

多体問題の計算科学

Computational Science for Many-Body Problems

#12 Large sparse matrices and quantum
statistical mechanics

14:55-16:40 July 4, 2023

1. Numerical methods clarified emergent concepts
2. Excitation spectra
3. Conjugate gradient
4. Typicality approach
5. Appendix A and B

1. Numerical Methods Clarified Emergent Concepts in Many-Body Problems

Important Applications of Lanczos Method and Exact Wave Functions

Emergent concepts in many-body physics has been verified by using Lanczos and exact wf

Fractional quantum Hall effect

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

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

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

-Verification of Laughlin-Jastrow wave function

Thermalization of isolated quantum systems

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

- Linear responses of strongly correlated electrons
- Frustrated magnetism
- Haldane gap

Background

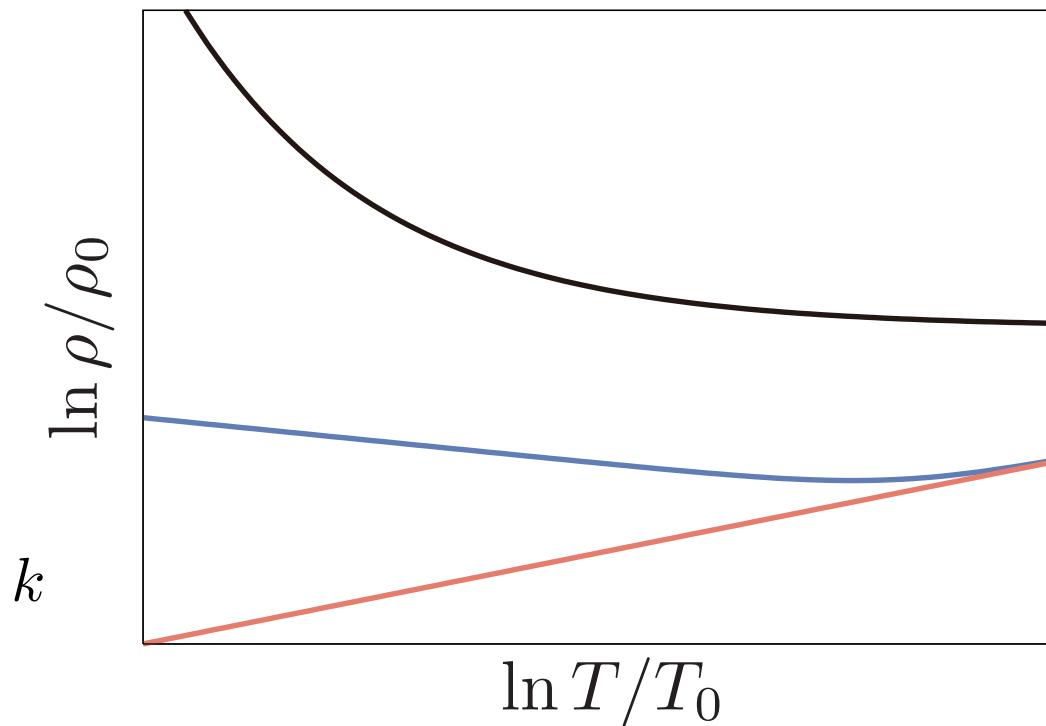
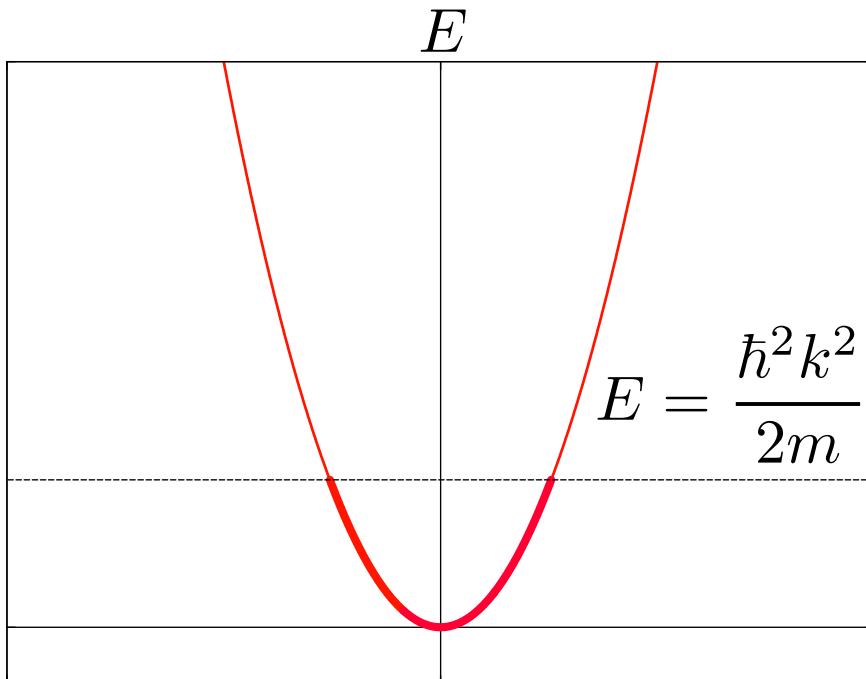
Classification of gapped quantum phases

Nobel Prize in 2016

“Topological phase transitions and
topological phases of matter”

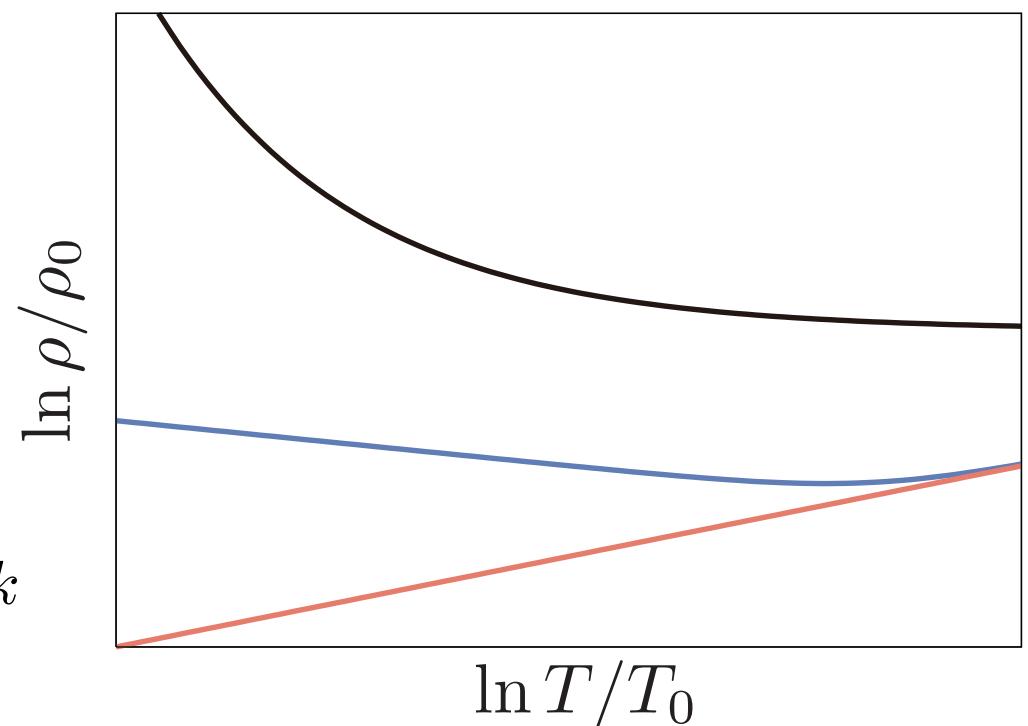
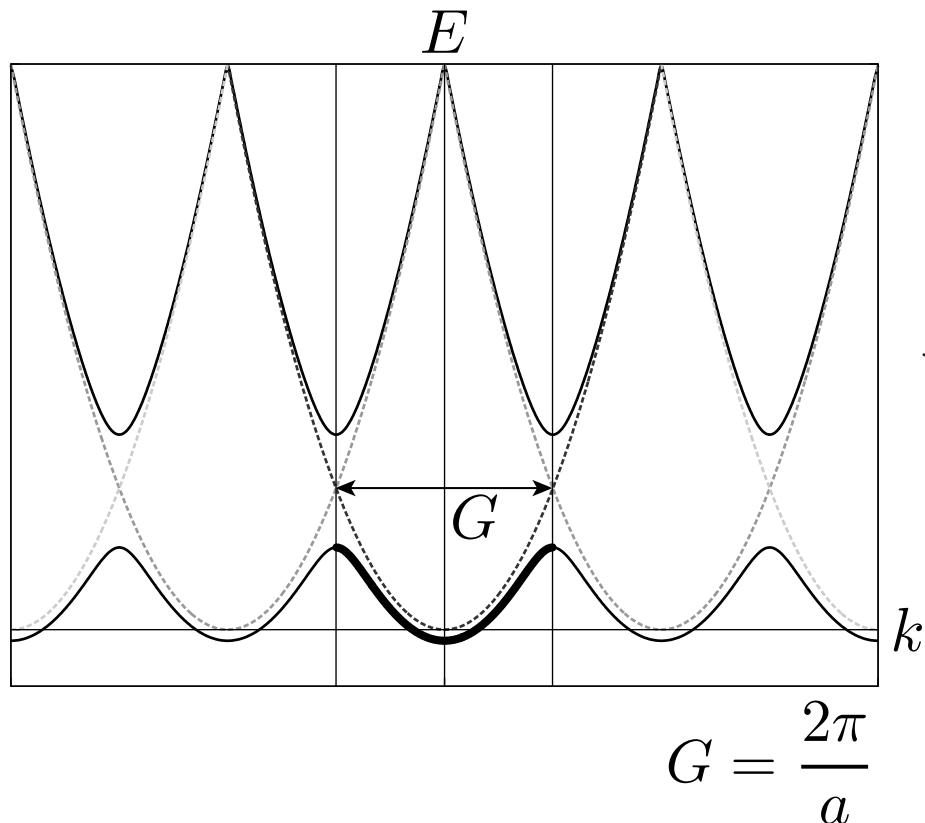
Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
- Semiconductor • Band insulator
- Mott insulator



Classification of Crystalline Solids from Electric Transport

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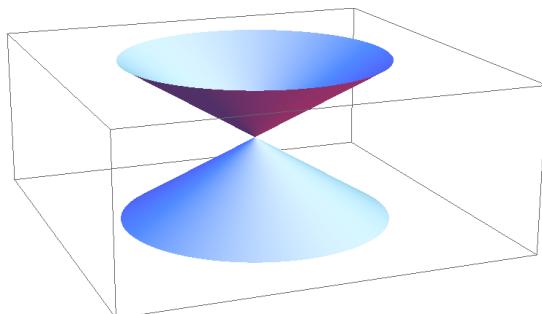
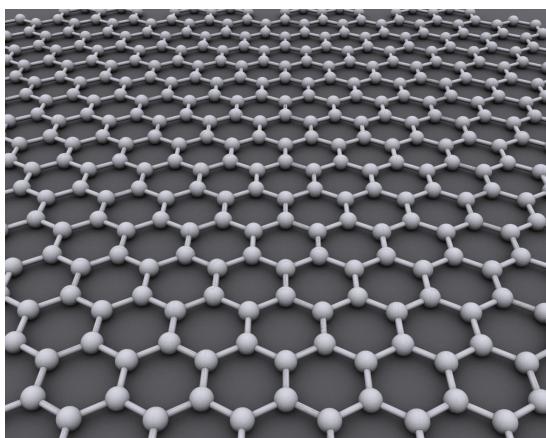


Classification of Crystalline Solids from Electric Transport

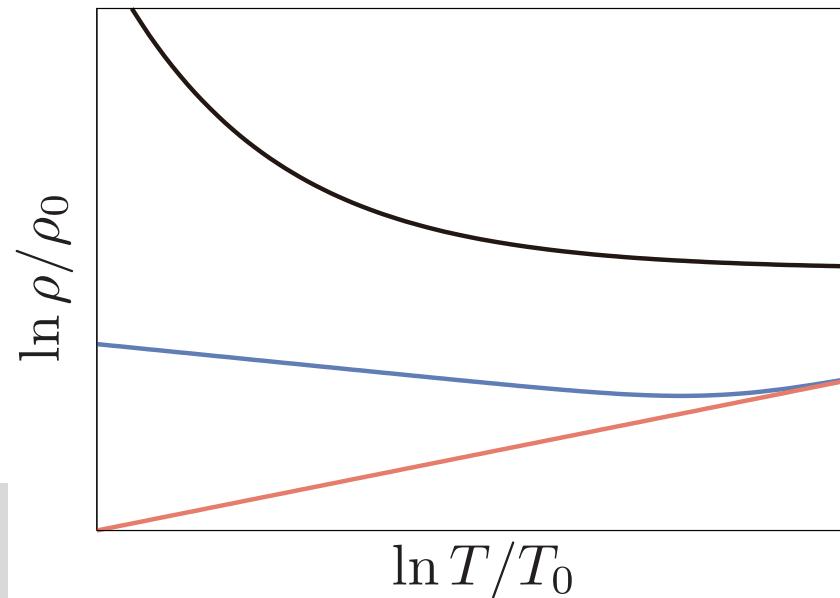
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Example of zero gap semi.

2 D Dirac: Graphene

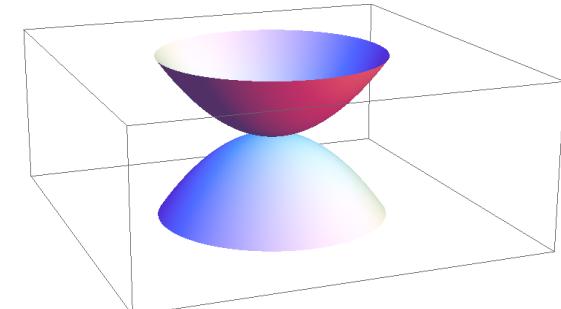


Castro Neto, Guinea, Peres, Novoselov, & Geim,
Rev. Mod. Phys. 81, 109 (2009)



3 D Dirac:
 Cd_3As_2 , Na_3Bi

HgTe, α -Sn (gray tin)



Classification of Crystalline Solids from Electric Transport

- Metal
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- Mott insulator

Y. L. Chen, *et al.*, Science 325, 178 (2009)

Trivial insulator

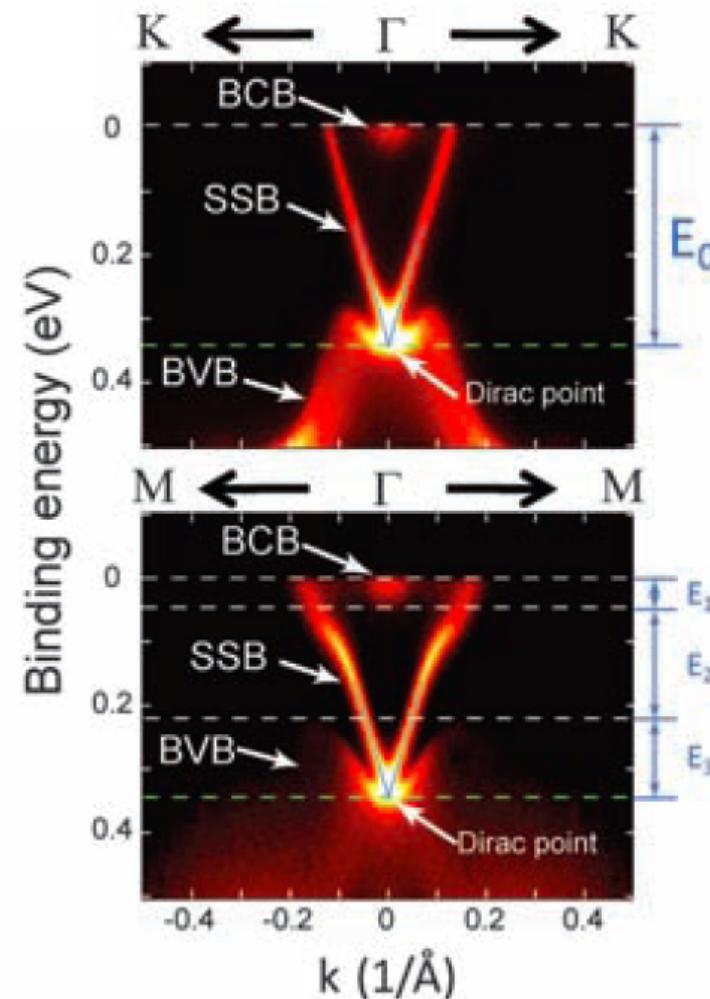
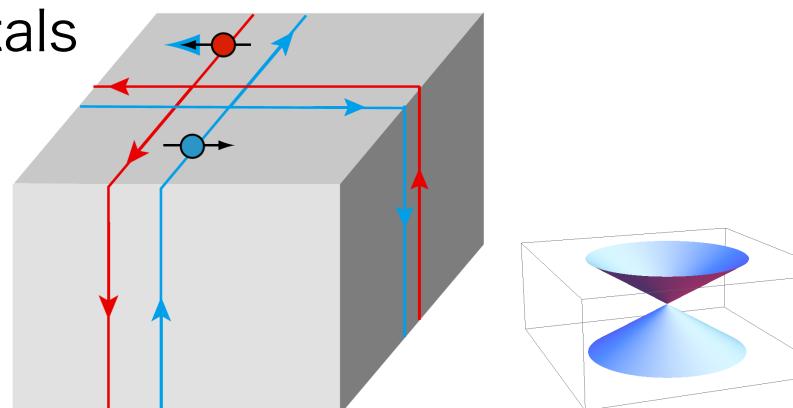
Si

Topological insulator

Bi_2Te_3

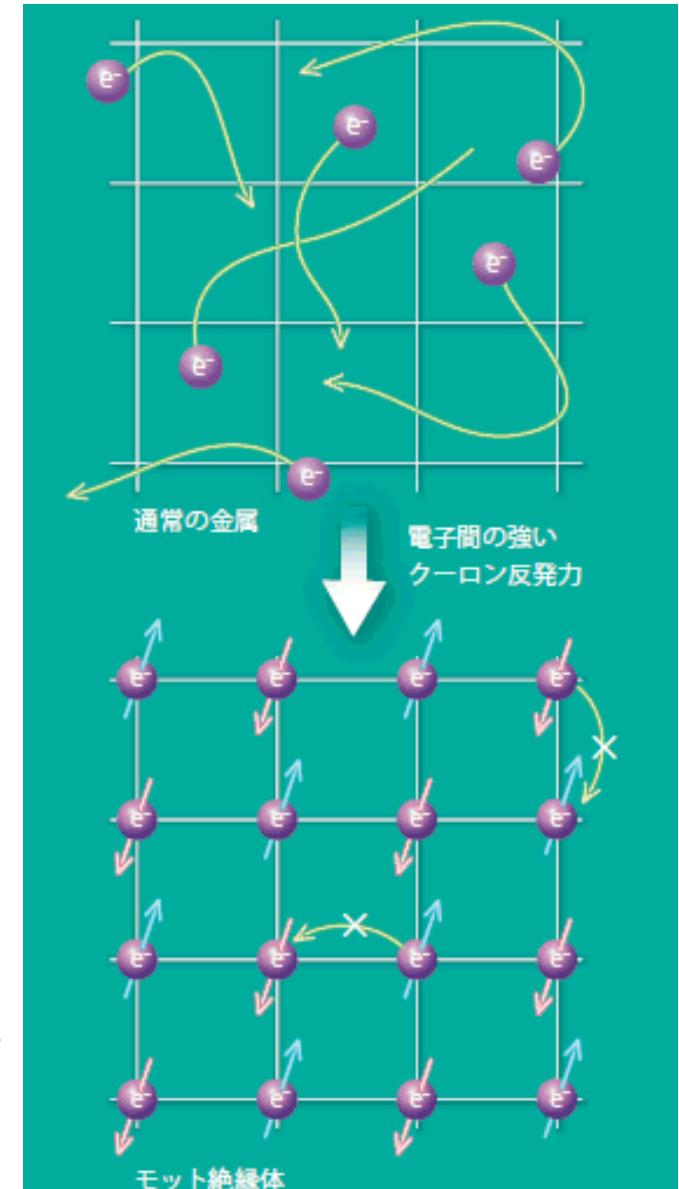
Thermoelectric

Surface metals



Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
- Band insulator
- Mott insulator



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Spin Angular Momentum Coupling

-An electron has $S=1/2$ ((spin angular momentum) = $h/4\pi$)

-Origin of magnetism due to total angular momentum of many electrons in solids

Example of spin angular momentum coupling:

Rare earth gadolinium Gd^{+3} $S=7/2$

-Classical Heisenberg spins obtained in $S \rightarrow +\infty$ limit

$S=1$ consists of two $S=1/2$

$$|m_z = +1; S = 1\rangle = |\uparrow\uparrow\rangle$$

$$|m_z = 0; S = 1\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|m_z = -1; S = 1\rangle = |\downarrow\downarrow\rangle$$

Spin Operators for $S=1$ Quantum Spins

Matrix representation for $S=1$

$$\hat{S}^x \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & +1 & 0 \\ +1 & 0 & +1 \\ 0 & +1 & 0 \end{pmatrix}$$

$$\hat{S}^y \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\hat{S}^z \doteq \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

\hat{S}^x	+1	0	-1
+1	0	$+1/\sqrt{2}$	0
0	$+1/\sqrt{2}$	0	$+1/\sqrt{2}$
-1	0	$+1/\sqrt{2}$	0

\hat{S}^y	+1	0	-1
+1	0	$-i/\sqrt{2}$	0
0	$+i/\sqrt{2}$	0	$-i/\sqrt{2}$
-1	0	$+i/\sqrt{2}$	0

\hat{S}^z	+1	0	-1
+1	+1	0	0
0	0	0	0
-1	0	0	-1

$S=1$ Heisenberg Model

Haldane gap

F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983); Phys. Lett. 93A, 464 (1983).

-Theoretical prediction on excitation gap:

Gapless: $S = 1/2, 3/2, 5/2, \dots$

Gapful: $S = 1, 2, 3, \dots$

cf.) AKLT I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki,
Commun. Math. Phys. 115, 477 (1988).

$$\Delta(S) = \begin{cases} 0.41048(6) & \text{for } S = 1 \\ 0.08917(4) & \text{for } S = 2 \\ 0.01002(3) & \text{for } S = 3 \end{cases}$$

S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

→ Symmetry Protected Topological (SPT) state

$S=1$ Heisenberg Model

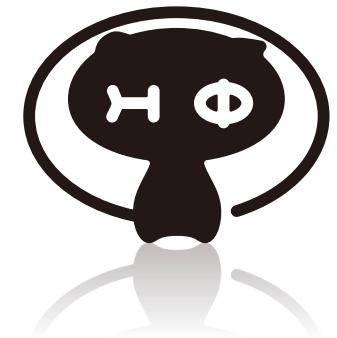
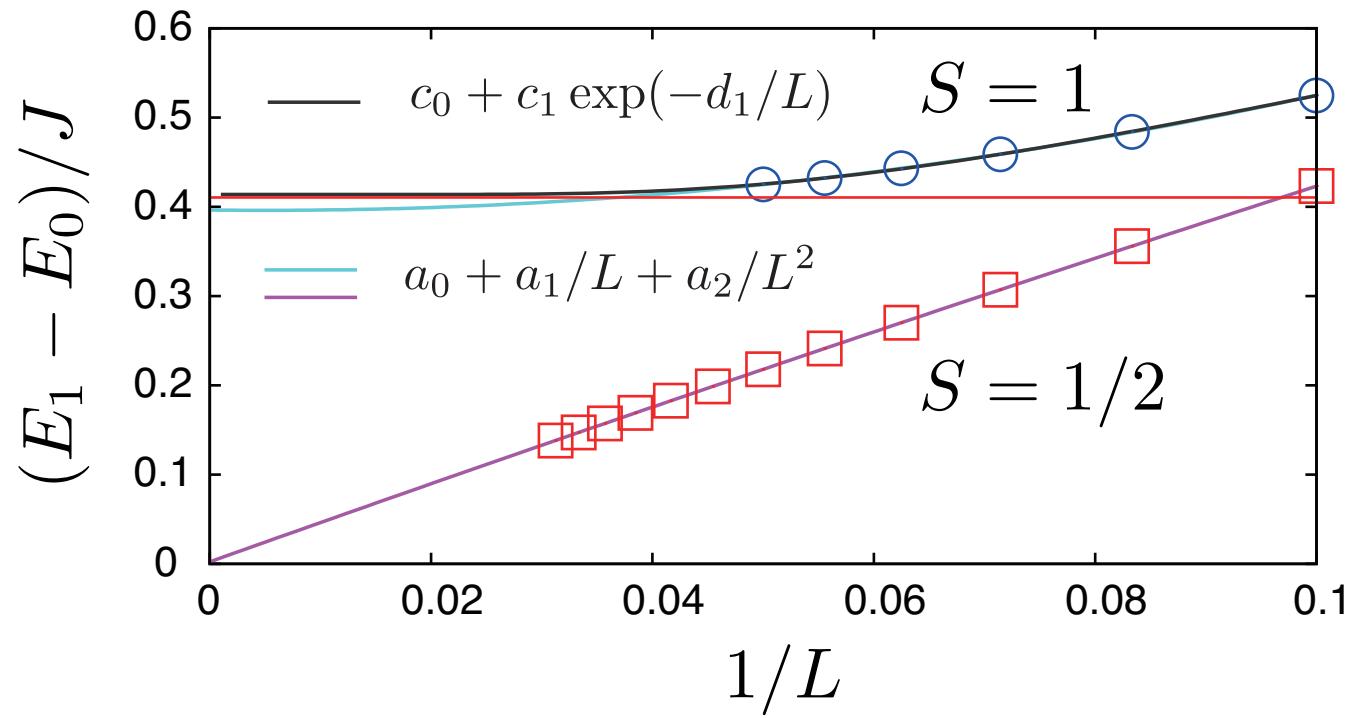
Edge states

Please see the lecture slide of Haldane

https://www.nobelprize.org/nobel_prizes/physics/laureates/2016/haldane-lecture.html

$S=1$ Heisenberg Model

Haldane gap



ED: $S=1$ up to 22 sites

O. Golinelli, Th. Jolicoeur, and R. Lacaze, Phys. Rev. B 50, 3037 (1994).

QMC: S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

2. Excited States: Linear Responses or Dynamical Correlations in Many-body Electrons

An Example: Dynamical Spin Structure Factor

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

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

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

Representation by using Green's function

$$\begin{aligned} S(\vec{Q}, \omega) &= - \lim_{\delta \rightarrow 0+} \frac{1}{\pi} \text{Im} \sum_{\alpha=x,y,z} \sum_m \frac{\langle 0 | \hat{S}_{-\vec{Q}}^\alpha | m \rangle \langle m | \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle}{\omega + i\delta - E_m + E_0} \\ &= - \lim_{\delta \rightarrow 0+} \frac{1}{\pi} \text{Im} \sum_{\alpha=x,y,z} \sum_m \langle 0 | \hat{S}_{-\vec{Q}}^\alpha \frac{1}{\omega + i\delta - \hat{H} + E_0} | \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle \end{aligned}$$

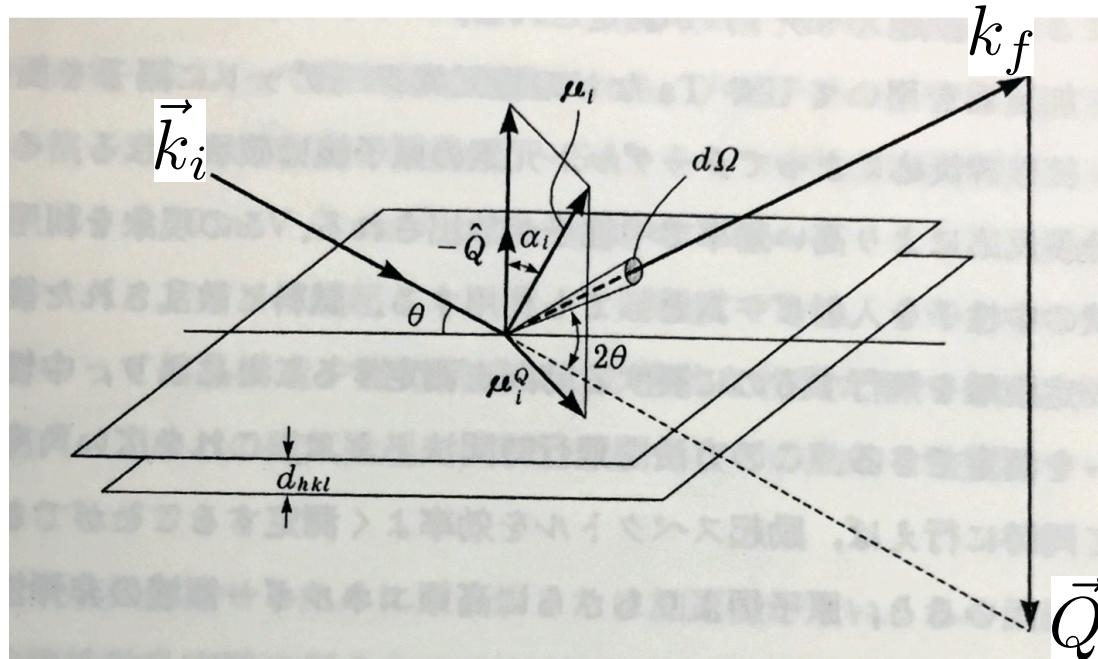
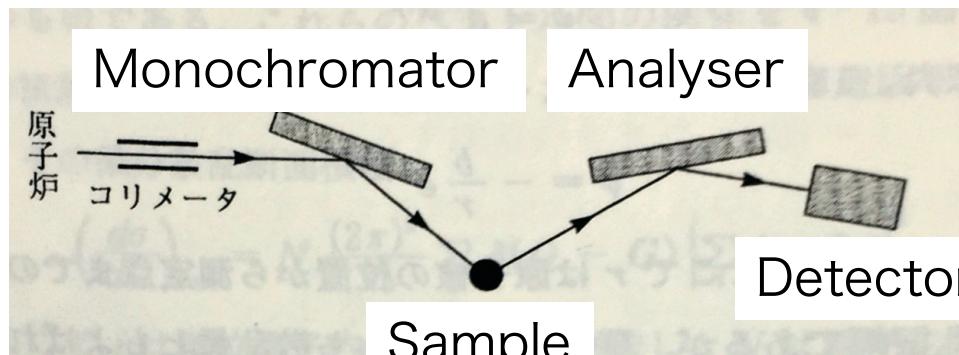
Corresponding Experiment: Neutron Scattering

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

Nuclear reactor

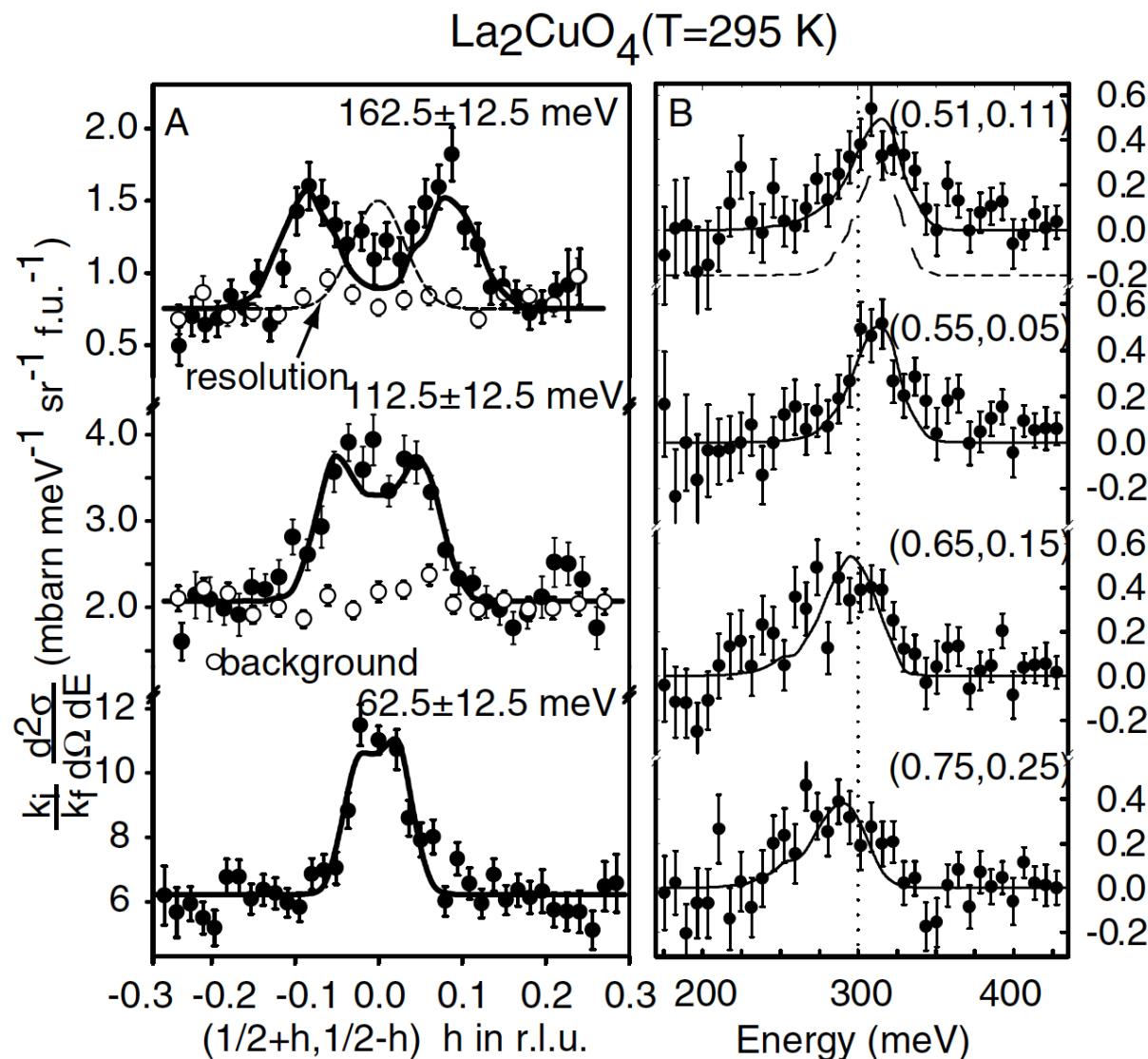
$$\vec{k}_i - \vec{k}_f = \vec{Q}$$

$$E_i - E_f = \omega$$



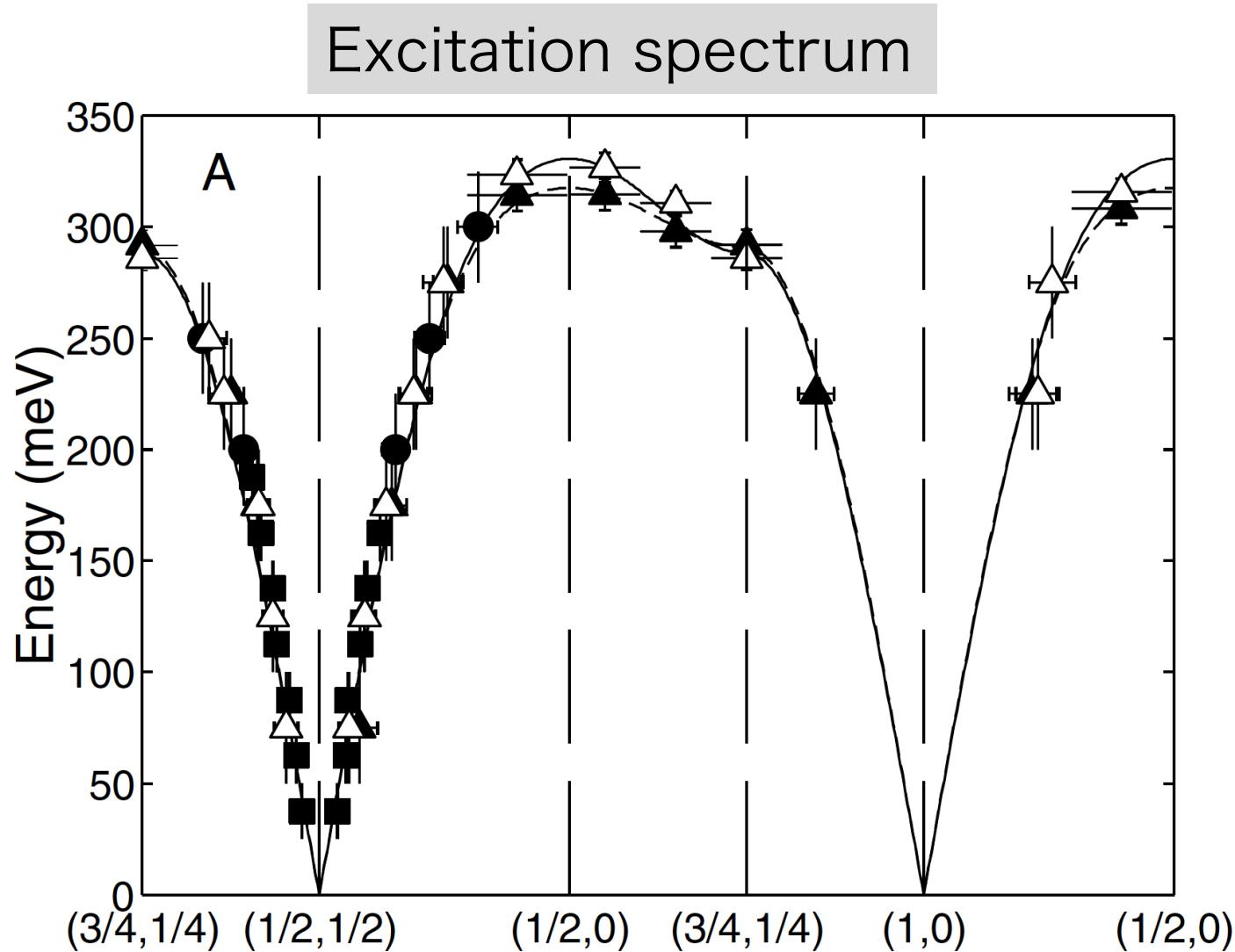
Inelastic Neutron Scattering Measurement of La_2CuO_4

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



Inelastic Neutron Scattering Measurement of La_2CuO_4

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



Simulating Spectroscopy Measurements

Linear response of ground state $|\psi\rangle$

Green's function

$$G_{\hat{O}}(z) = \langle \psi | \hat{O}^\dagger (z \mathbf{1} - \hat{H})^{-1} \hat{O} | \psi \rangle$$
$$z \rightarrow \omega \quad (z \in \mathbb{C}, \omega \in \mathbb{R})$$

Excitation spectrum $-\frac{1}{\pi} \text{Im} G_{\hat{O}}(\omega + i\delta)$

Example of **perturbation & response**:
Magnetization of spins under **magnetic fields**

$$\hat{H}_{\text{ex}} = e^{i\omega t} B_z \left(\frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^z \right)$$
$$\hat{O} = \frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^z$$

Excitation Spectra

Lanczos steps with initial vector defined as

$$|\phi_0\rangle = \hat{O}|\psi\rangle / \sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle} \quad (\text{multiplying excitation operator to g.s.})$$

Lanczos' tridiagonal matrix

$$z\mathbf{1} - H \doteq z\mathbf{1} - H_{\text{td}} = \begin{bmatrix} z - \alpha_0 & -\beta_1 & 0 & 0 & \cdots \\ -\beta_1 & z - \alpha_1 & -\beta_2 & 0 & \cdots \\ 0 & -\beta_2 & z - \alpha_2 & -\beta_3 & \\ 0 & 0 & -\beta_3 & z - \alpha_3 & \\ \vdots & \vdots & & & \ddots \end{bmatrix}$$

→ Excitation Spectrum

$$\begin{aligned} \langle\psi|\hat{O}^\dagger(z\mathbf{1} - \hat{H})^{-1}\hat{O}|\psi\rangle &= \sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle} \{(z\mathbf{1} - H)^{-1}\}_{00} \\ &= \frac{\sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle}}{z - \alpha_0 - \frac{\beta_1^2}{z - \alpha_1 - \frac{\beta_2^2}{z - \alpha_2 - \dots}}} \end{aligned}$$

Continued Fraction

Representation for inverse of a matrix
by Grassmann number

$$\frac{\int \psi_\ell \bar{\psi}_m e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]}{\int e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]} = (M^{-1})_{\ell m}$$

Continued Fraction

Representation for inverse of a matrix
by Grassmann number

$$\frac{\int \psi_1 \bar{\psi}_1 e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]}{\int e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]} = (M^{-1})_{11}$$

An example for 2x2 matrix

$$\begin{aligned} & \int e^{-\bar{\psi}_1 M_{11} \psi_1 - \bar{\psi}_1 M_{12} \psi_2 - \bar{\psi}_2 M_{21} \psi_1 - \bar{\psi}_2 M_{22} \psi_2} d\bar{\psi}_2 d\psi_2 d\bar{\psi}_1 d\psi_1 \\ &= \int M_{22} e^{-\bar{\psi}_1 \left[M_{11} - \frac{M_{12} M_{21}}{M_{22}} \right] \psi_1} d\bar{\psi}_1 d\psi_1 \end{aligned}$$

$$(M^{-1})_{11} = \frac{1}{M_{11} - \frac{M_{12} M_{21}}{M_{22}}}$$

Continued Fraction

General matrices: Schur complement

$$M = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & 0 & 0 & 0 \\ M_{21} & M_{22} & M_{23} & \cdots & 0 & 0 & 0 \\ 0 & M_{32} & M_{33} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & M_{m-2,m-2} & M_{m-2,m-1} & 0 \\ 0 & 0 & 0 & \cdots & M_{m-1,m-2} & M_{m-1,m-1} & M_{m-1,m} \\ 0 & 0 & 0 & \cdots & 0 & M_{m,m-1} & M_{m,m} \end{bmatrix}$$

Continued Fraction

General matrices: Schur complement

Integrating m th component

$$M/M_{m,m} = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & 0 & 0 \\ M_{21} & M_{22} & M_{23} & \cdots & 0 & 0 \\ 0 & M_{32} & M_{33} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & M_{m-2,m-2} & M_{m-2,m-1} \\ 0 & 0 & 0 & \cdots & M_{m-1,m-2} & M'_{m-1,m-1} \end{bmatrix}$$

$$M'_{m-1,m-1} = M_{m-1,m-1} - \frac{M_{m-1,m} M_{m,m-1}}{M_{m,m}}$$

Continued Fraction

General matrices: Schur complement

Integrating m th and $(m-1)$ th components

$$(M/M_{m,m})/M_{m-1,m-1} = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & 0 \\ M_{21} & M_{22} & M_{23} & \cdots & 0 \\ 0 & M_{32} & M_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & M'_{m-2,m-2} \end{bmatrix}$$

$$\begin{aligned} M'_{m-2,m-2} &= M_{m-2,m-2} - \frac{M_{m-2,m-1}M_{m-1,m-2}}{M'_{m-1,m-1}} \\ &= M_{m-2,m-2} - \frac{M_{m-2,m-1}M_{m-1,m-2}}{M_{m-1,m-1} - \frac{M_{m-1,m}M_{m,m-1}}{M_{m,m}}} \end{aligned}$$

→ Iteratively, continued fraction form is obtained

2-1.

Alternative Approach to Green's Function

Green's Function by Solving Linear Equations

Green's function

$$G^{AB}(\zeta) = \langle 0 | \hat{A}^\dagger (\zeta - \hat{H})^{-1} \hat{B} | 0 \rangle$$

-Lanczos/Arnoldi methods

$$\begin{aligned} |\lambda\rangle &= \hat{A}|0\rangle \\ |\rho\rangle &= \hat{B}|0\rangle \\ |\chi(\zeta)\rangle &= (\zeta - \hat{H})^{-1}|\rho\rangle \end{aligned}$$

$$\rightarrow G^{AB}(\zeta) = \langle \lambda | \chi(\zeta) \rangle$$

→ Linear equations

$$(\zeta - \hat{H})|\chi(\zeta)\rangle = |\rho\rangle$$

-CG-type methods, ...

Green's Function by Krylov Subspace Method

Searching solutions in Krylov subspaces

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \text{span}\{|\rho\rangle, (\zeta - \hat{H})|\rho\rangle, \dots, (\zeta - \hat{H})^{n-1}|\rho\rangle\}$$

-Lanczos/Arnoldi methods, **CG-type methods**, ...

Initial: $|\chi_0(\zeta)\rangle = |\rho\rangle$

For $n=1, 2, \dots, m$

Find $|\chi_n(\zeta)\rangle$ in $\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle)$

$$|\rho_n(\zeta)\rangle = (\zeta - \hat{H})|\chi_n(\zeta)\rangle - |\rho\rangle$$

CG-type method

A. Frommer, Computing 70, 87 (2003).

Collinear residuals $|\rho_n(\zeta)\rangle \propto |\rho_n(\zeta')\rangle$

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathcal{K}_n(\zeta' - \hat{H}, |\rho\rangle)$$

→ Seed switch

S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang, & T. Fujiwara,
J. Phys. Soc. Jpn. 77, 114713 (2008).

Library $K\omega$ (released) by Dr. Kawamura (ISSP)

3. Conjugate Gradient Method

Linear Equations

Algorithm for linear equations
instead of eigenvalue problems

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

A simple method: Gradient descent/steepest descent

Solving a linear equation is mapped onto
finding a minimum of a cost function

For symmetric matrix A

$$f(\vec{x}) = \frac{1}{2}\vec{x}^T A \vec{x} - \vec{b}^T \vec{x}$$

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b}$$

$$\vec{x}_{k+1} = \vec{x}_k - \alpha \vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}$$

-Only local information is utilized,
and thus often captured by local minima

Conjugate Gradient Method

M. R. Hestenes & E. Stiefel, J. Res. Natl. Bur. Stand. 49, 409 (1952).

Find an approximate solution in a Krylov subspace

$$\vec{x}_k = \sum_{j=0}^{k-1} a_j \vec{p}_j$$

Conjugate basis set $\{\vec{p}_k\}$ $\vec{p}_i^T A \vec{p}_j = 0 \ (i \neq j)$

Additional constraint: Find orthogonal residual vectors

$$\vec{r}_k = \vec{b} - A \vec{x}_k$$

Orthogonal basis set $\{\vec{r}_k\}$ $\vec{r}_i^T \vec{r}_j = 0 \ (i \neq j)$

Conjugate Gradient Method: Algorithm

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

For symmetric matrix A

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

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

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

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

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

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

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

M. R. Hestenes & E. Stiefel,
J. Res. Natl. Bur. Stand. 49, 409 (1952).

The algorithm generates

-Conjugate basis set $\{\vec{p}_k\}$

-Orthogonal basis set $\{\vec{r}_k\}$

←A Krylov subspace

CG method finds an approximate solution
of the linear equation in a Krylov subspace

Sketch of Proof for CG Method 0.

Induction

Assume $\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k\}$ is orthogonal basis set

$$\vec{r}_i^T \vec{r}_j = 0 \quad (i \neq j, i \leq k, j \leq k)$$

Assume $\{\vec{p}_0, \vec{p}_1, \dots, \vec{p}_k\}$ is conjugate basis set

$$\vec{p}_i^T A \vec{p}_j = 0 \quad (i \neq j, i \leq k, j \leq k)$$

Prove \vec{r}_{k+1} satisfies $\vec{r}_j^T \vec{r}_{k+1} = 0 \quad (j \leq k)$

Prove \vec{p}_{k+1} satisfies $\vec{p}_j^T A \vec{p}_{k+1} = 0 \quad (j \leq k)$

Sketch of Proof for CG Method 1.

Ansatz

$$\begin{aligned}\vec{x}_{k+1} &= \vec{x}_k + \alpha_k \vec{p}_k \\ \rightarrow \vec{r}_{k+1} &= \vec{b} - A\vec{x}_{k+1} \\ &= \vec{r}_k - \alpha_k A\vec{p}_k\end{aligned}$$

Requirement

$$\begin{aligned}\vec{r}_k^T \vec{r}_{k+1} &= 0 \\ \rightarrow \vec{r}_k^T \vec{r}_{k+1} &= \vec{r}_k^T \vec{r}_k - \vec{r}_k^T \alpha_k A\vec{x}_{k+1} = 0 \\ \rightarrow \alpha_k &= \frac{\vec{r}_k^T \vec{r}_k}{\vec{r}_k^T A\vec{p}_k} \\ \left\{ \begin{array}{l} \vec{p}_k = \vec{r}_k + \beta_{k-1} \vec{p}_{k-1} \\ \vec{p}_{k-1}^T A\vec{p}_k = 0 \end{array} \right. &\quad \text{← assumption} \\ \rightarrow \alpha_k &= \frac{\vec{r}_k^T \vec{r}_k}{\vec{r}_k^T A\vec{p}_k} = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A\vec{p}_k}\end{aligned}$$

$$\begin{aligned}\vec{r}_j^T \vec{r}_{k+1} &= \vec{r}_j^T \vec{r}_{k+1} - \alpha_k \vec{r}_j^T A\vec{p}_{k+1} \\ &= -\alpha_k \vec{p}_j^T A\vec{p}_{k+1} \quad (\vec{p}_j = \vec{r}_j + \beta_{j-1} \vec{p}_{j-1}, \vec{r}_j^T \vec{r}_{k+1} = 0) \\ &= 0 \quad (j < k)\end{aligned}$$

Sketch of Proof for CG Method 2.

Ansatz &
Requirement

$$\left\{ \begin{array}{l} \vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k \\ (\vec{p}_k^T A) \vec{p}_{k+1} = 0 \end{array} \right. \rightarrow (\vec{p}_k^T A) \vec{p}_{k+1} = (\vec{p}_k^T A) \vec{r}_{k+1} + \beta_k (\vec{p}_k^T A) \vec{p}_k = 0$$
$$\rightarrow \beta_k = -\frac{\vec{p}_k^T A \vec{r}_{k+1}}{\vec{p}_k^T A \vec{p}_k}$$
$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$
$$\rightarrow A \vec{p}_k = \frac{\vec{r}_k - \vec{r}_{k+1}}{\alpha_k}$$
$$\beta_k = -\frac{\vec{p}_k^T A \vec{r}_{k+1}}{\vec{p}_k^T A \vec{p}_k} = -\frac{(\vec{r}_k - \vec{r}_{k+1})^T \vec{r}_{k+1}}{\alpha_k \vec{p}_k^T A \vec{p}_k}$$
$$= \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k} = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$
$$\vec{p}_j^T A \vec{p}_{k+1} = 0 \quad (j < k)$$

Variation of CG Method

Variation of CG method:

- A : symmetric \rightarrow Conjugate Gradient

- A : hermitian \rightarrow Conjugate Gradient ($T \rightarrow +$)

- $A + \sigma I$: symmetric A and complex σ

\rightarrow Conjugate Orthogonal Conjugate Gradient (COCG)

- $A + \sigma I$: hermitian A and complex σ

\rightarrow Bi-Conjugate Gradient (BiCG)

An important application:

-Calculation of eigenvectors after the Lanczos method

Inverse iteration: $(\hat{H} - E_m)\vec{v}_{k+1} = \vec{v}_k$

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

3-1.
SD vs CG

Numerical Algorithm Is Not Originally for Modern Computers

-Gauss-Seidel & Jacobi method for linear equations
(19th century)

-Krylov's original work

*"On the numerical solution of the equation by which,
in technical matters, frequencies of small oscillations of
material systems are determined"*

(1931)

-ZND detonation model calculated by hand
for designing nuclear bomb @LANL
(1940's)

Many modern numerical algorithm is based on
algorithm before the invention of modern computers

One of the Simplest Example of Linear Equations

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

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

$$\vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Analytical solution

$$\vec{x} = A^{-1}\vec{b}$$

$$\begin{aligned}\vec{x} &= A^{-1}\vec{b} \\ &= \frac{1}{3} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 2/3 \\ -1/3 \end{pmatrix}\end{aligned}$$

Steepest Descent

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

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b} \quad \vec{x}_{k+1} = \vec{x}_k - \alpha \vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}$$

Formal solution

$$\begin{aligned}\vec{x}_{k+1} &= \vec{x}_k + \alpha(\vec{b} - A\vec{x}_k) \\ &= (1 - \alpha A)\vec{x}_k + \alpha\vec{b} \\ &= (1 - \alpha A)^2\vec{x}_{k-1} + \alpha\vec{b} + \alpha(1 - \alpha A)\vec{b} \\ &= \dots \\ &= (1 - \alpha A)^{k+1}\vec{x}_0 + \alpha\vec{b} + \alpha(1 - \alpha A)\vec{b} + \dots + \alpha(1 - \alpha A)^k\vec{b} \\ &= \alpha \frac{1 - (1 - \alpha A)^{k+1}}{1 - (1 - \alpha A)} \vec{b} \\ &= A^{-1}[1 - (1 - \alpha A)^{k+1}]\vec{b}\end{aligned}$$

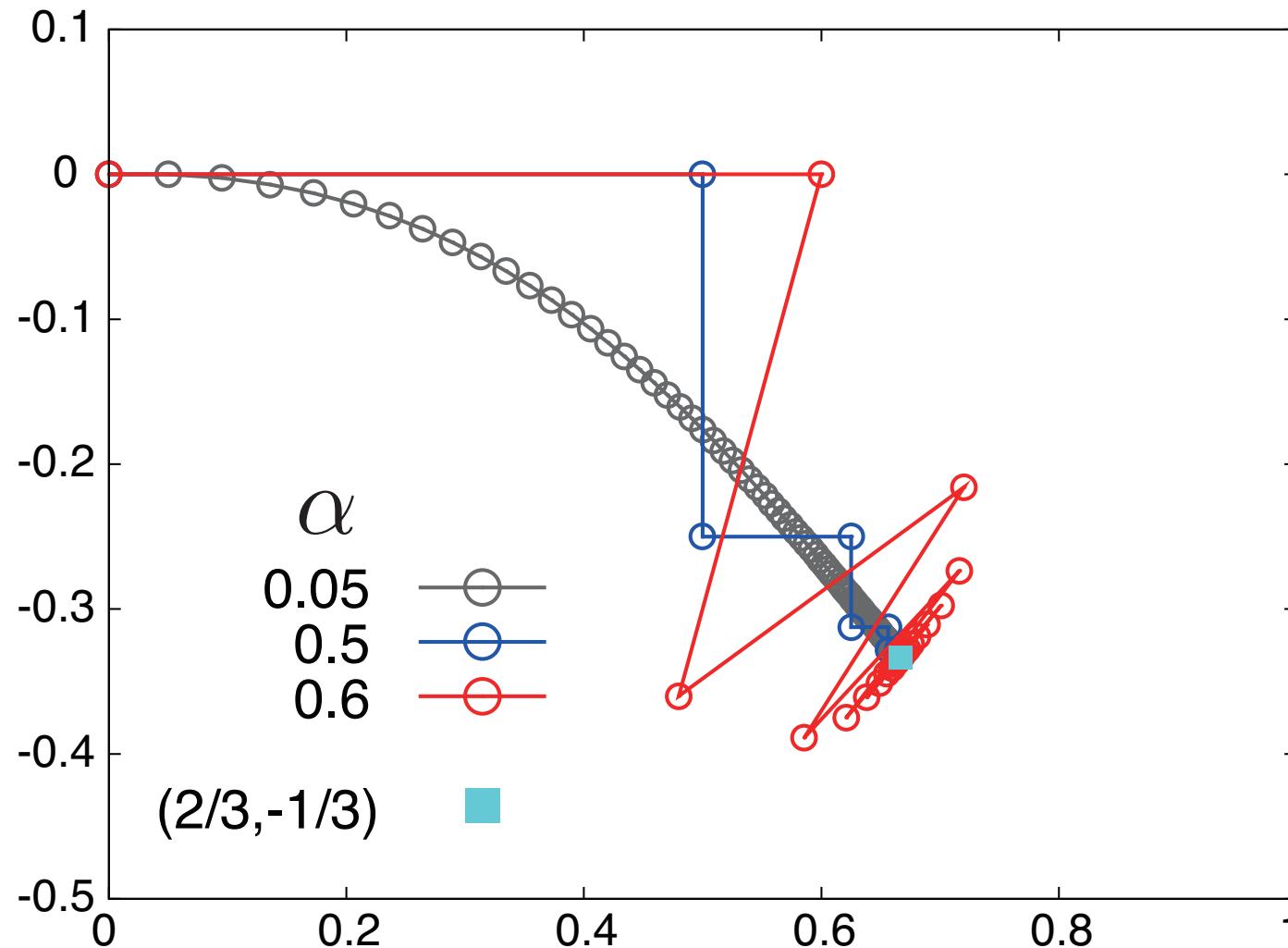
SD finds the exact solution only when $(1 - \alpha A)^{k+1}\vec{b} = \vec{0}$

Slow Convergence of Steepest Descent

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

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b}$$

$$\vec{x}_{k+1} = \vec{x}_k - \alpha \vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}$$



Conjugate Gradient

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

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

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

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

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

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

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

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

1st Step of CG

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

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

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

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

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

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

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

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

$$\vec{x}_0 = \vec{0}$$

$$\vec{p}_0 = \vec{r}_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\alpha_0 = \frac{1}{(1, 0) \begin{pmatrix} 2 \\ 1 \end{pmatrix}} = \frac{1}{2}$$

$$\vec{x}_1 = \vec{0} + \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix}$$

$$\vec{r}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix}$$

$$\beta_0 = \frac{\vec{r}_1^T \vec{r}_1}{\vec{r}_0^T \vec{r}_0} = \frac{1/4}{1} = \frac{1}{4}$$

$$\vec{p}_1 = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ -1/2 \end{pmatrix}$$

2nd Step of CG

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

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

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

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

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

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

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

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

$$\begin{aligned}\vec{x}_1 &= \vec{0} + \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix} \\ \vec{r}_1 &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} \\ \vec{p}_1 &= \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ -1/2 \end{pmatrix}\end{aligned}$$

$$\alpha_1 = \frac{1/4}{(1/4, -1/2) \begin{pmatrix} 0 \\ -3/4 \end{pmatrix}} = \frac{2}{3}$$

$$\vec{x}_2 = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix} + \frac{2}{3} \begin{pmatrix} 1/4 \\ -1/2 \end{pmatrix} = \begin{pmatrix} 2/3 \\ -1/3 \end{pmatrix}$$

$$\vec{r}_2 = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} - \frac{2}{3} \begin{pmatrix} 0 \\ -3/4 \end{pmatrix} = \vec{0}$$

CG finds the exact solution at the 2nd step!

3-2. Shifted Krylov Subspace Method

Collinear Residual

A. Frommer, Computing 70, 87 (2003).

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

$$\vec{r}_0 = \vec{b} \text{ if } \vec{x}_0 = \vec{0}$$

$$(A + \sigma \mathbf{1})\vec{x}^\sigma = \vec{b}$$

$$\vec{r}_0^\sigma = \vec{b} \text{ if } \vec{x}_0^\sigma = \vec{0}$$

Shift invariance of Krylov subspace

$$\text{span}\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k\} = \text{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \dots, \vec{r}_k^\sigma\}$$

CG-type methods find a new residual vector

$$\vec{r}_{k+1} \perp \text{span}\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k\}$$

$$\vec{r}_{k+1}^\sigma \perp \text{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \dots, \vec{r}_k^\sigma\}$$

Shift invariance of Krylov subspace

$$\text{span}\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k, \vec{r}_{k+1}\} = \text{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \dots, \vec{r}_k^\sigma, \vec{r}_{k+1}^\sigma\}$$

$$\vec{r}_{k+1} \propto \vec{r}_{k+1}^\sigma$$

Details of Collinear Residual 1.

Coefficient

A. Frommer, Computing 70, 87 (2003).

$$\vec{r}_k^\sigma = (1/\pi_k^\sigma) \vec{r}_k$$

$$\vec{x}_k = q_{k-1}(A) \vec{b}$$

$$\vec{r}_k = p_k(A) \vec{b} \quad (= \vec{b} - Aq_{k-1}(A) \vec{b} = \vec{b} - A\vec{x}_k)$$

$$p_k(t) = 1 - tq_{k-1}(t)$$

$$q_{k-1}(t) = \sum_{m=0}^{k-1} d_m t^m$$

$$\vec{r}_k^\sigma = p_k^\sigma(A + \sigma \mathbf{1}) \vec{b}$$

$$p_k^\sigma(A + \sigma \mathbf{1}) \vec{b} = (1/\pi_k^\sigma) p_k(A) \vec{b}$$

$$\rightarrow p_k^\sigma(t + \sigma) = (1/\pi_k^\sigma) p_k(t)$$

$$\pi_k^\sigma = p_k(-\sigma) \quad (\text{since } p_k^\sigma(0) = 1)$$

Details of Collinear Residual 2.

A. Frommer, Computing 70, 87 (2003).

Recurrence formula for residual vectors

$$\begin{aligned}\vec{p}_{k-1} &= \frac{1}{\beta_k}(\vec{r}_k - \vec{p}_k), \quad A\vec{p}_k = \frac{1}{\alpha_k}(\vec{r}_k - \vec{r}_{k+1}) \\ \rightarrow \vec{r}_k &= \vec{r}_{k-1} - \alpha_{k-1}A\vec{p}_{k-1} = \vec{r}_{k-1} - \frac{\alpha_{k-1}}{\beta_k}A(\vec{r}_k - \vec{p}_k) \\ &= \vec{r}_{k-1} - \frac{\alpha_{k-1}}{\beta_k}A\vec{r}_k + \frac{\alpha_{k-1}}{\alpha_k\beta_k}(\vec{r}_k - \vec{r}_{k+1}) \\ \rightarrow \vec{r}_{k+1} &= -\alpha_k A\vec{r}_k + \left(1 - \frac{\alpha_k\beta_k}{\alpha_{k-1}}\right)\vec{r}_k + \frac{\alpha_k\beta_k}{\alpha_{k-1}}\vec{r}_{k-1} \\ \rightarrow p_{k+1}(t) &= -\alpha_k t \cdot p_k(t) + \left(1 - \frac{\alpha_k\beta_k}{\alpha_{k-1}}\right)p_k(t) + \frac{\alpha_k\beta_k}{\alpha_{k-1}}p_{k-1}(t) \\ \rightarrow \pi_{k+1}^\sigma &= \left(1 + \alpha_k\sigma - \frac{\alpha_k\beta_k}{\alpha_{k-1}}\right)\pi_k^\sigma + \frac{\alpha_k\beta_k}{\alpha_{k-1}}\pi_{k-1}^\sigma\end{aligned}$$

Shifted CG: Algorithm

Initial $\vec{r}_0 = \vec{b}$, $\alpha_{-1} = 1$, $\rho_{-1} = +\infty$,
 $\pi_0^\sigma = \pi_{-1}^\sigma = 1$, $\vec{p}_{-1}^\sigma = \vec{x}_{-1}^\sigma = \vec{0}$

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

-Seed equations

$$\rho_k = \vec{r}_k^T \vec{r}_k$$

$$\beta_{k-1} = \frac{\rho_k}{\rho_{k-1}}$$

$$\alpha_k = \frac{\rho_k}{\vec{r}_k^T A \vec{r}_k - \beta_{k-1} \frac{\rho_k}{\alpha_{k-1}}}$$

$$\vec{r}_{k+1} = \left(1 + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}\right) \vec{r}_k - \alpha_k A \vec{r}_k - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} \vec{r}_{k-1}$$

-Shifted equations

$$\pi_{k+1}^\sigma = (1 + \alpha_k \sigma) \pi_k^\sigma - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} (\pi_{k-1}^\sigma - \pi_k^\sigma)$$

$$\vec{p}_k^\sigma = \frac{1}{\pi_k^\sigma} \vec{r}_k + \beta_{k-1} \left(\frac{\pi_{k-1}^\sigma}{\pi_k^\sigma} \right)^2 \vec{p}_{k-1}^\sigma$$

$$\vec{x}_k^\sigma = \vec{x}_{k-1}^\sigma + \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \alpha_k \vec{p}_k^\sigma$$

Shifted CG: The Simplest Example

$$(A + \sigma \mathbf{1})\vec{x}^\sigma = \vec{b} \quad A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \quad \vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

	Seed equations	Shifted equations
0th step	$\rho_0 = 1$	$\pi_1^\sigma = (1 + \sigma/2)$
	$\beta_{-1} = 0$	$\vec{p}_0^\sigma = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
	$\alpha_0 = 1/2$	$\vec{x}_0^\sigma = \frac{1}{2 + \sigma} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
	$\vec{r}_1 = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix}$	
1st step	$\rho_1 = 1/4$	$\pi_2^\sigma = 1 + 4\sigma/3 + \sigma^2/3$
	$\beta_0 = 1/4$	$\vec{p}_1^\sigma = \begin{pmatrix} 1/\{2 + \sigma\}^2 \\ -1/\{2 + \sigma\} \end{pmatrix}$
	$\alpha_1 = 2/3$	$\vec{x}_1^\sigma = \begin{pmatrix} \{2 + \sigma\}/\{3 + 4\sigma + \sigma^2\} \\ -1/\{3 + 4\sigma + \sigma^2\} \end{pmatrix}$
	$\vec{r}_2 = \vec{0}$	

$$(A + \sigma \mathbf{1}) \vec{x}^\sigma = \vec{b}$$

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

$$\vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Analytical solution

$$\begin{pmatrix} 2 + \sigma & 1 \\ 1 & 2 + \sigma \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{(2 + \sigma)^2 - 1} \begin{pmatrix} 2 + \sigma \\ -1 \end{pmatrix}$$

Numerical solution

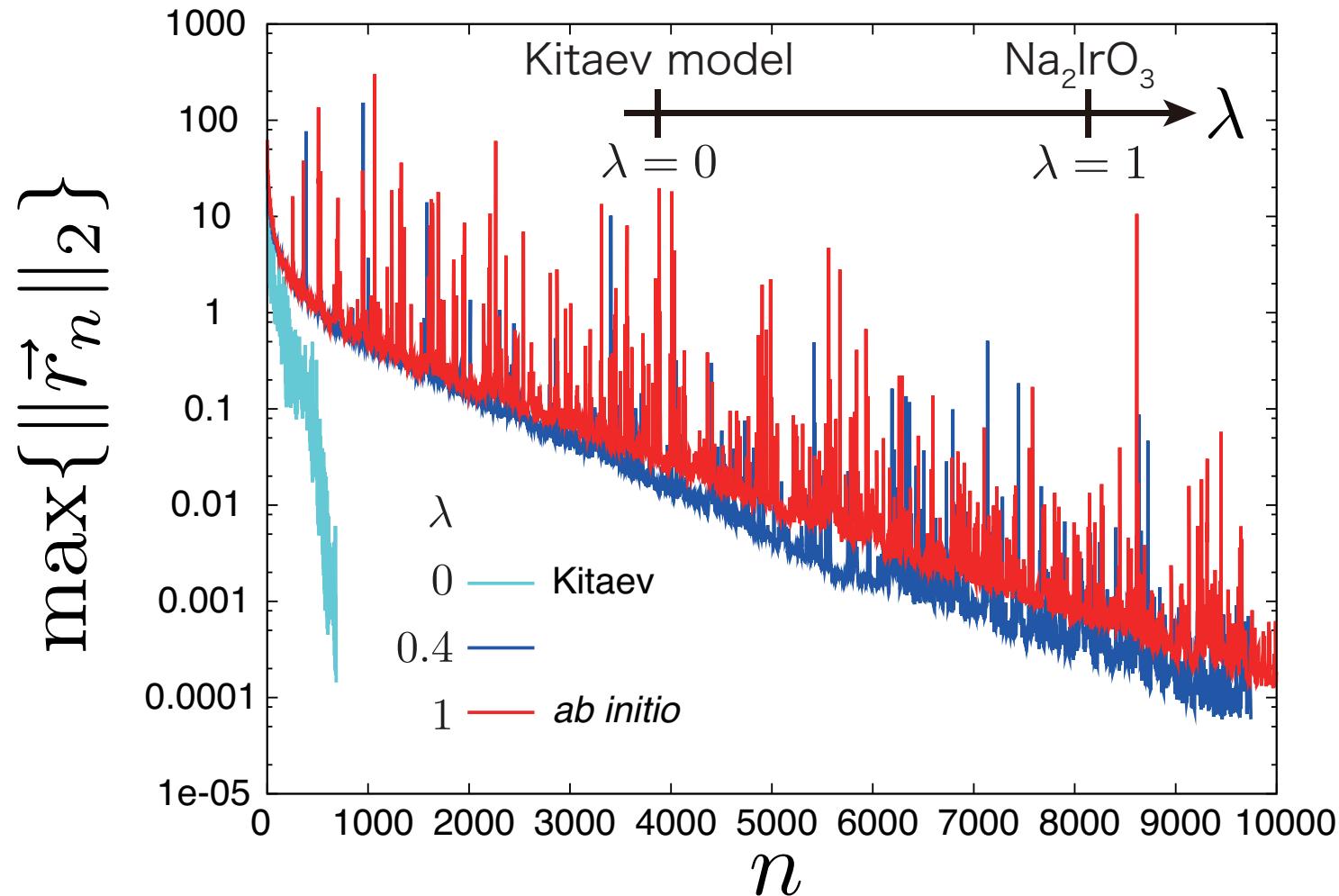
$$\vec{x}_1^\sigma = \begin{pmatrix} \frac{2 + \sigma}{3 + 4\sigma + \sigma^2} \\ -\frac{1}{3 + 4\sigma + \sigma^2} \end{pmatrix}$$

Shifted CG finds
the set of solution!

Convergence of Krylov Subspace Method

Krylov subspace method
finds a solution within N_H steps

An example of shifted BiCG for $N_H=16,777,216$



Important Notice 1

Lanczos method

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

Pros

- Simple to implement
- Cheap memory cost

Cons

- Eigenvectors are not directly obtained

Important Notice 2

CG method

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

-Linear equations

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

-Eigenvalues and eigenvectors

Locally optimal block CG (LOBCG):

A. V. Knyazev,

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

LOB(P)CG

Algorithm of LOBCG

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

Target of Tuning: LOB(P)CG

Algorithm for implementation

Initial condition: m orthogonal initial vectors $\mathbf{x}_0^{(i)}$
 $\mathbf{p}_0^{(i)} = \mathbf{0}$ ($i = 1, \dots, m$) $\mathbf{X}_0^{(i)} = A\mathbf{x}_0^{(i)}$ ←matrix-vector product

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

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

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

$$\mathbf{W}_k^{(i)} = A\mathbf{w}_k^{(i)} \quad \text{←matrix-vector product}$$

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

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

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

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

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

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

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

Until convergence

Important Notice 3

Shifted Krylov subspace method

- Same accuracy as CG obtain for same # of steps
- Solve many shifted equations with
nearly same costs for a single equation

4. Typicality Approach

Finite Temperature: Heat Capacity

Spread of energy distribution

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

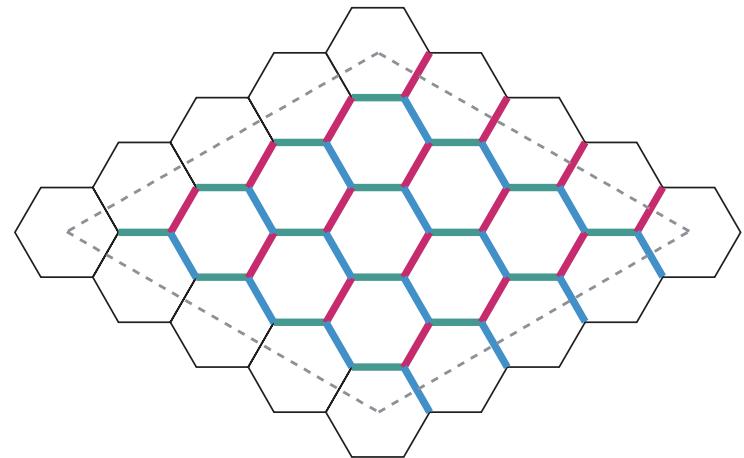
-Average with Boltzmann distribution

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

Complexity $\mathcal{O}(N_{\text{H}}^3)$

Memory $\mathcal{O}(N_{\text{H}}^2)$

32 site cluster of Na_2IrO_3



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

Hamiltonian
 $\sim 3 \times 10^8 \text{ TB!}$

$|n\rangle \sim 69 \text{ GB}$

Canonical Ensemble

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

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

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

Is it necessary? Answer is No

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

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

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).

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

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

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

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).

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

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

Exponentially 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 $T = +\infty$): $|\Phi_0\rangle = (\text{Random vector})$
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
- Krylov subspace method reproduces statistical mechanics

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

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

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

Every eigenstate contained
in a random vector with
equal probability

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

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

See also Jin *et al.*, JPSJ 90, 012001 (2021).

<https://journals.jps.jp/doi/full/10.7566/JPSJ.90.012001>

4-1. Combination of Shifted Krylov Method and Typicality Approach

An Alternative to Spectral Projection

T. Kato, Progress of Theoretical Physics 4, 514 (1949).

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

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

Discretized by Riemann sum

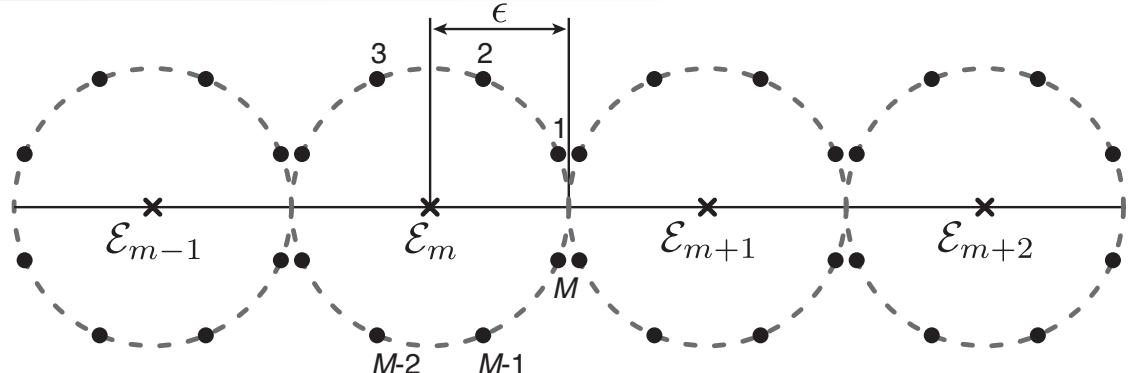
T. Sakurai and H. Sugiura,
J. Comput. Appl. Math. 159, 119 (2003).
T. Ikegami, T. Sakurai, and U. Nagashima,
J. Comput. Appl. Math. 233, 1927 (2010).

$$\hat{P}_{\gamma,\rho,M} = \frac{1}{M} \sum_{j=1}^M \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}}$$
$$\theta_j = 2\pi(j - 1/2)/M$$

Probability Distribution by Typical Pure States

$$|\phi_{\beta,\delta}^m\rangle = \hat{P}_{\mathcal{E}_m, \epsilon, M} |\phi_\beta\rangle$$

$$\delta = (E_0, \epsilon, M)$$



$$\mathcal{E}_m = E_0 + (2m - 1)\epsilon$$

$$|\phi_j\rangle = \frac{w_j}{z_j - \hat{H}} |\phi\rangle \quad \text{by (shifted) CG method}$$

$$\rightarrow \hat{P}|\phi\rangle = \sum_j |\phi_j\rangle$$

N. Shimizu, Y. Utsuno, Y. Futamura, T. Sakurai, T. Mizusaki, and T. Otsuka,
Physics Letters B 753, 13 (2016).

Probability distribution

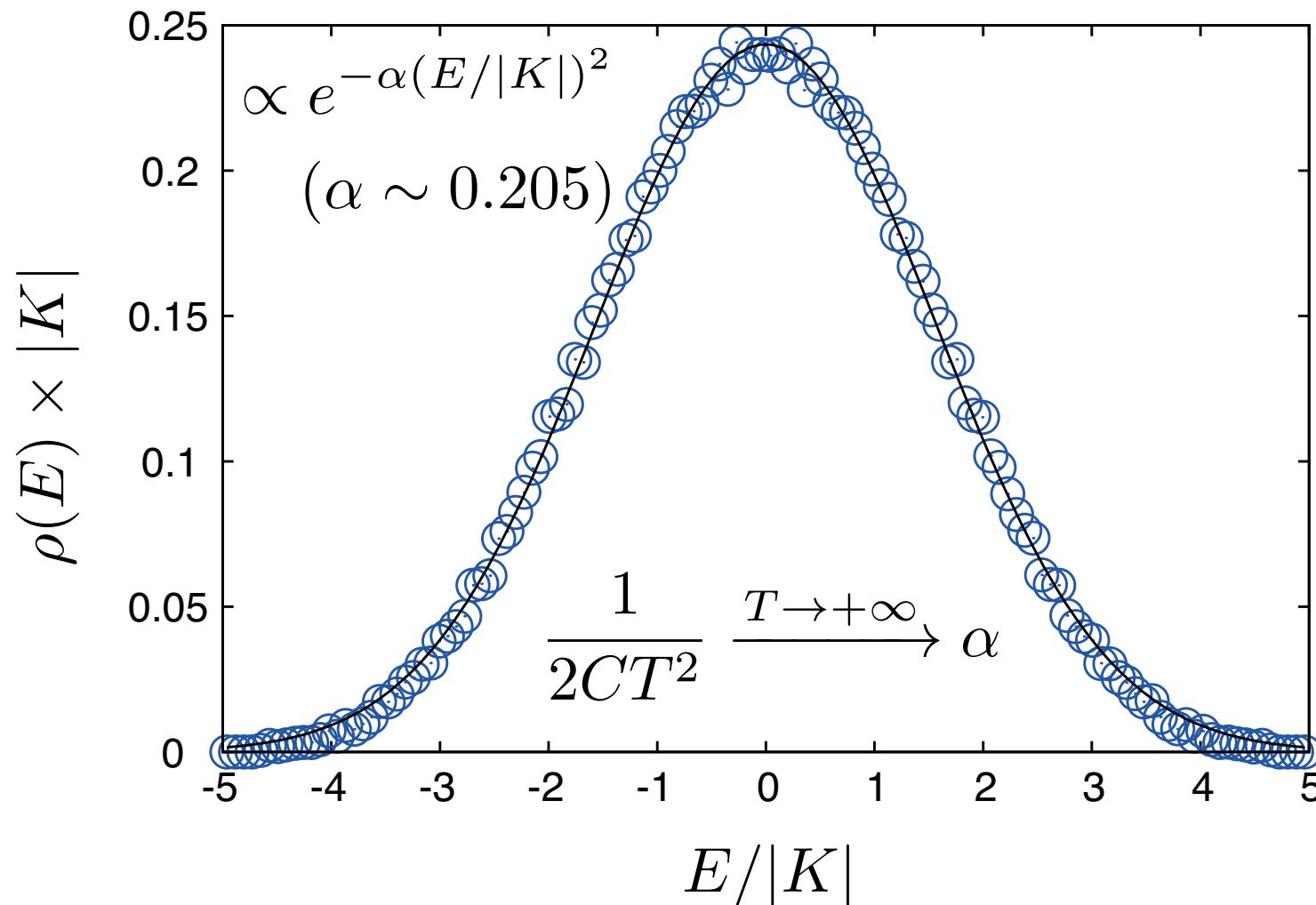
$$\tilde{P}_\delta(\mathcal{E}_m) = \langle \phi_{\beta,\delta}^m | \phi_{\beta,\delta}^m \rangle$$

An Example of Density of State

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

A. Kitaev, Annals Phys. 321, 2 (2006).

$$2^{24} = 16,777,216$$



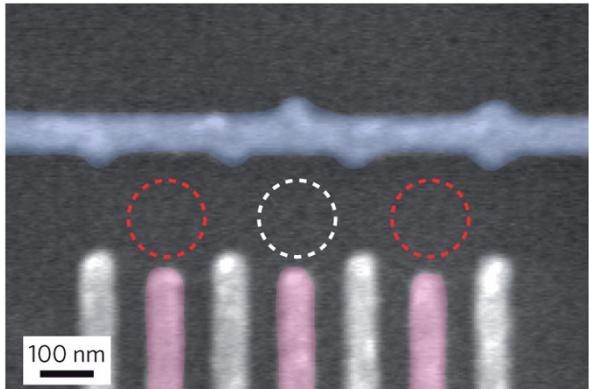
Appendix A

Numerical Implementation

Quantum Many-Body Problems

An example: 3 Quantum dots

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

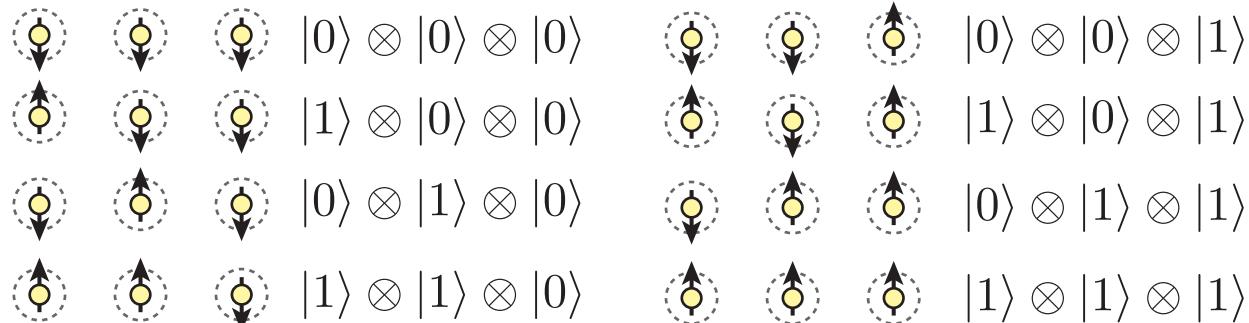


Quantum dot:

- 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)



States represented by superposition

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

Quantum Many-Body Problems

N Quantum dots

One-body problem:

$$\rightarrow \text{Number of states} = 2 \times N$$

N-body problem:

$$\rightarrow \text{Number of states} = 2^N$$

Further example: N=12



One-body problem \rightarrow Number of states = $2 \times N = 24$

N-body problem \rightarrow Number of states = $2^N = 4096$

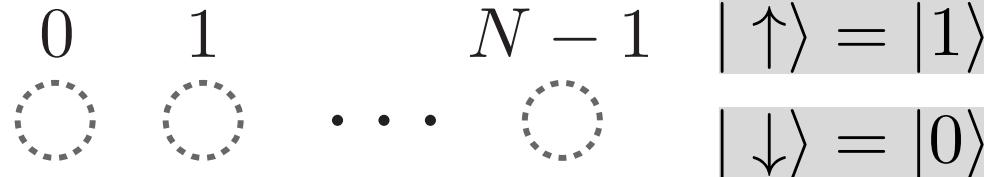
Extreme example: N=36

One-body $\rightarrow 2 \times N = 72$

N-body $\rightarrow 2^N \sim 6.9 \times 10^{10}$

Quantum Many-Body Problems

Mutual Interactions



1. Operators acting on a single qubit

A two dimensional representation of Lie algebra SU(2)

$$[\hat{S}_j^x, \hat{S}_j^y] = i\hat{S}_j^z$$

$$[\hat{S}_j^y, \hat{S}_j^z] = i\hat{S}_j^x$$

$$[\hat{S}_j^z, \hat{S}_j^x] = i\hat{S}_j^y$$

$$\hat{S}_j^+ = \hat{S}_j^x + i\hat{S}_j^y$$

$$\hat{S}_j^- = \hat{S}_j^x - i\hat{S}_j^y$$

$$\begin{aligned}\hat{S}_j^x |\uparrow\rangle &= (+1/2) |\downarrow\rangle \\ \hat{S}_j^x |\downarrow\rangle &= (+1/2) |\uparrow\rangle \\ \hat{S}_j^y |\uparrow\rangle &= (+i/2) |\downarrow\rangle \\ \hat{S}_j^y |\downarrow\rangle &= (-i/2) |\uparrow\rangle \\ \hat{S}_j^z |\uparrow\rangle &= (+1/2) |\uparrow\rangle \\ \hat{S}_j^z |\downarrow\rangle &= (-1/2) |\downarrow\rangle\end{aligned}$$

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

Quantum Many-Body Problems

Mutual Interactions



Fock space of N qubits:

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

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

Operators acting on N-quibit Fock space:

$$\hat{S}_j^a, \hat{S}_j^a \hat{S}_{j+1}^a : \mathcal{F} \rightarrow \mathcal{F}$$

$$\hat{S}_j^a \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}_j^a \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j}$$

$$\hat{S}_j^a \hat{S}_{j+1}^a \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}_j^a \otimes \hat{S}_{j+1}^a \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j-1}$$

Quantum Many-Body Problems

Quantum entanglement

Example: Two qubits



- Superposition
- Utilized for quantum teleportation
- cf.) EPR “paradox”

Mutual interactions between two qubits

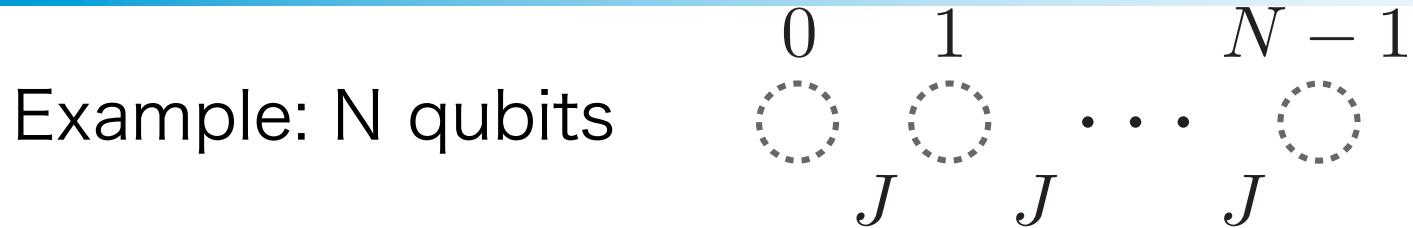
$$\hat{H} = J \sum_{a=x,y,z} \hat{S}_0^a \hat{S}_1^a \quad (J \in \mathbb{R}, J > 0)$$

→ Superposition



$$|1\rangle \otimes |0\rangle - |0\rangle \otimes |1\rangle$$

Hamiltonian Matrix



N-qubit Fock space:

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

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

Mutual interactions among N qubits:
Hamiltonian operator

$$\hat{H} : \mathcal{F} \rightarrow \mathcal{F}$$

$$\hat{H} = J \sum_{j=0}^{N-1} \sum_{a=x,y,z} \hat{S}_j^a \hat{S}_{\text{mod}(j+1, N)}^a$$

Vectors in Fock Space

Correspondence between spin and bit

2^N -dimensional Fock space:

$$\mathcal{F} = \left\{ \sum_{n_{N-1}=0,1} \cdots \sum_{n_1=0,1} \sum_{n_0=0,1} C_{n_{N-1} \dots n_1 n_0} |n_{N-1}\rangle \otimes \cdots \otimes |n_1\rangle \otimes |n_0\rangle \right\}$$
$$(C_{n_{N-1} \dots n_1 n_0} \in \mathbb{C})$$

$$|\uparrow\rangle = |1\rangle$$

$$|\downarrow\rangle = |0\rangle$$

Decimal representation of orthonormalized basis

$$|I\rangle_d = |n_{N-1}\rangle \otimes \cdots \otimes |n_1\rangle \otimes |n_0\rangle$$

$$I = \sum_{\nu=0}^{N-1} n_\nu \cdot 2^\nu$$

Wave function as a vector

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

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

Vectors and Matrices in Fock Space

Inner product of vectors

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

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

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

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

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

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

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

Example: Two Spins

Decimal representation of orthonormalized basis

	1 st site	0 th site	
$ 0\rangle_d$	$=$ $ \downarrow\rangle$	\otimes	$ \downarrow\rangle$
$ 1\rangle_d$	$=$ $ \downarrow\rangle$	\otimes	$ \uparrow\rangle$
$ 2\rangle_d$	$=$ $ \uparrow\rangle$	\otimes	$ \downarrow\rangle$
$ 3\rangle_d$	$=$ $ \uparrow\rangle$	\otimes	$ \uparrow\rangle$

Example: 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:

$$\hat{S}_j^+ |\downarrow\rangle = |\uparrow\rangle$$

Ladder operators

$$\hat{S}_j^+ = \hat{S}_j^x + i\hat{S}_j^y \quad \hat{S}_j^+ |\uparrow\rangle = 0$$

$$\hat{S}_j^- = \hat{S}_j^x - i\hat{S}_j^y \quad \hat{S}_j^- |\downarrow\rangle = 0$$

$$\hat{S}_j^- |\uparrow\rangle = |\downarrow\rangle$$

Hamiltonian Matrix

$$\hat{H} = J \left(\hat{S}_0^x \hat{S}_1^x + \hat{S}_0^y \hat{S}_1^y + \hat{S}_0^z \hat{S}_1^z \right)$$

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

4 by 4 Hamiltonian matrix

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

A-1. Itinerant $S=1/2$ Fermion

Creation and Annihilation Operators

$\hat{c}_{i\sigma}$: Annihilate spin σ at i th site/atom

$\hat{c}_{i\sigma}^\dagger$: Create spin σ at i th site/atom

Anticommutation rule
(Fermi statistics)

$$\hat{c}_{i\sigma}\hat{c}_{j\tau}^\dagger + \hat{c}_{j\tau}^\dagger\hat{c}_{i\sigma} = \delta_{i,j}\delta_{\sigma,\tau}$$

$$\hat{c}_{i\sigma}\hat{c}_{j\tau} + \hat{c}_{j\tau}\hat{c}_{i\sigma} = \hat{c}_{i\sigma}^\dagger\hat{c}_{j\tau}^\dagger + \hat{c}_{j\tau}^\dagger\hat{c}_{i\sigma}^\dagger = 0$$

Vaccum

Vaccum: Kernel of annihilation operators $\hat{c}_{i\sigma}$

$$|0\rangle = \prod_{i,\sigma} |0\rangle_{i\sigma} \quad |0\rangle_{i\sigma} \in \text{Ker}(\hat{c}_{i\sigma})$$

Pauli principle: $\left(\hat{c}_{i\sigma}^\dagger\right)^2 |0\rangle_{i\sigma} = -\left(\hat{c}_{i\sigma}^\dagger\right)^2 |0\rangle_{i\sigma} = 0$

Fock Space

Fock Space

Basis

$$\hat{c}_{i\sigma}^\dagger |0\rangle, \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger |0\rangle, \prod_i \hat{c}_{i\uparrow}^\dagger \prod_j \hat{c}_{j\downarrow}^\dagger |0\rangle, \dots$$

Hermitian conjugate

$$(\hat{c}_{i\sigma}^\dagger |0\rangle)^\dagger = \langle 0| \hat{c}_{i\sigma}, (\hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger |0\rangle)^\dagger = \langle 0| \hat{c}_{j\downarrow} \hat{c}_{i\uparrow}$$

Actions of Operators and Inner Product in Fock Space

Example of multiplication of operators to bases

$$(\hat{c}_{3\sigma}^\dagger \hat{c}_{3\sigma}) \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}^\dagger |0\rangle = 0$$

$$(\hat{c}_{1\sigma}^\dagger \hat{c}_{1\sigma}) \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}^\dagger |0\rangle = \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}^\dagger |0\rangle$$

$$(\hat{c}_{5\sigma}^\dagger \hat{c}_{1\sigma}) \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}^\dagger |0\rangle = -\hat{c}_{5\sigma}^\dagger \hat{c}_{2\sigma}^\dagger |0\rangle$$

Example of inner product

$$(\langle 0 | \hat{c}_{1\sigma} \hat{c}_{2\sigma}) \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}^\dagger |0\rangle = 1$$

Comparison between Fock space and linear algebra

Scalar obtained through vector-matrix-vector product

$$\langle 0 | \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} \hat{H} \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger |0\rangle \longleftrightarrow \vec{u}^T A \vec{u}$$

Implementation of Fock Space

Bit representation of electrons: Order of sites matter

Example: Two-site Hubbard model

$$\hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle = |1\rangle_{0\uparrow} \otimes |1\rangle_{0\downarrow} \otimes |0\rangle_{1\uparrow} \otimes |0\rangle_{1\downarrow}$$

$$\hat{c}_{0\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle = |1\rangle_{0\uparrow} \otimes |0\rangle_{0\downarrow} \otimes |0\rangle_{1\uparrow} \otimes |1\rangle_{1\downarrow}$$

$$\hat{c}_{0\downarrow}^\dagger \hat{c}_{1\uparrow}^\dagger |0\rangle = |0\rangle_{0\uparrow} \otimes |1\rangle_{0\downarrow} \otimes |1\rangle_{1\uparrow} \otimes |0\rangle_{1\downarrow}$$

$$\hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle = |0\rangle_{0\uparrow} \otimes |0\rangle_{0\downarrow} \otimes |1\rangle_{1\uparrow} \otimes |1\rangle_{1\downarrow}$$

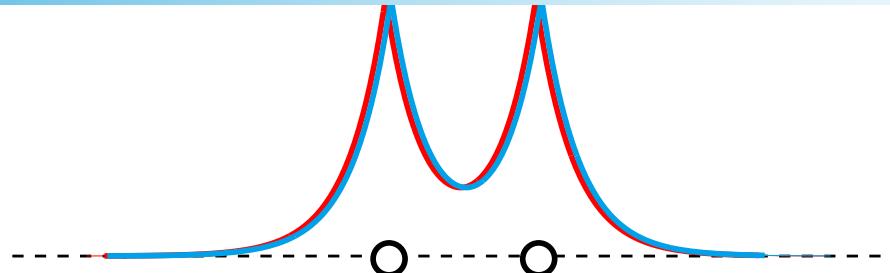
Bit rep. is not enough: Fermionic sign is necessary

Example: Tunneling

$$\begin{aligned} (\hat{c}_{1\downarrow}^\dagger \hat{c}_{0\downarrow}) \hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle &= -\hat{c}_{1\downarrow}^\dagger \hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow} \hat{c}_{0\downarrow}^\dagger |0\rangle \\ &= -\hat{c}_{1\downarrow}^\dagger \hat{c}_{0\uparrow}^\dagger |0\rangle \\ &= \hat{c}_{0\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle \end{aligned}$$

A-2.
2-Site Hubbard Model

2-Site Hubbard Model



Hubbard model

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}_{0\sigma}^\dagger \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^\dagger \hat{c}_{0\sigma}) + U \sum_{j=0,1} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}$$

Example 3:

Create 4 by 4 Hamiltonian matrix with following 4 bases

$$\hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle$$

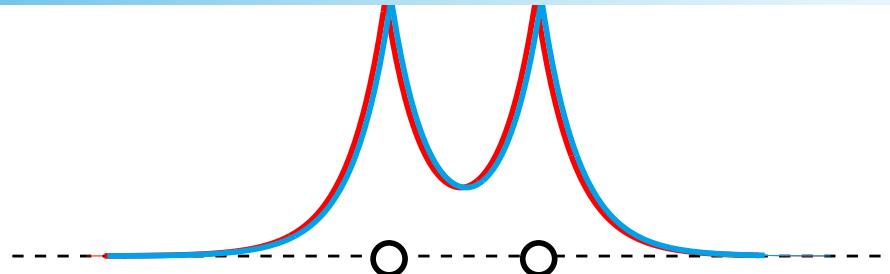
$$\hat{c}_{1\downarrow}^\dagger \hat{c}_{0\uparrow}^\dagger |0\rangle$$

$$\hat{c}_{1\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle$$

$$\hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle$$

Be careful about
the order of the operators!

2-Site Hubbard Model



Hubbard model

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}_{0\sigma}^\dagger \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^\dagger \hat{c}_{0\sigma}) + U \sum_{j=0,1} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}$$

Answer of Example 3:

4 by 4 Hamiltonian matrix with the following 4 bases

$$\begin{array}{l} \hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle \\ \hat{c}_{1\downarrow}^\dagger \hat{c}_{0\uparrow}^\dagger |0\rangle \\ \hat{c}_{1\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle \\ \hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle \end{array} \quad \hat{H} \doteq \begin{bmatrix} +U & +t & -t & 0 \\ +t & 0 & 0 & +t \\ -t & 0 & 0 & -t \\ 0 & +t & -t & +U \end{bmatrix}$$

A-3.

Let's Solve 2-Site Hubbard
Model by $H\Phi$

$\text{H}\Phi$

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 [3]: 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. Comput. 23, 517 (2001).

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

[Open source program package \(latest release: ver.3.5.1\)](#)

License: GNU GPL version3

Project for advancement of software usability in materials science by ISSP

$\text{H}\Phi$ <https://www.pasums.issp.u-tokyo.ac.jp/hphi/en/>

MatriApps LIVE! <http://cmsi.github.io/MateriAppsLive/>

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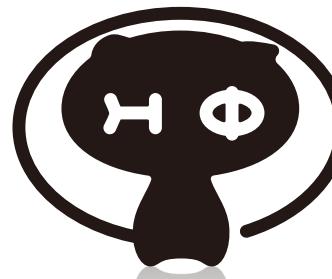
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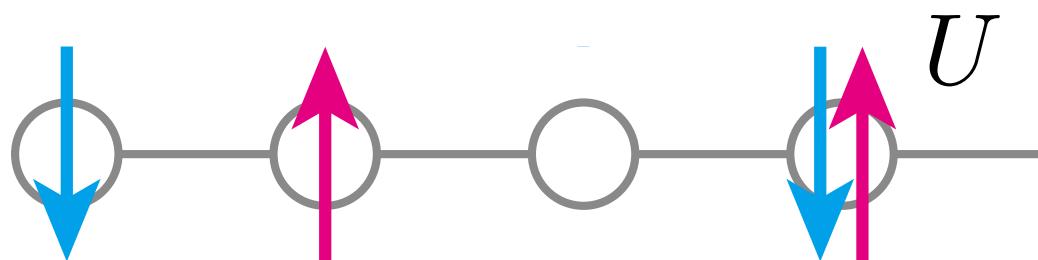
“Project for advancement of software usability in materials science” by ISSP

Target Hamiltonian

- Standard Hamiltonian 1

Itinerant electrons: Hubbard-type model

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



Fermion Hubbard: Particle # & total S_z conserved

HubbardNConserved: Particle # conserved & total S_z not

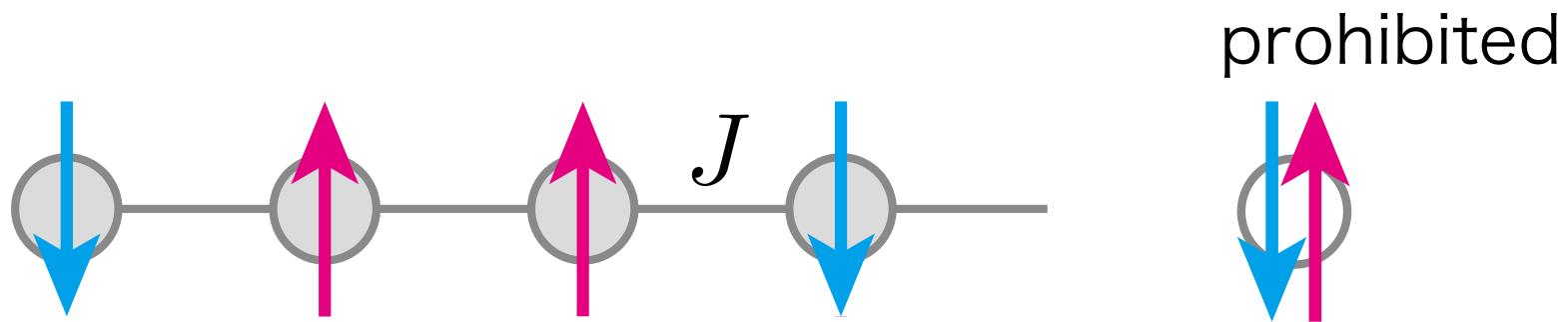
Fermion HubbardGC: Particle # & total S_z not conserved

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

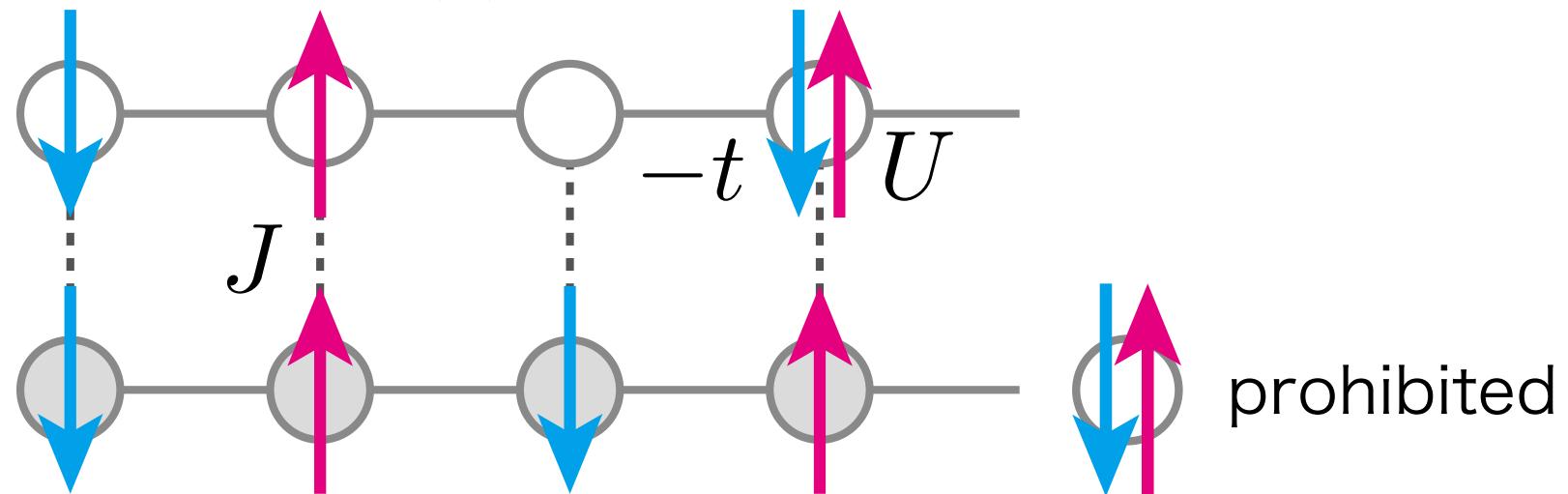
$S > 1/2$ can be simulated
if your memory is enough large

Target Hamiltonian

- Standard Hamiltonian 3

Mixture: Kondo-lattice-type model

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



Kondo Lattice: Particle # & total S_z conserved

Kondo LatticeGC: Particle # & total S_z not conserved

Standard input: Simplified input for typical lattice models

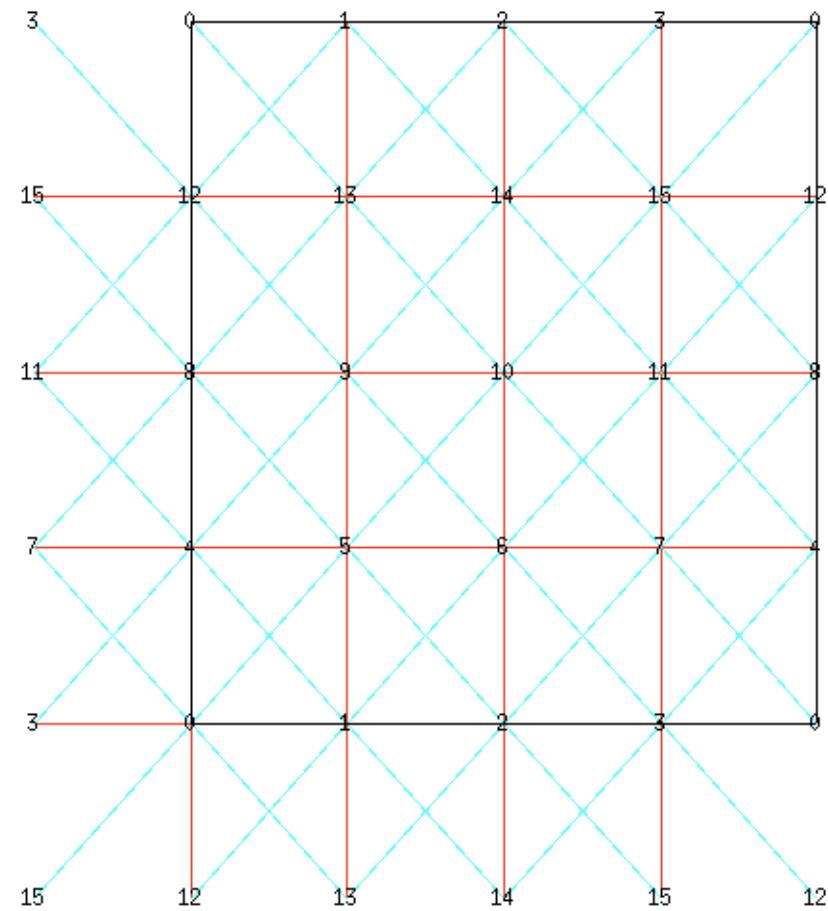
Hubbard	$H = -\mu \sum_{i=1}^N \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^\dagger c_{i\sigma} - \sum_{i \neq j} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j} V_{ij} n_i n_j$
Quantum spins	$H = -h \sum_{i=1}^N S_i^z + \Gamma \sum_i S_i^x + D \sum_i S_i^z S_i^z + \sum_{i,j} \sum_{\alpha,\beta=x,y,z} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta$
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

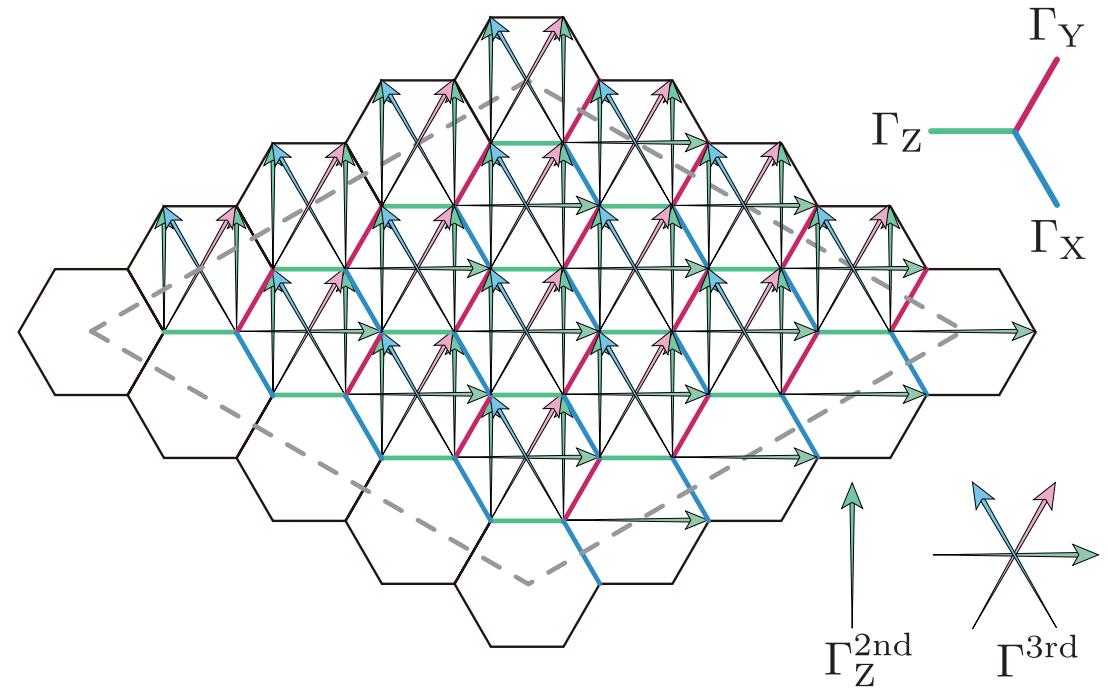
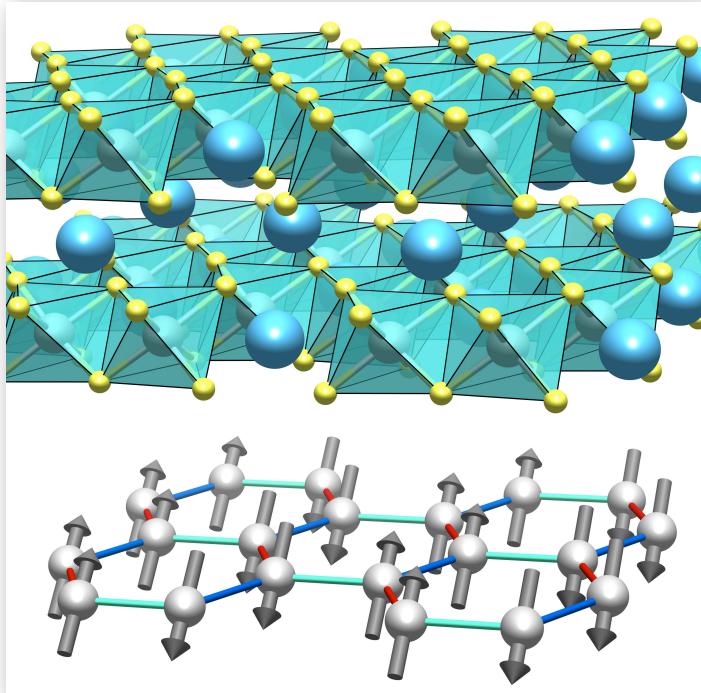
$$\langle H \rangle, \langle H^2 \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$$

-Dynamical Green's function is also available

An Example of Expert Input: *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

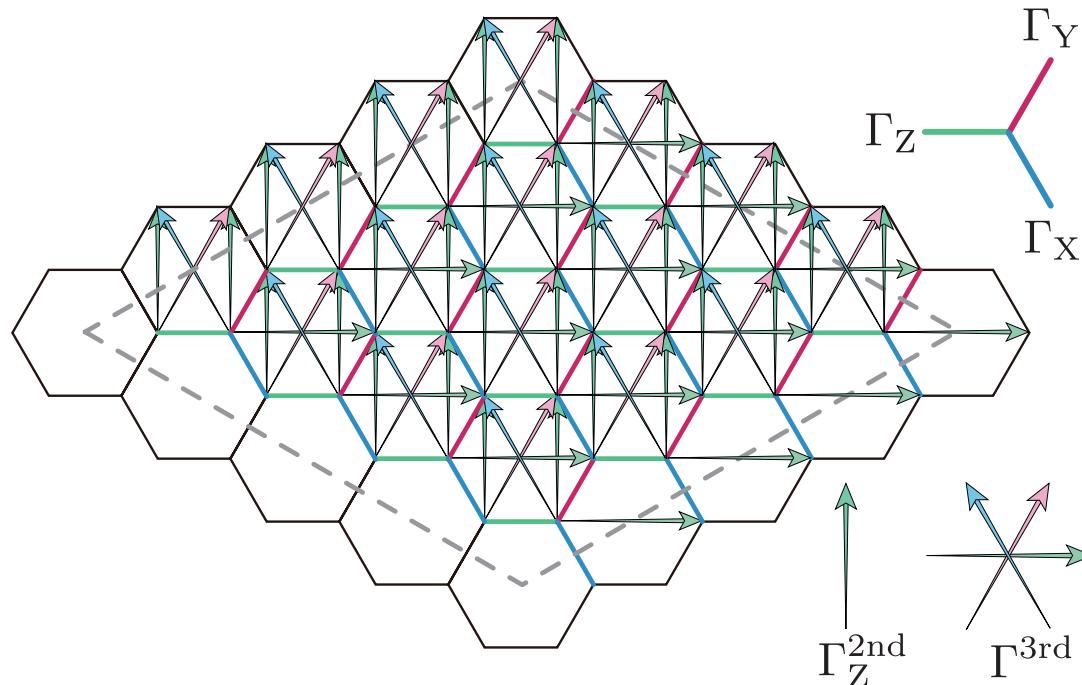


An Example of Expert Input: *Ab Initio* Spin Hamiltonian

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

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

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



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

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

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

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

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

cf.) RESPACK

Overview of Software ΗΦ

- Language: C
- Compiler: C & Fortran compiler
- Library: BLAS, LAPACK, Kw (distributed with ΗΦ)
(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

2-Site Hubbard Model

An example of the input file for 2-site Hubbard model

StdFace.def (arbitrary file name is acceptable)

```
L = 2
model = "FermionHubbard"
//method = "Lanczos"
//method = "TPQ"
method = "FullDiag"
lattice = "chain"
t = 0.5
U = 8.0
nelec = 2
2Sz = 0
```

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}_{0\sigma}^\dagger \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^\dagger \hat{c}_{0\sigma}) + U \sum_{j=0,1} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}$$

Large U/t Limit

Energy spectrum 2-site Hubbard model (total $S_z = 0$)

$$E = 0, +U, \frac{U \pm \sqrt{U^2 + 16t^2}}{2}$$

$$\frac{U \pm \sqrt{U^2 + 16t^2}}{2} = \begin{cases} U + \frac{4t^2}{U} + \mathcal{O}\left(\frac{t^3}{U^2}\right) \\ -\frac{4t^2}{U} + \mathcal{O}\left(\frac{t^3}{U^2}\right) \end{cases}$$

Low energy state \rightarrow 2 spins

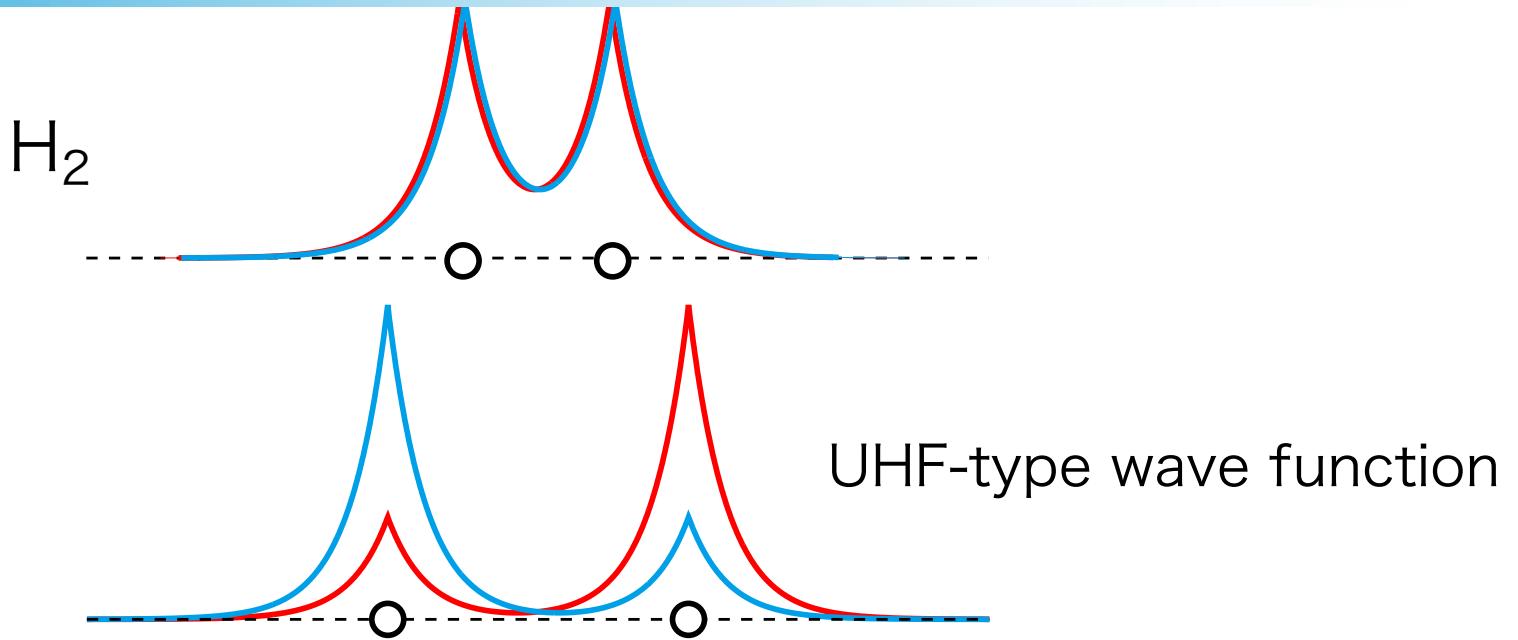
$$E = 0$$

$$\frac{1}{\sqrt{2}} \hat{c}_{0\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle + \frac{1}{\sqrt{2}} \hat{c}_{0\downarrow}^\dagger \hat{c}_{1\uparrow}^\dagger |0\rangle$$

$$E = -\frac{4t^2}{U} + \mathcal{O}\left(\frac{t^3}{U^2}\right)$$

$$\propto \hat{c}_{0\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle - \hat{c}_{0\downarrow}^\dagger \hat{c}_{1\uparrow}^\dagger |0\rangle + \frac{2t}{U} \left(\hat{c}_{0\uparrow}^\dagger \hat{c}_{0\downarrow}^\dagger |0\rangle + \hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow}^\dagger |0\rangle \right) + \mathcal{O}\left(\frac{t^2}{U^2}\right)$$

Hydrogen Molecule



Hubbard model

cf.) Chiappe *et al.*, Phys. Rev. B 75, 195104 (2007)

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}_{0\sigma}^\dagger \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^\dagger \hat{c}_{0\sigma}) + U \sum_{j=0,1} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}$$

Heisenberg model or J -coupling $\hat{H} = J \left(\hat{S}_0^x \hat{S}_1^x + \hat{S}_0^y \hat{S}_1^y + \hat{S}_0^z \hat{S}_1^z \right)$



$$J = 4t^2/U$$



Singlet ground state

Appendix B

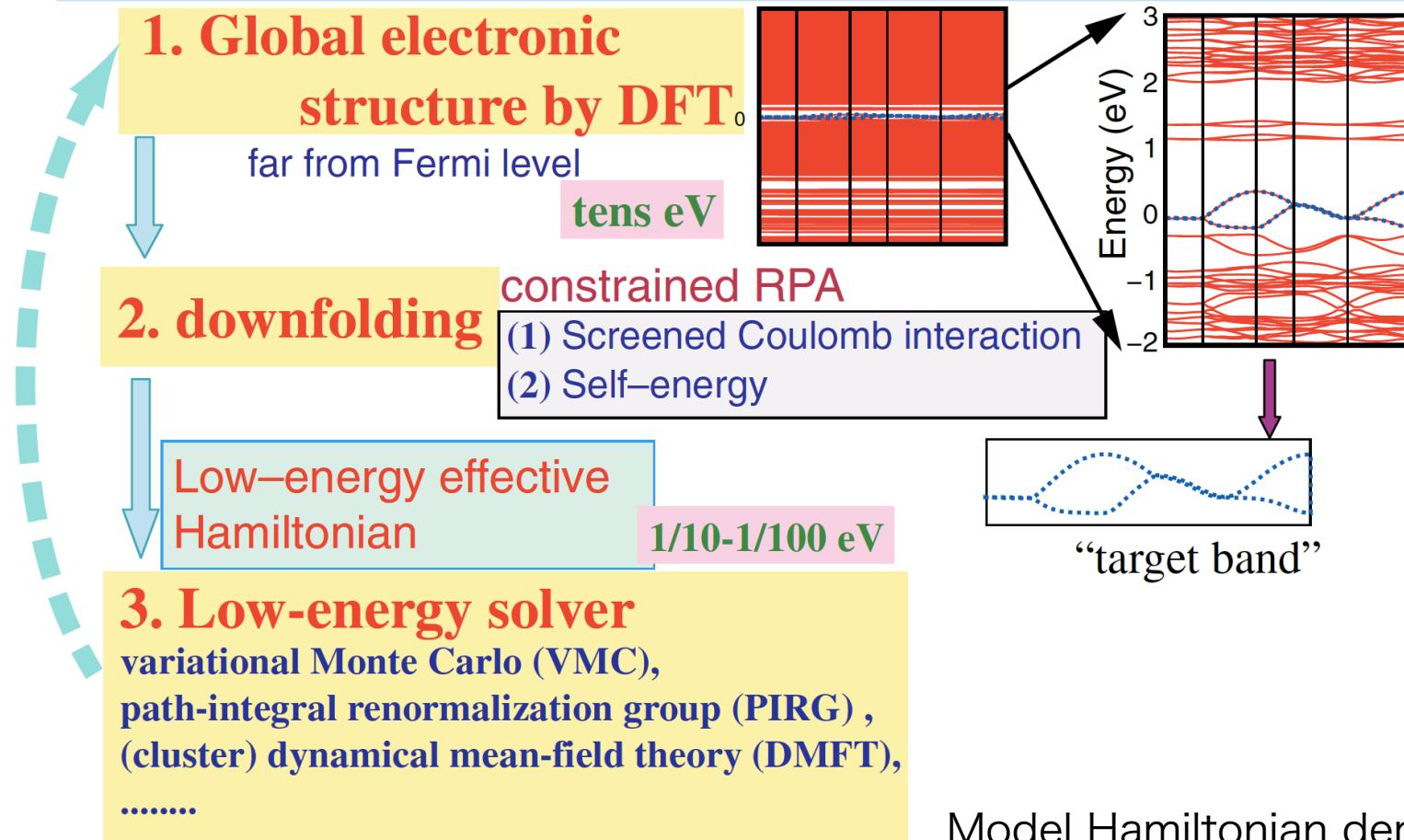
Lattice Model of Solids

Target of Model Calculations

- Ising model
 - Rare earth magnets
- Heisenberg model
 - Transition-metal oxides
- Hubbard model (Gutzwiller, Kanamori)
 - Itinerant magnets, Mott insulators
- $t-J$ model
 - Cuprate superconductors
- Kondo model and Anderson model
 - Magnetic impurities in alloys
 - Rare earth alloys

Model Construction

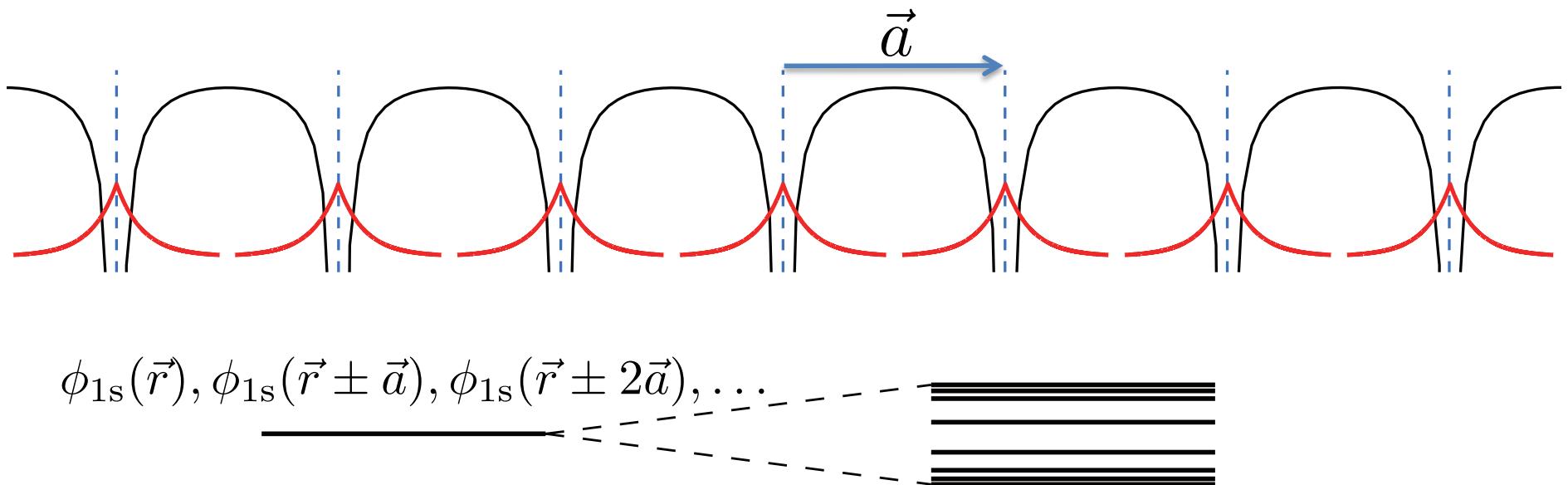
Schematic procedure of three-stage scheme
thanks to energy hierarchy structure



Model Hamiltonian derived by
DFT+DMFT, Wannier+cRPA
G. Kotliar, et al., RMP 78, 865 (2006)
M. Imada & T. Miyake, JPSJ 79, 112001 (2010)

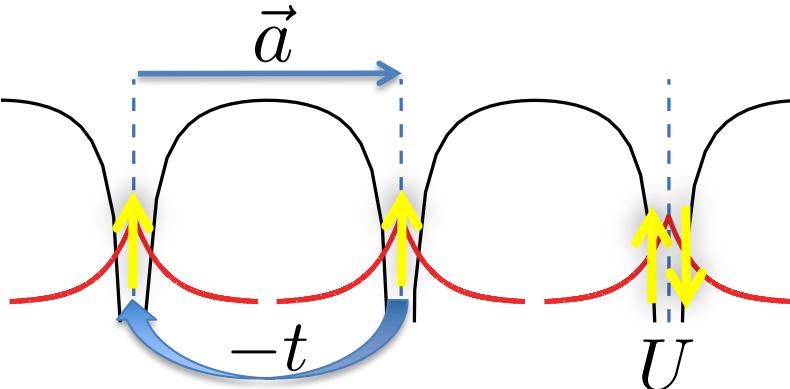
Model of Many-Body Electrons

One of the simplest many-body electrons in Crystalline solids: Hydrogen solid



Gedankenexperiment of F. N. Mott

One of the Simplest Model: 1D Hubbard Model



$$\phi_{1s}(\vec{r}), \phi_{1s}(\vec{r} \pm \vec{a}), \phi_{1s}(\vec{r} \pm 2\vec{a}), \dots$$

-Tunnelling among neighboring 1s orbitals

$$-t = \int d^3r \phi_{1s}^*(\vec{r}) \frac{-\hbar^2}{2m} \nabla^2 \phi_{1s}(\vec{r} - \vec{a})$$

-Intra-atomic Coulomb in 1s orbitals

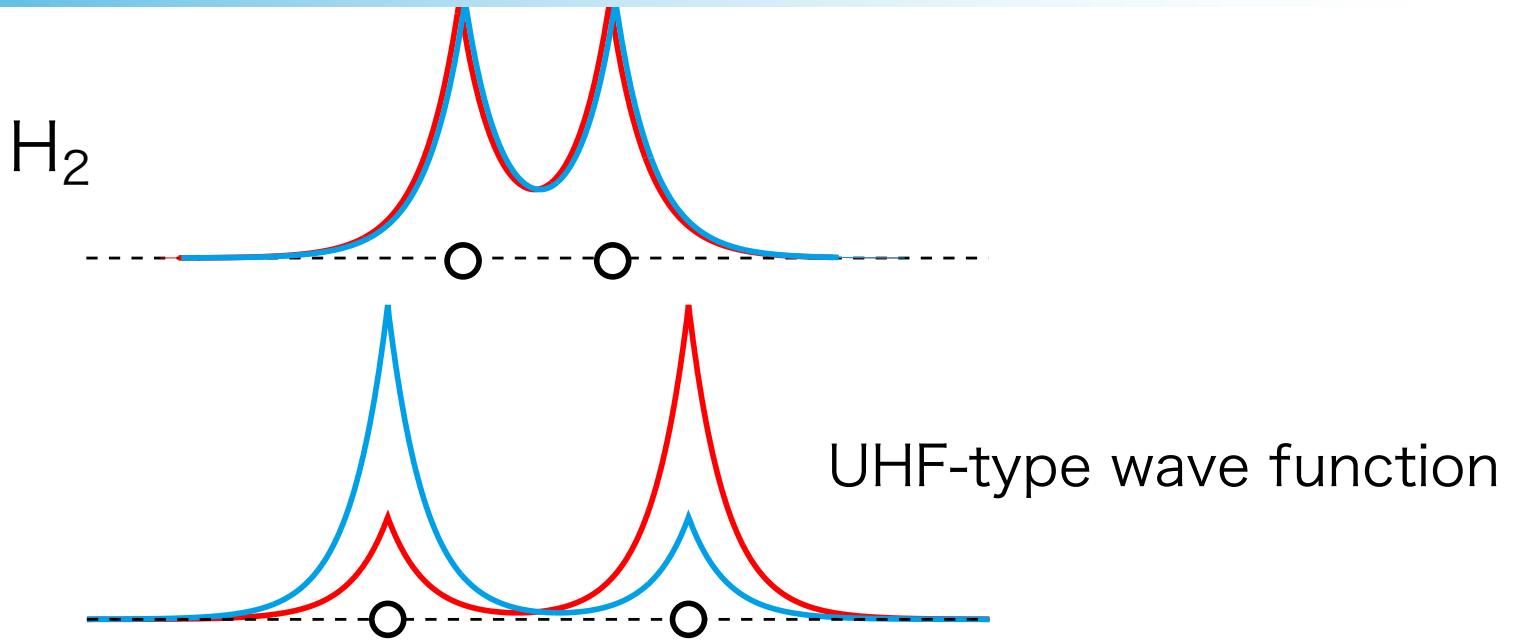
$$U = \int d^3r \int d^3r' \phi_{1s}^*(\vec{r}) \phi_{1s}^*(\vec{r}') \frac{e^2}{|\vec{r} - \vec{r}'|} \phi_{1s}(\vec{r}') \phi_{1s}(\vec{r})$$

1D Hubbard model (periodic boundary condition, L site)

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

cf.) Bethe ansatz, Tomonaga-Luttinger liquid

Hydrogen Molecule



Hubbard model

cf.) Chiappe *et al.*, Phys. Rev. B 75, 195104 (2007)

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}_{0\sigma}^\dagger \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^\dagger \hat{c}_{0\sigma}) + U \sum_{j=0,1} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}$$

Heisenberg model or J -coupling $\hat{H} = J \left(\hat{S}_0^x \hat{S}_1^x + \hat{S}_0^y \hat{S}_1^y + \hat{S}_0^z \hat{S}_1^z \right)$



$$J = 4t^2/U$$

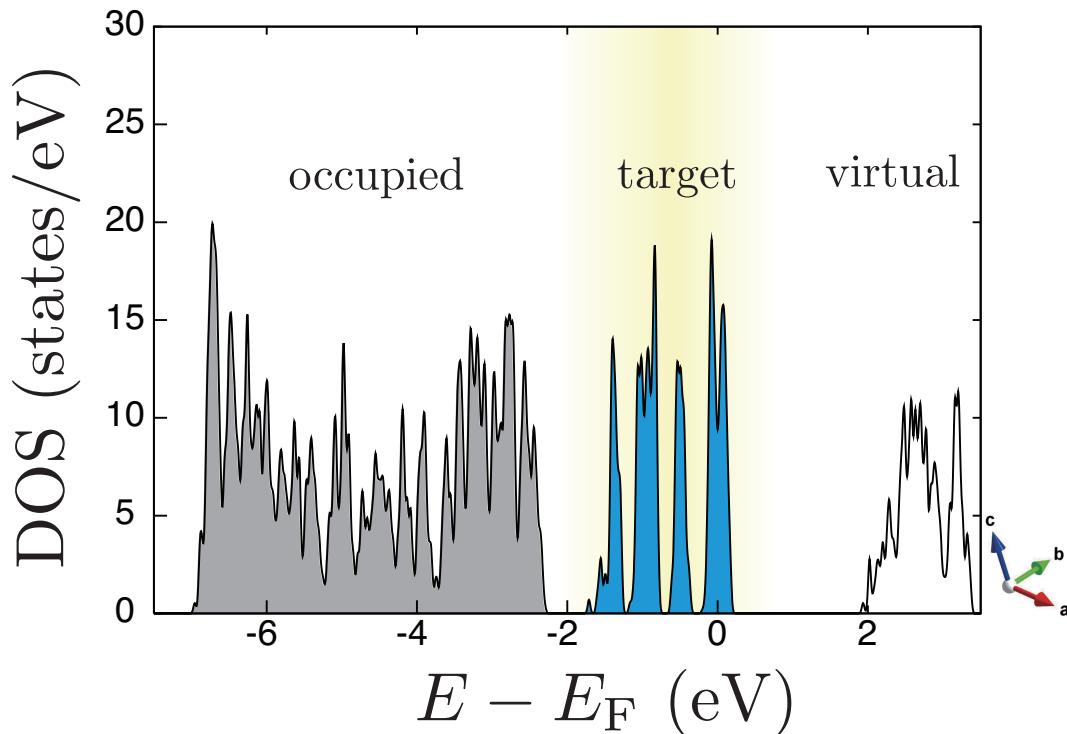


Singlet ground state

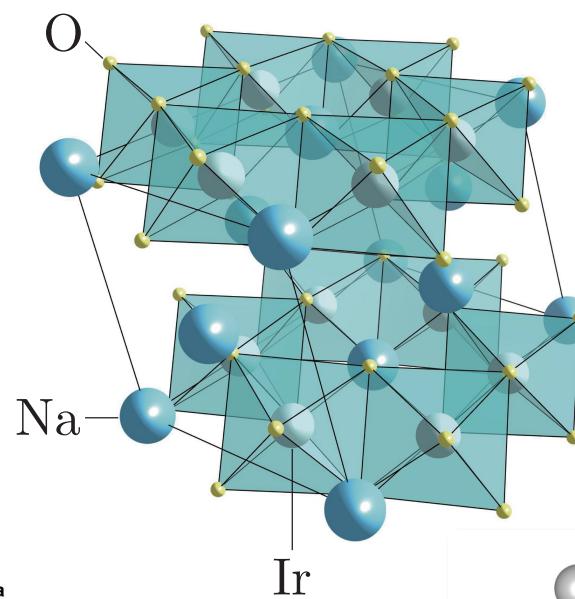
Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

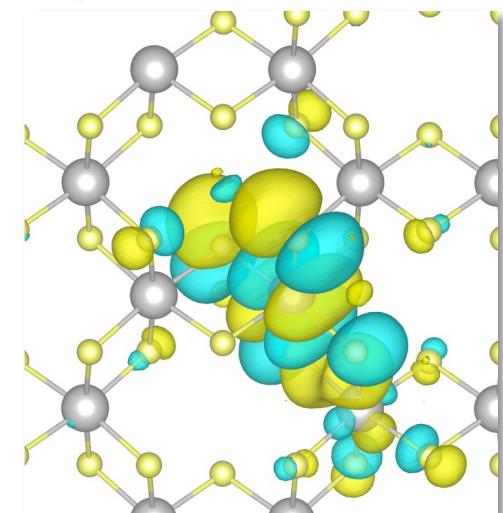
DFT result for energy spectrum



Souza-Marzari-Vanderbilt



Na_2IrO_3



- Effective Coulomb interactions in target space
Renormalization due to
infinite virtual particle-hole excitations

← Constrained random phase approximation

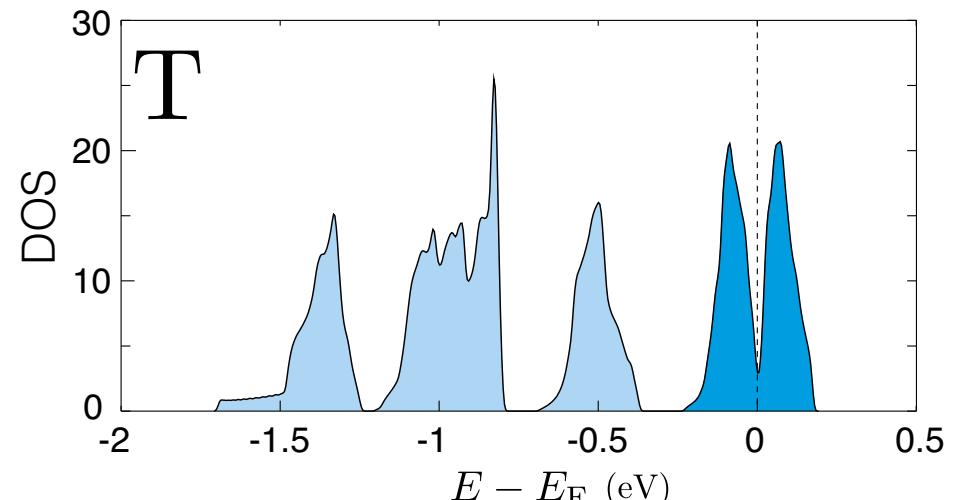
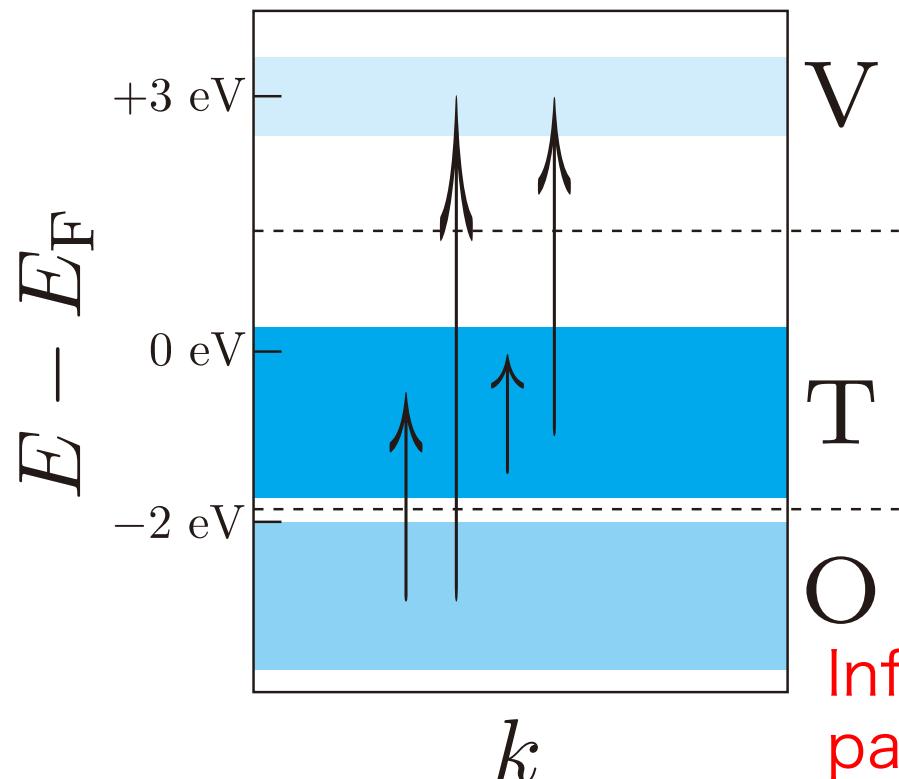
Imada & Miyake, J. Phys. Soc. Jpn. 79, 112001 (2010)

Constrained RPA Estimate on Coulomb Interaction of t_{2g} -Hubbard

$$W^{\text{cRPA}} = \frac{V}{1 + V\chi^{\text{cRPA}}} \leftarrow \text{Dielectric constant}$$

$$\chi^{\text{RPA}} = \chi_{O \rightarrow T} + \chi_{O \rightarrow V} + \chi_{T \rightarrow T} + \chi_{T \rightarrow V}$$

$$\chi^{\text{cRPA}} = \chi_{O \rightarrow T} + \chi_{O \rightarrow V} + \cancel{\chi_{T \rightarrow T}} + \chi_{T \rightarrow V}$$



Infinite number of RPA-type
particle-hole excitations

2nd Report Problems

Please solve 1-1., 2-1-1., & 2-1-2..

You may solve 2-2. and 3-1.
optionally to get additional score

Report 2

Problem 1: Monte Carlo for quantum systems

1-1 (compulsory).

- Evaluate statistical errors in a 2-point distribution function $g(r)$ of liquid helium 4 at each distance r .
- Obtain the relationship between the statistical errors and numbers of Monte Carlo samples (and confirm the error is proportional to $1/N_{MC}^{1/2}$, where N_{MC} is the number of Monte Carlo samples).

You may use McMillan's variational Jastrow wave function and variational parameters given in [sample_vmc_helium4.ipynb](#).

- Be careful about definition of the statistical errors
standard deviation of the MC averages
given by independent Markov chains (10 Markov chains may be enough)
Not statistical errors within a single Markov chain!

Report 2

Problem 2: Krylov subspace method

2-1-1 (compulsory).

- Implement Lanczos method for the 1D Hubbard model and obtain the ground-state energy (the lowest eigenvalue) E_0 for 6 electrons and 6 sites at $U/t = 8$.
- In Lanczos method, you may use Lapack to diagonalize small tridiagonal matrices.
- Illustrate convergence of E_0 obtained at each Lanczos step.
- Obtain E_0 by Lapack and compare with the solution by Lanczos.

2-1-2 (compulsory).

- Obtain U/t dependence of E_0 by Lanczos for $0 < U/t < 16$.

2-2 (Optional).

- Implement LOBCG method for the 1D Hubbard model.
- Confirm that the code can calculate E_0 and the corresponding eigenvector for 6 electrons and 6 sites at $U/t = 8$.
- Obtain the 2nd and 3rd lowest eigenvalues.
- Compare them with the solution by Lapack.

Report 2

Problem 3: Open source software

3-1 (optional).

- Solve the following problems. You may use HΦ.
Estimate the energy difference between the lowest and 2nd lowest eigenstates of the 1dimensional $S=1/2$ and $S=1$ Hesenberg models with periodic boundary conditions.
- Use several L (number of spins) and extrapolate the gap to thermodynamic limit ($L \rightarrow \infty$). Please compare the extrapolated values with other results in the literature.
You may use $a+b/L+c/L^2$ or $a+b \exp(-cL)$.
- Illustrate the extrapolations.

- The code you wrote should be included
(a jupyter notebook is recommended).
- Deadline: 7/31

Report 2

Deadline for Report 2:
-2023/7/31

Please submit your report through ITC-LMS
(web page for the reports will be opened).

If you have any trouble, please contact us via email:
YAMAJI.Youhei@nims.go.jp

Lecture Schedule

- #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

7/11 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.