多体問題の計算科学

#13

2017/7/11

Computational Science for Many-Body Problems

Numerical Methods for Quantum Many-Body Problems

1. Steepest descent vs conjugate gradient
2. Shifted Krylov subspace method
3. Numerical implementation
4. Itinerant fermions and HΦ
5. Parallelization
6. Other numerical methods
7. Report problems

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

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

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

Formal solution

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

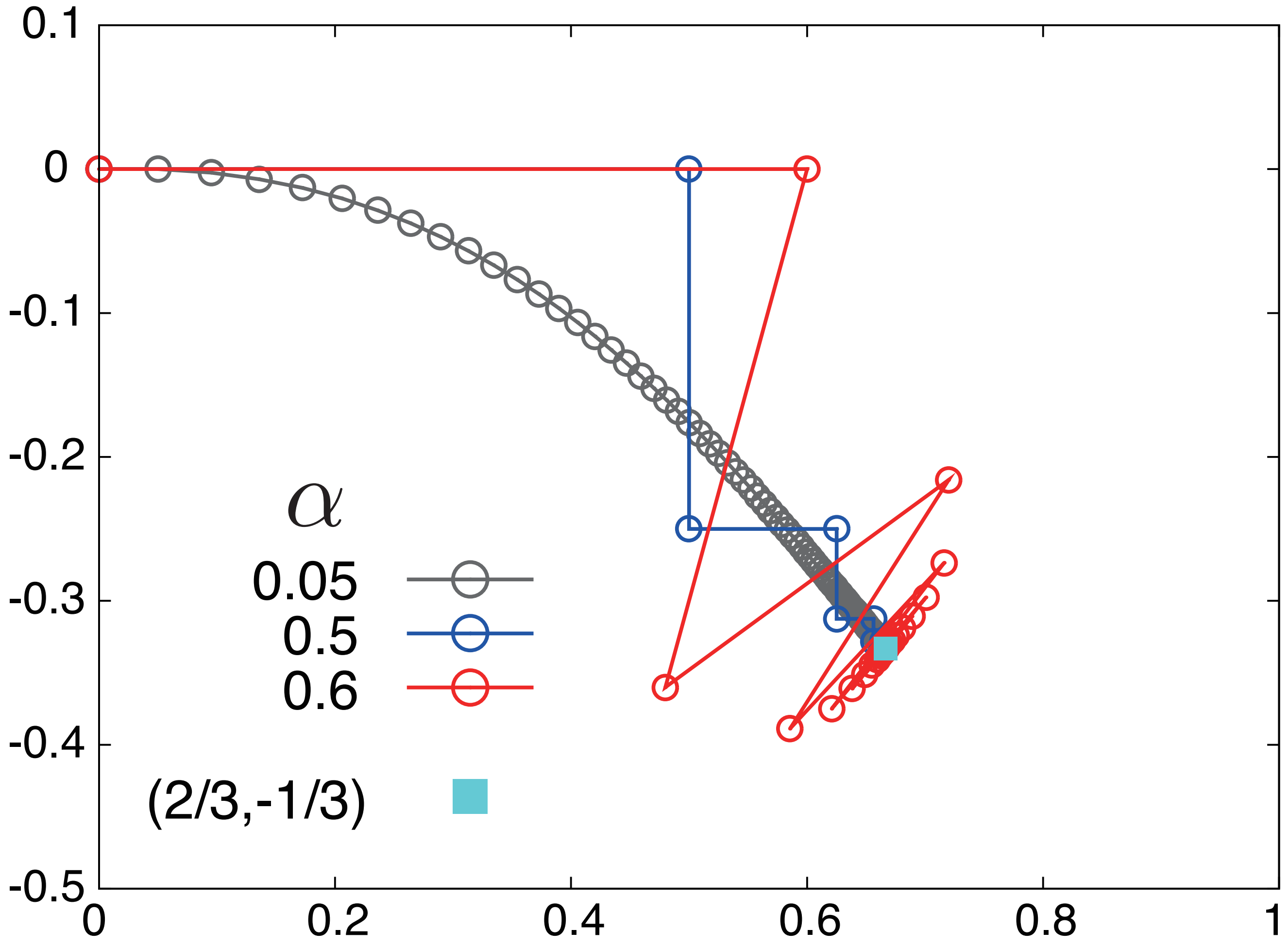
SD finds the exact solution only when $(1-\alpha A)^{k+1}\vec{b} = \vec{0}$

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 $k = 0, 1, \ldots, m$

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

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

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

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

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

1st Step of CG

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

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

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

$$\begin{aligned}
\alpha_k &= \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k} \\
\vec{x}_{k+1} &= \vec{x}_k + \alpha_k \vec{p}_k \\
\vec{r}_{k+1} &= \vec{r}_k - \alpha_k A \vec{p}_k \\
\beta_k &= \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k} \\
\vec{p}_{k+1} &= \vec{r}_{k+1} + \beta_k \vec{p}_k
\end{aligned}$$

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

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

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

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

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

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

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

2nd Step of CG

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

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

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

$$\begin{aligned}
\alpha_k &= \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k} \\
\vec{x}_{k+1} &= \vec{x}_k + \alpha_k \vec{p}_k \\
\vec{r}_{k+1} &= \vec{r}_k - \alpha_k A \vec{p}_k \\
\beta_k &= \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k} \\
\vec{p}_{k+1} &= \vec{r}_{k+1} + \beta_k \vec{p}_k
\end{aligned}$$

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

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

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

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

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

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

CG finds the exact solution at the 2nd step!

Shifted
Krylov Subspace Method

Shifted CG

Find a set of the solutions

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

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 $k = 0, 1, \ldots, m$

-Seed equations

$$\begin{aligned}
\rho_k &= \vec{r}_k^T \vec{r}_k \\
\beta_{k-1} &= \frac{\rho_k}{\rho_{k-1}} \\
\alpha_k &= \frac{\rho_k}{\vec{r}_k^T A \vec{r}_k - \beta_{k-1} \frac{\rho_k}{\alpha_{k-1}}} \\
\vec{r}_{k+1} &= \left(1 + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}\right) \vec{r}_k - \alpha_k A \vec{r}_k - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} \vec{r}_{k-1}
\end{aligned}$$

-Shifted equations

$$\begin{aligned}
\pi_{k+1}^\sigma &= (1 + \alpha_k \sigma)\pi_k^\sigma - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} (\pi_{k-1}^\sigma - \pi_k^\sigma) \\
\vec{p}_k^\sigma &= \frac{1}{\pi_k^\sigma} \vec{r}_k + \beta_{k-1} \left(\frac{\pi_{k-1}^\sigma}{\pi_k^\sigma}\right)^2 \vec{p}_{k-1}^\sigma \\
\vec{x}_k^\sigma &= \vec{x}_{k-1}^\sigma + \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \alpha_k \vec{p}_k^\sigma
\end{aligned}$$

Shifted CG: The Simplest Example

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

Seed equations

Shifted equations

0th step

$$\begin{aligned} \rho_0 &= 1 \\ \beta_{-1} &= 0 \\ \alpha_0 &= 1/2 \\ \vec{r}_1 &= \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} \end{aligned} \qquad \begin{aligned} \pi_1^{\sigma} &= (1+\sigma/2) \\ \vec{p}_0^{\sigma} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \vec{x}_0^{\sigma} &= \frac{1}{2+\sigma}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{aligned}$$

1st step

$$\begin{aligned} \rho_1 &= 1/4 \\ \beta_0 &= 1/4 \\ \alpha_1 &= 2/3 \\ \vec{r}_2 &= \vec{0} \end{aligned} \qquad \begin{aligned} \pi_2^{\sigma} &= 1+4\sigma/3+\sigma^2/3 \\ \vec{p}_1^{\sigma} &= \begin{pmatrix} 1/\{2+\sigma\}^2 \\ -1/\{2+\sigma\} \end{pmatrix} \\ \vec{x}_1^{\sigma} &= \begin{pmatrix} \{2+\sigma\}/\{3+4\sigma+\sigma^2\} \\ -1/\{3+4\sigma+\sigma^2\} \end{pmatrix} \end{aligned}$$

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

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

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

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

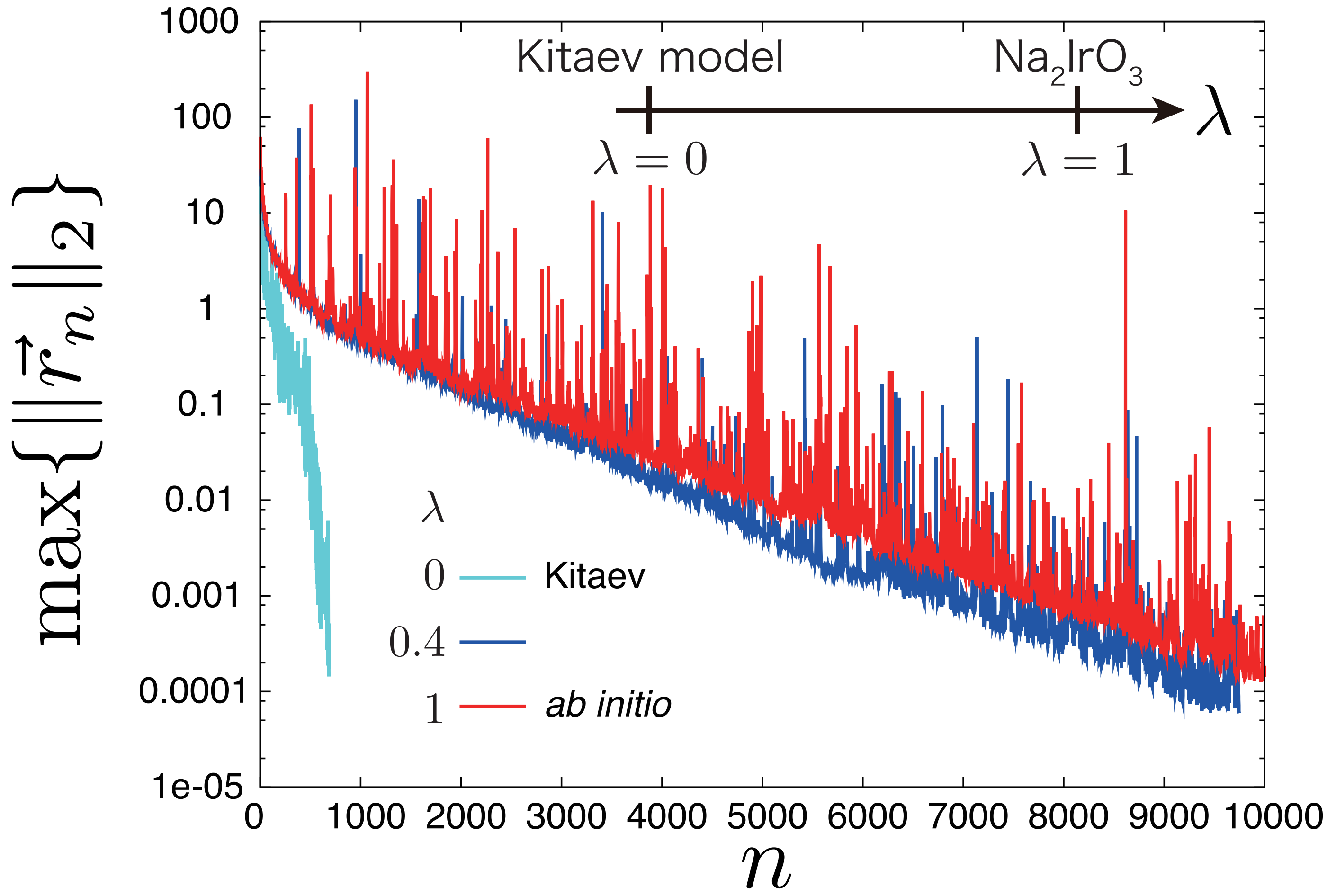
$$\vec{x}^{\sigma}_1 = \begin{pmatrix} \dfrac{2+\sigma}{3+4\sigma+\sigma^2} \\ -\dfrac{1}{3+4\sigma+\sigma^2} \end{pmatrix}$$

Shifted CG finds
the set of solution!

Convergence of Krylov Subspace Method

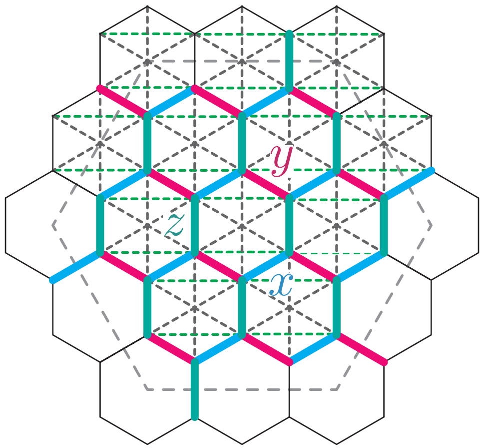
Krylov subspace method
finds a solution within N_H steps

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

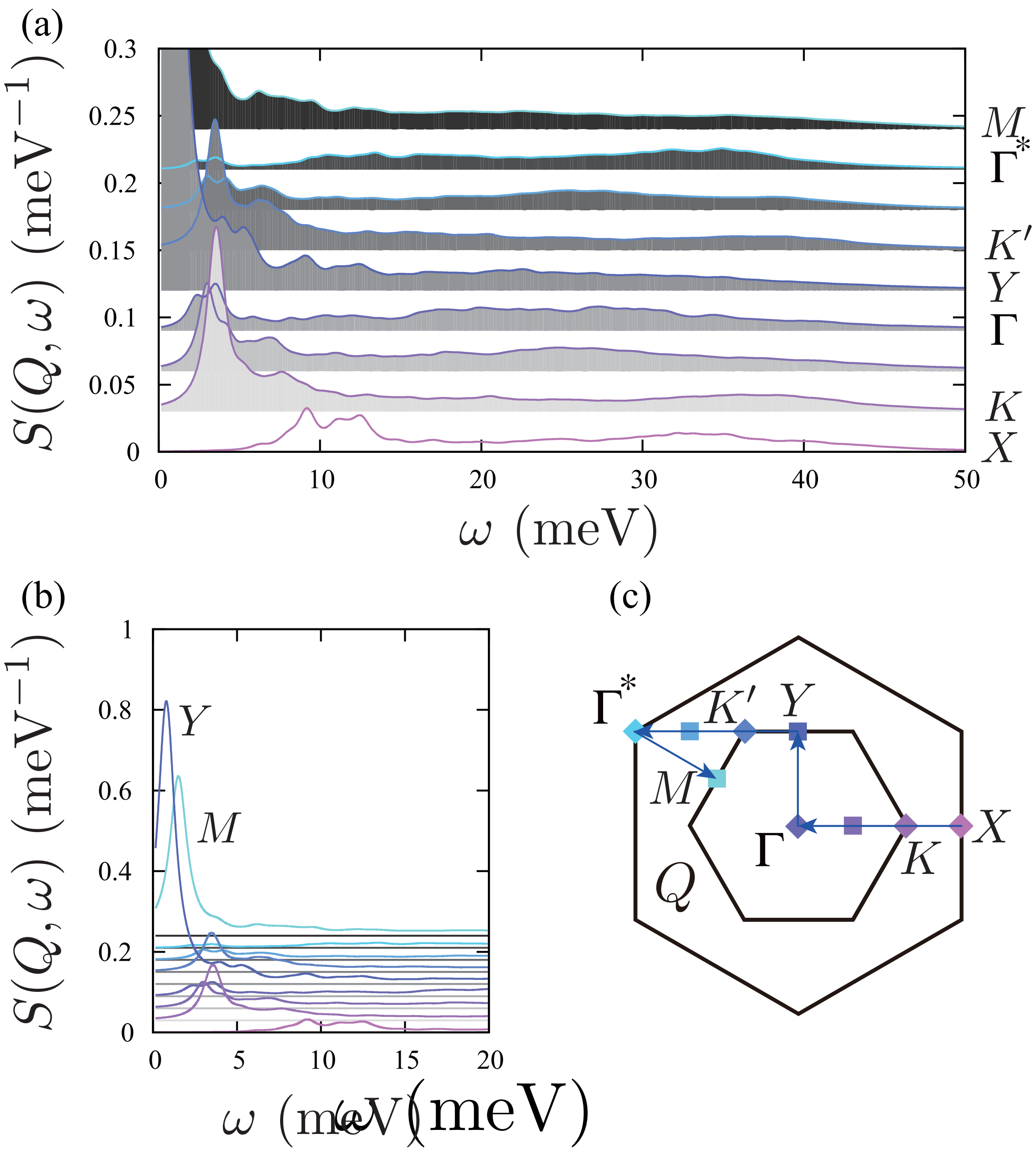


Dynamical Spin Structure Factors

Na_2IrO_3



N_H=16,777,216

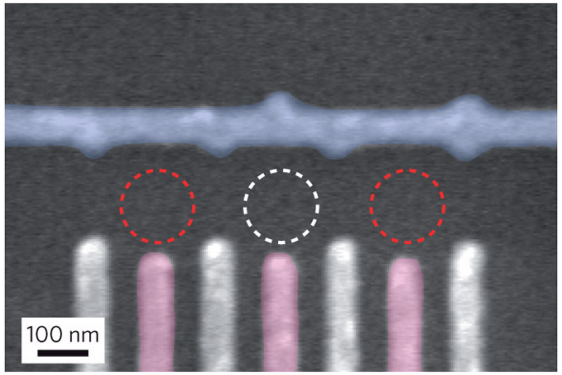


Numerical Implementation

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:
$\rightarrow$ Number of states = 2^3 (factor 2 from spin)

$|0\rangle \otimes |0\rangle \otimes |0\rangle$ $\quad |0\rangle \otimes |0\rangle \otimes |1\rangle$

$|1\rangle \otimes |0\rangle \otimes |0\rangle$ $\quad |1\rangle \otimes |0\rangle \otimes |1\rangle$

$|0\rangle \otimes |1\rangle \otimes |0\rangle$ $\quad |0\rangle \otimes |1\rangle \otimes |1\rangle$

$|1\rangle \otimes |1\rangle \otimes |0\rangle$ $\quad |1\rangle \otimes |1\rangle \otimes |1\rangle$

States represented by superposition

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

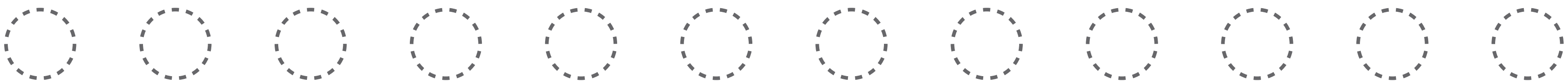
Quantum Many-Body Problems

N Quantum dots

One-body problem:
→ Number of states = $2 \times N$

N-body problem:
→ Number of states = 2^N

Further example: N=12



One-body problem→ Number of states = $2 \times N = 24$
N-body problem→ Number of states = $2^N = 4096$

Extreme example: N=36

One-body→ $2 \times N = 72$
N-body→ $2^N \sim 6.9 \times 10^{10}$

Quantum Many-Body Problems

Mutual Interactions

$0 \quad 1 \quad \cdots \quad N-1$

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

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

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

$$\overset{0}{\bigcirc} \quad \overset{1}{\bigcirc} \quad \cdots \quad \overset{N-1}{\bigcirc}$$

Fock space of N qubits:

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

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

Operators acting on N-quibit Fock space:

$$\boxed{\hat{S}^a_j, \hat{S}^a_j \hat{S}^a_{j+1} : \mathcal{F} \to \mathcal{F}}$$

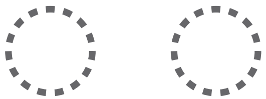
$$\hat{S}^a_j \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}^a_j \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j}$$

$$\hat{S}^a_j \hat{S}^a_{j+1} \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}^a_j \otimes \hat{S}^a_{j+1} \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j-1}$$

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

Example: N qubits

N-qubit Fock space:

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

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

Mutual interactions among N qubits:
Hamiltonian operator

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

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

Vectors in Fock Space

Correspondence between spin and bit

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

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

2^N-dimensional Fock space:

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

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

Decimal representation of orthonormalized basis

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

Wave function as a vector

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

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

Vectors and Matrices in Fock Space

Inner product of vectors

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

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

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

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

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

Hamiltonian matrix

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

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

Example: Two Spins

Decimal representation of orthonormalized basis

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

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:
Ladder operators

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

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

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

4 by 4 Hamiltonian matrix

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

Itinerant S=1/2 Fermion

Creation and Annihilation Operators

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

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

Anticommutation rule
(Fermi statistics)

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

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

Vaccum

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

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

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

Fock Space

Fock Space

Basis

$$\hat{c}^\dagger_{i\sigma}\left|0\right\rangle, \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{j\downarrow}\left|0\right\rangle, \prod_i \hat{c}^\dagger_{i\uparrow}\prod_j \hat{c}^\dagger_{j\downarrow}\left|0\right\rangle, \dots$$

Hermitian conjugate

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

Actions of Operators and Innter Product in Fock Space

Example of multiplication of operators to bases

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

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

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

Example of inner prodcut

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

Comparison between Fock space and linear algebra

Scalar obtained through vector-matrix-vector product

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

Implementation of Fock Space

Bit representation of electrons: Order of sites matter

Example: Two-site Hubbard model

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

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

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

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

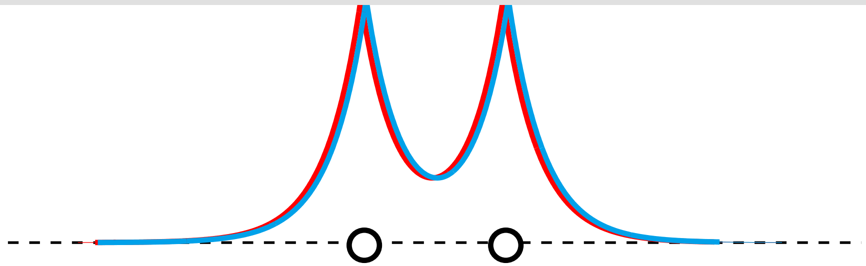
Bit rep. is not enough: Fermionic sign is necessary

Example: Tunneling

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

2-Site Hubbard Model

2-Site Hubbard Model



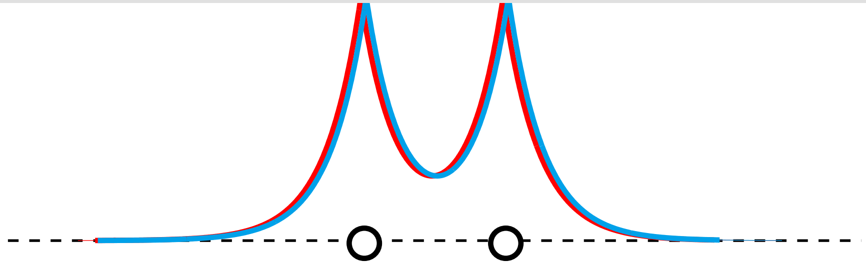
Hubbard model

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

Problem 3:
Create 4 by 4 Hamiltonian matrix with following 4 bases

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

2-Site Hubbard Model



Hubbard model

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

Answer of Problem 3:
4 by 4 Hamiltonian matrix with the following 4 bases

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

$$\hat{H} \doteq \begin{bmatrix} +U & +t & -t & 0 \\ +t & 0 & 0 & +t \\ -t & 0 & 0 & -t \\ 0 & +t & -t & +U \end{bmatrix}$$

Let's Solve
2-Site Hubbard Model by
HΦ

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 Sz = 0)

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

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

Low energy state → 2 spins

$E = 0$

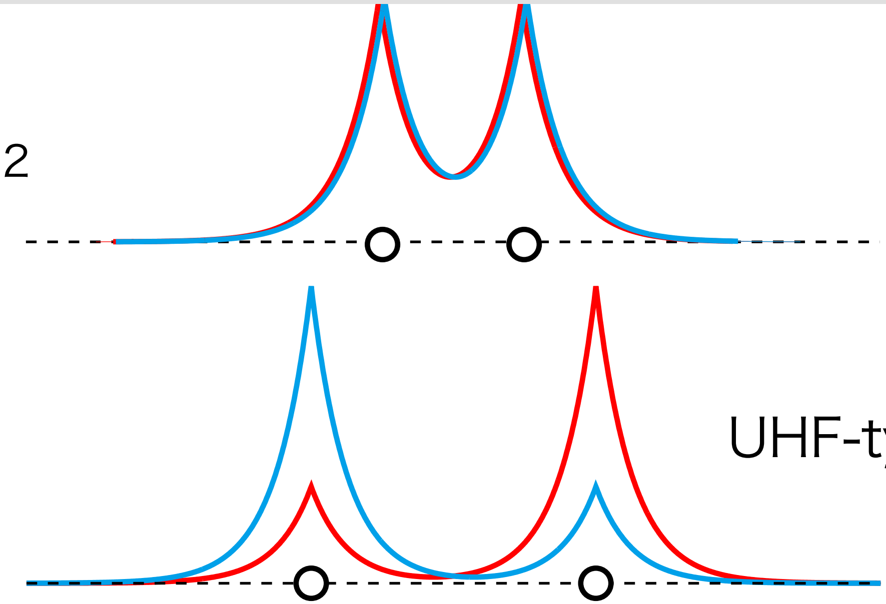
$$\frac{1}{\sqrt{2}} \hat{c}^\dagger_{0\uparrow} \hat{c}^\dagger_{1\downarrow} |0\rangle + \frac{1}{\sqrt{2}} \hat{c}^\dagger_{0\downarrow} \hat{c}^\dagger_{1\uparrow} |0\rangle$$

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

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

Hydrogen Molecule

H_2



UHF-type wave function

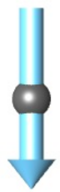
Hubbard model

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

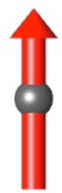
$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} \left(\hat{c}^{\dagger}_{0\sigma}\hat{c}_{1\sigma} + \hat{c}^{\dagger}_{1\sigma}\hat{c}_{0\sigma}\right) + U \sum_{j=0,1} \hat{c}^{\dagger}_{j\uparrow}\hat{c}_{j\uparrow}\hat{c}^{\dagger}_{j\downarrow}\hat{c}_{j\downarrow}$$

Heisenberg model or *J*-coupling

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



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



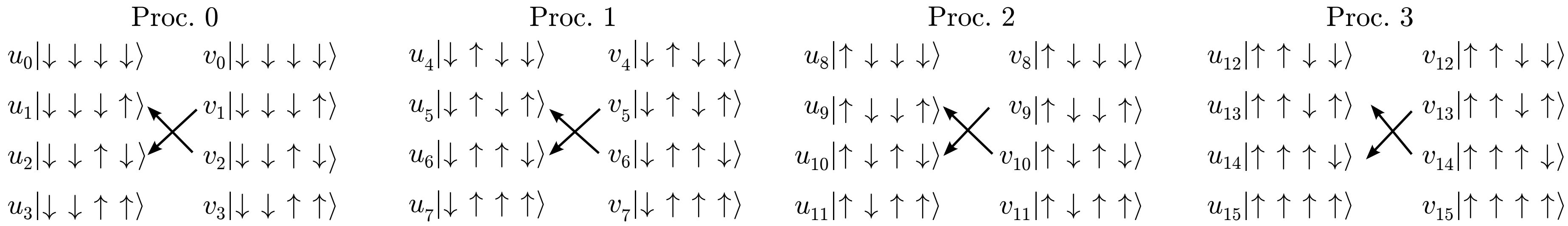
Singlet ground state

Parallelization

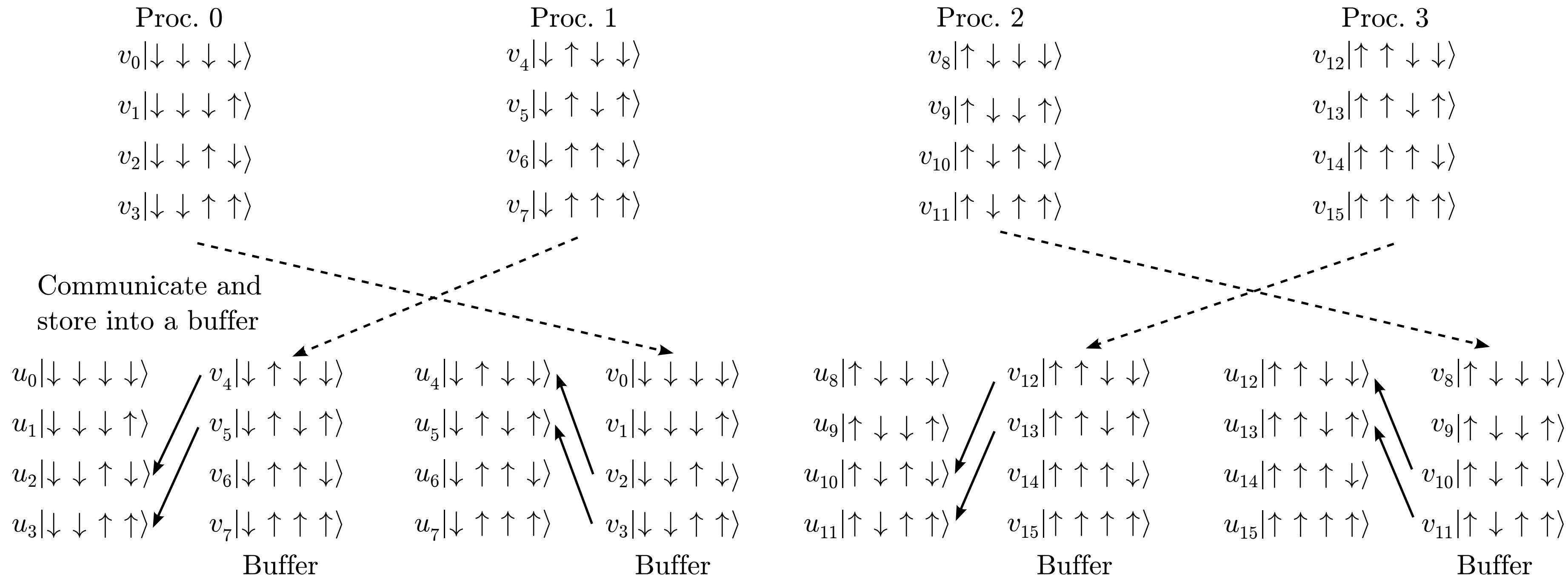
Parallelization

$|u\rangle = \hat{\mathcal{H}}|v\rangle \qquad N^{\mathrm{Local}}=2 \qquad N^{\mathrm{Total}}=4$

(a) $J(\hat{S}_0^+\hat{S}_1^- + \hat{S}_1^+\hat{S}_0^-)$

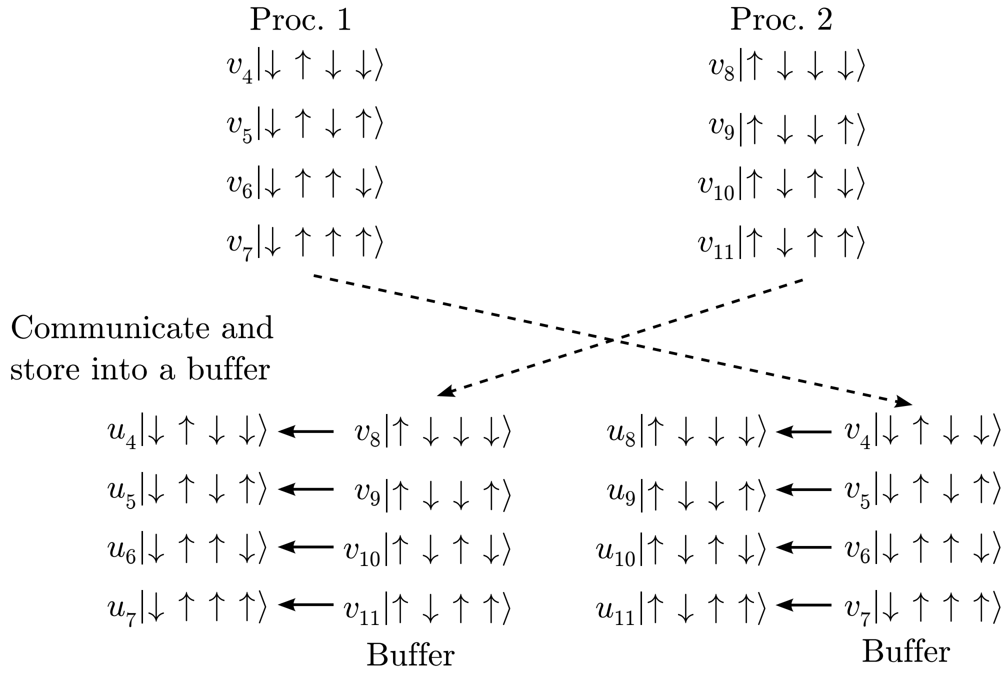


(b) $J(\hat{S}_1^+\hat{S}_2^- + \hat{S}_2^+\hat{S}_1^-)$



Parallelization

(c) $J(\hat{S}_2^+\hat{S}_3^- + \hat{S}_3^+\hat{S}_2^-)$



Other Numerical Methods

Other Numerical Methods

Ab initio

-Hartree-Fock theory*
-Density functional theory
 Local density approximation*
 Generalized gradient approximation*
 Hybrid functional*
 GW*
-Post Hartree-Fock (Quantum Chemistry)
 Møller-Plesset*/Configuration interaction/Coupled cluster

*Difficulties in describing Mott insulators

-Transcorrelated

Other Numerical Methods

Many-body

-Exact diagonalization

-Quantum Monte Carlo (QMC) method

BSS, continuous time,···

Variational Monte Carlo

Green's function Monte Carlo

Diffusion Monte Carlo

-Numerical renormalization group (NRG) method

K. Wilson

-Density matrix renormalization group (DMRG) method

S. White

-Matrix product and tensornetwork method

→ lecture in A term

-Dynamical mean-field theory

Combination

Report Problems

3rd Report

Please choose one of the two questions and solve it.
If you solve both, you will gain a bonus.

1. Solve the following questions. You may use HΦ.
   1-1. Solve the two site Hubbard model and obtain U dependence of the every energy eigenvalue.
   1-2. Estimate the Haldane gap of the S=1 Hesenberg model.
   - The Haldane gap is energy difference between the ground states in total S=0 and total S=1 sectors. You may obtain the the ground states in the total S=M by obtaining the ground state with total S_z=M.
   - Use several L (number of spins) and extrapolate the gap to thermodynamic limit ($L \to \infty$).
   - Illustrate the extrapolations.

   1-3. Examine convergence of the Lanczos method by focusing on the ground state energy of a hamiltonian you choose.
   - Show the Lanczos step dependence of the lowest energy.

3rd Report

2. Implement CG and shifted CG methods and solve the questions.
   2-1. Implement CG method.
   -Please include your code in the report.
   2-2. Solve linear equations. Please select a symmetric postive-definite matrix A with non-zero offdiagonal element. The vector b should not be the zero vector. Please choose A and $\boldsymbol{b}$ with N_{H} (linear dimension of A) > 5.
   -If you obtain the solution of $A\boldsymbol{x}=\boldsymbol{b}$ by Lapack and compare with the solution by CG, you will gain a bonus.
   -Illustrate convergence. You may plot step dependence of 2-norm of residual vectors $\boldsymbol{r}_k$.
   2-3. Implement shifted CG method.
   -Please include your code in the report.
   2-4. Solve the linear equations you used in question 2-2. with several shifts σ. Choose 5 different shifts at least.
   -Illustrate the 2-norm of the residual vectors for the shifted equations.

3rd Report

Deadline: 2017/7/31

Please submit your report through ITC-LMS
(web page for the reports will be opened) or
by sending the report as attached pdf files via email
to yamaji@ap.t.u-tokyo.ac.jp.

About installation of HΦ, please visit the webpage
MateriApps or HΦ's homepage.
How to construct an environment for using HΦ
http://qlms.github.io/HPhi/presentation/2017/Lecture2017/Hphi_install_manual_v2.0.1.pdf