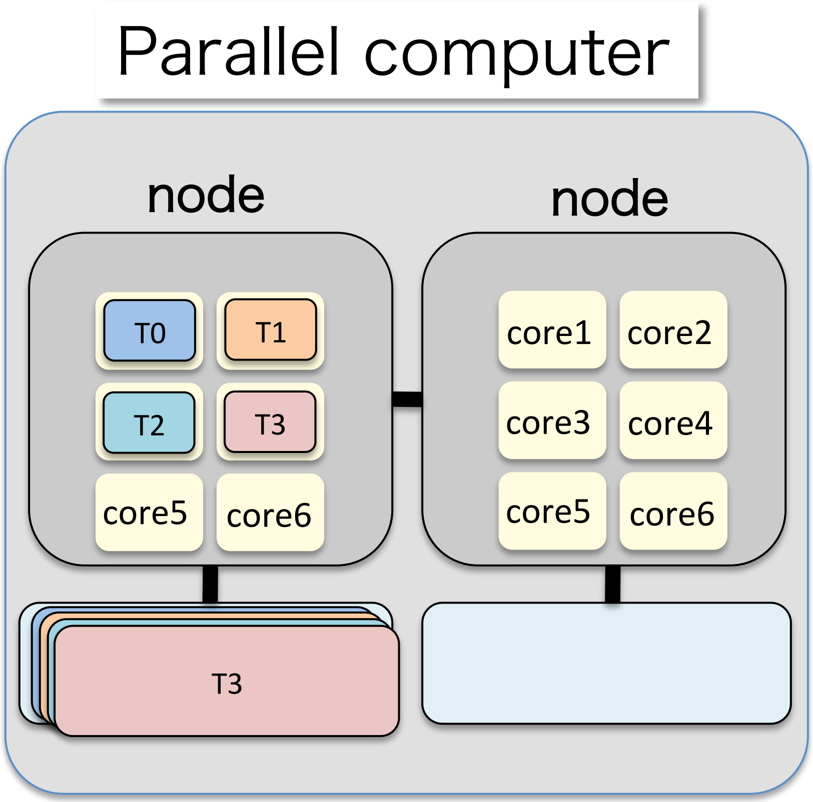
$\propto \sigma_O$

Parallelization of HΦ

Parallelization

- Hybrid parallel

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



Parallelization

- Hybrid parallel

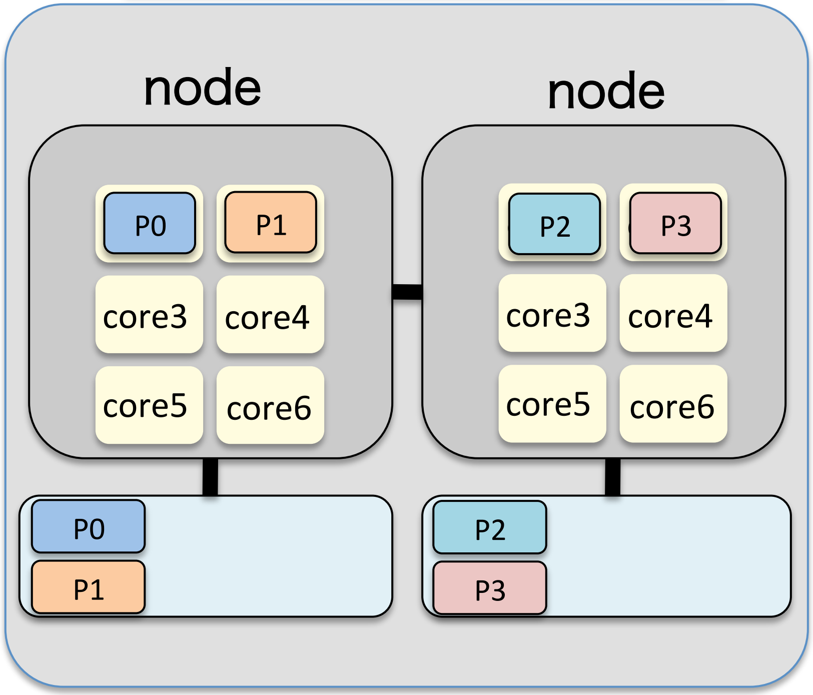
-Shared memory (OpenMP) Thread
-Distributed memory (MPI) Process

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

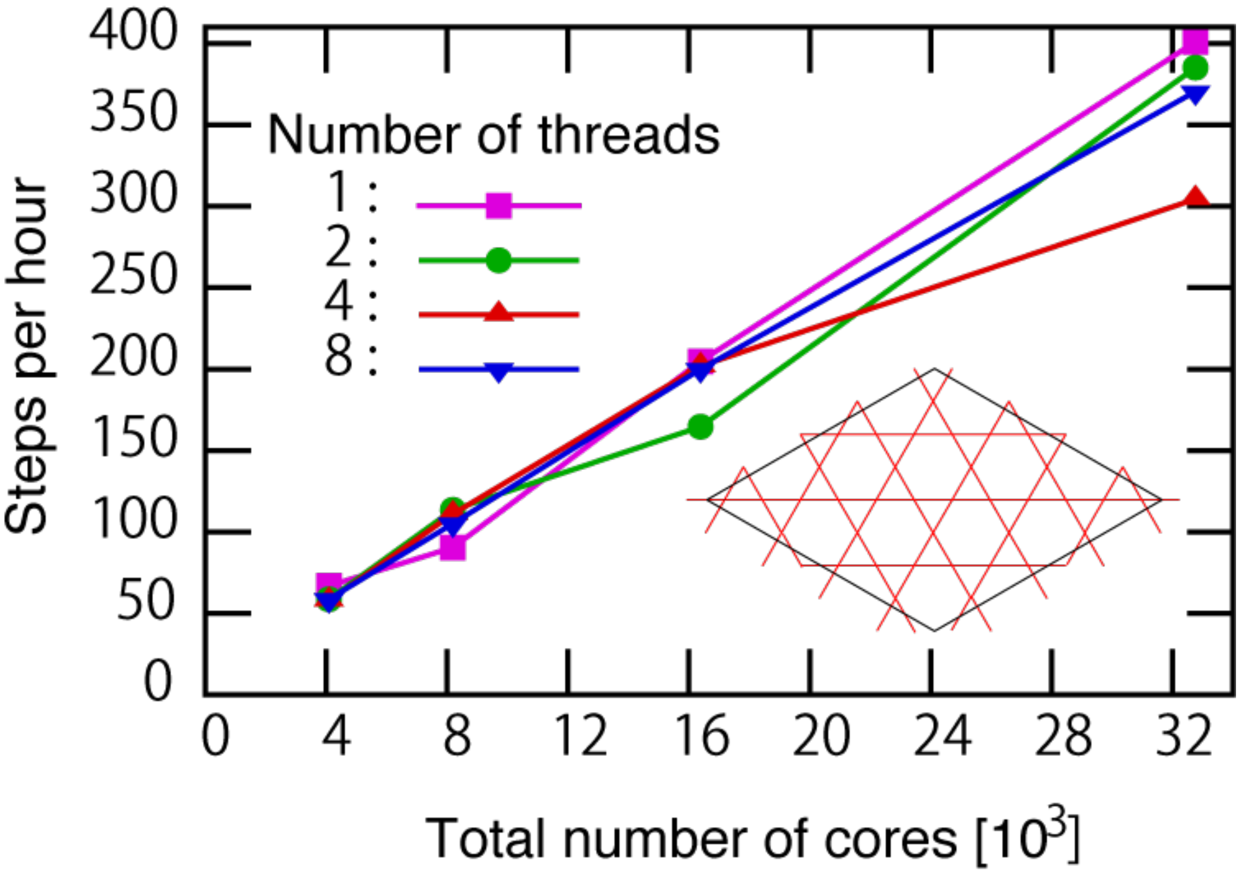
Example of MPI: 2 process

$$
\begin{array}{lcll}
|0\rangle & = & |\downarrow\downarrow\,\downarrow\rangle & \\
|1\rangle & = & |\uparrow\downarrow\,\downarrow\rangle & \\
|2\rangle & = & |\downarrow\uparrow\,\downarrow\rangle & \text{rank 0} \\
|3\rangle & = & |\uparrow\uparrow\,\downarrow\rangle & \\
\hline
|4\rangle & = & |\downarrow\downarrow\,\uparrow\rangle & \\
|5\rangle & = & |\uparrow\downarrow\,\uparrow\rangle & \\
|6\rangle & = & |\downarrow\uparrow\,\uparrow\rangle & \text{rank 1} \\
|7\rangle & = & |\uparrow\uparrow\,\uparrow\rangle &
\end{array}
$$

Parallel computer



Speedup



Lanczos method: Up to 6.87x10^{10} dimension
@K computer & ISSP supercomputer
From 4096 32768 cores: Parallelization efficiency 80%

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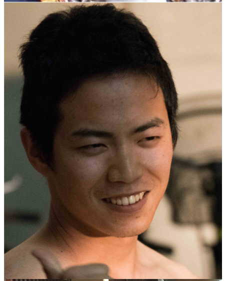

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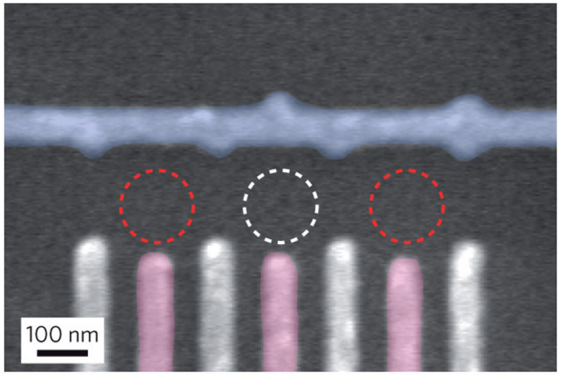
Appendix: Formulation of Quantum Many-Body Problem

Quantum Many-Body Problems

An example: 3 Quantum dots

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



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

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

↓ ↓ ↓	$\|0\rangle \otimes \|0\rangle \otimes \|0\rangle$	↓ ↓ ↑	$\|0\rangle \otimes \|0\rangle \otimes \|1\rangle$
↑ ↓ ↓	$\|1\rangle \otimes \|0\rangle \otimes \|0\rangle$	↑ ↓ ↑	$\|1\rangle \otimes \|0\rangle \otimes \|1\rangle$
↓ ↑ ↓	$\|0\rangle \otimes \|1\rangle \otimes \|0\rangle$	↓ ↑ ↑	$\|0\rangle \otimes \|1\rangle \otimes \|1\rangle$
↑ ↑ ↓	$\|1\rangle \otimes \|1\rangle \otimes \|0\rangle$	↑ ↑ ↑	$\|1\rangle \otimes \|1\rangle \otimes \|1\rangle$

States represented by superposition

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

Quantum Many-Body Problems

Mutual Interactions

Operators acting on
a single qubit

A two dimensional representation of Lie algebra SU(2)

$$[\hat{S}^x_j, \hat{S}^y_j] = i\hat{S}^z_j$$
$$[\hat{S}^y_j, \hat{S}^z_j] = i\hat{S}^x_j$$
$$[\hat{S}^z_j, \hat{S}^x_j] = i\hat{S}^y_j$$

$$\hat{S}^x_j|0\rangle = \frac{1}{2}|1\rangle$$
$$\hat{S}^x_j|1\rangle = \frac{1}{2}|0\rangle$$
$$\hat{S}^y_j|0\rangle = \frac{i}{2}|1\rangle$$
$$\hat{S}^y_j|1\rangle = -\frac{i}{2}|0\rangle$$
$$\hat{S}^z_j|1\rangle = \frac{1}{2}|1\rangle$$
$$\hat{S}^z_j|0\rangle = -\frac{1}{2}|0\rangle$$

Vectors in Fock Space

Correspondence between spin and bit

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

2^N-dimensional Fock space:

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

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

Decimal representation of orthonormalized basis

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

Wave function as a vector

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

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

Vectors and Matrices in Fock Space

Inner product of vectors

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

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

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

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

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

Hamiltonian matrix

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

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

Example: Two Spins

Decimal representation of orthonormalized basis

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

Problem: Find 4 by 4 Hamiltonian matrix that describes

$$\begin{aligned}\hat{H}/J &= \hat{S}_0^x\hat{S}_1^x + \hat{S}_0^y\hat{S}_1^y + \hat{S}_0^z\hat{S}_1^z \\ &= \frac{1}{2}\left(\hat{S}_0^+\hat{S}_1^- + \hat{S}_0^-\hat{S}_1^+\right) + \hat{S}_0^z\hat{S}_1^z\end{aligned}$$

Useful transformation:
Ladder operators

$$\begin{aligned}\hat{S}_j^+ &= \hat{S}_j^x + i\hat{S}_j^y \\ \hat{S}_j^- &= \hat{S}_j^x - i\hat{S}_j^y\end{aligned}$$

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

Answer of the Problem

$$\hat{H} = J\left(\hat{S}^x_0 \hat{S}^x_1 + \hat{S}^y_0 \hat{S}^y_1 + \hat{S}^z_0 \hat{S}^z_1\right)$$

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

4 by 4 Hamiltonian matrix

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

Answer of the Problem 2: Energy Spectrum of the Two Spins

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

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